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

Summary of Reviewer Comments on Hydrogen Production and Delivery Subprogram:

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

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



Hydrogen Production and Delivery Funding by Technology:

Majority of Reviewer Comments and Recommendations:

In general, the reviewer scores for the production and delivery projects were high to average, with scores of 3.9, 3.1 and 1.9 for the highest, average and lowest scores, respectively. The scores are indicative of

the technical progress that has been made over the past year for DOE competitively selected and Congressionally directed projects. Recommendations and major concerns for each project category are summarized below.

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

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

Biomass Gasification: Two projects in this area were reviewed. Both projects are researching the potential of central plant, low temperature, single step, aqueous phase reforming of hydrolyzed biomass. The project scores ranged from 2.3 to 3.0. Projects scoring higher were noted as having significant technical advancements since last year and to have a focused project plan, which was followed closely.

Solar-Driven High Temperature Thermochemical: Two presentations and two posters were reviewed in this topic area. The projects were favorably rated for their collaborative efforts and technical skills and abilities of the researchers. Recommendations for improvement included ensuring that the calculation of overall system efficiency is consistent for each cycle, completing all material balances, and identifying and resolving waste disposal issues.

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

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

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

Hydrogen from Coal: The projects reviewed in this area received mostly favorable ratings from the reviewers. Reviewers observed that the projects were in alignment with DOE HFCIT and Hydrogen from Coal Program goals and objectives. The reviewers suggested that the projects need to advance the technology to the point where experiments using actual or close to actual gas streams are being performed. Specifically, the reviewers noted that the membranes need to be tested in the presence of impurities. The membranes also need to go through additional testing to assess long-term durability and stability.

Hydrogen Production Using Nuclear Energy: In general, the projects reviewed in this area were scored favorably. Reviewers approved of the breadth of collaboration for some projects and the well-focused approach of other projects. The projects were judged to be well aligned with the program's goals. As in 2008, reviewers recommended that materials and cost drive research. Specific recommendations were made to understand durability and degradation of the high temperature electrolytic cells.

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

Project # PD-02: Bio-Derived Liquids Reforming

Yong Wang: Pacific Northwest National Laboratory

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

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

- This project is split into two parts: 1) aqueous phase reforming catalysts and 2) ethanol steam reforming catalysts. Relevance for this project is high in that it directly supports Virent Energy System's aqueous phase reforming project as well as non-precious metal ethanol catalyst work.
- Finding an energy efficient and cost effective way to convert biomass to a useful energy carrier is critical to DOE's mission.
- The project addresses the stated goal of the program.

Question 2: Approach to performing the research and development

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

- The project has useful research towards cost reduction, both with regards to capital as well as O&M, but does not necessarily have the most important research.
- The basic catalyst development approaches in the project are strong.
- The use of Pt and Ru as the catalyst for the aqueous-phase reforming (APR) process is questionable when the project itself recognizes the need to identify 'base' metal catalysts as a critical need to meet the cost-effectiveness barrier.
- This project is in contrast to the ethanol stream reforming (ESR) work where a base metal is identified.
- Branch points and go/no-go decisions should be built into the project's approach.
- It is unclear why glycerol is being used instead of one of the sugars produced by hydrolysis. The usage of glycerol will create issues different from those found with using hexoses or pentoses.

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

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

- The project shows outstanding progress toward DOE's program and/or project goals.
- The investigation of Re/Pt catalysts on carbon supports is relevant, focused, and a solid achievement.

- Experimental determination of Rh catalyst lifetime at lower space velocity (~20,0000/hr) is an important finding. However, the project cost impact on system needs to be addressed.
- The project's process work is well done. A good start on the economics of the chemical plants is apparent.
- The project team should look at or conduct sensitivity analysis on economics. An EtOH value of \$1.07/gallon is very unrealistic.

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

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

- The project seems to have work in common with Virent Energy Systems, but nothing as identifiable as collaboration. Virent Energy Systems seem to be disconnected and not part of the development team. The partners in this project do not seem to be integrated and it is not clear if they add substance to the technical development path.
- The project team's interaction with Virent Energy Systems is relevant and productive.
- It appears there is only modest interaction with Ohio State University (OSU).
- The level of collaboration in this project does not make the best use of the DOE complex. The relationship with Virent Energy Systems appears to be mostly one way.
- The project team needs collaboration with commercial entities that have fuels and catalyst/process experience and expertise, i.e., an energy company or catalyst vendor.
- "Collaboration with Ohio State on ethanol steam reforming has been minimal in the past and we have had discussions to specifically increase this interaction" and "Initial discussions were held on collaborative work".
- Regarding the above quoted statements, neither constitutes reasonable progress in a year. Discussions are not considered collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The project team appears to be addressing late stage commercialization barriers, but it is unclear where the commercialization partner is. Addressing such late stage issues if there is no commercialization plan does not make sense.
- A future plan for this project is solid.
- The project team is looking to find ways to "Improve hydrogen productivity and selectivity by exploring additives that may retard dehydration pathway to acids on Pt-Re/C." This is vital but it would be constructive for the team to provide more specifics on this issue.
- The project's coking mechanisms are well established but knowing them is unlikely to help in coke reduction. Time would be better spent empirically exploring catalyst compositions and process conditions.
- The project team should not work on pressure swing adsorption (PSA) issues. This issue is outside the scope of the project and the expertise of the investigators.
- A systematic investigation of steam:ethanol ratio needs to be conducted.

Strengths and weaknesses

Strengths

• The project team's basic science investigation of new catalyst systems under representative operating conditions is a strength.

Weaknesses

- The project team conducted economic analysis to determine hydrogen cost, but catalyst lifetime assumptions are not defined.
- The lab results in this project indicate that carbon deposition on Co catalyst is substantially higher than on Rh. Lifetime testing is needed to determine real-word effects. Limited Co-based catalyst lifetime has traditionally been a fundamental problem but is not addressed in this project.

- The number of moles of hydrogen produced per each mole of glycerol should have been presented. Selectivity was not defined in this project.
- The project has no real industrial collaboration.

Specific recommendations and additions or deletions to the work scope

• The project team should consider switching from using glycerol to real sugars.

Project # PD-03: Hydrogen Generation from Biomass-Derived Carbohydrates via the Aqueous-Phase Reforming Process

Bob Rozmiarek; Virent Energy Systems, Inc.

Brief Summary of Project

The overall objectives of this project are to 1) design a generating system that uses lowcost sugars or sugar alcohols that can meet DOE's hydrogen cost target of \$2 to \$3/gge for 2017; and 2) fabricate and operate an integrated 10 kg of H₂/day generating system. The 2009 objectives were to 1) continue fundamental development and analysis to increase the thermal efficiency of the aqueous-phase reforming (APR) system; 2) continue development of the APR catalyst and reactor system that converts glucose to hydrogen; 3) complete hydrogenation fundamental study and interact with PNNL on data exchange and fundamental surface science study; 4) operate reactor development pilot plant



(scale-up testing); 5) develop initial process flow diagram and catalytic reactor design for 10 kg/day demonstration system; and 6) review techno-economic performance of the APR system.

Question 1: Relevance to overall DOE objectives

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

- This project is especially relevant as the team pushes toward less-treated biomass. However, the application of refined biomass has to be questionable versus use of those molecules directly as fuel.
- The project directly targets the objective of low-cost renewable hydrogen. Aqueous reforming is an important pathway for the team to explore.
- This project addresses one of DOE's preferred pathways. Efficient conversion of biomass to hydrogen or other liquid fuel is critical to DOE's mission.
- This project aims at producing hydrogen from a renewable source and has the potential to meet DOE's production target.
- The project team addresses DOE's program goal but uses a convoluted route. A direct cellulose to hydrogen route is preferable to control costs.

Question 2: Approach to performing the research and development

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

- The project team had a good identification of barriers they faced in 2008. The team's approach is difficult to judge because of the secrecy.
- This program lends itself to a relatively straight-forward approach. They have clearly articulated a game plan: approach is very good.
- The project team's investigation of basic catalyst science to determine reaction rates and improve catalyst is solid.
- The project team has a good approach as it is important to have a wide range of feedstocks for hydrogen production. The lack of a gas compression step is also useful/productive.
- The project team's fundamentals to improve H₂ yield was a good study.

- The project's approach to address fundamental catalyst issues especially reactor design and system design is good.
- The project team needs to address impurities expected in sugars and their effects on catalyst performance.
- The team needs to address where the \$0.064/pound glucose number comes from. This number seems low.

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

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

- The project's gross 10% reduction of cost is a little disappointing (from \$6.50 with a \$3.00 target). The team should have explained how the 10% factors into the 60% needed to reach the target. The secrecy surrounding the project allows only superficial evaluation.
- The team has made significant technical progress. However, more defined metrics are needed regarding their efforts, such as the goal and threshold fuel conversions to meet price goal or the goal and threshold CO₂ and H₂ yields.
- The project has been successful but it has no method in place to evaluate it. The important results are mentioned as "exclusive work-wide licenses, ... multiple new patent applications, ... solid trade secret position." There is a lack of real data in the report.
- If the program has been as successful as claimed, there should be no need for government funding.
- The project's 10% reduction in H₂ costs is not encouraging as the process needs about 50% reduction improvement to meet DOE targets. It is unclear if the low yield is due to catalyst performance or inherent thermodynamics.
- This program is due to end in September 2009. To this date questions remain such as what the status is of 10kg/day reactor? Has it been designed or is it running now? Is it designed for continuous operation? How long has it operated continuously? The team should do a sensitivity analysis on economics to identify critical parameters and examine sensitivity on sugar price.
- The project's reaction network study should be published. This is important information discovered with government funds and needs to be shared with the entire biomass community.

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

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

- This project seems very well integrated with the University of Wisconsin (UW) Madison folks.
- It is difficult to evaluate the extent of interaction with PNNL and UW. Archer Daniels Midland Company (ADM) is listed as a collaborator but no examples or explanations of contributions are provided.
- ADM is listed as a collaborator but their contribution is not identified. PNNL and the University of Wisconsin appear to be suppliers rather than partners.
- The project has good collaboration with ADM and University of Wisconsin. The project team should consider additional collaborations with a catalyst company and a system design/integrator with expertise in design for manufacturing and assembly (DFMA).
- The project team would benefit from interaction with an entity that has industrial experience/expertise such as an energy company or catalyst vendor.

Question 5: Approach to and relevance of proposed future research

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

- The approach to and relevance of proposed future research is very superficial due to the project's secrecy. It is unclear how the team plans address the magnitude of the gap. It is also not clear why a larger unit should be built when issues remain for reducing cost to the \$3.00 target.
- This program seems ripe for 50 or 50+% cost share.
- The team should address impurities expected in sugars, especially if the sugars used are produced from lignocellulosic biomass due to their effect on catalyst performance.
- This project closing therefore there is no relevance of proposed future research.

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Strengths and weaknesses

Strengths

- The project team tried to commercialize something, which is the right place to lead this R&D.
- The project team has a seemingly good coordination of catalyst development theory with test.

Weaknesses

- The project team and the project itself is under secrecy, which makes it difficult to pinpoint weaknesses.
- The project's "bio liquid to hydrogen" concept seems to be a weak approach.
- The team's emphasis seems to be on the hydrogenation reaction. While hydrogenation of glucose to sorbitol is necessary, they also need to examine the actual H₂ production reaction. This concern is not adequately conveyed in the presentation.
- Heat transfer is very important factor in reactor design and needs to be addressed. There is very little information on heat transfer which could be the dominant cost/sizing factor.
- This project needs a space velocity and/or example of reactor size for a given H₂ production rate. The reactor may be very large. It is currently hard to assess its size.

Specific recommendations and additions or deletions to the work scope

• The project team needs to add intermediate metrics to define targets conversions/yields so that yearly progress may be assessed.

Project # PD-04: Investigation of Reaction Networks and Active Sites in Bio-Ethanol Steam Reforming over Co-based Catalysts

Umit S. Ozkan, Hua Song, Xiaoguang Bao, and I. Ilgaz Soykal; Ohio State University

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

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

- The project's development of non-precious metal catalysts for the ethanol reformation is an enabling technology as it substantially lowers catalyst cost.
- The team's identification of a non-noble metal catalyst is key to providing cost effective electrolysis processes for producing hydrogen. The need for this is evident in many applications of DOE's program.
- This project addresses DOE's program goals well.

Question 2: Approach to performing the research and development

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

- This project has very well designed R&D to optimize catalyst.
- The team's description of the systematic approach to catalyst synthesis is very good.
- The project team's interdisciplinary approach is excellent. The amount of analytical data being collected and used is significant.
- It would be helpful to see some formal process to the problem of examining the entire data collection as a whole. It is recognized that this is a difficult challenge.
- This project recognizes the importance of catalyst synthesis to a greater extent than other projects.
- This project also has a good mix of catalyst characterization techniques.
- The team effectively explored the use of diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), Raman and isotopes.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

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

• The team's research is outstanding. The project's progress would also be outstanding if there were numerical benchmarks. For example, what is "high" and what has actually been achieved?

- The project tasks are clearly identified with progress succinctly laid-out. The project's goals should be more clearly identified, e.g., while a target space velocity is shown, lifetime goals and achievements are not listed.
- "One of the best performing catalysts" is listed as Co/CeO₂ hexamethyldisilane (HMDS) in the project. Substantial exploration of dopants, support structure, etc. was conducted by the team, but the "best" catalyst is not defined by it critical attributes. It is described only as generic Co/CeO₂.
- Substantial progress in understanding reaction networks seems to have been achieved.
- The catalyst characterization in this project is very impressive. Linkages of characterization to performance should be strengthened.
- The project uses a flow diagram to illustrate the process. The questions that remain are what are the initial estimates of the cost and what are the cost drivers?
- The slides for this project contained far too much information. It was difficult to follow the presentation because of the overwhelming amount of data presented on each slide.
- The team has a good understanding of mechanism developed. They have a good publication and presentation record.

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

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

- Collaboration within the team is outstanding, which is clearly an important factor for this effort. Critical insights and contributions coming from partner institutions are not transparent.
- This project has very good partners. The difficulty with explaining collaborations in detail is difficult; however, it would be helpful to see an example of the team building or synergy of the team.
- This project has a good involvement of industry, government labs, and various entities in university.

Question 5: Approach to and relevance of proposed future research

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

- The project's future work is logical in the micro sense of work progress, but maybe not in big picture. This "understanding" seems way ahead of development. Either this project needs a commercialization partner (if it is commercializable) or it needs a very close linkage with economics to verify that work is addressing the critical issues.
- Future work is detailed and specific for this project. However, longevity studies are the most important element.
- The project's kinetic rate expression determination is of value, but only of the most promising catalyst(s). There was no mention of down-selecting to a top contender for detailed examination.
- The future work plan for the team and project is rational but would be improved by branch points that are driven by discovery.
- More information on effects of varying steam:ethanol ratio is needed. A question that remains is what is the minimum steam ratio?
- The project needs sensitivity analysis to economics. How the decreasing steam ratio effects cost needs to be addressed.

Strengths and weaknesses

Strengths

- Technical catalyst development team activity is superb in this project.
- The team's three-leg approach is well thought-out.
- Each page of the team's presentation contained a very nice and succinct summary of the main message or concept learned.
- The project researcher did a good job of summarizing very complicated results.
- A 3-D yield graph showing various product yields at various temperatures is particularly effective. The team should make this a standard way to portray data.
- The project has good characterization and good work on exploring synthesis space.

Weaknesses

- The project relationship to actual process development needs is not revealed in talks. If there is no process development/commercialization need, this terrific work could be just a waste.
- Regarding the presentation, there were too many graphs on pages which created confusion/clutter without adding meaningful information.
- More focus needs to be placed on lifetime studies. Non-precious metal catalysts are desirable for their lower cost but that cost advantage is erased if the catalyst needs to be frequently replaced due to deactivation.
- More tests should be conducted at higher space velocities and at lower steam:ethanol ratios. Lower steam:ethanol ratios have a beneficial effect on system cost- but only if they do not adversely impact performance/lifetime.

Specific recommendations and additions or deletions to the work scope

No recommendations were made for this project.

Project # PD-05: Distributed Reforming of Renewable Liquids Using Gas Transport Membranes

U. (Balu) Balachandran, T.H. Lee, C.Y. Park, Y. Lu, J.E. Emerson, J.J. Picciolo, and S.E. Dorris; Argonne National Laboratory

Brief Summary of Project

The overall objective of this project is to develop a compact, dense, ceramic membrane reactor that enables efficient and cost-effective production of hydrogen by reforming bio-derived liquid fuels using pure oxygen formed by water splitting and transported by the membrane. Objectives over the past year were to optimize the performance of the oxygen transport membrane and demonstrate reforming of ethanol. Membrane technology provides the means to attack barriers to the development of small-scale hydrogen production technology.



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 2.6 for its relevance to DOE objectives.

- This project applies to barriers related to low-cost production.
- DOE's FY08 change to ethanol differentiates this project from the work done by Eltron Research.
- The PI is attempting to respond to the needs of the DOE Hydrogen Program, however, this work appears to be an attempt to adapt long term, on-going projects and concepts to fit the goals and objectives of the program. This approach may not be the most practical route to achieve the program goals. DOE and the PI need to consider if these novel approaches have any real benefit over current (or potential future) methods of hydrogen production. A reasonable cost analysis needs to be developed, not simply H2A. If this work is continued, it should be considered a long term fundamental effort, which is appropriate for a national laboratory, However, there should be no expectation that this will be developed in near timeframe (the page 8 schedule is not reasonable).
- This project seems to be using a difficult path (dual membranes) to do something that is nearly commercial today. It is not convincing that the big picture goal (ethanol to hydrogen) makes any sense in the base case.
- Given that the Hydrogen Program has already declared success in methane steam reforming, it is unclear how much benefit is to be gained by this process. A combined two membrane system seems to be complex.
- This project's focus is the use of oxygen transport membrane (OTM) and it appears to be funding long term OTM research with hydrogen money.
- This project's benefits are stated in increased conversion. There is a need to get a third party to assess increased capital cost and complexity and see if there are economic benefits.

Question 2: Approach to performing the research and development

This project was rated 2.2 on its approach.

- This project's economics should be completed on the potential savings prior to experimental program. While this project would reduce reactor size it will not affect the balance of the plant, and thusly only reduce a fraction of the cost of a reformer.
- This PI has suggested an extremely complicated and high-energy approach for the production of hydrogen and it is apparently based on simple ethanol reforming. It is not clear that there is any benefit over standard reforming technology. The proposed design (page 5) incorporates two membrane technologies that are still not

developed and using them in this combined approach is likely not practical. The temperatures required for these materials are too high for any general use. Although not specifically mentioned, there are other numerous material issues (for example seals) that will also be a problem with this approach. Costs were not specifically addressed but, with the exotic materials and complicated engineering approach, it is likely that this approach will never meet the DOE cost targets.

- Work is scattered in this project. The team needs to focus on the proof of concept (POC) experiments and the key data needed for economic evaluation.
- The team's approach is unique and for that reason may be pursued. However, the work on OTM has been extensive at ANL and future work extends quite a way out. This technology may simply be too complex to have a good hope for success.
- Although this project focuses on OTM, hydrogen transport membrane (HTM) is mentioned several times. It needs to be determined whether it is realistic to use two membranes, i.e., whether temperatures, gas compositions, etc. are matched in two membranes. The team needs to model an entire system.
- The project needs to carry out reforming at realistic conditions, i.e., air as oxygen source and varying steam ratios in fuel gas. The team's approach indicates good membrane expertise, but investigators need to learn more about reforming.
- This project ignores seal problems that typically kill membrane applications.

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

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

- A technical accomplishment of this program is having/creating stable membranes for up to 1000 hours.
- This project's technical progress since beginning this work in 2005 has been minimal. Flux rates are still minimal and need to be improved. There is no information on the hydrogen membrane at this time. Temperatures are very high and need to be much lower (around 400°C) but, all the tests in this project are still at 700° 900°C. It is likely that the solid membranes will not function at this lower temperature. There has been little work on the reforming reaction. Only a gas phase conversion at high temperature, which produced a variety of products. This tends to suggest that it will probably not be possible to produce an alternate stream of high-purity/high-pressure CO₂, which is also a goal of this approach. The need to add more steam at this point is also a negative aspect that leads to increasing costs. Adding pure oxygen for the reforming. The concept of combining all these processes into one reactor is overly aggressive. In particular, expecting a single section of the reactor to allow oxygen ion recombination, ethanol reforming and hydrogen dissociation is not realistic all occur under different conditions. In addition, the work has not considered the effects of conducting an actual reaction, with heat and volume changes, near and in the OTM. These changes can be significant and result in destruction of the membrane (oxygen separation alone with no reaction is a much simpler system).
- The team's work has identified some minor improvements to the membrane structure.
- The chart on page 7 shows an average of 35% progress- this is troubling. Instead of focusing on the POC and data needed for concept evaluation, researchers seem to be working on improving the membrane.
- Some good progress has been made in improving the performance of the OTM.
- The rest of the project's milestones are far from being met.
- Considering the limited funding of this project, the team has had good progress.
- There needs to be a strategy to reduce byproducts in this project as well as a need to move to realistic reforming conditions as soon as possible.

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

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

- This project will benefit from collaborations mentioned in their future plans.
- The project has minimal outside collaboration and it is all academic or their sponsor. If this work is to ever get to some kind of scale-up or commercialization, there needs to be some industry perspective, and this is lacking.

- Collaboration does not seem to be the main thrust of this project. The most important collaboration is Directed Technologies, Inc. (DTI) to understand the project's targets and needs, and this collaboration does not appear to be well integrated.
- Collaboration with other institutions appears to be fairly minimal.
- Very little collaboration is seen in this project. The team needs to partner with someone who practices steam/autothermal reforming commercially to identify important issues.
- This project should also partner with sources for scale-up options.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.2 for proposed future work.

- It is not apparent that this project has any clear direction and is primarily Edisonian in nature. The PI needs to establish clear targets, goals and milestones as well as document these accomplishments. In particular, the PI needs to develop a plan to define a reasonable operating target for the process. The temperatures suggested in the presentation for reasonable ethanol reforming are still too high (550°C, page 15) for an acceptable conversion process.
- The team needs to focus on POC and on data needed for economic evaluation.
- The proposed forward plan for the project extends too far to make an assessment.
- The project should have outlines a set of more quantifiable forward milestones.
- The team needs to settle on a membrane and focus on reforming.

Strengths and weaknesses

Strengths

- The team's skills with OTMs are a strength.
- The team's expertise in OTMs is a strength.
- The project has good OTM expertise.

Weaknesses

- The project's target production rate is not included in presentation.
- This project has a lack of focus. There is too much work on advancing OTM and not enough on critical program needs.
- The project has slow progress in other aspects of their work.
- The project is too nascent to provide a good H2A analysis.
- The team needs to focus on seals, reforming, and good modeling.

Specific recommendations and additions or deletions to the work scope

- The team needs to address the safety aspect of a failure of OTM resulting in rapid mixing of oxygen stream with ethanol.
- DOE needs to consider this as a fundamental study on solid oxide "oxygen" transport membranes and, if work is to be conducted, the work should focus on improving oxygen flux from air. This work has been ongoing for some time with little advancement. Adding complications such as reforming is not benefiting this development. In addition, DOE should not be expecting any breakthroughs, even minor. in the near future.
- This project feels like it is using technology in search of an application. That is, using the cover of an ethanol to find a hydrogen application because this was and area where funding was available to continue base advancement of the OTM membrane. DOE needs to focus this group on getting the critical data needed to identify if the use of this application makes any sense or choose to advance the membrane for its own sake.
- At some point, module-scale modeling will probably be needed to understand the potential hydrogen pressure that might be achieved.

Project # PD-06: Zeolite Membrane Reactor for Water-Gas-Shift Reaction for Hydrogen Production *Jerry Y.S. Lin, Henk Verweij, Peter Smirniotis, and Junhang Dong; University of Cincinnati*

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

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

- The project's lower reactor costs support DOE objectives.
- This is a standard zeolite modification project that attempts to develop a hydrogen separation membrane. It is unlikely that this approach will ever meet the DOE purity targets whether separation is based on size or preferential adsorption. In either case the H₂ purity will be low.
- The only concern for this project is that membranes fundamentally give hydrogen at low pressure, which is a poor fit with hydrogen manufacturer (or distribution). However, this project could be a very good fit to a coupled reforming/fuel cell, which could be appealing in power cycles or home combined heat and power (CHP).
- The project's H₂ purification from water-gas shift (WGS) reaction through a membrane is useful technology but not game-changing.

Question 2: Approach to performing the research and development

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

- Chemical Vapor Deposition (CVD) of Silica to narrow pores.
- The project is focusing on modifying the exposed surface pore sizes. This may improve separation and it is a reasonable effort for and academic project.
- The team should have a more explicit description of its approach, but its steps to (1) make the membrane work; (2) make the WGS cat work; and then (3) put them together was outstanding.
- It is not clear why sulfur tolerance is required or was tested in this project. Presumably sulfur would have been removed upstream prior to the reformer step.
- This is primarily a membrane development project, which is an appropriate focus but is not broad enough in scope.
- The project's pore decoration approach to tailoring pore size is a good approach.

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

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

- Tubular reactor tested for one week.
- The team's work has produced some interesting results. Slide 12 suggests that the purity can be improved (for whatever reason which is not clear). In addition, there appears to be evidence that there is some sulfur tolerance with the catalyst materials being developed. These are all good achievements for a project of this nature.
- The project's objectives are quantitatively stated and achieved.
- It is noted that the quantitation of objectives is taken from page 4, which is not actually described as the target for the project. This should be more explicit.
- It would have been good for the team to show thermodynamic equilibrium of the WGS reaction under the conditions tested (slide 17).
- Progress in membrane improvement through constricting pore opening is a reasonable approach in this project. It would be interesting to know if large scale synthesis if uniform membrane materials is economic.
- The project has great selectivity for zeolite membrane. There is a need to know selectivity for H₂/H₂S in membrane.
- Does the statement "Chemically stable in H₂S, thermally stable at ~400°C" mean that membrane is stable in H₂S at 400°C? The report also mentions a one month stability. Is degradation being seen after one month, or is this just the maximum time tested?

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

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

- This project's University focus could be improved by increasing collaborations with industries.
- The PI's have put together a well qualified team and have included an industrial perspective for the work (page 19). This is a good collaborative effort between three universities.
- The team's work highlights critical accomplishments by partners (Si CVD of zeolites) on pg 12-13.
- The project seems to have good collaboration with OSU on modifying porosity.
- This is mostly pretty fundamental work.
- More attention to overall energy balances is needed assuming this is a steam methane reforming reaction followed by WGS and membrane.
- Also, partners that provide more of the business possibilities and process sense would be recommended for this
 project.
- This project needs industrial collaboration to determine if the membrane is commercially feasible and also needs to look at costs.

Question 5: Approach to and relevance of proposed future research

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

- Benefits of a combined sulfur tolerant catalyst and the separation capability of hydrogen to be demonstrated on long term study is seen in this project.
- The project's future plans are reasonable and appropriate. This project has shown some promise with the recent technical advances and the future work will build on these accomplishments. This is a good project and approach for a collaborative university effort.
- All proposed items by the project team are excellent, however there is a need to focus on: (1) proof of concept which is subsequently needed for combined membrane & catalyst; and (2) advances beyond this proof need to be economically driven. What are the features that need to be improved to make the technology attractive?
- The project appears to have a reasonable technical forward plan. It would be good to know the metrics that are being aimed for in future work and to get an estimate of H₂ delivery costs as well as what assumptions are made to define that cost.
- Why is this project doing disk membranes?
- This project should get an industrial partner (Pall?) to work with regarding cost issues.

Strengths and weaknesses

Strengths

- This project has had some good technical success and provided some interesting gas separation results. This is a project that is worth future funding at a reasonable level.
- This project shows superb collaboration, clear targets, good science and execution.
- This project has a good membrane development team.

Weaknesses

- This project's economics should be completed to determine if this reactor product (~94%) would result in reduced PSA costs for purity required for fuel cell use.
- This project's low WGS pressure as well as uncertainty that comes from the unknowns of combining the WGS with the membrane can be a weakness.
- The team might gain from more catalysis focus and a commercialization partner.

Specific recommendations and additions or deletions to the work scope

• In this project it would be beneficial to see if the mechanism for separation could be determined. Separation by size is actually very unlikely. These molecules are mostly space and, even though the kinetic diameters appear somewhat different, these molecules are basically the same size. It is not clear if the surface modification changed the adsorption capability of both CO₂ and H₂, but this is a possibility. It does not appear to be simply Knudsen diffusion as the CO₂ permeance appears to go to almost zero. The research has provided a good opportunity to study the mechanism for gas separation in these modified materials which would be a good project for a Ph.D. student.

Project # PD-07: High-Performance, Durable, Palladium Alloy Membrane for Hydrogen Separation and Purification

Jim Acquaviva; Pall Corporation

Brief Summary of Project

The objective of this project is the development, demonstration and economic analysis of a Pd-alloy membrane that enables the production of 99.99% pure hydrogen from reformed natural gas at a cost of \$2-3/gge by 2010. The objectives for the past year were to 1) fabricate a series of membranes covering a specific range of alloy composition and functional layer thickness; 2) optimize the membrane formation process; 3) test the membranes in pure gas streams prior to water-gas shift (WGS) testing; 4) complete the equipment needed for extended WGS testing; 5) obtain initial WGS test results; and 6) initiate the techno-economic modeling as soon as the combined membrane reactor model is available from Directed Technologies.



Question 1: Relevance to overall DOE objectives

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

- This project is very relevant towards the goal of making hydrogen for fuel cells and storage.
- This project is directly addressing the DOE targets for hydrogen production. They are developing supported Pd and Pd alloy membranes on a porous support. This work, and recent work by other researchers, has indicated that this approach can meet the DOE targets (as presented in Slide 5).
- The project aligns with DOE Hydrogen Production element needs by developing and demonstrating a costeffective Pd-based hydrogen separation membrane. The Pall Corporation is well aware of DOE's targets and barriers.

Question 2: Approach to performing the research and development

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

- This project has an adequate approach to perform research and development.
- The project's coating method looked good, and alloy choice was okay, but might be too expensive. The project should also attempt to look at membranes with some of the Au replaced by Ag. A membrane with 15% Ag and 5% Au might be expected to have more flux and durability than one with 11% Au and also may cost less. More effort should be put into durability issues like resistance to cycling and start up.
- This project is a standard Pd/Pd alloy membrane development approach. It is a reasonable approach for metallic membrane development. The researchers appear well aware of the standard problems and are working to correct and improve on these issues.
- The team's work has provided a good compact design for a membrane unit capable of producing 100 kg/day hydrogen. This is a big benefit in that scale-up to larger sizes will only require addition of these compact units. Cost estimates appear reasonable and within DOE goals and targets.
- The project and team's approach is sound and straightforward, starting from development of a thin-film Pdbased membrane supported on a substrate, to experimental evaluation of hydrogen separation/purification from reformate gases. In the project objective slide, the program shifts the feedstock from the natural gas reformate

(in 2008 AMR meeting) to the ethanol reformate (this year AMR meeting). Pall should address justification of the change and effects of changes, from the standpoint of the cost of feedstock, compositions of reformates, and impurity on the membrane performance and cost of hydrogen.

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

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

- It is hard to evaluate the technical accomplishments in this project because the fundamentals of the process were not presented.
- This project seemed to have achieved most if not all of their goals. They claim to be making progress with quality control, and cycling. More work on these issues is needed. Funding for this project should be kept.
- The team's work has shown some good technical progress. Flux rates are good (200 300 scfh/ft²) and this includes tests with mix gas (including steam). This was the next step in developing these materials (it was time to move beyond pure gas diffusion). The work has had good success and will likely improve in the next year. This project has also demonstrated good stability of the membranes over moderate time frames (slide 19 approximately 100 hours). In addition, the work has demonstrated the ability to produce constant thickness pure and alloy membranes on the 1 3 micron level.
- The Pall Corporation did a great job on reducing the membrane cost while achieving a high H₂ flux goal. Pall also did excellent job on scaling tubes to 12 inches long. The durability test of 100 hours is much shorter than the target of 2 years. It would be much more informative if the project shows the optimum alloy thickness and Au content based on the lab results.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- The project team has good collaborations with prestigious institutions.
- This team is working with all the right people.
- The research team is adequate and includes a university, national lab and industry entity. The team is well qualified and has the expertise to further develop these membrane materials.
- This project has a good team involving industry and academics.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- This project has a good sequence of planned activities.
- The team did not present a particularly clear sense of where they hoped to go next.
- The future direction for this project is reasonable and appears to be following the original work plan. The work appears to be on schedule and within budget. It also appears to be a well managed effort with clear targets and milestones.
- The project work for next year should include testing in the presence of sulfur or other impurities. Impurities could "kill" the membranes and their effect needs to be determined in the near future. Also, additional improvements that are necessary or if the impurity effects are so severe that these membranes will not be able to be used for H₂ separation need to be determined.
- This is a good project worth continuing.
- The project's future work to evaluate the membrane durability, membrane formation process improvement, device operating procedure development, testing matrix, and techno-economic analysis refinement, are very sound. The program should also investigate the effects of feedstock impurity and hydrogen embrittlement of the membrane, and possible solutions.

Strengths and weaknesses

Strengths

- This project has good collaborations and plans.
- This project is relevant, well done and has good results.
- The team has achieved good technical accomplishments during the past year. This appears to be a good project that could meet the DOE targets and is work worth continuing.
- The project has good membrane fabrication capability though the yield rate and thin film quality are unknown.
- Good collaboration among teams is seen.
- This project provides a great means to produce hydrogen with high purity.

Weaknesses

- There is very weak project rationale and the team needs to consider how this could make sense.
- More needs to be done in this project and the team did not present a particularly clear road-map for the future.
- In this project no weaknesses were identified.
- This project lacks study on the feedstock impurity effects on the membrane performance.
- It is unclear if this project is applicable to H₂ central production.
- The lack of information on the hydrogen embrittlement issue and Pd-based alloy coarsening issue after a long period of operation is apparent in this project.

Specific recommendations and additions or deletions to the work scope

- The team should work with modelers to try to evaluate under what conditions this project would make sense.
- The team should consider looking at membranes with some of the gold replaced by silver. There is a need for more effort to be put into durability issues like resistance to cycling and start up. More work should be done with Doug Way, employing his electrolysis techniques.
- The team needs to address the quality assurance plan for membrane fabrication.
- Membrane durability/life and impurity tolerance are the two key factors to be addressed in this project.

Project # PD-08: Solar Cadmium Hydrogen Production Cycle

Bunsen Wong, Lloyd Brown, and Bob Buckingham; General Atomics Roger Rennels and Yitung Chen; University of Nevada, Las Vegas

Brief Summary of Project

The overall objective of this project is to demonstrate the feasibility and economics of a solar cadmium hydrogen cycle. Objectives are to 1) validate the key reaction steps with experiments; 2) establish design concepts for process steps based on experimental data; and 3) integrate process design concepts and solar field design into a flowsheet for a solar hydrogen plant.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **2.3** for its relevance to DOE objectives.

• This program has taken a different



- direction and this technology is on a different path to the program's goals.
- The objective of this project is to show the feasibility and economics of a solar cadmium cycle for hydrogen production, and therefore, this project supports the Hydrogen Program. There are several (over 140 thermo-chemical cycles investigated since 1955 but the question remains- why this Cd cycle? Is there anything new and exciting here? The uniqueness of this proposed Cd cycle project is not explained. In what way is this cycle better than the 140+ other cycles already investigated?
- The project's big picture "solar to H_2 " is very good.
- A \$3/kg target for H₂ manufacturer out in the middle of the desert is an economic challenge, and this is well above that.
- The project's concept of hydrogen production using solar driven processes pertains to the DOE Fuel Cells Subprogram.
- The project's use of such a dangerous and toxic material in such large volumes may not be feasible. It is not clear that this project would pass an environmental impact review or if the local community would accept it due to toxicity concerns. They should focus on materials with lower toxicity.
- The project addresses renewable hydrogen with solar.
- This project has significant health consequences and challenges of design during scaling up of the design. The project should be evaluated for hazards, and in this reviewer's estimate, it won't be a safe and feasible system. Cadmium has been banned by many nations, as it is a highly toxic and carcinogenic material. This process requires large quantities of the material while using very large, complex and difficult to seal environment.
- This project supports DOE goals for hydrogen production by thermochemical means but because of the high temperature of the main reaction and the need for high-flux solar, it is restricted in its applications.

Question 2: Approach to performing the research and development

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

- The project has a good approach.
- CdO decomposition, Cd vapor quenching, and hydrogen production are key steps for hydrogen production. Decomposition of CdO is going to be studied using a number of carrier gases. It is not clear how the decomposition rate is influenced by the carrier gas.
- The project is well focused on proof of concept (POC) demonstration and on key measurements needed to complete H2A guidance.

- The team fails to address a major barrier to this process which is toxicity.
- The team's examination of the reactions rates was effective.
- The project needs more work, perhaps modeling, to validate the rapid quench assumption. This seems to be a critical part of the process and should be further studied.
- The project is very high risk using so many novel, untested technologies.
- There needs to be testing the specific pieces of the scheme at larger scale.
- There is a need for clarification regarding how process steam is generated at night.
- Regarding the solar collector: how do cross beams reduce solar flux and utilization?
- Regarding air use: how does the team plan on handling entrained cadmium in emissions? Nitrogen would be effluent even under stoichiometric conditions.
- Regarding reaction time on CdO regeneration, the team should consider catalyzing this process or using a substrate to improve transport limitations of the process. The reaction appears to be equilibrium or kinetically limited. The team may want to look for promoters or catalysts.
- The project's need for a carrier gas is a handicap that impacts efficiency. The use of air as a carrier gas introduced problems with back reaction. The need for a quench to recover the cadmium is also an inefficiency that effectively eliminates a pathway for heat recovery.

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

This project was rated 3.1 based on accomplishments.

- The project team demonstrated the CdO decomposition at temperatures less than 1150°C. They also studied the effect of carrier gas on decomposition rate and found air is the best carrier gas. The team also demonstrated two pathways to use either molten or solid Cd to produce hydrogen. Progress is being made in modeling of Cd vapor quench.
- The project has done an extensive demonstration of POC.
- The team has acquired key data for economic analysis.
- The team has enabled/completed economic analysis
- The development of the thermogravimetric analyzer (TGA) in this project to measure oxygen reaction rates at the high temperatures was a significant accomplishment which can be applied to other systems.
- The reactor design in this project was very innovative.
- The cost analysis in this project uses unrealistic numbers and still cannot achieve the \$2-3/kg hydrogen cost target. For example, the heliostat costs are much too low.
- The CdO Cycle appears to be well characterized by the team.
- Significant experimental progress has been made in the laboratory especially with regard to producing hydrogen via steam oxidation of molten cadmium. However, yields are low and it is not clear that the introduction of a tumbling reactor filled with ceramic media can be supported by the energy budget. Rotating equipment filled with media are power hogs.

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

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

- The team is collaborating with the University of Nevada, Las Vegas (UNLV). The required slide explaining the collaboration was not presented or included in the package, and therefore what was done under this collaboration is not clear.
- My belief, from previous exposure, is that their collaboration may be outstanding, but the PI did not highlight who is doing what pieces.
- The working relationship between UNLV and General Atomics seem good.
- No collaborations were listed.
- While collaborations are satisfactory, it is clear that a more practical design is required for the solar reactor. The design showing a fluidized bed at the bottom and Cd vapor recovery via quenching at the top offers too much opportunity for the back reaction to occur. The CdO decomposition step and the quenching step should occur

very close in both space and time. A team member with capabilities to design a simple solar receiver needs to be added. The current design is too complex.

Question 5: Approach to and relevance of proposed future research

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

- The team may want to redirect work since program goals have changed.
- The project's CdO decomposition using a simulated solar source will be done in the future. The Cd-O₂ reaction is very important and therefore the PI is planning to study the effect of quench rate on recombination reaction.
- Given economics that are well above target, there is a need to engage some kind of limit analysis or process brainstorm to identify what (if anything) could possibly change to enable a step change in the cost. Then focus R&D in those areas in this project.
- The team's future plans should include identifying a critical path for development which will enable the technology to achieve the cost targets. The project does not seem focused. Identifying the critical path will help the PI focus the work to the most important areas.
- In this project, additional work on quenching should be done.
- Questions regarding relative sizing of solar collector vs. thermal storage, i.e., how much thermal storage is there, one day, one week, how does storage size impact collector costs, when system shuts down, and how long and expensive to start up should be considered.
- The team should create an Aspen-like process model including all equipment such as heat exchangers, pumps, etc., and project cost.
- Future work needs to address a simpler less energy intensive method for the hydrogen production step. Future work should also address a simpler design for a solar receiver.

Strengths and weaknesses

Strengths

- The team completed a preliminary flow design for the solar Cd cycle and studied the Cd-O₂ reaction rate. The PI seems to love the thermochemical reaction cycles. General Atomics is well known for its effort in developing thermochemical reaction cycles for hydrogen production.
- This is a beautifully executed program with focus on POC and key data for economic analysis (would hire these guys again in a heartbeat).
- The chemical cycle selected can store the activated Cd enabling 24 hour hydrogen production.
- General Atomics has a great deal of experience in chemical cycles.
- This cycle, relative to the others, has the potential for high efficiency.
- The project's two step reaction is among the greatest strengths. The use of a molten metal in the hydrogen production step is also a plus. The dark color of the CdO at high temperature is also a plus that allows for direct interaction between the solar flux and the reactant.

Weaknesses

- Economic analysis using helium as a carrier gas is questionable when the experiments have shown that air is the best carrier gas. It is wrong to use 1% back reaction rate for the economic analysis when the experiments are showing back reaction rates as high as 30 percent. The question remains: is this done because the economic analysis look good if a 1% back reaction is used? Also, how difficult is to pump liquid Cd and are there pumps to do this job?
- This specific technology in this project is emerging as just too expensive.
- The cadmium is very toxic in this project.
- The team's cost analysis shows the hydrogen cost targets could not be achieved even with the optimistic assumptions.
- Safety practices and assumptions in this project need to be externally verified.
- There is a very serious concern about the safety of this project, and questions of if the risks justify the rewards perceived.
- The high temperature required for the CdO decomposition step limits the available heat sources to high-temperature solar and, as experts in solar receiver design will explain, the higher the temperature of the main

reaction, the less efficient the solar receiver. The use of rotating equipment filled with ceramic media will reduce the overall energy efficiency due to frictional losses.

Specific recommendations and additions or deletions to the work scope

- The team should delete the analysis using He as a carrier gas unless advantages of using He is clearly explained. They should modify the economic analysis using more realistic figures for the back reactions. Questions regarding the toxicity of Cd, in particular Cd vapor, still remain.
- As discussed above, the need to identify if there are potential step-outs that could make step-changes in the economics.
- It is recommended that the team examine a different chemical cycle.
- The team should look at nitrogen as quench gas as it is much cheaper than helium and less prone to leakage. They should go ahead with engineering hazard analysis. With such a complex process involving reducing gases, solid transport, and hydrogen, it's never too early to look for problems.
- The project should place more effort on design of the solar receiver.
- The team should replace the rotating machinery with an alternative approach to producing hydrogen from liquid metal.

Project # PD-09: Solar High-Temperature Water-Splitting Cycle with Quantum Boost

Ali T-Raissi, C. Huang, N.Z. Muradov, S. Fenton, P Choi, D.L. Block, and J. Baik; Florida Solar Energy Center Robin Taylor and Roger Davenport; Science Applications International Corp. David Genders; Electrosynthesis Company, Inc.

Brief Summary of Project

The objectives of this project are to 1) evaluate photo/thermo-chemical water splitting cycles that employ the visible portion of the solar spectrum for production of hydrogen; 2) select a cycle that has the best potential for cost-effective production of hydrogen from water DOE target of \$3.00/kg H2); 3) demonstrate technical feasibility of the selected cycle using solar input in a bench-scale reactor; 4) demonstrate pre-commercial feasibility via a fully integrated pilot-scale solar hydrogen production system; and 5) perform economic analysis of the selected cycle.



Question 1: Relevance to overall DOE objectives

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

- This is a good project.
- The focus of this project is to conduct research on a new sulfur family of thermochemical water splitting cycle for large-scale hydrogen production using solar energy. More specially, the goal of this project is to evaluate the sulfur-ammonia (SA) water splitting cycle. This project is relevant to the DOE Hydrogen Program.
- The project's solar driven thermochemical cycles aligns with the Hydrogen Program RD&D objectives.
- DOE's MYPP indicates that the Solar Program will be reducing heliostat costs. It is unclear why this project is examining that aspect. It seems that improving the chemical process is enough scope.
- This seems like a complex process to produce H₂ to meet the DOE targets. The solar thermochemical cycle proved uneconomic and it is not clear how adding an electrochemical piece will make it cheaper. What assumptions were made to reach that conclusion?
- The researchers have done a very good job at determining the performance and potential economics of this system. However, this does not seem to be in line with the process requirements for the DOE targets.
- The overall goal of producing hydrogen using thermochemical methods is satisfactory in this project. However, as originally conceived, the splitting of the solar beam is too complex to be practical at high throughputs.
- The project fully supports the intent of the Hydrogen Program. The PI acknowledges that the cost objectives will be challenging, but possible, to meet.

Question 2: Approach to performing the research and development

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

- The project's approach was not explained clearly. What is RY'09 stand for? RY'09 appears in two slides describing this project's objectives. It is not clear why two schemes (photocatalytic & electrolytic) are evaluated for hydrogen production. Did the PI do a down-selection in previous year to come up with these two schemes?
- The PI exhibited flexibility in changing their approach when it became clear that their original approach would not be able to achieve the cost goals.
- The PI worked on heliostat cost reduction when the Hydrogen Program MYPP indicated that the Solar Program will be working on heliostat cost reduction.

- The project's shift to change from a purely solar driven process to a hybrid process was a good decision.
- The honest comment that the solar cycle approach is unlikely to meet targets and was down-selected was appreciated. Much of the project's work done on the solar thermochemical is now converting to the electrochemical + thermochemical cycle and little data is available to assess its promise.
- The project has a very creative idea for spectrum splitting. The concept appears to make more favorable economics of the design.
- The initial combined photochemical/thermochemical approach, which was novel and interesting, was abandoned in favor of a hybrid thermochemical/electrochemical approach and that was then modified to include a molten salt step. This project has gone off track and now has the flavor of a project aimed at screening different thermochemical cycles. The novel aspect was the combination of a photochemical step and a thermochemical step. Abandoning the photochemical step has placed this cycle in competition with other cycles that are simpler and have been under investigation longer. It is not clear that the latest embodiment has any advantage over what's gone before.
- The presentation delineated all barriers and how they are being addressed. Novel approaches are being utilized to address the most critical barriers in this project.

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

This project was rated 2.7 based on accomplishments.

- The project's technical progress appears to be good but the costs of electrodes may prohibit feasibility.
- The photoreactor system was evaluated in this project. The central receiver system was optimized to deliver energy. The team has completed the half-scale prototype glass reinforced heliostat and demonstrated drive system features and controls.
- The team's work on the electrochemical aspect of the project was appropriate.
- The PI was working on heliostat which the Hydrogen Program MYPP indicates is the responsibility of the Solar Program.
- Changing to potassium from zinc and eliminating the solids was a positive development of this project.
- The team needs to continue decreasing the cell potential of the electrolyzer.
- There has been only fair progress toward meeting goals, given the shift in project focus. Many unanswered questions remain.
- There are problems with 24/7 operation given solar availability.
- Modest progress has been made in this project. However, some barriers appear to have been neglected. In the chemical equations, aqueous ammonium sulfate is shown being produced in one step but solid ammonium sulfate is used in the subsequent step. How did this go from an aqueous solution to solid material? There have been a number of sulfate cycles proposed over the years and every one of them suffered a large energy penalty associated with the recovery of the solid sulfate from an aqueous solution. This was not addressed in the presentation nor the slides and can be a real show stopper if it is necessary to boil off excess water. This needs to be addressed.
- Significant progress has been made on production and efficiency targets, but it is not clear if the cost barrier can be overcome in this project.

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

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

- The project has used a good variety of partners with diverse interest levels.
- SAIC is the lead in this project. Electrosynthesis Company, Inc is the industrial partner. Their collaborative roles are defined in this project.
- The project appears to have a strong team with good interaction.
- It appears that the project has a reasonable set of collaborators.
- This is a good team collaboration with the solar and electrochemistry experience necessary for the project's success.
- Good collaboration among team members is providing new approaches to solve problems.

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<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.9 for proposed future work.

- The project is not slated for future funding, although results so far appear promising.
- The PI had too many slides in his presentation.
- The team is focusing on the important aspects of the process.
- The forward plan for this project is very general and does not seem to specifically address key challenges.
- The project's proposed work is too heavily weighted toward solar receiver development considering the early stage of development of the chemistry. More effort needs to address the electrochemical cell and getting current density up and voltage down. For all practical purposes, this cycle is now in competition with the hybrid sulfur (HyS) cycle and so needs to show equal or better operational parameters for the electrochemical cell, than the HyS electrochemical cell, for this cycle to be considered competitive.
- Barriers are clearly identified and are being addressed by the team.

Strengths and weaknesses

Strengths

- The team members seem to know what they are doing.
- The PI has shown great flexibility in changing their approach in order to reduce cost.
- They have a strong team.
- Project execution is very thorough and clean. This team has done very good work.
- This project has a good team.
- Continued innovation has led to improvements in this project.

Weaknesses

- The efficiency of this process can not be high. It can only be in the range of about 22 percent. The ammonia and sulfur cycle has been well studied for several decades and others have proven that it is a difficult process to optimize and get better efficiency. The question remains: why are these investigators going back to this cycle?
- The PI had too many slides (35 slides) for a 20-minute presentation. The presenter did not have time to explain the collaborations and the future plans. This talk was poorly organized.
- A hybrid cycle requires electricity which will need to be generated on-site or brought in from the grid. In order to achieve 24/7 operation, as the PI indicated was a goal, they will need to be connected to the grid.
- The cost figures assume operation in the desert and therefore underestimate the cost of water and permitting (mostly the water rights cost). It is unlikely that the team would be able to get the water rights for this system in an area which has very little water available.
- This project deals with a complex process with many hurdles remaining. This does not seem to rank at the top of the thermochemical projects.
- The project has too many steps in the cycle requiring a separate reactor.
- The project has too many different chemical reagents needed in its latest embodiment; zinc, potassium, and ammonium sulfates. The HyS cycle uses only one, that being sulfuric acid.
- Much work needs to be done on the electrochemistry of this project.

Specific recommendations and additions or deletions to the work scope

- The sulfur ammonia cycle has been researched for several decades and proven to be difficult to optimize. This project should be dropped.
- The heliostat work is needed, but not sure if this is the right project for it. The Hydrogen Program has very little resources. Those resources should be focused on developing the chemical cycle and not the heliostat. The Solar Program's budget request is very large and they should have enough resources to address the heliostat costs.
- The team should identify the critical path which would enable the technology to become economically as well as technically viable.
- The team should carry out the proposed plan expeditiously. The team should hone down on the real technical challenges.
- The solar receiver work can wait. The team should solve the problems with the electrochemical cell first.

Project # PD-10: Solar-Thermal Ferrite-Based Water Splitting Cycles

Alan W. Weimer, Jonathan Scheffe, and Melinda M. Channel; University of Colorado, Boulder

Brief Summary of Project

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



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

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

- The project's big picture of solar to H₂ is okay, but concerns about the relevance of a process with a target cost of \$4/kg at plant gate out in the dessert remain.
- The basis of this project being solar driven thermochemical processes is relevant to the DOE Hydrogen Program.
- The project's process attempts to use a potentially low-cost substrate.
- This project is relevant for turning high-temperature heat available from a solar receiver into hydrogen. However, it is not compatible with high-temperature nuclear.
- The project fully supports the Hydrogen Program objectives for solar thermochemical hydrogen production.

Question 2: Approach to performing the research and development

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

- If the project's economic basis is unsupported ferrite, then the proof of concept (POC) should be done to measure conversion levels with unsupported ferrite. If materials basis is the atomic layer deposition (ALD) (which is <5% ferrite), then the economics need to be evaluated assuming that all that carrier (95%) is going through the solar furnace absorbing heat. This is a major weakness of the project's approach.
- The team is using less toxic materials than other cycles.
- The project's operating temperature of less than 1300°C has some materials which can work compared to other cycles which require temperatures greater than 1500°C.
- The ALD approach to fabrication may be very expensive considering the quantity that is required for this project.
- The team needs to increase the cycle life testing.
- For this to be economical, the process needs to operate 24/7 which will require activated material storage, without the material deactivating. This needs to be studied and should be prominent in the scope of the project.
- The project's ferrite cycle appears promising.
- The project calls for hundreds (thousands?) of cycles to assure particle integrity.
- Was thermal storage for night operation considered in economics calculations? Project costs need a more detailed break down.

- Energy storage is not addressed in this project. The question remains: how does this process work around the clock?
- Is 1200°-1400°C a realistic temperature range for this project? Has this been demonstrated or projected from a laboratory project?
- The project's approach is good with respect to using a small number of steps to accomplish hydrogen production. It is handicapped, however, in that it requires the transport and handling of solid materials, as opposed to liquids and gases as are typical of other cycles. It also is limited by the need to remove oxygen under vacuum.
- The project focused on a narrow scope of materials science objectives.

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

This project was rated 2.7 based on accomplishments.

- The team's description of the objectives is superficial at best, therefore measurement against objectives is nearly impossible. Furthermore, if there is a general need is for some POC within an economic framework, then there is a total disconnect here as the economic guidance materials are different from research materials in a way that is critical to the analysis.
- For the economic analysis the team should not assume that an oxygen credit and the capital cost seems too low (especially for the heliostats). This analysis should be re-done.
- Initial tests in this project are well done.
- This project requires more cycle and lifetime tests are needed, especially for the ALD coated substrates.
- Good work was done by the team in evaluating ferrites.
- ALD shows improved kinetics in this project.
- ZrO₂ is not addressed in the ASPEN model. The team should show how substrate thermal cycling affects the process.
- What is the degradation mechanism or hypothesis of what is causing the degradation in this project. What can be done to address this degradation?
- Good technical progress is shown in this project but more thought should be placed in the design of a solar receiver able to do large scale throughput. A relatively simple design for a solar receiver was shown, suitable for proof of concept but not a design conducive for high throughput in this project.
- Progress is being made in addressing materials and cost barriers for this project. The solar field design appears to be specified but not validated.

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

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

- The project team's collaborations are mentioned at the end of the presentation but there is no indication of how they fit into the critical progress of the program.
- The project team has strong interactions both nationally and internationally.
- The team has good publications regarding this project.
- This project can improve by including an engineering partner with experience with large projects to better estimate costs.
- This is a good team but needs U.S. collaborators.
- This is a good team and strong collaborations are evident.

Question 5: Approach to and relevance of proposed future research

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

• All the project plans are ALD, but all the economics are based on unsupported ferrite and require high (35%) conversion. This is a total mismatch because the solar field is a key cost, and ALD materials require solar energy to be wasted heating the >95% carrier. The project should not continue until this mismatch is resolved.

- The team needs to increase the cycle life studies.
- The PI needs to include work on how the team will enable 24 hour operation. This can be achieved by thermal storage or activated material storage. This should be a major focus of the work. Without 24 hour operation it is extremely unlikely that the process will be able to achieve the DOE cost targets.
- The project should concentrate on stability of materials upon multiple cycling.
- The team should include attrition testing for moving bed work.
- Proposed work with zinc looks promising in this project.
- It is not clear how future work identified is aimed at overcoming barriers.

Strengths and weaknesses

Strengths

- This project has a cycle that contains and uses less expensive materials and less toxic materials compared to other cycles.
- This project may be able to operate 24/7, but the project team needs to verify this claim.
- This project uses simple chemistry and has well defined reactions.

Weaknesses

- The ALD is not just an issue of particle cost and needs to be addressed.
- High utilization of solar flux is critical for this project because the heliostat field is very expensive. The use of solar flux to heat carrier must be included in the economics. Proposing high-carrier solids while doing economics on zero-carrier solids is not unacceptable for this project.
- The cost assumptions in this project presume that cheap water is available in the desert. The water rights and water cost in arid regions are much more difficult and expensive to attain than what is assumed in the economic models.
- The team needs to demonstrate that their coated substrates will not disintegrate.
- The assumption that ALD can be economical at the scale of production that is required needs to be validated by the team.
- The team has not included enough studies on 24/7 operation.
- The team has not presented a critical path which leads to achieve the technical and economic DOE targets.
- The project and team needs a support for the ferrite to make this work well.

Specific recommendations and additions or deletions to the work scope

- This project needs cycle life testing to validate that the team can use the supported material.
- The team needs to identify a critical path which will enable the pathway to meet the technical and economic DOE Targets.
- Further work in this project is recommended to addresses how the proposed reaction can be accomplished in a high throughput reactor.

Project # PD-11: R&D Status for the Cu-Cl Thermochemical Cycle

Michele Lewis; Argonne National Laboratory

Brief Summary of Project

The objective of this project is to develop a commercially viable process for producing hydrogen based on a thermochemical cycle that meets the DOE cost and efficiency targets. The Cu-Cl cycle was chosen and the current Aspen flowsheet indicates that it is possible to meet the targets if assumptions can be validated. Features that promote meeting targets include: 1) the 550°C maximum temperature reduces demands on materials; 2) yields near 100% in hydrolysis and oxychloride decomposition without catalysts (no recycle streams in these reactions); 3) conceptual process design uses commercially practiced processes; and 4) preliminary H2A analysis indicates H₂ production costs are within range of 2025 target if assumptions validated.



Question 1: Relevance to overall DOE objectives

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

- This project has both nuclear and solar sources of heat that are relevant to DOE's program goals.
- The project's thermochemical water splitting aspect supports the Fuel Cells Subprogram objectives.
- This is another thermochemical cycle-based project co-funded by DOE, EERE and the Office of Nuclear Energy (NE). It appears to have the potential to meet targets by 2025 but may require some real breakthroughs.
- ANL scientists have been developing the Hybrid Copper-Chlorine Cycle for thermochemical production of hydrogen for a number of years.
- The project's temperature range of this process matches up well with medium and high-temperature advanced nuclear reactors and could also be adapted to moderate temperature solar, which make this almost a universal cycle.

<u>Ouestion 2: Approach to performing the research and development</u>

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

- The project has a good approach to adapt commercially available solutions to unit operations.
- The minimization of copper (Cu) crossover is dependent on anion exchange membrane, which may have a lifetime issue.
- The thermochemical cycle in this project requires low temperature (550°C).
- The project team is focusing on the correct areas.
- The team should develop a credible critical pathway to achieve DOE's cost and technology targets in a timely manner.
- The approach to work on the separate reactions seems appropriate in this project. The use of the ultrasonic nebulizer seems to have helped progress. Numerous breakthrough technologies seem to be required to make this a viable process. This project must still be considered in its early stages despite several years of work.
- The overall approach of this project is good. However, the report does not clearly state how the different steps of the process, such as hydrolysis, oxychloride decomposition, electrolysis, and separation will be completed

with appropriate modeling, design, process control, construction and testing. Some of the unit operations are shown as conceptual designs of the process. A more definitive approach needs to be presented.

• The cycle this project uses has several material handling problems. The approach is well focused on solving those problems but suffers due to the use of non-standard methods. In particular the use of an ultrasonic nozzle does not bode well for a scale-up to high throughputs.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

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

- Good progress has been made on many of the technical issues in this project. Progress on the electrochemical step appears to be slowing as the team has pushed end date forward.
- The team has created a conceptual design based on many industrial processes.
- The cost estimate of this project was based on the conceptual design and it did not achieve the \$2-3/kg H₂ cost target. It is highly likely that the cost will increase more so as the process gets refined.
- No analysis was completed to identify what the project needed to implement or do to achieve the cost goals.
- The project team needs to significantly improve the electrochemical step to achieve reasonable life and decrease costs.
- The team needs to demonstrate that the particles will not sinter, aggregate, etc. over time under the high-temperature conditions. They need to do a cycle life / durability test.
- It is hard to assess how much technical progress has actually been made, and how much is relying on future developments in this project.
- The primary focus of this project is on hydrolysis with modeling and demonstration of high yield and free flowing Cu₂OCl₂ powder. Yet, no model has been presented on how to optimize (1) the particle size distribution of the powder; (2) heat and mass transfer rates; and (3) process parameters for both high yield and good flow properties. It is anticipated that as the size of the droplets produced by ultrasonic nebulizer is decreased, the hydrolysis reaction yield will be improved with the increasing surface area but the fine powder produced in this way will be cohesive as a dry powder.
- Excellent progress has been made in defining the chemistry and developing approaches to mitigate side reactions in this project. The development of a membrane to prevent copper ion crossover is a significant achievement.

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

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

- The project has a good cross-border program including a multitude of universities. It is well leveraged with other programs using their own funding.
- The project team's collaboration with partners, other than Atomic Energy of Canada, Ltd., is good.
- The collaboration with Atomic Energy of Canada, Ltd. was important to the success of the project. The lack of cooperation has impacted the project significantly by slowing the progress.
- The list of collaborators seems strong and appropriate in this project. It is not known, however, how well the PI is managing all the collaborations.
- The complexity of this multi-stage process requires a strong collaborative approach and the authors are giving their best efforts in maximizing the DOE investments by jointly working on the problem with other groups. However, the details of the collaborative efforts are not sufficiently presented. The team needs to show how the current technological barriers in each of these processes will be solved by the different groups working on the Cu-Cl cycle.
- This project has an excellent international team.

Question 5: Approach to and relevance of proposed future research

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

• This project has a great unknown of future funding.

- Back up plans in case of the project's failure, such as not being able to find a stable anion exchange membrane, should be identified.
- Titanium is not stable in HCl unless it is used in combination with Pd to create an alloy, Ti-Pd. As an alternative the project team should look at De Nora Tech, an Italy-based company that has a branch in Ohio that can coat titanium with RuOx, which is stable to HCl.
- The project team needs to consider cycle life and integrated experiments.
- The team needs to identify a critical path and show that it is possible to achieve the cost targets.
- The project's forward plan is reasonable, but many good things need to happen.
- The team provided a good general description of the future work plan, but the objectives are not stated with specifics.
- Proposed work in this project will continue to address issues with chemistry and separations. However, the project should also begin looking at scale-ups to larger sizes.

Strengths and weaknesses

Strengths

- The project has a very good team to address the problems in bringing about this technology.
- This project is well managed.
- The project implements and uses a low temperature process.
- A potentially strong team is heading this project.
- This project has a good team.
- The authors have an excellent track record in this field. The proposed Cu-Cl cycle is one of the most promising processes for hydrogen conversion at a moderate temperature (435° 500°C). Their collaborative efforts with Atomic Energy of Canada Ltd. and Nuclear Energy Research Initiative Consortium (NERI-C) have a good chance for success.
- The international team of investigators is this project is its greatest strength. Also, the fact that all the reactions can be performed at temperatures below 600°C is a very big plus.

Weaknesses

- The project's anion exchange membranes are not nearly as stable as cation or Nafion® type membranes. What is the back up plan in case these do not work? What data supports the anion exchange membrane reducing crossover?
- The materials used in this project are very caustic.
- The team has not identified a critical path to achieve the cost goals.
- The project has had relatively slow progress and many remaining hurdles.
- The report lacks some the specifics on (1) the technical barriers being solved; (2) modeling studies; (3) process optimization; (4) material engineering components related to heat exchangers, corrosion resistance, and mixing; and (5) cost reduction steps.
- Side reactions, particularly the production of chlorine, are a problem that still needs to be addressed in this project. The need to remove water to concentrate products is also a weakness although the use of electrodialysis is a step forward.

Specific recommendations and additions or deletions to the work scope

- The project should consider increasing membrane efforts.
- The project teams should have a back up plan if no me membrane becomes available. For example, can you use electrode cycling to remove Cu build-up?
- The project teams should consider putting more effort on materials compatible with a very corrosive environment.
- As part of the close out, the team should identify a critical path that would enable them to achieve the target costs. If a reasonable path cannot be identified then that should be noted.
- The team needs to demonstrate cycle life of the materials.
- The authors should submit specific objectives for their proposed studies. This project merits further funding.
- This project needs to begin addressing scale-up to large sizes and throughputs. In particular, what will production scale equipment look like?

Project # PD-12: Sulfur-Iodine Thermochemical Cycle

Paul Pickard; Sandia National Laboratories Ben Russ; General Atomics

Brief Summary of Project

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

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

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

This project addresses the big picture of



- H_2 from nuclear or solar, but a concern remains about the project's relevance when cost targets are so high for H_2 at the plant gate.
- This project is aimed at DOE EERE and NE objectives. Cost targets should have been mentioned.
- The S-I cycle is one of the most promising methods for producing hydrogen. This is due to the rate of hydrogen production as well as the efficiency of production can compete with the currently used steam methane reforming (SMR) process but with no carbon footprint. Once the material engineering issues are resolved, the project has a strong potential to reach DOE goals on producing hydrogen in a commercially viable process.
- This project fully supports DOE's objectives but is not necessarily critical since there are other approaches to both sulfur (S) and iodine (I).
- This project addresses hydrogen production in particular and thermochemical hydrogen production in general. Until credible and reviewed production costs of this process are available, it will not be possible to assert whether or not this is critical to the Hydrogen Program.
- The project's cycle is a good match with both the Nuclear Program and the Solar Program.

Question 2: Approach to performing the research and development

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

- The absence of a sulfur scrubber, which prevented fully integrated operation, seems like a flaw in the project's approach.
- The project's approach appears to be reasonable. This is a very challenging project to manage all three reactions safely.
- The project's interface unit allows separate operation which lowers coupling between unit operations.
- The success of the S-I cycle using its fluid-based "closed loop" process depends upon overcoming the current technological barriers involved in the decomposition of H₂SO₄ and HI in a highly corrosive chemical environments at a high temperature. Fabrication of appropriate materials that are both chemically and thermally stable is needed for reaching the DOE goals. The approach of this project is targeted in overcoming this challenge at a reasonable cost.
- The focus of the research for this project has been on the development of lab scale experimental setups for each of the three reactors and on testing their performance both separately and after integration of the three units.
- The project's integrated laboratory scale (ILS) should be essential to planning for pilot scale and would permit adequate data to support pilot design and decision-making whether or not to proceed to pilot. Production rate of

100 I/hr is barely adequate to support design and decision to move from ILS to pilot scale-up. The Bunsen reactor design performance is inadequate to provide feed to HI reactor. The project's testing regime is inadequate to demonstrate Bunsen reactor performance.

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

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

- The project would have been "outstanding" if the objectives had been detailed in the discussion. Objectives are not stated in enough detail to enable more than a "ran ILS" check mark. Nonetheless, there has been a lot of work accomplished.
- Some major enabling accomplishments in this project appear to have been made over this period.
- The Bayonet reactor design is enabling for H_2SO_4 to SO_2+O_2
- The Bunsen reaction is most challenging but appears to have been resolved in this project.
- In this project, no control feedback is seen between stages as of yet.
- Given that the project is complete, it would have been appropriate for the team to give some estimation of the hydrogen delivery cost with this technology.
- Significant progress has been made in this project on each of the three reactor operations and their interconnection for producing hydrogen according to the integrated lab scale units design. Both corrosion and separation problems have been addressed; however, more emphasis is needed in these two areas with respect to the scaling up process for industrial application. For example, stability of the glass lined stainless steel (SS) during thermal cycling in a highly corrosive environment could be a serious problem in large scale installations. Availability and cost of these components for installations and plant maintenance may determine the overall success for commercial application.
- Is hydrogen is not detected in HI decomposer? Is the hydrogen infusing with the reactor vessel?
- This project has a very good subsystem integration process.
- The project's progress is excellent. The full integration of the test section was never achieved. This shortfall requires that either the current ILS facility be "upgraded" or retrofitted to permit truly integrated operation or another integrated test system be constructed and run.
- Much good work has been accomplished in this project but significant progress has not been made in overcoming many of the materials issues associated with corrosion. The process of extractive distilling HI from phosphoric acid is a handicap that saps efficiency.

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

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

- In this project three partners build skids, which are all then integrated at General Atomics. This is evidence of a good collaborative effort.
- The collaboration between General Atomic and Sandia National Laboratory is a good one.
- The project work reflects an exemplary cooperation between different organizations. The authors could explore possible cooperative studies with the Japanese Atomic Energy Research Institute since this institute is in the process of building a large scale plant using the S-I cycle for hydrogen production.
- Three institutions were in close coordination to achieve the ILS construction and operation. Nevertheless, there appeared to be inadequacies in overall supervision and decision-making authority to deal with both institutional and international issues. Adequate centralized supervision and decision-making authority would likely have resulted in better progress and more useful operational information.
- This project has an excellent international team.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.2 for proposed future work.

- This project's future research was not identified even as a speculative next stage.
- This project is complete.
- The current project has been successfully completed. While further research will be continued, no specific plan for future research has been presented.
- This project is complete.
- No proposed future work was provided. If the ILS accomplishments had been sufficient to move to the next phase, perhaps no proposed future work would be necessary in light of the planned Nuclear Hydrogen Initiative (NHI) down-select this summer. It is likely that there will be insufficient information to effect a down-select among the three candidates and the ILS effort has significant deficiencies so additional work would appear appropriate.
- Reactive distillation may be a good solution for the problem of HI concentration in this project. Also, control systems need to be addressed and operation of all sections simultaneously should be addressed. More attention needs to be paid to cross contamination.

Strengths and weaknesses

Strengths

- This project has a competent team.
- Both General Atomics and Sandia National Laboratory have been doing pioneering research in this field since the invention of the S-I cycle by General Atomics. The project has been well planned and executed. The results are impressive and the presentation was excellent.
- This team has done excellent process integration work.
- The Sulfur Iodine thermochemical cycle is the most studied thermochemical hydrogen production cycle. This feature should serve to help identify priority and focus in the production enterprise. The process shares a similar high temperature step with the hybrid sulfur process, permitting resource sharing. Finally, the process is susceptible to operating with both solar and nuclear thermal sources, allowing some flexibility in future operation.
- This project has a good team with much experience.
- The chemistry in this project is well understood.
- The maximum temperature below 1100°C in this project makes for a good match with several advanced heat sources.
- The S-I Cycle can be easily scaled to large sizes and throughputs.

Weaknesses

- There are ongoing technical challenges. This is a difficult project.
- The project has no economics provided.
- Specific recommendations along with a cost analysis have not been provided for nuclear hydrogen technology decisions. An alternative application of solar radiation concentrators was not considered for the S-I cycle.
- ILS proved insufficient to answer many questions, especially with regard to truly integrated operation that would assist in pilot plant design and, instead, would answer many questions regarding the actual chemical process costs that are important to understanding true hydrogen cost at the gate. Reduced time and money makes this process vulnerable to premature down-selection.
- This project has three chemical reactions and one difficult physical separation in cycle requiring significant process equipment.
- This project has corrosion caused by HI which is a materials issue that is expensive to overcome.

Specific recommendations and additions or deletions to the work scope

- Funding for this project should continue for studies on large scale design, catalysis, separation of the reaction products, removal of the product gases, stability of the candidate materials, and a comprehensive cost analysis.
- From the perspective of the EERE R&D program, renewed effort in operating the ILS or modifying the ILS to permit fully integrated study of the cycle would be essential before further investments in the cycle implementation under solar power would be justified.
- This project should have continued funding.

Project # PD-13: Hybrid Sulfur Thermochemical Cycle

William A. Summers; Savannah River National Laboratory

Brief Summary of Project

The overall objective of this project is to develop and demonstrate the hybrid sulfur thermochemical process as a viable option for large-scale hydrogen production using nuclear energy. The objectives for fiscal year 2009 are focused on improving performance and operating lifetime of the SO₂-depolarized electrolyzer using a proton exchange membrane-type cell. Hightemperature portions of HyS Cycle are common with Sulfur Iodine Cycle and are being developed in parallel with this project. System design and economics have been performed in conjunction with industry to ensure relevance and to establish realistic performance and cost goals.



Question 1: Relevance to overall DOE objectives

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

- In this project, if the heat can be driven with solar heat, the electrolysis system efficiency would be good for not only fuel cells but industrial H₂ customers.
- Regarding the big picture of this project, H₂ from solar/nuclear is good. However concerns about relevance of this program deal with costs. This project has H₂ cost of \$5/kg at plant gate which are far from market.
- This project has a novel approach. However, the team's approach to DOE cost targets is an issue. These cost targets should have been mentioned in the presentation.
- The project's hybrid thermochemical process has a strong potential for large scale hydrogen generation with efficiency close to 40% or better.
- The project is fully supportive of DOE program objectives, but not necessarily critical because there are other thermochemical cycles that could provide solar-powered hydrogen production. As cost projections become more firmly grounded in data, the essential nature of the project will be clarified.
- This particular thermochemical cycle has elements that are common to several other alternative cycles and progress made here may have applications beyond this Hydrogen Program.

Question 2: Approach to performing the research and development

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

- This program is indeed highly focused, but only on the SO₂-depolarized electrolyzer using a proton exchange membrane (PEM) type cell, and in particular crossover. No or little work has been done on integration into a prototype of breadboard system in this project.
- This project has an excellent focus on proof of concept (POC) issues and on data needed for economics.
- It is not clear what the DOE targets are for H₂ costs, but they should have been included in the presentation. This information would be needed to compare costs with economics proved in end of packet slide.
- The project team's overall approach on the development of the process in collaboration with other federal laboratories, universities, and industrial partners is very good. Specific objects are well planned in some areas. While the sulfur crossover problem has been has been given the needed attention, corrosion problems due to the presence of high concentration of H₂SO₄ (close to 50%) have not been addressed adequately.

- The project's SO₂-depolarized electrolyzer (SDE) reactor formed the focus of the work during the past year. The project also included the use of SNL Bayonet design permitted essential program focus on SDE. The project plan is comprehensive and permits high visibility for management purposes. The question that always remains is whether additional external expertise in electrolyzer design and tests would accelerate progress and reduce costs.
- The project has identified key barriers to efficient electrochemical cell operation and has designed approaches to overcome the barriers. Progress is being made through innovative electrochemical cell design.

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

This project was rated 3.3 based on accomplishments.

- This project provides a very innovative solution for sulfur crossover. Instead of relying on material advances (membrane or electrode) they have identified conditions that allow minimum crossover.
- The project has well defined goals and is nearly accomplishment all of them.
- It is unclear what the durability of the system and membrane under an extended run time.
- Regarding slide 10, was the reversible potential reduced by 87% or was the 87% referring to the water case?
- The project's accomplishments toward overcoming some of the major barriers suggest the overall feasibility of the process used. More integrated laboratory scale investigations are needed for solving the remaining technical problems and for scaling up studies.
- The project's apparent resolution of sulfur crossover is a major step forward. How good the solution actually is remains to be seen. Additional testing will be required before the electrolyzer is selected for integrated testing.
- Durability testing for this project remains as an outstanding requirement before transition to ILS testing would be appropriate.
- The project has shown success in reducing sulfur crossover from anode to cathode and their approach was successfully demonstrated in 200 hours of testing. These cells demonstrated no sulfur buildup in the separator which was a failure mechanism in previous work. This, by itself was a great accomplishment. However, there is still concern about the small amount of sulfur dioxide that is still getting through the membrane separator to form hydrogen sulfide in the cathode. Hydrogen sulfide in the hydrogen exhaust stream should be a concern even at levels of a few hundred parts per million and should not be taken lightly.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- The project team holding a workshop amongst the various and highly diverse (government, university, industry) partners is commendable.
- This project has many collaborations. Some are "core" collaborations without whom progress could not have been made and are well recognized in the presentation. Some more peripheral collaborations are also acknowledged.
- This project seems to have a good combination of partners.
- The project's collaboration is excellent.
- The project has an excellent team of collaborators. In particular, teaming with Giner for electrochemical cell design was a good move.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- Strongly endorse running an integrated system.
- The project team had a fairly superficial description of future plans which is perhaps due to fitting the situation of waiting for a down-select decision.
- The project's future plans should include extended durability tests at a reasonable scale.
- The project's overall approach for future research is stated without sufficient details.

- Future plans are hostage to program continuation, but the program has taken steps to plan for them eventually. Electrolyzer selection should be the level 1 milestone so that all the button testing can terminate and resources can be directed to integrated lab scale testing.
- There are issues that still need to be addressed in this project at a fundamental level. Two of these are the cell voltage and the small levels of sulfur crossover that is still occurring. These are passed over as being only minor annoyances but they may become significant issues as the system is scaled up.
- The program needs to demonstrate long term durability of the electrolyte membrane.

Strengths and weaknesses

Strengths

- The project's use of electrolysis to depolarize SO₂ is a good one.
- The team has come up with a clever solution to minimize crossover.
- The project has a strong team of diverse backgrounds.
- The project appears to have a competent team focusing uniquely on a combination of thermal and electrochemical approaches. Good progress is shown.
- The project work is undertaken by a team of well qualified engineers and scientists and the progress to date shows a strong potential for success.
- The project's process is susceptible to operation with both solar and nuclear thermal power sources and shows promise of meeting DOE cost goals. The process is similar in its high-temperature step with regards to the sulfur iodine process so that resources are partially process-shared.
- The project has only two chemical steps in the cycle.
- The project's sulfuric acid decomposition is well developed and presents no serious materials problems.
- The electrochemical cell development leverages advancements being made in PEM fuel cells.

Weaknesses

- It is unknown if the special operating conditions can hold over the 40k hour target for lifetime. No data were given on preliminary outcomes, or whether small amounts of crossover are still occurring after, for example, 1,000 hours.
- There is no correlation between level of sulfur impurity and lifetime.
- Issues regarding durability of the system and whether 50 hours without sulfur buildup is adequate are significant.
- The overall feasibility of a commercially viable hybrid process for producing hydrogen needs to be established by comparing the hybrid cycle with other processes of hydrogen generation.
- The electrolyzer design, extended testing and costing remain as critical elements for assessing utility of this process relative to competitors. Time and money are running out so that there is a possibility of premature down-select in this project.
- The use of an electrochemical cell limits the cost savings that can be realized by scale-up to industrial size equipment. Increasing the cell size by a factor of 10 increases costs by a factor of 10, unlike the cost savings that might be realized by scaling up chemical reactors.
- The need for concentrated acid coming from the electrochemical and going into the acid decomposition reactor has a significant impact on efficiency.

Specific recommendations and additions or deletions to the work scope

- The project team should work with Pickard of SNL/GA/CEA team on integrating into a full system.
- The team needs to determine what happens during an uncontrolled shutdown of the electrolyzer (gas feed on, loss of power to electrolyzer). Is the effect reversible or permanent?
- Durability testing needs to be done in this project.
- The project is innovative and deserves additional funding unless a comparative cost analysis does not support further advancements.
- The addition of long term durability tests to the program is recommended.

Project # PD-14: High Temperature Electrolysis System

Steve Herring; Idaho National Laboratory

Brief Summary of Project

The overall objectives of this project are to 1) develop an economical method for the CO₂-free production of hydrogen in centralized facilities; and 2) configure the plant for the integration of heat and electricity from a nuclear reactor and for interactions with the grid to accept or supply power as wind/solar sources vary. The objectives for the past year were the 1) construction and operation of the threemodule Integrated Laboratory Scale (ILS) experiment for long-duration (>1,000 hrs); 2) organization and sponsorship of a workshop on solid oxide electrolysis cell (SOEC) degradation with experts from the solid oxide fuel cell/SOEC community; 3) characterization of degraded cells to



determine silicon/chromium transport, delamination and destabilization of electrolyte; 4) tests of short stacks and button cells of other designs and from other manufacturers; and 5) building of capability to simultaneously run five small tests.

Question 1: Relevance to overall DOE objectives

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

- The overall objective of this project is to develop an economical method for the CO₂-free production of hydrogen in a centralized facility. This project supports the DOE Hydrogen plan (nuclear hydrogen initiative).
- Ability to switch H₂ production to aid in grid stability is a good feature of this project.
- The solar-thermal is a good fringe benefit.
- The general project concept is responsive to the Hydrogen Program. The work is attempting to develop a hightemperature process and ILS for hydrogen production using nuclear (or solar) heat/power. The PI understands the goals and objectives of the program and is working to attain those goals/targets. The project appears to be following the agreed upon work scope by DOE and INL.
- This is an ongoing project for generating hydrogen from steam by using high-temperature SOECs in stack formation. The team of researchers lead by the PI at INL has been working on this process for more than six years and the project has reached a stage for pilot plant development with a goal for producing hydrogen with optimized efficiency, cost and durability. The project is very relevant in reaching the goals of DOE for hydrogen production.
- This project fully supports program objectives, but other electrolytic processes are possible with which to produce hydrogen. Cost and operational issues will need to be resolved before the level of critical support to program objectives can be assessed.
- Although funded through the Nuclear Hydrogen Initiative, this work has a much broader appeal. Large-scale, high-efficiency water electrolysis can have applications in intermittent and renewable energy storage as well as hydrogen production.

Question 2: Approach to performing the research and development

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

- The approach of this project is to develop energy-efficient, high-temperature SOECs for hydrogen production from steam. Nuclear heat will be used. The approach is to increase the SOEC stack durability but unfortunately the performance of the stack degrades too fast. Twenty percent per 1000 hr is a high rate. This project is not making good progress.
- The team's use of solid oxide electrolyzers could significantly reduce the capital costs for the production of H₂.
- The project has a very good approach with regard to building test systems and analysis of failure mechanisms.
- The project's approach is based on a relatively old principle (25+ years) that has been researched by numerous investigators over the years. The principle may be applicable in some small scale applications (e.g., oxygen sensors) but expansion to a relatively large scale may be extremely difficult. Ceramic materials are inherently difficult to deal with (fabrication, sealing, etc.) and these problems are compounded exponentially with multiple stack units. The investigator appears aware of the issues and is taking steps to address them. The approach is acceptable for identifying and solving the necessary issues. Another issue concerning the approach is the incomplete conversion of the water/steam feed which will require additional separation and polishing. This could be a major cost issue in and overall larger system. The presenter failed to discuss this issue and simply stated that the membrane separation will be employed. This is not an answer and will not to work well at this time either. Condensing the stream may be an approach; however, it is not clear how much conditioning will be required for the water reactant which may become another cost issue.
- A comprehensive approach is presented both in terms of overall goal and specific objectives. The goals for efficiency, cost, and durability are not expressed in quantitative terms. The aims are to design and construct a 200 kW pilot plant for producing hydrogen in a commercial scale. This will be a major breakthrough in CO₂-free hydrogen generation if successful.
- The project plan seems adequately focused on the discovery of an acceptable cell design. However, it appears that inadequate design practices are applied to cell test stand configuration. Test stands should be designable before construction and implementation.
- The approach for this project is satisfactory and is addresses many barriers simultaneously. However, the jump to a multi-kilowatt size demonstration may have been premature since there are still some materials issues that have not been solved.

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

This project was rated 2.8 based on accomplishments.

- The project demonstrates hydrogen production rates up to 5.6 Nm³/hr in the ILS facility. Long-term cell degradation is a serious issue. Degradation has been characterized well but the approach to over come the degradation is not clear.
- The project team has had very good progress with actual skid system on meeting goals with respect to production of hydrogen.
- The project's lifetime/degradation appears to limit impressive initial outputs compared to other, far more complex technologies.
- The project has been ongoing since 2003 and the technical progress is somewhat limited. The work does demonstrate some hydrogen production (slide 9) although still at moderate levels. Of major concern are the materials issues (element transfer, delamination, etc,- see slide 10 for example). These are well know problems, and this work does not appear to have made any significant advancements in solving these problems. Until these issues are properly addressed, building larger scale test units has no purpose. In addition to the problems specifically mentioned, seals will be a major problem. The PI and team should consider a revised approach to address these problems before attempting to demonstrate a scaled up unit.
- The project has accomplished several milestones. One of their integrated lab scale production unit was able to produce 0.5 kg H₂/hr for 1000+ hours. Previously experienced corrosion-related problems were solved. SOEC stacks were designed and tested. While these major advancements have been made, a serious problem with respect to long term durability of the cells was noticed. Extensive tests and analysis were performed to identify the problem for developing an appropriate solution.
- However, in view of the team's focus mainly on the cell degradation problem, many of their stated objectives were not addressed. Analysis with respect to efficiency and cost were not presented. Safety analysis was not addressed.

- Testing regimen for long periods exceeds the regimens for both HS and sulfur iodide SI. However, more time should be spent exploring detailed causes of cell degradation and establishing fixes to assure an operational concept in support of down-select. Until then, less time should be spent in long term durability testing.
- Excellent progress has been made in this project especially regarding the production of 1/2 kilogram of hydrogen per hour from it's demonstration stacks is noteworthy. Although the degradation rate is at least an order of magnitude too high, these barriers have been overcome by the solid oxide fuel cell developers using similar materials and technology and need only be addressed by the current program to be solved as well for the electrolysis cell.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- The project has very good collaboration (see slide 12). The presenter explained the contributions and roles of these collaborators. Good to see collaborations with NERI projects.
- It is not clear in the presentation which team member contributed various results or segments of the program.
- INL has assembled a diverse and talented team with good experience in this particular area however, INL needs to better utilize this group to solve the fundamental problems associated with this approach rather than spending money on multiple test units. Based on the presentation, INL seems to have neglected the expertise of Ceramatec, who has a good track record with high-temperature ceramics development. They need to more fully incorporate this knowledge and experience into the materials development effort.
- The team work in this project is very impressive. The authors presented how the different components of the project were investigated by respective team members from national laboratories, academic institutions, and private enterprises.
- Broad collaboration exists in the project. However, reliance on only Ceramatec might prove to be a weakness. It was not made apparent that parametric requirements were established and industrial RFP sought. There could be a reason for this "sole source", but, if so, it was not made apparent.
- The partners are well coordinated. The inclusion of Ceramatec as a partner is good since it allows the program to tap into solid oxide fuel cell expertise.

Question 5: Approach to and relevance of proposed future research

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

- How is the project team going to solve the degradation problem(s)? The project's future plan does not address this important issue. It is mentioned that the PI is going to collaborate with SECA SOFC manufacturers. SECA program has been talking about the degradation issues for very long time yet there seems to be no solution is in sight.
- The team's roadmap for degradation is relevant.
- If one or all of these mechanisms in the project are confirmed, what are possible solutions?
- Which of these potential mechanisms are show-stoppers?
- This category is not relevant for this project. Continuation depends on a down-selection. However, the PI should recognize the need to solve the materials issues rather than focusing on building a larger scale ILS.
- The team's future work is described clearly and appears to be well planed for the project goal.
- Too many options are left open for future work on this project, even given continuation beyond down-select.
- Future plans of this project are focused on overcoming materials issues that limit lifetime and reduce performance. Should this work continue to be funded, it is suggested that the participants survey one or more of the other SOFC developers. Several claim high-temperature electrolysis cells based on SOFC designs with much better durability that reported by the current program. It would be advantageous to shorten development time by bring the best of them on board this program.

Strengths and weaknesses

Strengths

• This project has a very strong team as well as a long list of publications & presentations.

- This project team provides a very simple and elegant way to produce low-cost H₂.
- This project has had great initial output.
- The project's thermal balance is easy to maintain, aiding scale-up.
- The PI and the team members are highly experienced and qualified to complete the project. The project appears to be close to demonstrating a commercially viable hydrogen production process.
- This project has some similarities to previous NHI approaches but high-temperature electrolysis (HTE) should be simpler. It is also, however, apparent that both operational management of electrolyzers and scale-up issues are different between hybrid sulfur and HTE.
- The project's demonstration of multi-kilowatt stacks is a strength.
- The technology/processes described in this project have performed well enough to operate at the thermal neutral voltage.
- This project has a good team with much experience in developing similar technology.

Weaknesses

- This project neither shows nor offers a clear approach to solve the degradation problem.
- The team faces the basic weakness of SOFC -- interconnects and durability applies to SOEC.
- The accelerated degradation rate of SOEC compared to SOFC is worrisome, implying either extreme conditions for current known SOFC failure modes, or some yet to be discovered failure mode not common with SOFC.
- The project's approach has major materials issues.
- The team's lack of cost analysis and operational features along with the project's durability problem are of major concern.
- The believed simplicity and reduced potentials for HTE relative to conventional electrolysis was not emphasized in the process description; such was also not evident in the work presented.
- Performance degradation is this project's main weakness. The team is attributing performance degradation to materials issues such as chromium diffusion into the electrodes, strontium migration into the electrolyte, delamination at or near the electrode/electrolyte interface, and silicon migration from the seals. These should have been addressed before moving to multi-kilowatt stacks. These are issues that plagued the SOFC developers several years ago that they seem to have overcome using sub-kilowatt, bench-scale experiments before moving on to multi-kilowatt demonstrations.

Specific recommendations and additions or deletions to the work scope

- Issues relating to drastic degradation of cell performance must be addressed before moving forward.
- Agree with large focus on durability.
- The work needs to focus on addressing the materials problems in a logical method. Stop all production tests and address the real development problems which are mainly the materials.
- The project should receive continued funding if the team members clearly establish that they could resolve the durability and other materials-related problems and reach their goals in terms of efficiency, cost of production, and scale-up design.
- The team needs to address the materials and performance degradation issues. This should be the main focus of the research going forward.

Project # PD-15: Technoeconomic Boundary Analysis of Photobiological Hydrogen Producing Systems *Brian D. James, George Baum, Julie Perez, and Kevin Baum; Directed Technologies, Inc.*

Brief Summary of Project

Directed Technologies conducted a technoeconomic boundary analysis and defined and evaluated four different H₂ production approaches: 1) photosynthesis with algae and bacteria; 2) water algae fermentation; 3) lignocellulose fermentation; and 4) microbial electrolysis. These approached included multiple system embodiments and system integrations. Concept feasibility, performance and cost and resultant \$/kgH₂ were estimated.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

Overall Project Score: 3.4 (3 Reviews Received)

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

- Longer-term renewable methods for hydrogen production are critical if this energy carrier is to succeed in the market. Photobiological hydrogen production has been assessed many times over the last 15 years. However, there is only limited bench scale data for many of the systems identified in this analysis. It would have been of value if error bars had been provided on the costs to determine the relative accuracy of the analysis.
- This project has a critical need in the field. Although, without an economic basis it is very hard to focus the team's research efforts.
- This project aligns well with DOE's goals to develop a cost-effective system for biological hydrogen production.

Question 2: Approach to performing the research and development

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

- Better discussions on how this team's work influences the research approach were needed especially regarding whether to set priorities or eliminate research pathways.
- The project team looked at both a series of different organisms and a set of different approaches for growing these organisms. The set of both organisms and reactor systems seemed comprehensive. Sizes were appropriately normalized for comparison in terms of the amount of hydrogen produced. The team took into account cycling times for some of the batch reactors vs. continuous growth. They also considered the issues associated with mixed gases (hydrogen and oxygen). The project team considered the reactor design, the materials and amounts of materials required. They also considered the mixing and flowing issues. They also constructed a bill of materials for each case.
- The team's approach is logical and appropriate. Systems used in this project for technoeconomic boundary analysis were carefully designed.

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

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

• The team has a reasonable systems analysis approach for this project. An improvement would have been to use a previous study conducted 5 years ago and assess if the technology and costs have been reduced as a result of government support. It would also be beneficial to determine if the high-priority barriers with the greatest cost impact had been included in the research funding.

- The project team was able to compare costs for each of the systems. The oxygen tolerant systems were cheapest but these result in gas mixtures. The amounts of hydrogen that can be created using each of the system dramatically changes. The algal system has a rather low amount of output. The cellulose systems were better. The microbial electrolysis cell (MEC) was the best option but requires energy input and needs acetate as an input. Overall costs for this project were dominated by infrastructure. There was no apparent benefit for using integrated systems. A key issue is that the lignocellulose system was much higher in total costs than the other systems.
- Progress for this project has been very good. Although the three integrated systems studied did not reduce the cost of biological hydrogen production, they provided guidance for designing better integrated systems in the future.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- Excellent investigators are involved in the work, but more discussion could have been presented on roles, responsibilities and if issues arose over cost or technical factors. Light could have been shed on how the team resolved these issues due to limited amounts of quantified data.
- The project team had some of the major groups in this area providing information about the algal and fermentation systems.
- The investigator collaborated closely with the Bio-hydrogen Working Group and other university investigators, resulting in a successful project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- The team's future research included the validation of costs, however, this should have been discussed in the initial work and any additional systems analysis should refine or reduce the assumptions. The project team could have benefited from using consultants with waste water treatment experience and algal producers for high-value food additives. This would allow them to perform and independent validation of the approach and then use their assessment to determine where this work should focus.
- This team has shown no future work. The project is essentially completed.
- The project's proposed future work is appropriate.

Strengths and weaknesses

Strengths

- This project has a good team of knowledgeable experts.
- The project uses reasonable technologies to bracket potential concepts.
- This project addresses a critical question that should drive much of the science.
- The team considered both a range of organisms and a range of bioreactor types.
- This project shows strong teamwork.

Weaknesses

- This project lacks sufficient information on assumptions.
- There is not enough information on the range of outputs, plus or minus 50%, 100% or more in this project.
- The project has had no outside independent review.
- There are undoubtedly additional factors in this project that need to be considered, particularly in terms of some of the inputs like water into the system, but this is an excellent initial model that can be expanded.
- There were too many assumptions used for the boundary analysis in this project.

Specific recommendations and additions or deletions to the work scope

• The cost for waste algae fermentation is too high in this project. This approach should be abandoned.

Project # PD-16: Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures *Tasios Melis; University of California, Berkeley*

Brief Summary of Project

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



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

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

- The project goals are well aligned with DOE's program targets for maximizing light utilization efficiency and hydrogen production in microalgal cultures.
- The project's focus on minimizing chlorophyll antenna size to maximize solar conversion efficiency is relevant to improve solar to hydrogen conversion efficiency.
- The success of this project is instrumental in feasibility of photobiological hydrogen production.
- Findings from this research can potentially be applied to other phototrophs to develop efficient photobiological hydrogen production.
- The work in this project aligns well with the need for a longer-term renewable hydrogen production technology, and photobiological hydrogen production that has been hampered by light sensitivity.
- A key issue in large-scale growth of algal cultures is going to focus on the penetration of light into the culture. While this can be remedied by mixing or simply by using a smaller thickness of growth culture, these approaches have disadvantages in terms of energy consumption and the distribution of energy to different organisms in the culture.
- The project aligns well with DOE's efforts to develop a cost-effective system for photobiological hydrogen production.

Question 2: Approach to performing the research and development

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

- The project has a very good approach, using a random mutagenesis technique and high throughput screening method to obtain mutants with truncated antenna size and with increased rate of photosynthetic activity (O₂ evolution).
- Systematically obtaining mutants with reduced levels of antenna size and increased light utilization efficiency validates the effectiveness of this project's approach.
- Both the tla1 and tla2 genes are important in regulating chlorophyll antenna size. The homology comparison suggested that other phototrophs may use the same strategy. This approach therefore has immense applications expanding beyond the current organism used in this study.

- In the accomplishments summary, the PI focused on plans instead of accomplishments, specifically with the down regulation of the tla1 gene. The PI also indicated the team had advanced the biochemical and biophysical analyses but had difficulty with the molecular analysis. There was however, insufficient information on the effectiveness of this work.
- The team's approach is standard but effective. They are looking at random mutagenesis of the organism and isolating mutations that decrease the antenna size. The team has a rather unique ability to make these measurements.
- Random mutagenesis combined with high throughput screening was employed in this project to identify green algae mutants with a smaller Chl antenna size. The approach is well-focused on specific technical barriers and it is very effective.

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

This project was rated **3.8** based on accomplishments.

- The progress toward the project's goals is excellent.
- The team systematically demonstrated the truncation of antenna size which has potential to meet the 2010 target
- The project's accomplishments included the cloning of the tla1 gene and determined that tla1 is a hydrophilic protein. Work is underway to determine a sub cellular localization of the protein, which is a novel discovery.
- The team managed to overcome the complication that antibody raised against Tla1 also cross-reacted with D2 protein. The team has also since identified the C-terminus of D2 protein displaying antigenecity toward the tla1 antibody. This is verified by using mutants deficient in D2 protein.
- The project team has cloned the tla2 gene and work is underway to characterize the protein to gain a more indepth understanding as to its role in regulating antenna size in Chlamydomonas.
- This is the first demonstration of two different genes that regulate the chlorophyll antenna size in photosynthesis, which signifies the importance of the team's work.
- This is a 5-year research project and, based on the data, the team has successfully accomplished a significant reduction of antenna size and light sensitivity. However, the PI stated that it made the DOE target for utilization efficiency of solar light, however all the information presented is on the original mutant tla1 and nothing on tla_x or tla_{new} except for the two graphs.
- The project team has isolated three mutations that greatly decrease the antenna size which is evidence of achieving the goals set by the team. The first mutation has been characterized in some detail. This was complicated by the fact that, as it turns out, D2 of PSII has a common epitope with the gene product of the gene that was mutated. The team has worked through this and understood the cross reactivity of the antibody in detail. They are currently in the process of characterizing the second mutation and will move to the third. The team has demonstrated that the decreased antenna size increases the photosynthetic conversion efficiency and decreases the sensitivity to photoinhibition.
- The team has made good progress in FY08. The tla2 gene was cloned and the tla1 immunoblot problem was solved. The project has reached the DOE target beyond 2015.

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

This project was rated 2.7 for technology transfer and collaboration.

- Very little collaboration is shown in this project. Coordination amongst different partners may have and can potentially expedite the research progress.
- Technology transfer was initiated in this project with UC Berkeley's Office of Technology issuing a nonexclusive license for the commercial use of tla1 gene.
- The team does not appear to have much collaboration on this work.
- There were no collaborations on this project but none were necessary to satisfy the scope of work.
- This project is a sole source effort.

Question 5: Approach to and relevance of proposed future research

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

- The project's sub-cellular localization of the tla1 protein is underway.
- A clear plan is laid out for future research in this project, including characterization of the tla2 gene.
- The next step in this project is to characterize genes conferring the phenotype in tlaR strain.
- Most of the team's proposed work is focused on whether tla_{new} is stable and can be replicated to demonstrated repeated results with 25% efficiency.
- The project team will continue to characterize the second and third mutations that they have discovered.
- Proposed work for cloning genes from the tlaR strain is appropriate. However, the investigator did not propose further plans to study biological functions of tla1 and tla2 proteins.

Strengths and weaknesses

Strengths

- The investigator has demonstrated superior progress toward well-defined goals.
- The investigator has a collection of mutant organisms with truncated antenna sizes and, based on these mutants, novel genes were identified. The outcomes reveal how chlorophyll antenna sizes are regulated for the first time in Chlamydomonas.
- The team's research is very valuable in guiding the design of other phototrophs with improved light conversion efficiency via down-regulating of antenna size.
- The investigator's laboratory is well equipped to determine chlorophyll antenna size.
- The team has a good PI and demonstrated accomplishments.
- This project has a well defined problem to solve which is directly applicable to large scale growth.
- The project team has demonstrated that mutations that result in decreased antenna size can be found and can also improve photosynthetic efficiency and stability to high light levels.
- The investigator is an expert in photosynthetic systems of Chlamydomonas.

Weaknesses

- Even though mutants with truncated antenna sizes displayed higher photoconversion efficiency (O_2 evolution), it is not yet determined if hydrogen production is similarly improved, especially at high light intensity.
- The truncated antenna mutants would be less competitive compared to the wild type and therefore pose an issue with contamination when scaling up.
- The project has insufficient data and descriptions on advanced mutants.
- Ultimately, this project needs to be coupled to hydrogen production values in order to be critically evaluated.
- In this project, no data was presented to show increased hydrogen production in the tla1, tla2, and tlaR mutants.
- The investigator did not address the questions about the proposed biological functions of tla1 and tla2 proteins from previous reviews. A biological function study is essential to reveal regulation mechanisms of the Chl Antenna Size, which may lead to a rational design of better algae mutants.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PD-17: Biological Systems for Hydrogen Photoproduction

Maria L. Ghirardi; National Renewable Energy Laboratory

Brief Summary of Project

The overall objectives of this project are to 1) develop and optimize aerobic photobiological systems for the production of hydrogen from water; 2) utilize the sulfur-deprivation platform to address biochemical and engineering issues related to photobiological hydrogen production; and 3) integrate photobiological with fermentative organisms to more efficiently utilize the solar spectrum and the substrates/products from each reaction.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



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

- This project, which is based on biological hydrogen, supports DOE's RD&D objectives.
- This project is relevant because it creates an integrated photobiological/fermentative system.
- Key issues in this project are oxygen tolerance ability to optimize the sulfur deprivation system and the integration with the fermentation system. In principle, this could become an important approach to generating biomass from biomass derived from photosynthetic microbes.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- The team's approach was clearly presented as logical stepwise steps.
- The project's milestones should be better defined.
- The project team is trying to improve oxygen tolerance via a rational design of the enzyme or by expressing heterologous hydrogenases or through random mutagenesis. The rational mutagenesis relied on finding the pathway that oxygen uses to reach the cofactors. However the hydrogenases appear to be heterogeneous in their oxygen effects, making this hard to evaluate. They are also introducing bacterial hydrogenases in algae and looking at the stability of these to oxygen.
- The project team is currently looking at sulfur deprived organisms and their ability to convert light. They have been looking recently at immobilized systems in films. It is not clear how relevant this is to scaled systems, though it provides some fundamental understanding of the system

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

This project was rated 2.3 based on accomplishments.

- The team is proceeding in a stepwise manner.
- With the considerable funding for this project, more progress was expected.
- The team has been developing the high-volume throughput screening tests since 2007. More details on their progress are needed.
- The team's antenna and sulfur deprivation work seem very similar to what was done by Professor Melis at UC Berkeley.

- Initial project work on integrating the fermentative and algal systems was interesting. The team needs to include information on any treatments made to the algal biomass/water mixture prior to feeding it to the fermentative system. Purified proteins and algal lipids seem like an expensive fuel.
- Results of using fermentation products for feed in a photosynthetic system were encouraging, but more details about pretreatments, etc. are needed.
- The team has had difficulty analyzing the rational mutagenesis results because of the heterogeneous hydrogenase issues. They have not yet been able to assay the other approaches for improving oxygen sensitivity.
- The project's sulfur deprivation of immobilized algae in films shows 1% conversion efficiency. Hydrogen production takes place in the presence of oxygen because the film protects the hydrogenase. ATPase mutants improve the hydrogen production, which is an interesting observation.
- For the integrated system, first the team looked at whether the spent algal biomass can be used by fermentative system. They see increased hydrogen production when algal biomass is provided. Both the lipid and protein are fermented and utilized for hydrogen production. At the moment, the team is working at very small scale.

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

This project was rated 2.7 for technology transfer and collaboration.

- It appears that the team has had collaboration between partners.
- The PI should identify areas that the partners collaborated more clearly. It is difficult to determine what was done by partners and what was done by NREL.
- The project team has a set of collaborators with expertise in the different tasks.

Question 5: Approach to and relevance of proposed future research

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

- The project team's future plans are the same as in previous years. Since progress has been made, it would seem reasonable to adjust the plans.
- The project has continued work on the same issues. Basic research with long term goals have been accomplished however, this project is not going to reach production scales any time soon.

Strengths and weaknesses

Strengths

- This is a long-term project that is well funded and has many partners.
- The project team is exploring the fundamental understanding of hydrogenase structure and function, particularly with regard to oxygen tolerance.
- The team is also characterizing the conditions that allow hydrogen production, particularly when some oxygen is present.

Weaknesses

- Progress in this project seems slow or at least unclear. For example, they have been working on developing high-volume throughput screening tests for several years and it is not clear what progress has been made. The challenges and progress should be better identified.
- The near term milestones are inadequate for this project. "Test the performance of immobilized ATPase mutants" does not seem very ambitious. The milestones should include some performance targets as well as "testing" a number of organisms. There are no milestones for the high-volume screening process development, which has been identified for the last several years as an important component of this program. Milestones should be added.
- There is no indication, at this point, how this work could be scaled and no real understanding of how to increase the hydrogen production to a point that will be useful at scale.
- This project is early stage exploratory work, which is not a weakness, but it makes extrapolation to any kind of useful system essentially impossible.

Specific recommendations and additions or deletions to the work scope

- The PI has reported making an impressive number of presentations 19. This is over one conference a month, which is a lot of travel. Their resources and time would be better utilized if they limited their conference attendance to only the premiere conferences.
- The project team's milestones need to be focused on achieving technical targets. "Testing an organism" is a weak milestone.

Project # PD-18: Fermentative and Electrohydrogenic Approaches to Hydrogen Production

Pin-Ching Maness; National Renewable Energy Laboratory Bruce Logan; Pennsylvania State University

Brief Summary of Project

The long-term objective of this project is to develop direct fermentation technologies to convert renewable lignocellulosic biomass resources to hydrogen. The near-term objectives of this project are to 1) optimize bioreactor performance for the cellulosedegrading bacterium Clostridium thermocellum; 2) identify key metabolic pathways to guide generic engineering to improve hydrogen molar yield; and 3) integrate microbial electrolysis cell (formerly BEAMR: bio-electrochemically assisted microbial reactor) process to improve hydrogen molar yield.



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

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

- This project aligns to DOE's Hydrogen Program.
- The project team is trying to convert lignocellulose directly to hydrogen without going through sugar. This is much simpler than going through a monomeric sugar. They are also coupling this to a microbial electrolysis cell (MEC) step that uses the byproducts of the fermentation. If economic ways of using biomass have to be made then this is probably required.

Question 2: Approach to performing the research and development

This project was rated 3.7 on its approach.

- The project team has a step-wise approach.
- The team is using a single bacterium for the degradation of cellulose. This bug can use cellulose as a carbon source and it also works at high temperature. The byproducts of the fermentation are used in an MEC which seems like a well thought through approach.

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

This project was rated 3.7 based on accomplishments.

- The project team has made good progress towards the DOE targets.
- The team's integrated system surpasses the DOE hydrogen production targets.
- Comparing the project's MEC efficiency based on electricity to water electrolysis is not a fair comparison since the MEC is decomposing an organic compound and the electrolyzer is decomposing water. Electrolyzers that decompose organic compounds use much less power to produce hydrogen than the process of water electrolysis does. To be consistent with other technologies, the only efficiency number of merit is the one that includes the lower heating value of the organic material.
- The hydrogen production rate in this project is very slow and needs to be increased dramatically in order for this technology to be viable.

- The project team is observing hydrogen production using corn-Stover, and they are able to see greater H₂ production than CO₂. They have looked at the effects of metabolic pathway inhibitors to see if blocking certain pathways will increase hydrogen production. This aspect points to the use of metabolic engineering at the points that the inhibitors work. They have looked at several inhibitors and can see the predicted increases in hydrogen production. The team is in the process of developing the genetic system for this work.
- For the MEC system, the project team has looked at a synthetic mixture of byproducts, and optimized the system for the individual substrates and then combined the organisms. They are now getting more hydrogen energy out than the electrical energy they are putting in.
- Overall, the project is getting almost 10 moles of hydrogen per hexose. This is more than twice the goal.

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

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

- There appears to be good collaboration between the partners in this project.
- The team has developed new collaborations with Oakridge to work towards the metabolic engineering. The fundamental collaboration between the fermentation work and the MEC is excellent.

Question 5: Approach to and relevance of proposed future research

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

- The team's proposed future work should also consider ways to increase the production rate (kg H₂/day and kg H₂/ volume).
- The project team's focus is on metabolic engineering based upon the inhibitor studies. They will continue to improve the efficiency of the MEC output, which seems like an excellent approach.

Strengths and weaknesses

Strengths

- This project has a strong team with good communication.
- The team has meaningful milestones, which indicate substantial thought being put into the process. As a result, the team has developed a plan to achieve its goals.
- The project's integrated process better utilizes the feedstock.
- This project has a very good combination of novel fermentation with MEC technology.
- The systematic inhibitor study to help guide the metabolic engineering was excellent in this project.
- The project results in terms of molar yields are quite impressive.

Weaknesses

- This project requires a relatively expensive feedstock.
- Maintaining the feed mixtures will be a significant challenge for this team.
- Hydrogen gas produced is not pure; therefore purification technologies will be required in this project. Unless the project team can produce the hydrogen under pressure, which is difficult, the compression costs will be high.
- It would be good for the team to start working on predicting the effects of scaling output and considering the roadblocks involved in the scaling process.

Specific recommendations and additions or deletions to the work scope

• Over the past year the team presented on 11 occasions, which would consume a significant amount of time and resources. It is recommended that they limit their conference attendance to the most prestigious conferences in order to better utilize their funds and time.

Project # PD-19: Development of Water Splitting Catalysts Using a Novel Molecular Evolution Approach Neal Woodbury, Arman Ghodousi, Trent Northen, Matt Greving, Pallav Kumar, Bharath Takulapalli, Nicolas Yakubchak, James Allen, JoAnn Williams, Trevor Thornton, Stephen Johnston, and Zhan-Gong Zhao; Arizona State University

Brief Summary of Project

The objectives of this project are to 1) develop a novel approach to creating molecular catalysts for redox reactions based on high throughput synthesis on electrodes; 2) mimic nature's approach to water splitting; and 3) reduce the overpotential by 30%. Specific objectives for fiscal year 2009 are to 1) optimize high throughput peptide synthesis on CombiMatrix Arrays; 2) optimize the multielectrode measurements of water splitting on the CombiMatrix Arrays; and 3) demonstrate several rounds of optimization for catalytic activity.



Question 1: Relevance to overall DOE objectives

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

- While this project is relevant to renewable hydrogen production, it implements and uses very fundamental research and it is not certain that it should belong in Basic Energy Sciences (BES).
- This project is critical to DOE's objective of improving efficiency of hydrogen production through improved catalysts.
- This project addresses the viability of direct renewable hydrogen production.

Question 2: Approach to performing the research and development

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

- It appears this project has a trial-and-error approach and a more systematic approach might be needed. Quite a bit of optimization is needed to yield of peptide synthesis and to prevent/minimize effects of side chain protecting groups during synthesis. It is unclear what the technical targets are.
- The project's approach is developing a broad range of catalysts using a peptide synthesizer. This involves a large amount of trial and error to see which formulations will work.
- The project's selection of the CombiMatrix as basis for evaluation is good approach.

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

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

- This project does not show any significant breakthroughs from previous to this year. The research needs to be more focused on addressing key issues.
- Much progress has been made in producing and testing numerous formulations in this project. Automation allows mass throughput.
- The team faces difficulty in overcoming noise in results and is limiting. No specific results were shown and preferred catalysts were presented.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- The project team had good collaborations with CombiMatrix and others.
- Coordination with CombiMatrix as equipment supplier has been good for the project.
- A strong industry partner has been good for this project.

Question 5: Approach to and relevance of proposed future research

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

- The project team needs to focus on addressing key issues and addressing key targets.
- The remaining work on this project intends to close-out research performed to date.

Strengths and weaknesses

Strengths

• This project has strong industry partners and a good technical approach.

Weaknesses

• The team needs to overcome the problem of noise in results in order to differentiate between peptides.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PD-20: High-Capacity, High Pressure Electrolysis System with Renewable Power Sources *Martin Shimko; Avalence LLC.*

Brief Summary of Project

The electrolyzer development project goals are to 1) achieve at least a 15x increase in the gas production rate of a single highpressure 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 for a full scale plant (300 kg/day, 750 kW) that meets the 2017 DOE cost target of \$3.00/gge.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



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

- This project takes a very unique (but very challenging) approach to high-pressure hydrogen production. When successful, downstream mechanical compression stages will be reduced and possibly eliminated to help reduce the cost of delivered hydrogen gas.
- This project focuses on high-pressure electrolysis from potentially renewable sources for cost effective hydrogen generation.
- The electrolysis of water is a currently available hydrogen production technology. The challenge for the project to meet the Hydrogen Program and DOE energy goals is to develop the technology for it to produce hydrogen at a cost such that a hydrogen fuel cell vehicle could be competitive with a gasoline-based vehicle. The cost of electricity accounts for 50-75% of the cost of the hydrogen from electrolysis. It is doubtful that the cost of electricity can be substantially reduced. Therefore the only way to meet the DOE cost targets is for substantial electrolyzer capital cost reduction. It is, at best, unclear that the Avalence, LLC's technology approach can achieve the required capital cost reduction.
- In order for electrolysis to be a low greenhouse gas (GHG) emitting technology, the electricity used must be produced predominantly from renewable or non-carbon emitting technology. This could be realized in a large located at a central electrolysis facility near or at a wind-farm or other low GHG emitting electricity production facility. The Avalence technology seems to be targeted for distributed production and appears to be not well suited to large central scale production. For distributed electrolysis to use low GHG emitting electricity, the U.S. grid would need to use predominantly renewable or other low GHG emitting electricity production. This is a goal of DOE but, practically, will take a very long time to achieve.
- This project focuses on improving efficiency and cost of high-pressure electrolysis systems.

Question 2: Approach to performing the research and development

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

- It is good to see that the 2008 goal of 6500 psi wrapped cell demonstration has been reduced to 2500 psi in 2009. In this project, many of the same design challenges still exist a year later. This seems to indicate that the project may need additional resources to overcome these barriers.
- This project appears to be mostly engineering and optimization and not much innovative and novel approach. The 2500 psig is still not a high enough pressure where a hydrogen compressor can be eliminated. It is important that work needs to concentrate on 6500 psig system for H₂ fueling applications for vehicles.

- Nowhere in the project goals is cost reduction nor a cost target specifically mentioned. This is the key goal for electrolysis-based hydrogen production for the DOE Hydrogen Program. The project milestones include a "go/no-go" decision 2 years into this 4.5-year project, based on electrolyzer performance and cost but there is no quantification of these targets.
- The project goals state that a full-scale production unit would produce only 300 kg H₂/day. DOE expects distributed forecourt refueling station hydrogen production units to need to produce 1500 kg/day. It would take five 300 kg/day units to achieve this. The costs would thus scale linearly rather than a single 1000 or 1500 kg/day full-scale unit that would have an economy of scale advantage and thus have a better chance of meeting the DOE cost targets. For large central scale hydrogen production, the larger the base electrolyzer unit the lower its cost based on the same economy of scale argument. The Avalence technology by nature is difficult to scale-up to large base electrolyzer units.
- The approach of using multiple concentric tubular "cells" to obtain some advantage for high-pressure operations is novel but very challenging.
- There are four slides in the presentation devoted to discussing using hydrogen as an energy storage system that includes an electrolyzer and fuel cell. Although this is an interesting concept worth pursuing, it is not part of this Avalence project.
- The project focused on addressing engineering challenges of the high-pressure system.

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

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

- The project drawings of the various options for the 1000 psi single cell are encouraging but no evidence was provided that construction of the actual test cell has begun (other than the valving control panel). One question raised on slide 14 was to settle on a design pressure (2500 vs. 6500). A staged approach is recommended where starting at lower pressures would first be achieved before moving on. The identification, testing, tube forming and joining of sheet membrane materials are listed as two accomplishments. Details surrounding that work would strengthen the presentation and should have been shared.
- This project appears to be mostly for practical engineering design activities and more progress towards a scalable 6500 psig system should be seen. Also, work on how the system can be integrated with renewable sources and manage supply and demand should be shown.
- Not enough progress is observed with this project in working towards meeting DOE's cost target.
- This is a relatively new project. It was initiated in May 2008 and is currently on track vs. its planned schedule of accomplishments.
- The project has identified membrane materials; shown that it can be formed into tubes; seam sealed and has initiated the construction of a test cell.
- Steady progress has been made toward objectives of this project.

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

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

- A team member from MIT was not shown in this year's partner list. Has their collaborative work been completed or was some other conflict keeping them from assisting with the two-phase fluid design? It was unclear from the slides and presentation how any particular partner was assisting to overcome the project barriers.
- Not much collaboration with other institutions was observed in this project.
- Avalence is partnering with HyperComp, which is experienced in high-pressure wrapped composite vessels. This is a good collaboration. The project team is also partnering with the Hydrogen Energy Center and MaineOxy but it is not clear what these collaborations offer.
- It would seem that there would be other very fruitful collaborations that could add to the capabilities of Avalence to increase the probability of a successful project.
- The project has good coordination and interaction amongst its partners.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

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

- There seems to be a couple of options with regard to the single cell design and the design pressure of this project. It is unclear what criteria will be used to select a winner, unless both designs are going to be fabricated and tested against each other. It is suggested that the team throw a couple simple IV curves up at different pressures.
- The team needs to also address any potential challenges associated with the 6500 psig system (other than the hose leaking issue observed so far).
- The project's current system is looking at around 300 kg/day. There is a need to focus more attention on addressing any potential scale-up issues (to 1500 kg/day for forecourt and larger for central production).
- There is no slide that is titled Future Work Plan, but the Project Technical Objectives and Program Schedule do provide an overall work plan that is well organized.
- More detailed information on the work plan for the next 12 -18 months leading to the "go/no-go" decision point would be very helpful for this project.
- Future work continues current activities in this project.

Strengths and weaknesses

Strengths

- The project's unique design is a plus but there seems to be up-coming challenges. The electrochemical (high) pressure goals will be valuable in reducing mechanical compression stages downstream.
- This is a relatively new project. It was initiated in May 2008 and is currently on track vs. its planned schedule of accomplishments.
- This project has identified membrane material; shown it can be formed into tubes; seam sealed and has initiated the construction of a test cell.
- There is no slide that is titled Future Work Plan but the Project Technical Objectives and Program Schedule do provide an overall work plan that is well organized.

Weaknesses

- The team should provide a clearer indication of where the project is with regards to objectives and timeline. Regrettably very few details are provided on the year's accomplishments.
- It is unclear that the Avalence technology approach can achieve the required capital cost reduction targeted by the DOE Hydrogen Program. The basic tubular design is well suited for high-pressure operation but this design and operating pressure are relatively expensive. This design is also not well suited for scale-up to a large base (>1000 kg-H₂/day) electrolyzer. Thus, the project could lose the potential capital cost savings resulting from economy of scale to meet the production quantities sought by the DOE program.
- In order for electrolysis to be a low GHG emitting technology, the electricity used must be produced predominantly from renewable or non-carbon emitting technology. This could be realized in a large central location at an electrolysis facility near or at a wind-farm or other low GHG emitting electricity production facility. The Avalence technology seems to be targeted for distributed production and appears to be not well suited to large central scale production. For distributed electrolysis to use low GHG emitting electricity, the U.S. grid would need to use predominantly renewable or other low GHG emitting electricity production. This is a goal of DOE but practically will take a very long time to achieve.
- Nowhere in the project goals is cost reduction nor a cost target specifically mentioned. This is the key goal for electrolysis-based hydrogen production for the DOE Hydrogen Program. The project milestones include a "go/no-go" decision 2 years into this 4.5-year project, based on electrolyzer performance and cost but there is no quantification of these targets.
- It would seem that there would be other very fruitful collaborations that could add to the capabilities of Avalence to increase the probability of success of this project.

Specific recommendations and additions or deletions to the work scope

- Cell degradation was discussed during the Q&A with an answer of "No cell degradation". This seems impossible. Running the cell over 5,000 50,000 hours will degrade the cell in some manner, so perhaps more sensitive voltage measurements should be made to quantify.
- This project should develop a detailed cost estimate assuming success of their design. This should be compared with the DOE cost targets for Distributed and Central Production to determine if this electrolysis technology approach should be pursued.

Project # PD-21: PEM Electrolyzer Incorporating an Advanced Low Cost Membrane

Monjid Hamdan; Giner Electrochemical Systems, LLC

Brief Summary of Project

The overall project objective is to develop and demonstrate an advanced low-cost, moderate-pressure proton exchange membrane (PEM) water electrolyzer system to meet DOE targets for distributed electrolysis, by developing a 1) highefficiency, low-cost membrane; 2) long-life cell-separator; 3) lower-cost prototype electrolyzer stack and system; and 4) prototype electrolyzer system at the National Renewable Energy Laboratory. Objectives for fiscal year 2008-2009 are to 1) develop a low-cost, high-efficiency, highstrength membrane with electrochemical performance comparable to thin Nafion® (N1135) and high strength to allow operation at 300 psig and 80-90°C; 2)



initiate cell-separator development; and 3) complete preliminary system design and development of lower-cost components.

Question 1: Relevance to overall DOE objectives

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

- Improving capital cost and system efficiency of PEM electrolysis is vital to bring reliable and low-tech electrolyzers to distributed/home fueling stations.
- This project's focus on hydrogen production helps in addressing issues with capital cost and system efficiency.
- This project has clearly defined targets.
- Electrolysis of water is a currently available hydrogen production technology. The challenge for this project is to develop technology to produce hydrogen at a cost such that a hydrogen fuel cell vehicle could be competitive with a gasoline-based vehicle. The cost of electricity accounts for 50-75% of the cost of the hydrogen from electrolysis. It is doubtful that the cost of electricity can be substantially reduced. Therefore the only way to meet the DOE cost targets is for substantial electrolyzer capital cost reduction and to improve the electrolyzer efficiency. The approach that Giner Electrochemical Systems, LLC. (GES) is taking has the opportunity to substantially reduce electrolysis capital costs and improve efficiency.
- In order for electrolysis to be a low GHG emitting technology, the electricity used must be produced predominantly from renewable or non-carbon emitting technology. This could be realized in a large central electrolysis facility located near or at a wind-farm or other low GHG emitting electricity production facility. The Giner PEM technology could be scaled to reasonably large base electrolysis units suited for this purpose. For distributed electrolysis to use low GHG emitting electricity, the U.S. grid would need to use predominantly renewable or other low GHG emitting electricity production. This is a goal of DOE but practically will take a very long time to achieve.
- Project addresses several key objectives in the area of electrolysis improvement.

Question 2: Approach to performing the research and development

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

- This project has a strong technical team and partnerships working to overcome the project challenges. After demonstrating ~1200 psi without a pressure dome why is it required for a 'mere' 300 psi stack? The O&M impact of the N₂ purge and frequency of the dome will be interesting to ask about next year.
- The team is addressing the low-cost membrane, durability and high efficiency of their project technology.
- This project is addressing key issues, which are durability with Dimension stable membrane (DSM) and cost with Bi Phenel Sulfone, H form (BPSH).
- This project lays out a logical approach to targets (from inside out) membrane to stack to integrated system.
- Given the fact that the stack pressure is relatively low, going with a round design might not be a best fit in terms of system layout (the system is in a rectangular box).
- The Giner research is targeted to: develop a high-efficiency low-cost membrane, a long life lower cost cell separator, and to reduce the cost and improve the efficiency of the BOP. These are exactly the improvements needed for PEM-based electrolysis to meet the DOE Hydrogen Program cost targets.
- Giner has and continues to do detailed cost estimates to ensure their approach can lead to achieving the DOE cost targets. Initial economic analysis results are promising.
- Giner could increase their probability of success of achieving the DOE cost targets if they put some more thought and effort into trying to target larger and larger cell/base electrolyzer sizes.
- This is a well-focused project aimed at reducing cost and improving efficiency of PEM water electrolyzer systems.

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

This project was rated 3.8 based on accomplishments.

- The team appears to be making steady progress towards an alternative membrane for their stacks. While the slope of the cell voltage on slide 10 appears to be 'zero' there has to be some cell degradation. Extrapolating from 1000 hours (milestone met) to 50,000 hours seems a bit of a stretch. As new lower cost BOP materials are selected it will be interesting to see if GES can also drive the temperature range from 50°C towards the 90°C to take advantage of the efficiency boost.
- This project has a good durability testing progress 1,000 hrs at 80°C without degradation (DSM). They also have a 71 75% stack efficiency lower heating value (LHV).
- Good progress has been made in addressing safety, durability and costs in this project.
- Giner has successfully developed a Dimensionally Stable Membrane (DSM) based on a novel design incorporating perfluorosulfonic acid (PFSA) ionomer in an engineering plastic support. Lab testing has demonstrated improved performance over Nafion membranes and projects to >45,000 hour lifetime. They also have initial promising results on a Bi-Phenyl-Sulfone-based membrane. Both these membranes can be substantially lower cost than Nafion.
- Giner has developed a lower cost cell separator that looks promising in initial lab tests and is in progress on working with vendors to reduce the cost and improve the efficiency of the BOP.
- The project team is making excellent progress toward stated objectives of project.

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

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

- The Parker Hannifin Corporation and Virginia Polytechnic Institute and State University (VT) seem to be strong partnerships for the project's targeted tasks.
- The project has good collaborations with Virginia Tech for low-cost membrane development and Parker Hannifin Corp. for system and component development.
- Giner is collaborating with Virginia Tech University on new polymer membranes and with Parker Hannifin Corp. on the BOP issues. These are key additions to Giner's in-house capabilities for success in this project.
- There could be additional collaborations that would further enable this project.
- Good collaboration with industry and university partners to take advantage of strengths available for incorporation into project.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 3.5 for proposed future work.

- The project team's focus on hydrogen drying is an excellent area for cost and efficiency improvement. Stack/BOP would ideally handle higher temps 80-90°C. Next year it would be interesting to hear more about how the hydrogen drier has been improved and how the 97% efficiency was determined. More information should be shared on any new deionized (DI) water level sensing process or device in the phase separator.
- The project team should focus some efforts on system integration, power electronics and testing to address durability and operational issues.
- The team should consider leveraging parallel fuel cell MEA development for synergies.
- The future work plan for this project is brief but clear. A more detailed work plan would be helpful.
- Future work is well planned to continue current excellent progress to address electrolyzer costs and efficiency issues.

Strengths and weaknesses

Strengths

- The project's strong technical teams and partnerships are making progress. The PI did an excellent job highlighting the technical accomplishments.
- The Giner research is targeted to: developing a high-efficiency, low-cost membrane, a long life lower cost cell separator, and reducing the cost and improving the efficiency of the BOP. These are exactly the improvements needed for PEM-based electrolysis to meet the DOE Hydrogen Program cost targets.
- Giner has and continues to do detailed cost estimates to ensure their approach can lead to achieving the DOE cost targets. Initial economic analysis results are promising.
- Giner has successfully developed a Dimensionally Stable Membrane (DSM) based on a novel design incorporating PFSA ionomer in an engineering plastic support. Lab testing has demonstrated improved performance over Nafion membranes and projects to >45,000 hour lifetime. They also have initial promising results on a Bi-Phenyl-Sulfone-based membrane. Both these membranes can be substantially lower cost than Nafion.
- Giner has developed a lower cost cell separator that looks promising in initial lab tests and is in progress on working with vendors to reduce the cost and improve the efficiency of the BOP.

<u>Weaknesses</u>

- Why is the dome used in this project? The team needs to present a better answer to stack degradation rather than saying it is "low."
- Giner could increase their probability of success of achieving the DOE cost targets if they put some more thought and effort into trying to target larger and larger cell/base electrolyzer sizes.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PD-22: Photoelectrochemical Hydrogen Production: DOE PEC Working Group Overview *Eric L. Miller; University of Hawaii at Manoa*

Brief Summary of Project

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



and analytical techniques, for optimizing future PEC materials and devices; and 4) explore avenues toward manufacture-scaled devices and systems.

Question 1: Relevance to overall DOE objectives

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

- DOE's PEC working group is playing a critical role in accelerating the developing of the PEC technology, which is one of the key pathways in DOE's renewable hydrogen production goals.
- PEC is a potentially long-term hydrogen producer and therefore does very little to bring down cost of hydrogen in the next 10-15 years to meet the overall DOE objectives. However, the potential impact of PEC is very high.
- The working group is effectively coordinating theoretical, modeling, and experimental efforts directed towards meeting the DOE multi-year PEC hydrogen production targets.
- This group multiplies the effectiveness of this technology development by increased information flow between teams, thus allowing a wide search of materials without overlap of efforts.
- The high-risk/high-payoff search for the Holy Grail, providing direct storage of solar energy in a transportable hydrogen energy carrier is fully supportive of program objectives. Establishing cost effectiveness remains to be done in order to assess level of importance of the process to program objectives.

<u>Ouestion 2: Approach to performing the research and development</u>

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

- The PEC working group approach to problem solving is outstanding. Their combination of theory, experiment and analysis is what will be needed to solve this challenging problem.
- The close coordination between various team members is helping accelerate the development and avoiding repetition.
- Lessons learned and development of the material library will be critical to development of this project in the long term.
- White papers approach is pretty good for current and future developments of this project.
- This summary of PEC work showed a good cross-section of the working being conducted. The standardized test protocol is a valuable tool at this (early) point in the project.

- The presentation should provide information on the budget for managing/administrating the PEC Working Group. The use of White Papers to document current research status is good, but it is unclear what the status/availability of the white papers is from the presentation, or what kind of collaboration is being achieved within each task force. The development of standardized testing and reporting protocols is critical, so it is very good that progress is being made here.
- The project's integrated feedback loop using all technical tools available with tight inclusion of the technical experts is characteristic of this project. No other material development project has integrated the levels of sophistication and depth of inquiry than this project. Flow charting of critical parameters assessment to permit "go/no-go" decisions is superior for this project. This feature is partly characteristic of the process physics and partly due to highly interactive management of distributed work.

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

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

- The team needs to look at the progress of the whole group in a structured format, rather than a list. For example, divide the work into class of materials (similar to hydrogen storage) program with "go/no-go" decision points and/or conditions identified to allow the group to move on from something that is non-practical.
- Generally, this group has made steady progress on materials and developing capabilities.
- Steady progress is being made to identify and characterize candidate materials in this project.
- The team's rate of progress is partially hampered by budget and partially by the broad scope of materials under consideration. Future down-selection efforts may help speed progress on most promising materials.
- The project appears to continue to pursue incremental improvements of inadequate materials even though dramatic changes are essential to meeting cost performance metrics. It's always hard to move people away from things they know into unknown, and it's impossible to demand instant invention of new materials that would surely be better than current materials.

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

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

- This project is an outstanding example of collaboration to deliver on common goals. Perhaps a good addition would be to get an industry entity involved for a different perspective.
- It is good to see a growing number of domestic and (more recently) international researchers involved in this project. Are there companies out there with brilliant materials people (GE, 3M?) that would be interested in collaborating on this?
- The purpose of this project is to foster collaboration on PEC hydrogen production R&D. All DOE-funded PEC projects are actively participating in the working group to share information and develop common testing and reporting protocols, and international collaboration is being achieved through the International Energy Agency (IEA).
- This project has every individual and every institution with the interest and skills related to the task have been invited to an open community for discussion of optional paths forward and decisions regarding focused funding and effort.

Question 5: Approach to and relevance of proposed future research

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

- The team's future work should also include an element on system development and cost estimation.
- The project's 'tool chest' is getting full enough that large amounts of material characterizations can be processed in the coming year. Perhaps the team should highlight any benchmarking the PEC Working Group has conducted with international community.
- Strong working relationships have been built in the PEC working group and good plans are in place to continue that work in the future. Future focus continues to be on coordinating efforts to develop and apply the PEC "tool

chest," to develop and apply screening protocols and test procedures, and to make down-selection decisions that will focus R&D on the most promising materials classes.

• Future work did not achieve "outstanding" category simply because a plan had not been developed that establishes a clear path toward different approach to discovering truly promising and revolutionary materials. Modeling and simulation remains about as difficult as synthesis and characterization so that more rapid screening of complex materials is still elusive. Planning might be improved by focusing effort on work-arounds for inadequate aspects of otherwise promising concepts. More effort should be implemented in developing theoretical screening of advanced materials. This is partly a DOE responsibility to provide more funding and partly a project responsibility to properly apply such funds.

Strengths and weaknesses

Strengths

- This project has good collaboration between outstanding researchers.
- Growing domestic and international collaboration for this project is promising.
- Collaboration and coordination between various stakeholder groups is a highlight of this project. The team's work is directed towards meeting DOE PEC targets.
- The direct conversion of solar energy to transportable stored energy is a strength reflected only in direct electrolysis. PEC is presumed to be more efficient and cost effective than direct electrolysis. Progress in PEC is also directly interesting to improved photovoltaics, so that there could be presumed spin-off benefits of the effort.

Weaknesses

- The project needs to get an industry view.
- Can DOE lure any material scientists from corporate America to help?
- Many years of this project's research efforts have been spent without notable progress toward adequate performance. This weakness might be turned into a strength through the project re-orientation to an integrated feedback loop between materials modeling/simulation, synthesis and characterization.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PD-23: Technoeconomic Boundary Analysis of Photoelectrochemical (PEC) Hydrogen Producing Systems

Brian James; Directed Technologies, Inc.

Brief Summary of Project

The objectives for this project are to 1) perform economic and technical analysis of H_2 producing systems including PEC H_2 production conceptual system designs and hydrogen cost calculations; and 2) identify key factors affecting cost estimates. Design features include 1) advancing implementation of new technology by designing physical systems tailored to PEC materials; 2) design of gas collection system for continuous operation; and 3) design of solar collection for maximum sunlight conversion.



Question 1: Relevance to overall DOE <u>objectives</u>

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

- The project team involved the cost estimates at an early stage to assess how close or far their approach was from being practical and competitive.
- For the team's progress to be measured towards hydrogen production cost targets, a cost basis must be established through modeling of current PEC "state-of-the art" systems. This modeling effort is essential for showing progress towards DOE cost goals and for identifying high-cost components that can be targeted with R&D.
- This project's analysis is critical to guiding researchers toward a feasible system application.
- The team's work is highly relevant to DOE program goals to establish "go/no-go" decision frameworks for the broad suite of possible activities. However, the foundation of the work is far more assumption-driven than fact-driven so that decisions based on this work are not yet possible.

Question 2: Approach to performing the research and development

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

- The team's approach to do economic analysis is fair; however a lot of assumptions were made about cost, system design and footprint possibilities.
- The team needs to involve an industry representative for feedback and input into the cost estimation process.
- The team needs to pay more attention to land use and site preparation costs. It should be a major component in the cost breakdown.
- The technoeconomic model is well designed in this project. Because these systems are still only conceptual, it is appropriate that the focus has been on two of the simpler material applications. The design effort included expert input at multiple steps.
- The process that was followed places limits on the scope of costs that may be associated with this technology.
- The project's approach framework is essentially what is needed, but the data essential to its useful application remains elusive. Consequently, more work is warranted until such time as real data becomes available.

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

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

- The project team achieved the goal of estimated produced cost from hydrogen after making certain design, system and cost assumptions.
- Regarding the 1 tonne per day (TPD) system, would this require many pumps because it includes a slurry mixing system? The only pump listed on the BOM is for water make-up. When the question was asked of where the slurry mixing pumps cost is captured, the response was essentially: "Included somewhere else." The sum of all of the costs on slide 7 (BOM) reaches the \$2,080,963 value, making it unclear how the pumps could have been added in to the capital cost of the 1 TPD system somewhere else,. The cost/operation of these pumps are not trivial based on 43 acres of slurry in bags.
- The project has an excellent first modeling of the economics of PEC systems. Results from the modeling should be helpful in future cost reduction efforts for hydrogen from PEC generation.
- While performing an outstanding analysis of concepts, half the project's concepts implemented have not been brought through a feasibility first (suspended colloids). Colloids have not shown ability to produce hydrogen or oxygen bubbles in any arrangement, and should not be considered for scale-up. Only spectrum adsorption appears to be operating in this technology embodiment. Electrochemistry and transport processes do not provide for a feasible scale-up in this reviewer's experience.
- The project's technical accomplishments in formulating the model framework and its general implementation are outstanding. Nevertheless, more data is necessary before barriers to useful application are surmounted. Some design options can be shown either inadequate or perhaps better than others, but all such decisions are premature until active materials are discovered.

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

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

- Good collaboration has been provided by the PEC group. They, however, need to involve an (energy) industry member.
- It is unclear how the partners contributed to the project's results.
- The project team has excellent collaboration through their work with the PEC Working Group. They directly drew status information and system design concepts from researchers in the PEC Working Group and included them in their models.
- This project has effectively involved the group of researchers associated with it.
- The task leaders were open to input and collaboration with concept leaders.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The project has a fair list of proposed work for completion as it is in the early stages of work.
- This BOP work seems premature without having at least one strong candidate material.
- The project is nearing completion, so preparation of a final report is the next step in their current contract. Future work to include new materials systems and fabrication methods as well as exploring new system concepts would be valuable additions to the techno-economic modeling of PEC systems.
- The work proposed by the team is reasonable.
- Incorporation of new data and some new processes can continue to support program planning for this project.

Strengths and weaknesses

Strengths

- The project has a strong background in H2A type economic analysis.
- This project will help measure progress towards and potential for meeting the DOE cost targets. The methodology was systematic and included good collaboration with outside experts.
- This project provides a decision framework to implement "go/no-go" directions.

Weaknesses

- The project team lacks an industrial background.
- Imagining what the 'winning' PEC material will look like is difficult enough without guessing what type of BOP/process will be required to take advantage of its unique properties.
- There is no validation effort on this model.
- The project is too heavily leaning on unproven technology (colloids). Among the PEC consortium, there appears to be significant disagreement that this is a remotely viable pathway.
- The following is not a problem for the analysis project, but a problem for the implementation of analysis findings: the team's effort should become more focused on discovering slurry particulates that would permit actual operation of the dual bed slurry concept.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PD-24: Characterization of Materials for Photoelectrochemical Hydrogen Production (PEC) *Clemens Heske; University of Nevada, Las Vegas*

Brief Summary of Project

The goals of this project are to 1) develop standardized testing and reporting protocols for PEC material/interfaces evaluation; and 2) publish the standardized PEC characterization techniques in a peerreviewed journal to reach a maximum number of people. The purpose and scope of the project is to 1) properly define the efficiencies (solar-to-hydrogen) that should be used for wide-scale reporting vs. efficiencies (incident photon conversion efficiency) that are useful for scientific, diagnostic purposes only; 2) describe proper PEC procedures for characterizing planar photoelectrode materials; 3) focus on single band gap absorber material only; and 4) describe the techniques, the knowledge



gained, the experimental set-up and procedure, the data analysis, and the potential pitfalls and limitations.

Question 1: Relevance to overall DOE objectives

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

- This project supplies a critical tool chest for the PEC development. The project is instrumental for analysis of PEC materials.
- The project is well aligned with the program goals of achieving system efficiency and life targets.
- Characterization of electrochemical properties is essential for hydrogen generation employing photoelectrochemical (PEC) electrolysis of water. The PEC process is the most direct method for producing hydrogen from water with no carbon footprint. Unlike the other CO₂-free hydrogen production processes, such as S-I cycle, Cu-Cl Cycle, hybrid cycle, and high-temperature SOEC electrolysis, where hydrogen production takes place in a highly corrosive chemical environment. The PEC process is relatively simple with respect to materials handling. The characterization of the photochemical electrodes for splitting water with only sunlight is of major importance in hydrogen generation.
- This project is a workhorse for the technology, and has done admirably to characterize and promote the understanding of the technology's inner workings.

Question 2: Approach to performing the research and development

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

- This project has a good approach to use a standardized characterization method set to disseminate it to the community.
- This project has good experimental capabilities and very powerful analysis toolkits.
- The project team should use well-established flow chart symbols for easier understanding of decision points versus other process steps. Glad to see that there seems to be a process/tracking for calibration of all the sensors.
- The team's approach is innovative and appears to be sufficient for achieving the desired results.
- The project has a comprehensive approach for characterizing the electrochemical properties of candidate materials is described.
- The project's technical approach is very reasonable.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 3.2 based on accomplishments.

- The project's progress was presented against milestones. There was no cost extension for another year requested which may represent some delay in timeline.
- The project appears to be successfully applying and developing state-of-the art measurement techniques and equipment to achieve the required experimental results.
- The project has shown good experimental results that can be explained fundamentally.
- The accomplishment reports analysis on candidate materials is an example of technical achievements made. A table showing the properties of the most promising materials analyzed, including metal oxides and compound semiconductors, would have been more useful.
- No details are given by the PI regarding the characterization of the chemical stability of the materials. This is one of the major issues in the PEC process.
- The progress report illustrates the experimental facilities available at UNLV with pictures. However, no details are given and contributions from other team members on experimental or theoretical analysis, such as density functional theory (DFT) calculations, are not discussed.
- The project's *in situ* characterization process is not elucidated.
- The team's analysis has been modified to fit PEC material characterization needs. Additional modifications are proposed to increase surface chemistry understanding.

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

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

- This project has very good collaborations between this group and rest of the PEC team, as also seen live during a previous UNLV visit.
- Are there any other places in the world conducting characterization testing on PEC material? If so, as this testing is still in the early phases, what have the researchers done to benchmark or reproduce work being conducted at other institutions?
- Collaboration appears to be excellent with all partners in this project.
- The collaboration is impressive but no specific details regarding how the characterization is performed as a team and how the each member of the team interacts with one another. The standardized PEC evaluation process should have been described cited as a reference.
- The project collaboration is admirable. This team has collaborated and improved fundamental understanding for the entire consortium.

Question 5: Approach to and relevance of proposed future research

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

- The teams should continue doing more of the same alongside developing new techniques, which is needed.
- The team's proposed future work looks reasonable and in line with program objectives.
- A future plan is included without any details on how researchers could have candidate material evaluated with guidance from the project team using the standardized test method developed under the project.
- The team will continue the excellent work they are already doing, plus adding ability to further understand surface chemistry of the PEC.

Strengths and weaknesses

Strengths

- The team, especially the group leader, has used powerful analytical techniques and technical expertise in this project.
- This project is providing a lot of feedback to the Standardized Test Protocol project.
- The project is well aligned with the program goals of achieving system efficiency and life targets.

- The team's approach is innovative and appears to be sufficient for achieving the desired results.
- The project appears to be successfully applying and developing state-of-the art measurement techniques and equipment to achieve the required experimental results.
- The project has shown good experimental results that can be explained fundamentally.
- Collaboration appears to be excellent with all partners.
- The PI is a highly competent researcher in material characterization related to the PEC process with an excellent track record in publication and presentations. Availability of a standardized test method for PEC material evaluation would be immensely valuable.

Weaknesses

- The project team's lab safety is a concern.
- The report lacks many specifics.

Specific recommendations and additions or deletions to the work scope

• The project team should clean up the lab area (papers, cardboard boxes, etc.) shown on slides 18 and 19. There are reports on top of devices obstructing device cooling/air flow (slide 18).
Project # PD-25: Nanostructured MoS₂ and WS₂ for the Solar Production of Hydrogen *Thomas F. Jaramillo; Stanford University*

Brief Summary of Project

The main objective of the project is to develop new photoelectrode materials with new properties that can potentially meet DOE targets (2013 and 2018) for usable semiconductor band gap, chemical conversion process efficiency, and durability. To date, there are no known materials that simultaneously meet these DOE targets. The project aims to quantum confine semiconductors through nanostructure to tailor their bulk and surface properties for photoelectrochemical cells. By synthesizing ~ 5 nm diameter MoS₂ nanoparticles, Stanford has tuned the band gap from 1.2 eV to 1.7 eV, a value very close to DOE's 2013 and 2018 targets of 2.3 eV and 2.0 eV, respectively.



Question 1: Relevance to overall DOE objectives

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

- The PEC materials development in this project is a key to PEC pathway success for hydrogen production.
- This project is well aligned with DOE's program goals of achieving high efficiency and durability at low cost.
- This work expands understanding of PEC base material behavior. The work done here is expanding the ability to find solutions to the PEC systems.
- This project is fully supportive of program objectives. Its approach is critical to for future success of photoelectrochemical hydrogen production enterprise. The project's exploration of alternative approaches to band gap and band edge modification in the search for appropriate configurations for efficient and inexpensive hydrogen production is crucial.

Question 2: Approach to performing the research and development

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

- The project's approach of quantum confinement is novel, unique and a distinct way to address the solution to search of right PEC material. In theory this should all work but the team needs to practically demonstrate it.
- The team appears to have a unique approach to solving some of the numerous PEC barriers.
- The team's approach is innovative and shows potential to be able to tailor material properties to achieve high efficiency and low cost (i.e., do not need Nobel metals). Durability was not addressed in this project.
- This is a very creative approach. This reviewer is interested in the handling and robustness of the system. Surface damage seems to be significant due to handling and exposure. This early in the project however, this should not be a huge concern. This technology may very well find application in a different area as well.
- The assessment of outstanding is certainly dependent on successful implementation of the project's approach.
- The study of alternative approaches to doping and alloying that modify band gap and band edge alignment while retaining intrinsic materials performance is an innovative and possibly important approach to acquiring dramatic improvements in poorly performing materials. "Outstanding" award in this project is dependent on additional assessment of the retention of quantum confinement effects for the various structural options presented. Some theoretical/analytic evidence of quantum confinement should be sought before moving to the synthesis/characterization phase in this project.

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

This project was rated 3.6 based on accomplishments.

- This project is a good demonstration of success in achieving the band gap with quantum confinement.
- Demonstration of success in various stages of the final process step by step is shown in this project. The project team now needs to do it all together and show the right behavior at the PEC level.
- The project has had good progress towards DOE's goals from the opposite direction.
- This project is showing significant progress towards meeting goal of 2.0 eV band gap for photo cathodes.
- There are a number of fundamental questions that still need to be answered (e.g., molecular nanowire orientation), but the project appears to be poised to answer most, if not all of them.
- The team has done very good work in the time and budget allocated.
- The project's synthesis of samples has been successful. MoS nanoparticles extended the MoS band gap from 1.2 eV to 1.7 eV. .Further development indicates band gap extension to over 2 eV. Developed AlO₃ frameworks for nanowires and demonstrated data essential to assuring electrochemical deposition of MoS₂ as nanowires inside AlO₃ framework. Nevertheless, it is not clear from analysis that nanowire configuration will retain quantum confinement effects.

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

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

- The PEC group has outstanding collaboration and approach for working together.
- More collaboration will be needed as this project progresses.
- This project appears to be very open in sharing both techniques and fundamental understandings of findings.
- The PI is a strong contributor to collaborative work and is one of the most articulate members of the working group.

Question 5: Approach to and relevance of proposed future research

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

- The team needs to demonstrate the success in terms of photoelectrochemical behavior of the synthesized materials.
- This is an ambitious project that would probably benefit from more time and funding.
- The project team should engage the theoretical group in assessing energetic isolation of nanowire building blocks to assess retention of quantum confinement. Such theoretical studies might identify either materials or processing particulars to assure such retention. The proposed future work did not address this feature.

Strengths and weaknesses

Strengths

- This project shows a different approach allowing much better control of material properties.
- This project is well aligned with DOE's program goals of achieving high efficiency and durability at low cost.
- The project's approach is innovative and shows potential to be able to tailor material properties to achieve high efficiency and low cost (i.e. do not need Nobel metals).
- This project is showing significant progress towards meeting goal of 2.0 eV band gap for photo cathodes.
- Absent miraculous discovery of a new material that meets all the requirements for band gap, band edge alignment, charge carrier generation, survivability and mobility, approaches such as promoted in this project will be essential to improving specific materials properties to improve overall material performance.

Weaknesses

• This project may construct and implement materials that are extremely expensive to manufacture by bulk techniques.

- Durability was not addressed in this project.
- There are a number of fundamental questions that still need to be answered (e.g., molecular nanowire orientation), but the project appears to be poised to answer most, if not all of them.
- More collaboration will be needed as the project progresses.
- The work presented suffers from a lack of theoretical performance modeling and molecular dynamics assessments of stable configurations of materials under nano-configurations. Virtually all planning has been based on observation of gross properties for nano-scale configurations. Such macro-scale properties do not assure the retention of other properties essential to performance.

Specific recommendations and additions or deletions to the work scope

- This is an ambitious project that would probably benefit from more time and funding.
- This project may benefit from modeling of light adsorption and bulk characteristics. Optical absorption rates would determine thickness of nano-materials required, and mechanical property of this layer would be of concern. Mechanical considerations should be accounted for.

Project # PD-26: Development of Hydrogen Selective Membranes/Modules as Reactors/Separators for Distributed Hydrogen Production

Paul KT Liu; Media and Process Technology Inc.

Brief Summary of Project

The objectives of this project are to 1) develop, fabricate and demonstrate field implementable hydrogen selective membranes/modules; 2) achieve process intensification of conventional hydrogen production; and 3) reduce cost for distributed hydrogen production. Specific objectives for fiscal year 2008-2009 are to 1) perform economic analysis; 2) conduct tests using the process development unit (PDU) testing facility at the University of Southern California and pilot testing unit at Media and Process Tech; and 3) fabricate field implemental membranes/modules for field testing by end users.



Question 1: Relevance to overall DOE objectives

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

- This project's objectives align with the Hydrogen Program RD&D mission goals.
- The PI is aware of the DOE technical goals and targets and the timeframe to achieve these targets. In particular, the PI has modified the direction to address the required purity targets that could not be achieved with the prior carbon molecular sieve (CMS) membranes.
- The project studies of separation purity and H₂ recovery are directly applicable to the DOE objectives.
- This program is aligned with DOE objectives but does not seem to provide any game changing technology.
- Development and evaluation of H₂ selective membranes and their evaluation are critically important in hydrogen production and delivery processes.
- This technology has potential to significantly reduce steam methane reforming (SMR) and gasification system complexity and cost.

Question 2: Approach to performing the research and development

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

- The project follows an engineering development path suitable for scale-up. The project in its development path has identified barriers and attempted to overcome the barriers.
- Some of the project's assumptions are ideal. Palladium is a well-known hydrogen transport material, but phase change and stability are issues that the project has not addressed.
- The PI should present the flux data in the DOE recommended unit, SCFH/f² at 100 psi trans-membrane ΔP at DOE-recommended operating temperature and pressure.
- Regarding the actual presentation, the different unit(s) presented only confuses the readers and presenting a ratio instead of independent performance data is further confusing.
- The PI is addressing a process intensification approach that involves incorporating both water gas shift and hydrogen separation. This is a preferred approach that could include cost reductions due to combining engineering process elements. In addition, the work is attempting to utilize a commercial membrane bundle as the Pd support. The bundle has already been demonstrated in other commercial applications. However, the use

of Pd has already been extensively researched and demonstrated limited separation/flux efficiencies and the use of a pure precious metal may have severe commercial limitations.

- The major improvement in this project is based on delivering super atmospheric pressure H₂ on the delivery side of the membrane. It is not clear what the innovation is exactly coating on a ceramic rather than metallic substrate?
- Design, fabrication, evaluation and economic analysis of H₂ selective membranes are the main objectives of the project. The specific approach taken to reach commercially viable processes is well presented. Process simulation, optimization, and field-testing methods are sufficiently described.

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

This project was rated 2.7 based on accomplishments.

- The major technical accomplishment of the project is supplying a module to the Ballard Corporation.
- It is not clear what membrane the project recommends, say for scale-up. Would the team use just the CMS or Pd-coated CMS.
- The project's experimental and economic studies are conducted on both types of membranes and presented interchangeably in a lumped mode and, thus, not readily comprehensible to the reader.
- How the technology can achieve high-pressure permeate stream without additional compression is unclear in this project. What the additional cost for high-P permeate stream is not discussed.
- Technically, the hydrogen flux rates are well below an acceptable limit for Pd membranes (slide 11). There have been numerous other investigations that show much higher flux rates (with both pure and mixed gases). In addition, these prior efforts have also addressed seals and leaks, which this work has not clearly considered (slide 13 suggests a poor H₂/N₂ ratio). The PI suggests a Pd level of 1 micron (on slide 13) but this is an unreasonable thickness because a defect free coating will not be achieved. There will be a significant error if cost estimates are based on this assumption (see chart 1, slide 11).
- The PI made good performance over the year. The team's achievement fell short in terms of permeance but they defend that since the cost much lower than the target, that the system meets the intent of the DOE objectives.
- The team's claim that they "need optimization" suggests that the results are not that much better than the competition. However, with fine-tuning, it can be better. There was no compelling reason for this technology to provide great improvement.
- The project accomplishments show successful separation performance of the relatively low-cost Pd membranes developed and evaluated in pilot scale units. Some of the barriers in reaching economic production of the membranes have been resolved. Field-testing appears promising. Cost analysis shows how the production costs can be minimized.
- What causes the CO₂ permeation and what is the CO breakthrough? Does this device need a further downstream clean up to provide transportation-grade hydrogen?

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

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

- The project team consists of the University of Southern California, Chevron ETC, a catalyst manufacturer (Johnson Matthey), and the Ballard Corporation. These collaborations provide the best opportunity to move the R&D product to market readiness.
- The project involves collaboration with both academics and industrial partners. During the past year, the PI has added the involvement of Ballard, which provides additional insight from an industrial fuel processing end user. The identified partners are well qualified to scale up and commercialize this technology if the larger scale pilot tests are successful.
- The project has good collaboration with industry and academia. It is not clear if all the pieces are being fully addressed by the partners.
- Collaborative efforts with academic faculty members and industrial professionals are well planned in this project.
- This project could benefit from a wider industry exposure. The team can possibly collaborate with European hydrogen production companies.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated 2.8 for proposed future work.

- The project is 95% complete, and ended June 30, 2008. The proposed future work, especially how it is funded, is not evident.
- The team's future work involves membrane/module fabrication for field test. This would be a good success story.
- The project's future work plan is acceptable. A pilot scale test is necessary; however, it is questionable if this membrane will have an acceptable flux level and function in a mixed gas environment.
- The project's future work seems reasonable especially the aim for commercialization.
- The team presented excellent plans for further development of the membranes, testing, and field evaluations.
- This project should consider impurities impact. For example breakthrough of sulfur species if any, effect of CO diffusion and H₂O permeation. What is the scaled-up expected reliability? At a small scale, good performance can be expected, but at scaled-up level, defects can be significant factor.

Strengths and weaknesses

Strengths

- The project's actual test data, collecting permeance and purity information and projecting into system context, is exactly what is needed.
- Apparently a good team is working together in this project.
- The project is on schedule and shows a strong possibility for successful completion.

Weaknesses

- The project's pressure/temperature cycling of bundles was conducted at 220°C rather than 350°C.
- Permeate not 100% H₂.
- The PI had a weak explanation of permeate pressures as well as how the steam purge is implemented.
- The quantification and explanation of electrical energy savings is poorly conveyed by the team.
- The diagrams on slide 17 do not appear correct: individual stage pressures do not add up to permeate pressure.
- The explanation of systems penalty due to added compressors was not clearly spelled out.
- The project had a lack of convincing data that DOE's targets can be achieved.
- Palladium-based membranes are relatively more expensive than carbon-based membranes under development by the project team.

Specific recommendations and additions or deletions to the work scope

- The team should report membrane performance in units consistent with DOE requirements.
- It is not clear that this project has demonstrated adequate technical targets to proceed to larger pilot scale testing. Larger scale testing may not be worth the cost.

Project # PD-28: A Novel Slurry Based Biomass Reforming Process

T.H. Vanderspurt, S.C. Emerson, R. Willigan, T. Davis, A. Peles, Y. She, J. MacLeod, G. Marigliani, and S. Seiser; United Technologies Research Center

Brief Summary of Project

The objectives of this project are to 1) illustrate through an initial feasibility analysis on a 2,000 ton/day (dry) biomass plant design that there is a viable technoeconomical path towards the DOE 2012 efficiency target (43% lower heating value) and assess the requirements for meeting the DOE's cost target (\$1.60/kg hydrogen); 2) demonstrate through preliminary results that an acid tolerant model sugar solution reforming catalyst with acceptable kinetics has been synthesized and that a viable technical path for scale up (mass production) of this catalyst in a costeffective way exists; 3) identify hydrolysis conditions for a simulated biomass system and viable techno-economic path towards



the achievement of the hydrolysis of the real biomass system; and 4) demonstrate through extensive test results an acid tolerant, long life, cost-effective biomass hydrolysis product reforming catalyst.

Question 1: Relevance to overall DOE objectives

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

- This project supports the overall DOE Hydrogen technology R&D program goal and the biomass utilization focus area.
- The team's work is attempting to produce hydrogen from a biomass source, which is a goal of the Hydrogen Program. The PI appears aware of the DOE technical and cost targets.
- The production of hydrogen is relevant however; parts of the project such as operating conditions and residence time seem risky.
- The development of a commercially viable process for the conversion of biomass to hydrogen is one of the DOE goals of hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **2.2** on its approach.

- Hopefully, the project's proposed proof-of-principle approach will work and be scalable. A 2,000 psig titanium liquid phase reactor is cost-prohibitive and operationally difficult. If it is assumed that a scaled-up practical unit will be operated by steam hydrolysis, then the pressure of saturated steam at 310°C is approx 1,400 psi. Additional slurry compression is highly energy intensive.
- The project team's approach is weak and vague. There does not appear to be any clear direction to this project. Since the last review, the investigators seem to have decided that their approach should be a base digestion of biomass coupled with high-pressure reforming (with the subsequent hydrogen separation that was not addressed). The work appears to be a laboratory scale curiosity due to it requiring a high pH base to digest a small amount of biomass (1%). This will not be practical at any scale outside the laboratory. In order to run this process, reasonably exotic materials will be necessary and this will likely be costly. The environment is so corrosive that it even destroys the catalyst and Ti basket (slide 11). Overall, the entire approach does not seem practical and likely has little chance to achieve any of the DOE targets and goals.

- The approach is novel and the results seem too good to be true. The project needs an independent assessment.
- A comprehensive approach is taken for developing an economic process for biomass reforming along with a cost analysis that includes the required initial investments. The objective is to produce hydrogen using a carbon-neutral gasification/reforming process followed by Pd-based membrane separation. Specific objectives are well described.
- This process calls for an extremely high-pressure high-temperature reactor, with 300°C water and reaction time on the order of 2-3 hours. This makes for an extremely expensive design. Construction methods would resemble steam turbines, where similar pressure and temperature are used, but at orders of magnitude larger scale. Cost projections are questionable. Effluent stream is not characterized in the liquid phase. Neither water usage of this process nor recycling strategy is addressed. The catalyst used does not appear to be reusable, and would be a consumable. Safety aspects of the reactor have not been addressed.

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

This project was rated 2.0 based on accomplishments.

- The project's claimed accomplishments are based on efficient and cost-effective separation of hydrogen by a hydrogen transport membrane(s) (HTM). But the selectivity, flux and cost performance of the United Technologies Research Center (UTRC) advanced concept HTM is unknown. Thus, the presented results are speculative. Delivering hydrogen at the claimed cost should be further examined by experiments and system analysis.
- The order of magnitude lower membrane cost and nearly order of magnitude lower capital claims are speculative, because the team has not provided experimental data or system analysis data.
- There appears to be little accomplishment on this project in the past year. The total results appear to be two experiments: 1) the reaction of 1 wt% yellow poplar and 2) the use of approximately 1.7 wt% ethanol. This is minimal work for a project of this size (\$3 million). The only results appear to be a picture of a clear liquid, that evidently represents complete conversion of the biomass into four products: H₂, CH₄, C₂H₆, and C₃H₈. This does not seem realistic from a chemical standpoint considering the complicated organic structure of the biomass. When questioned, the PI was unable to provide any comment on the overall material balance. This is a basic chemical principle and not being able to address this concept in some way is unacceptable technique. The only real data appears to be a plot on page 11, which provides little solid information. The work also advises some cost suggestions however, it is not clear what these are based on. These costs are mainly general assumptions with no clear technical basis and it is unclear that these have any real meaning. The presentation continues to mention modeling efforts (e.g., slides 6, 14 and 24) but modeling is worthless unless clear experimental results are obtained.
- This project is really a 3.5 rating, but a 4 was given based on full faith in the results described. The predicted H₂ selling price is well below targets and is outstanding if it can be achieved. However, the full conversion of even the lignin fraction of the wood is questionable. The pretreatment of some biomass sources might be required and an overall mass balance be carried out and described.
- The range of predictions on H₂ delivery capital costs, etc., suggest there are many unknowns still to be determined in this project.
- It is surprising that a ceria-zirconia-based catalyst will have the durability under aqueous base conditions.
- It was not clear how dilute the system was how much biomass per volume liquid.
- Technical accomplishments in this project include the establishment of proof-of-principle methods, economic analysis, design of new reactors and their performance assessments. Kinetic models of the reformers have been developed to demonstrate the feasibility of the methods proposed. Cost analysis results are very attractive for reaching the DOE goals much ahead of the DOE time schedule.
- Sufficient technical accomplishments to account for the funding level were not presented.

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

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

• UTRC is the prime on the project and the University of North Dakota Environment Energy Research Center (UND-EERC) is conducting the experiments and cost analysis studies.

- In the presentation, slide 16 suggests two direct collaborations in this project UND-EERC and an unidentified catalyst vendor. Neither seems to have any clear involvement in this work. In addition, the slide suggests leverage from another high-cost DOE project but neither appears to have provided any added value to this work. UTRC needs to actively involve other participants if this project is to have any success.
- Collaborations on hydrolysis studies and membrane development and vendor involvement are all good in this project.
- Collaboration with the UND-EERC is shown with their specific roles and project outcomes.
- This project seems to be working in a vacuum, only tapping into University of North Dakota.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.4 for proposed future work.

- For this project there has been, thus far, no FY09 funding and out-year funding is also unknown. Future work has been proposed including a 1 kWe demonstration unit for Phase 2.
- UTRC has demonstrated little success thus far, therefore, the future plans to simply continue on with the work seems to make no sense. In addition, it is not clear that there is any correlation to the established statement of work or work plan which should be the guiding document for the project. At a project of this size more effective project management from both UTRC and DOE is an absolute necessity.
- This project is good but uses a very aggressive plan to technology transfer.
- Future research plans are presented in detail for this project.
- No future work has been proposed.

Strengths and weaknesses

Strengths

- This project has a novel concept and surprisingly good results. This could be a game changer.
- The PI and the research team members are exceptionally qualified to reach the project goals.

Weaknesses

- This project demonstrates no clear strengths.
- The project data is sparse and accomplishment claims are speculative.
- There is a severe lack of project direction and management. The project has produced minimal results and a relatively high cost.
- At this point the project certainly raises eyebrows as no one has seen such results before. Project operation at such high temperature and pressure make aqueous base conditions dangerous.
- Because of the complexity of the economic assessment involving biomass conversion, the cost analysis should be rechecked by an independent source in collaboration with the project team. Biomass projects have significant concerns related to their actual efficiency and socio-economic impacts.
- No sufficient detail was given in order to determine that this is a feasible technology. This is a relatively simple proposed system, and for the funding and time allotted, should have been able to demonstrate better understanding of the process.

Specific recommendations and additions or deletions to the work scope

- The experimental result on the 100% conversion of yellow poplar to gas needs to be duplicated, a few times, using designed parametric experiments. The advanced concept HTM must be developed and proven first before making the hydrogen delivery price claims.
- DOE needs to seriously consider terminating this project immediately.
- The project team should get independent confirmation of overall mass balance and quantify reactor productivity in a flow system.
- Capital outlay and operational cost analysis and future plans merit further funding of the proposed studies.

Project # PD-30: Hydrogen Delivery Infrastructure Analysis

Marianne Mintz; Argonne National Laboratory

Brief Summary of Project

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



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

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

- This is a critical program. This project provides the ability to evaluate new developments in the total context of the program.
- The project and project tools are effectively used to evaluate numerous hydrogen delivery technologies as well as determine their costs and investigate least-cost pathways which directly supports many of the DOE program goals and objectives.
- The Hydrogen Delivery Scenario Analysis Model (HDSAM) has proven to be a very useful tool in estimating the costs and benefits of alternative delivery pathways and system configurations. Continued updates to the model are needed to incorporate new data, evolving technology improvements or operating strategies, and new technology options. The model permits analysis of options and trade-offs and can help to identify an optimized delivery infrastructure that can meet DOE cost targets.

Question 2: Approach to performing the research and development

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

- The project is well designed and does a good job addressing economic barriers, although it was not clear how rigorous the technical review was based on the presentation.
- In general it would have been nice to see more of the overall economic and technical barriers, although presentation time was very limited.
- The project team continues to work closely with industry to incorporate new data and reporting features that enhance the usefulness of the model and its ability to guide and inform the R&D efforts. The model documentation is excellent, assuring that all assumptions are transparent.

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

This project was rated 3.3 based on accomplishments.

• The project team's technical accomplishments this year were very good and the overall tool appears to be very useful to help answer key program questions concerning cost.

- It might have been possible to evaluate additional pathways if HDSAM were designed to be easier to modify or manipulate data (e.g., Excel is a very challenging tool to use for such a large data set).
- The project team's FY09 progress was strong, and the presenter clearly described the updates to the model since the last merit review. Inclusion of three new delivery pathways (700 bar fueling, cryo-compressed fueling, and high-pressure tube trailer) and station polishing steps was essential for modeling of current potential delivery pathway options.

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

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

- Overall, the project collaboration looks good, but it was not clear how well the project is coordinated with the Delivery Components Model work.
- The H2A modeling team continues to make strong use of outside collaborations for data gathering and QA, including the technical teams, industry members, researchers, Technology Validation Subprogram data, and others.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

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

- It would be nice to see chemical hydrides added to the list of delivery technologies being evaluated next year.
- Next steps for this project are reasonably well defined and seem in line with programmatic goals. How necessary is the fuel station footprint size analysis? The footprint makes little difference in the total delivery cost of hydrogen. The plan to allow for multiple markets, on the other hand, could greatly reduce the cost for delivery by reducing the seasonal storage needs. Releasing Version 2.1 of HDSAM (and corresponding documentation) which includes the updates made in the last year is important.

Strengths and weaknesses

Strengths

- The project has good continuity throughout.
- The project is well designed and does a good job addressing economic barriers.
- The technical accomplishments in this project this year were very good and the overall tool appears to be very useful to help answer key program questions concerning cost.
- Overall, the project collaboration looks good.

Weaknesses

- The project team should clarify how rigorous the technical review was based on the presentation.
- In general, it would have been nice to see more of the overall economic and technical barriers, although presentation time was very limited.
- It might have been possible to evaluate additional pathways if HDSAM were designed to be easier to modify and manipulate (e.g., Excel is a very challenging tool to use for such a large data set).
- The project team should clarify how well the project is coordinated with the Delivery Components Model work.

Specific recommendations and additions or deletions to the work scope

• Chemical hydrides should be added to the list of delivery technologies being evaluated next year.

Project # PD-31: H2A Delivery Components Mode

Olga Sozinova; National Renewable Energy Laboratory

Brief Summary of Project

The objectives of this project are to 1) update and maintain the Components Model of the H2A Computer Model; 2) support other models and analysis that include delivery costs; and 3) expand the Components Model by designing new components. Activities included the development of the H2A Delivery Components and Scenario Models.

<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

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

• This is a good program.



- The Hydrogen Delivery Components Model has become a well-used tool by the hydrogen community and is essential for cost analysis of hydrogen delivery components and systems on the basis of common and transparent assumptions. Continued updates to the model are needed to incorporate new data, evolving technology improvements or operating strategies, and new components. The components model also provides important cost data for use in systems-level and scenario analysis models.
- H2A Delivery components model has been critical to identify to key areas for R&D investment in the Delivery Technical Team program.

Question 2: Approach to performing the research and development

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

- The project approach appears to be on track with program's goals.
- The project approach seemed strong, although somewhat poorly communicated in the presentation.
- The team's approach of the modeling effort is good. Expansion of the model to correspond to new needs and developments in the program is aligned.

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

This project was rated 3.0 based on accomplishments.

- The project team appears to have good progress and has caught H2A glitches. The PI's notes at the back of the presentation with assumptions were appreciated.
- The project had significant progress in the last year, the most important of which was allowing for multiple runs through scripting in MATLAB. Progress on new hydrogen delivery options and components, including the addition of a refueling station tab for H2A Production; addition of cost data for rail delivery and 700-bar refueling; and cost analysis for short-distance, urban delivery pathways is important.
- The creation of an automated way to run HDSAM was very important for understanding the impact of many parameters and to more easily perform sensitivity analysis on those parameters.
- The project's technology accomplishments have been steady. The investigation into rail options is interesting but not particularly advantageous in terms of economics. It was confusing as to why 100,000's of model runs were needed for HyDS-ME. Is this project trying to use a model output to make a database for another model and, if so, why? Why not feed one model's results into the following model?

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- This project has a good use of partners. The team should consider having a rail company involved.
- The project has good collaboration with the H2A modeling team (ANL, NREL, PNNL, etc.). Regarding the railroad analysis, no railroad companies were included in discussions. The design of the train station could likely have been improved through interactions with railroad experts.
- There is good cooperation among the national labs and researchers and industry on getting the data together to build and calibrate this model.
- This project is our best product of the U.S. DOE Delivery Technical Team.

Question 5: Approach to and relevance of proposed future research

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

- The presenters should have access to and should use a laser pointer for presenting.
- The project's next steps seem logical and would be good for the Hydrogen Program. Continued refinement (and industry vetting) of the railroad delivery cost components are needed, as is the addition of cost components for cryo-compressed refueling and applications involving the "combined heat, hydrogen and power" pathway.
- The future work here is primarily driven by other projects areas that need modeling as they are developed. The cut in proposed funding will end progress.

Strengths and weaknesses

Strengths

• This project model allows H₂ Delivery Technical Team to focus resources on areas needing development and breakthroughs.

Weaknesses

• This project model needs calibration with actual installation costs to verify accuracy of predictions.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PD-32: Hydrogen Energy Station Analysis in Northeastern US and Hydrogen Sensors for Infrastructure

Eileen Schmura; Concurrent Technologies Corporation

Brief Summary of Project

The objectives of this project are to 1) investigate the potential dual use options, developing a hydrogen infrastructure; 2) analyze early market Hydrogen Energy Station (HES) fuel cell applications; 3) focus on the initial transition to a hydrogen economy, where less than one percent of vehicles will use hydrogen; 4) explore the indigenous energy with an emphasis on renewable feedstocks for hydrogen; and 5) identify the market readiness of the technologies and processes associated with HES biogas/fuel cell systems.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.3 for its relevance to DOE objectives.

- The majority of this presentation focused on HES analysis of stationary fuel cell sites powered by biogas (landfill and di-ester gas) in the northeastern U.S. corridor for combined heat and power (CHP) and combined heat, hydrogen, and power (CHHP). The secondary topic was on proposed evaluation of hydrogen sensors. It is hard to see the relevance of the two topics.
- The CHHP study is a very useful examination and it is very relevant to understanding the role of CHHP systems. The relevance rating for this project is good.
- Rationale or need for the H₂ sensor development is not clear. The relevance rating for this part is poor to fair.

Question 2: Approach to performing the research and development

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

- The project has no comparison of target or metrics of hydrogen sensor work for the currently available technology.
- The project has good cost analysis of CHP and CHHP approaches and the payback time for different classes of sites (biogas sites, big box/industrial sites, and coke gas production) and locations (from state to state).
- The project's hydrogen sensor studies appear to focus on evaluation of commercial sensor technology. It is unclear how will advance sensor technology.
- The project has a logical approach and is well laid-out.

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

This project was rated 2.0 based on accomplishments.

- This project confirms the government incentives required for hydrogen energy stations (HES).
- The project team has shown good progress on HES citing analysis but little or no progress on hydrogen sensor studies.
- The project's cost benefit analysis assumptions are unclear: \$7/kg or \$4/kg H₂, \$0.149/kWh or \$0.075/kWh electricity?

- This project's analysis seems to include free land fill gas. This is not accurate as the gas can be sold and therefore should have a cost to the CHHP system.
- The payback period is a simplified method of semi-quantitatively assessing the economics of a project but a discounted cash flow analysis should be conducted.
- It should be pointed out that the systems only look attractive because of the federal/state capital cost subsidies. A case should have been presented to show the economics without subsidies.
- The cost breakdown of HES & H₂ infrastructure equipment should be given by the project team.
- Benchmarks and goals for the H₂ sensor are not given. This is perhaps due to time constraints in the presentation. The PI did not adequate convey the progress of system and no mention was made of sensor cost which is critical. Discussions of why specific listed features are even needed were not included.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- Roles of collaborators are unclear in this project.
- This project has good collaboration regarding HES analyses. There is little or no collaboration in sensor work aside from what appears to a commercial off-the-shelf sensor.
- A list of collaborators is given but it is difficult or impossible to measure level of their interaction.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.7 for proposed future work.

- The project's funding is complete.
- No plans for future activities were presented.
- No future plans were discussed.

Strengths and weaknesses

<u>Strengths</u> No strengths were provided for this project.

Weaknesses

• This project has had little or no progress on sensor evaluation.

Specific recommendations and additions or deletions to the work scope

- The centrifugal compressors required for pipeline delivery, are projected to be the long-term low-cost option.
- Industrial compressors are one of the key barriers enabling cost effective hydrogen supply and distribution.
- This project is only relevant to central production and compression. This compression technology does not have a high enough compression ratio at 350 and 700 bar forecourt for production and compression.
- Various other compressor applications are outside of hydrogen and DOE program, and they should be explored.
- Improved compression vital to reducing delivery costs. Centrifugal compression for hydrogen represents major advance over existing compressors.
- This project is critical to selecting appropriate technologies for hydrogen delivery.

Project # PD-34: Oil-Free Centrifugal Hydrogen Compression Technology Demonstration

Hooshang Heshmat, Ph.D.; Mohawk Innovative Technology, Inc.

Brief Summary of Project

The objective of this project is to demonstrate key technologies needed to develop reliable and cost effective centrifugal compressors for hydrogen delivery. This project proposes to demonstrate that advanced and very highspeed, oil-free centrifugal compressors can meet hydrogen delivery needs. A key compressor stage will be designed, fabricated and tested to validate the concept and demonstrate overall system feasibility based upon advanced three dimensional aerodynamic designs combined with oil-free compliant foil bearings and close clearance compliant foil seals. Under this effort, compressor blade tip speeds and bearing and seal surface velocities exceeding state-of-art will be designed, built and evaluated.



Question 1: Relevance to overall DOE objectives

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

- The project's focus on centrifugal compressors required for pipeline delivery is relevant and projected to be the long-term low-cost option.
- Industrial compressors are one of the key barriers enabling cost effective hydrogen supply and distribution.
- This project is only relevant to central production and compression as this compression technology does not have a high enough compression ratio to 350 and 700 bar forecourt production and compression. However, it has various other compressor applications outside of hydrogen and DOE program and they should be explored.
- Improved compression is vital to reducing delivery costs. Centrifugal compression for hydrogen represents major advances over existing compressors.
- This project is critical to selecting appropriate technologies for hydrogen delivery.

Question 2: Approach to performing the research and development

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

- Contaminant-free hydrogen is required for low-cost fuel cell operation.
- The project team has an innovative high-speed super critical speed design.
- The team has a good approach to pick an established compressor design (NASA) and address the remaining issues with that design for prescribed application.
- Discharge pressures that the compressor technologies are aimed at (piston, guided rotor, centrifugal) is a bit confusing. The PI needs to make this clear as it is important for the intended application.
- The project team's use of computational fluid dynamics (CFD) modeling is a good approach.
- The project team needs to focus more on addressing potential H₂ leakage and durability issues.
- The team has a good use of simulation to address loads on shaft/bearings. The experiment correlates well with results.
- This project is sharply focused on demonstrating the feasibility and attributes of the centrifugal compressor technology as an input to a down-select.

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

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

- The project's initial frame design is a technical accomplishment.
- The project's analytical, multi-stage, and very high speed.
- The project's down-selected centrifugal vs. piston and guided rotor is a technical accomplishment.
- The project has had good progress on model-based design work.
- The project team needs to report progress on a more structured format including projections on life, cost and efficiency.
- The PI needs to set up a ranking system to evaluate the decision criteria shown (i.e., what are the most critical factors to address?). This needs to be developed in conjunction with DOE inputs.
- The PI needs to also address codes and standards issues and electrical area of classification requirements for H₂ applications.
- The project's 5% completion with \sim 50% of funding expended seems low.
- Objectives in this project are being achieved.

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

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

- Limited Collaboration is seen in this project.
- Good collaborations between Mitsubishi Heavy Industries (MHI) and Mohawk Innovative Technology, Inc. (MiTi), both being industrial players, is good.
- Perhaps the project team should consider having discussions with industrial gas compressor companies.
- Mitsubishi Heavy Industries is good partner for ultimate commercialization of this project.
- MHI is seamlessly incorporated into this project.

Question 5: Approach to and relevance of proposed future research

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

- Design fabrication and testing of concept is in the future plans of this project.
- There is a fair list of proposed work to accomplish this project's goals.
- The project team should consider addressing how the test will be set up to run the compressor on hydrogen.
- The project team should consider addressing safety codes and standards issues as well as durability.
- A timeline for the project's path forward should be shown. If funding is available, when would a compressor be seen?
- The project's future work is focused on supporting a down-select decision.

Strengths and weaknesses

Strengths

- The project's applications of lessons learned from the 70's by NASA are a strength.
- The project has good technical competency and industrial players.

Weaknesses

- The project's 500 tonnes per day (TPD) hydrogen compressors for hydrogen transport is a long-term application. The team should focus more on compressors at the forecourt.
- The project's low funding is a weakness.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PD-35: Development of a Centrifugal Hydrogen Pipeline Gas Compressor

Colin Osborne and Francis A. Di Bella; Concepts NREC

Brief Summary of Project

The objectives of this project are to 1) design and demonstrate an advanced centrifugal compressor for high-pressure hydrogen pipeline transport; 2) investigate alternative system sizes, design options, operating conditions and costs; 3) select a baseline design able to meet near-term applications; 4) identify critical areas of development and operational limitations; 5) design and test critical components under design conditions; 6) build and demonstrate full-scale components in an integrated compressor system; and 7) prepare a development plan for industrial pipeline applications.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

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

- The project's high-purity delivery of gas by pipeline is relevant.
- This project is relevant to DOE delivery program goals in compression cost reduction. Centrifugal compression would reduce down-time and O&M costs, which are typically significant for hydrogen compression and a significant barrier to hydrogen deployment.
- The development of lower cost compressors for hydrogen transportation via pipeline and other compression needs are essential for cost-effective delivery of hydrogen.
- This project is good at looking at current resources for developing compression solutions.

Question 2: Approach to performing the research and development

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

- The project team is "keeping their feet on the ground" with input from industry on requirements.
- The project's use of the shelf is state-of-the art.
- This project seems well designed to address DOE's technical barriers. Compression technology in the central plant must become more reliable and cheaper to enable central hydrogen production and pipeline hydrogen distribution. The project team is taking a very methodical approach to system design and is involving industry partners.
- The team's approach is good for objectives of the project. There is, however, a need to address the issue of hydrogen purity in more depth as design of preferred compressor advances.
- The PI moved too quickly through the technically detailed slides for comprehension.

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

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

• An accomplishment of this project is the "go/no-go" decision point on alternative systems design from phase one.

- The project team should provide a Gantt chart showing tasks and funding in order to better judge progress. It is unclear if the project is on track to meet the July 2009 "go/no-go" decision milestone. It is very good to see the project has developed cost modeling components that are compatible with the H2A models.
- The project's design of a system and end rotor seems novel and well thought out.

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

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

- The project has an excellent mix of industry, university, and national lab with interactions on design.
- The project team's inclusion of industrial gas partner is valuable.
- The team has good collaboration with both industry and materials researchers in universities and the national labs. Industrial collaboration is particularly important considering the potential commercial viability of the compressor technology in the short term.
- Collaboration with Praxair, Texas A&M University and HyGen Industries seems to yield good results int his project.

Question 5: Approach to and relevance of proposed future research

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

- Phase 2 includes detailed design.
- The project is following good practices to update economics as it moves to phase two.
- The project's materials issues are key to success.
- The project's future work seems to be well planned. Several "go/no-go" decisions are part of the plan, which is good, but the team does not appear to be linked to any particular technology performance targets.
- Much work needs to be done on this project. Materials testing, compressor design, and gearbox all require attention. Funding should continue for these tasks to be accomplished.

Strengths and weaknesses

Strengths

- The project's mix of partners, input from industry and selection of near term available materials are all strengths.
- The project has a good collaborative team.
- Take current compressor designs and components to determine if adequate hydrogen compression can be done.

Weaknesses

• This project has had too little progress especially if funding will end.

Specific recommendations and additions or deletions to the work scope

• The teams should consider availability of 70°F water at southern states compressor sites during the summer.

Project # PD-36: Advanced Hydrogen Liquefaction Process

Joe Schwartz and Jerry Jankowiak; Praxair

Brief Summary of Project

The overall objective of this project is to develop a low-cost hydrogen liquefaction system for 30 and 300 tons/day that meets or exceeds DOE targets for 2012. The objectives of this project are to 1) improve liquefaction energy efficiency; 2) reduce liquefier capital cost; 3) integrate improved process equipment invented since the last liquefier was designed; 4) continue orthopara conversion process development; 5) integrate improved ortho-para conversion process; and 6) develop an optimized new liquefaction process based on new equipment and new ortho-para conversion process.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

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

- This project is very good and recognizes/uses liquefaction is a key process for efficient distribution and storage.
- The project's reduced energy process required to make liquid hydrogen economically viable as a transportation fuel is relevant.
- The project's reducing cost and increasing efficiency of hydrogen liquefaction is critical to meeting Hydrogen Program objectives.

Question 2: Approach to performing the research and development

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

- The project adapted a new equation of state. Can the team just use the NIST software directly?
- The project's proprietary approach was not presented at meeting for review.
- The team's work is at too early a stage to evaluate effectiveness of approach. Also, presenter was not able to describe proprietary process.

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

This project was rated 2.5 based on accomplishments.

- The project team has relatively little accomplished. This project is in the planning stages only.
- The project's phase 1 feasibility is underway.
- The project team is building on previous work by EMTECH, Inc.
- The team is creating a new software package when an acceptable tool already exists. This seems to be a waste of effort.
- Evaluation of the ortho-para conversion process (25% of the program) is not possible because no useful information was provided in the review.
- Project is at an early stage; I'm giving it the benefit of doubt.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **1.3** for technology transfer and collaboration.

- No collaborations were listed in the project. This is partly justified by Praxair's dominant position.
- No collaboration or partners listed.
- No collaboration is evident.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- It is unclear what improvements will be incorporated into the system. The presentation seems vague, partly due to proprietary issues.
- The lack of information on plan for ortho-para conversion is a problem.
- This aspect of the project cannot be evaluated as no details were provided.
- This aspect of the project is hard to judge from information presented. The team's plan seems well laid out.

Strengths and weaknesses

Strengths

• This project has an important company leader in the field. The project has potential to greatly improve system efficiency and reduce cost.

Weaknesses

- Relatively little work is accomplished in this project. It is still in the earlier stages. Budget permitting, they have more to show in the future.
- Lack of collaborators and unwillingness of contractor to reveal critical details makes effective monitoring of the program impossible.

Specific recommendations and additions or deletions to the work scope

• If Praxair wants federal research money, they should be willing to be more open about their current performance figures. It is hard to evaluate progress and potential no details are provided.

Project # PD-37: Active Magnetic Regenerative Liquefier

John A. Barclay; Prometheus Energy Company

Brief Summary of Project

The objective of this project is to provide a validated engineering basis for an advanced hydrogen liquefier technology that meets or exceeds DOE's targets for both capital and energy efficiency. Prometheus Energy intends to apply their technical knowledge of and experience with active magnetic regenerative liquefaction to sequentially analyze, design, fabricate, test and validate three experimental hydrogen liquefier prototypes.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



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

- This project has excellent potential relevance, but it is unclear if this system can really compete against conventional chilling and expansion systems.
- This project was well presented and the materials are technically feasible. Good presentation.
- This project addresses high capital cost and low efficiency of current liquefaction technology.
- The team is addressing the key cost challenge of H_2 liquefaction to cost effectively supply H_2 at 700 bar.
- Using a non-compression technique is novel and worth investigating.
- The likely intended application(s) of this technology (central, forecourt or both) is unclear.

Question 2: Approach to performing the research and development

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

- The project team has a good, detailed plan. The advantage of a magnetic refrigeration system for cooling between ambient temperature and 20 K is questionable.
- The project has had good accomplishments in spite of its late start.
- Increasing figure of merit efficiency from 0.35 to 0.5 would be a major breakthrough in this project.
- Continuous adiabatic conversion vs. step wise processing is a good approach.
- The project's execution plan seems logical.
- The project team should develop interim targets (efficiency & cost reduction) for each stage (290 K to 120 K & 290 K to 20 K).

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

This project was rated 2.8 based on accomplishments.

- The project is behind schedule. The team has produced a design and calculated results.
- This project team has done very good work, technically on the right track.
- The project team has prototype parts on order but the cryocooler is in place.
- Significant progress in terms of actual testing due to company's ownership change is not seen and project is still in its early stages.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.2 for technology transfer and collaboration.

- No collaborations have been made other than with suppliers.
- The project team has good interest in licensing technology.
- Little collaboration is listed in this project.
- No significant collaboration with other institutions has been seen.

Question 5: Approach to and relevance of proposed future research

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

- The project team has interesting plans, but this may be an academic exercise. Is this process going to be efficient and competitive at large (station or production facility) scale?
- The project team will complete assembly tests by September 2009.
- This project's first of its kind liquefier is an excellent project for DOE to support.
- The project team should consider concentration on efforts to address any scale up issues and limitations (magnet).

Strengths and weaknesses

Strengths

• This project has an interesting concept and is good idea.

Weaknesses

- The project's progress seems slow, possibly due to contractual reasons.
- The presentation was hard to follow. It would have been helpful to see a schematic of the system with all relevant components. The figure that was presented does not illustrate the thermodynamics of the whole process.

Specific recommendations and additions or deletions to the work scope

• A detailed system analysis to calculate expected performance and evaluate advantages/disadvantages with respect to conventional liquefaction process is recommended.

Project # PD-38: Reversible Liquid Carriers for an Integrated Production, Storage and Delivery of Hydrogen *Bernie Toseland and Alan Cooper; Air Products and Chemicals, Inc.*

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

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

- In this project, how close is the liquid carrier fuel to actual conditions? It seems that the team has its own safety and hazard analysis that needed to be done differently from the full-scale fuel. This is necessary to perform but deflects from the full scale project.
- The project's liquid carriers have potential for low-cost hydrogen delivery.
- Liquid organic hydrogen carriers in this project are one of the key options to reduce Hydrogen supply, distribution, as well as retail and storage costs.
- Liquid hydrogen carriers offer potential paths to hydrogen using conventional infrastructure.

Question 2: Approach to performing the research and development

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

- This project is half-way complete and has shown good results so far.
- The project team's time is better spent investigating alternative materials vs. moving ahead with toxic / corrosive liquid.
- The team's use and approach of the LOHC compound is not to my liking. Why not find and use the real commercial one? Everything about this research is to find that unique material and using a non-commercially viable model material doesn't do any good. The dehydrogenation process is not generic enough to be applied to all different compounds.
- It is unclear if the OEMs like the concept of micro-reactor onboard.
- The project team had a good choice of reactor designs. The microchannel is promising and the team has done good flow simulation work.
- Good work with kinetics modeling can be seen in this project.

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

This project was rated 2.5 based on accomplishments.

• This project appears to be on track.

- Utilizing H₂ fuel for an internal combustion engine (ICE) does not take advantage of the increased efficiency of a fuel cell and would be economically undesirable.
- The project has not had good progress on the microchannel reactor development front. The efficiency (10 15%) is very low seems like a dead end and a huge practical challenge. The computational fluid dynamics (CFD) modeling conclusions are useful to understand but the team needs to demonstrate it practically.
- Systems modeling work progress is fair in this project.
- It is somewhat disappointing that no reactor design has been identified that achieves high conversion, but problem of maintaining catalyst in "wet" state is daunting.
- Are issues expected with autothermal carrier to be the same, greater, or smaller?
- The quantification of projected reactor size is a good addition to this project.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- Interaction between partners is not apparent in this project.
- The project has a good team of collaborators and right industry representatives in the project (OEM, IGC, Equipment Manufacturer).
- The project team's BMW collaboration is a good step. This collaboration adds the needed expertise from an automobile side. PNNL microreactor expertise has advanced this project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- This project's microchannel reactor milestones are shown with "go/no-go" phase gate.
- This project has had a fair proposed list of future work.
- Reasonable extension based on current results can be seen in this project.

Strengths and weaknesses

Strengths

- The project team identified the toxic and corrosive property of N-Ethyl Carbazole.
- The team's liquid carrier approach is unique and worth considering.
- The project shows a good approach and has a capable team.

Weaknesses

- The project team did not discontinue work on toxic and corrosive carrier.
- The team is using the model compound approach. Why not develop/use the real compound?

Specific recommendations and additions or deletions to the work scope

- The project team should compare the total weight and volume for liquid tanks and onboard dehydrogenation reactor vs. DOE targets for onboard storage.
- The team should consider the inclusion of autothermal material.

Project # PD-39: Inexpensive Delivery of Cold Hydrogen in High Performance Glass Fiber Composite Pressure Vessels

Andrew Weisberg, Salvador Aceves, Blake Myers, and Tim Ross; Lawrence Livermore National Laboratory

Brief Summary of Project

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



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>

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

- This project is a good match with the EERE program. It has had good technical progress in the one year time frame.
- This project reduced cost of storage and tube trailer delivery which is relevant to DOE's objectives.

Question 2: Approach to performing the research and development

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

- This project is well done.
- The team's selection of the operating regime to reduce delivery cost, while a good approach, should be reviewed in context of total cost.

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

This project was rated 3.0 based on accomplishments.

- Project appears to have good progress.
- The project team's progress towards trailer delivery targets could provide lower cost hydrogen in the near term.

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

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

- The project team has had collaboration between national labs and industry.
- The project team's "teaming with an innovator" has allowed fast progress towards goal.

Question 5: Approach to and relevance of proposed future research

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

• The project team should include updated cost review as part of transitions between phases.

Strengths and weaknesses

<u>Strengths</u> No strengths were provided for this project.

<u>Weaknesses</u> No weaknesses were provided for this project.

Specific recommendations and additions or deletions to the work scope

• The project team should consider the inspection of cylinders and potential build up of flammable gas mixture in closed container design.

Project # PD-40: Development of High Pressure Hydrogen Storage Tank for Storage and Gaseous Truck Delivery

Don Baldwin; Lincoln Composite Inc.

Brief Summary of Project

The objective of the project is to design and develop the most effective bulk hauling and storage solution for hydrogen in terms of cost, safety, weight, and volumetric efficiency. This will be done by developing and manufacturing a tank and corresponding ISO frame that can be used for the storage of hydrogen in a stationary or hauling application. The objective for the first year of this project (2009) is to design and qualify a 3,600 psi tank and ISO frame that will hold 510,000 in3 (~8,500L) water volume.



Question 1: Relevance to overall DOE <u>objectives</u>

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

- The project's high pressure storage and delivery of hydrogen, eliminating the need for additional compression at the stations is critical to the Hydrogen Program.
- The project aligns with DOE's Hydrogen Delivery element needs by design and development of cost-effective, high-pressure tanks for hydrogen bulk hauling and storage. Lincoln Composites is one of leading companies specializing in the high-pressure tanks development, and the company is well aware of DOE's targets and barriers.

Question 2: Approach to performing the research and development

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

- The project team should do more testing at 5000+ psig. There is not much value seen in 3600 psig tank activities. The team did not show a concrete plan to get to the 5000+ psig.
- The team's approach is sound and straightforward, starting from design and qualification of 3600 psi tanks to 5000 psi tanks. The cost reduction and risk mitigation are the driving forces.
- There is no innovation, and program risk is low.

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

This project was rated 3.3 based on accomplishments.

- The project team should consider more concentrated efforts on 5000+ psig tanks.
- The team needs to look into ambient temperature effects on tanks.
- Would like to see some work on addressing manufacturing of the tanks.
- It seems as if the program is delayed.
- The team has done a great job on development and qualification of the 3600 psi tank.

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

This project was rated **1.3** for technology transfer and collaboration.

- Collaboration in the area of testing to ensure the damage tolerance of the design to realistic scenarios is needed.
- It is suggested that the team consider collaborating with vehicle storage tank projects to see if any synergies can be leveraged. Also collaborations with industrial gas companies might be worthwhile.
- There is no collaboration seen in this project. The team should collaborate with other companies who have similar experience on high-pressure tanks development.

Question 5: Approach to and relevance of proposed future research

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

- The project team should consider looking into addressing any potential codes, standards and regulatory issues.
- Future work to develop and qualify the 3600 psi tanks and 5000 psi tanks are very sound in this project.

Strengths and weaknesses

Strengths

• The company has great fabrication capabilities and facilities.

Weaknesses

- Risk assessment and hazard analysis of tank accessories and corresponding interfaces, (such as pressure relief valves), is lacking and should also be performed.
- The cost of delivery of hydrogen in this project is unclear.

Specific recommendations and additions or deletions to the work scope

• Hydrogen's delivery infrastructure using high-pressure tanks is good for light use of hydrogen, but may not be applicable to daily/heavy use/transportation of hydrogen to H₂ refueling stations that particularly are located in metropolises. Under certain emergency situations (delivery truck involves an accident), a break or malfunction of the pressure relief valve or its interface to the tank may result in a release of 600 kg of H₂ at once. There is the potential that this could lead to a hazardous situation or possibly an explosion in population centers.

Project # PD-41: A Combined Materials Science/Mechanics Approach to the Study of Hydrogen Embrittlement of Pipeline Steels

P. Sofronis, I.M. Robertson, and D.D. Johnson; University of Illinois at Urbana-Champaign

Brief Summary of Project

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



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>

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

- This project has good relevance and much potential to characterize failure mechanisms in steel pipelines.
- The team's understanding of hydrogen embrittlement is critical to the design of hydrogen equipment.
- The project's study of pipeline steels is extremely important. Mechanistic understanding of the embrittlement processes is important for a hydrogen economy. Steel materials will likely be used throughout the hydrogen economy, whether in devices, in the existing pipeline network, or in pipelines repurposed for hydrogen.
- This project provides critical R&D to hydrogen pipeline delivery pathway and addresses potential hydrogen embitterment issue.
- I was unable to review due to a conflict.

Question 2: Approach to performing the research and development

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

- This project demonstrates a good combination of theory and experiments leading to better understanding.
- This project has a good blend of experimentation, characterization and modeling.
- Excellent fundamental work is shown in this project.
- The project is employing a sound mixture of modeling and experimental work. Models are validated with experimental data. This work increased the understanding of the fracture mechanics of pipeline steels in the presence of hydrogen. The methods developed in this project will have applications outside of pipeline steels.
- Significant amount of work was focused on simulation in this project. The project should have or build into some actual experiments to validate model.

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

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

- This project's progress has been delayed due to funding issues.
- The project team is developing knowledge to set safety standards based on science.

- The project team has had great progress on gaining a better understanding of the fracture mechanics, as seen in slide 14. Strong results are seen in the understanding of the change of stress intensity factor in a hydrogen environment. Substantial progress with this team was made in 2009 in both experimental and theoretical work.
- Actual experimental results should be represented in this project. As with any modeling/simulation effort, one learns the most through doing the experiments.

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

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

- This project has multiple collaborations with appropriate institutions.
- This project contains an excellent mix of partners and "active partnership".
- Coordination and relationship between University of Illinois at Urbana-Champaign and SNL is excellent in this project. Collaboration with various industry members, such as Secat, Inc. and DGS Metallurgical Solutions, Inc. is strong and contributes to the project through their understanding of pipeline microstructures. Also, the participation of the project with the Hydrogen Pipeline Working Group is excellent. Collaboration resulting from the working group team is extensive and should be continued. International and standards-related collaborations are valued and add to the depth of this project and the Hydrogen Program as a whole.
- Excellent collaborations with various institutions are seen in this project. The industrial gas companies and energy companies have localized hydrogen steel pipelines in operations. It would be worthwhile to learn about their experiences regarding hydrogen embitterment in steel pipelines.

Question 5: Approach to and relevance of proposed future research

This project was rated 3.5 for proposed future work.

- The project team has proposed appropriate work.
- The team is working on both testing and modeling to increase understanding of mechanisms involved.
- The team's plans are well focused, both combining theoretical and practical approaches.
- The team's future plans are well laid out. Continued efforts to validate simulation tools, in collaboration with SNL, are an excellent next step. The work continues to increase the base knowledge of hydrogen effects on pipeline steels, with an eye for a better understanding of hydrogen embrittlement in metallic systems in general.
- The project team should do experiments to validate simulation.
- The project team should seek data from existing, real world hydrogen pipeline networks (places like greater Houston area where local hydrogen pipeline network near refineries is in place).

Strengths and weaknesses

Strengths

- The project team is not only good but also a prestigious researcher.
- This project has a strong team with active partnerships.
- Good collaborations are apparent in this project.
- The team's experimental and theoretical method is very strong. Collaborations with other DOE projects and external groups should serve as a model for other research projects.

Weaknesses

• The project team should elaborate on the current status of the technology, i.e., how is this project enhancing knowledge?

Specific recommendations and additions or deletions to the work scope

• This project should be continued.

Project # PD-42: Fiber Reinforced Composite Pipelines

Dr. Thad M. Adams and G. Rawls; Savannah River National Laboratory

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

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

- This project could be important for long term delivery if challenges are addressed.
- This project is important for the cost-effective distribution of H₂.
- It is absolutely critical to understand the requirements for installing FRP for hydrogen service. This project begins to address that need.

Question 2: Approach to performing the research and development

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

- This project should focus on technical details (permeability, leakage, strength) rather than in regulatory aspects. If the technology succeeds, then the industry will get it through the regulations.
- This project shows analytical work framing code and safety issues with limited technical investigation. It is possible that the properties of the piping are know, but were not reported or analyzed.
- What about finite element analyses (FEA) for understanding the maximum bend radii? Is this known from natural gas usage? The change in leak rate reported was not interpreted, even if upon reflection, it seems inconsequential.
- The team should pay attention to accelerated test protocols for e.g. H₂ permeation or other pipe aging mechanisms.
- The team's approach seems a bit distributed among several tasks. The team should consider increasing focus on understanding what close requirements are needed by authorities with jurisdiction for installing FRP for hydrogen service. The team should focus on the aforementioned goals first.

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

This project was rated 2.3 based on accomplishments.

- This project has had reasonable accomplishments for the low budget allocation.
- The project's framing of the issues for adoption is well done.
- The team's technical depth and inspired analysis are both lacking.
- The project's accomplishments have been hampered due to the lack of funding. For the funding supplied, reasonable progress has been made.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- This project has good collaborations with key institutions.
- The project's extent of interaction with ASME is not totally clear.
- The project team should consider trials of these materials in an industrial gas setting (APCI, Praxair, Linde, Air Liquide), with appropriate controls. A high interest in this is assumed.
- Reasonable cooperation with ORNL, Fiberspar, Polyflow and ASME can be seen in this project.
- The project team should consider stronger cooperation with the Department of Transportation and ASTM to address requirements.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- This project has good future plans. They seem to be better aligned with technical issues than with regulatory issues.
- Not much can be said about future plans due to the halt in this project's funding.
- The involvement of an industrial gas stakeholder is encouraged.
- This project plan set if funding appears.

Strengths and weaknesses

Strengths

- This project has potential for future advantage if successful.
- The project has the knowledge of practical requirements, especially safety and codes.
- The project's examination requirements for FRP installation for hydrogen service are a strength.

Weaknesses

- The project needs a better evaluation of system cost and performance to better justify the work.
- The PI needs to be better informed about basic facts (safety factor for pipeline?).
- The project team's technical depth focused on outstanding issues which is a weakness.
- The project team needs a more focused approach for limiting requirements by authorities with jurisdiction.

Specific recommendations and additions or deletions to the work scope

- The project team should evaluate potential reduction in hydrogen delivery cost. How does this compare to other hydrogen delivery technologies?
- The project team should consider collaborating with key stakeholders and conducting field trials.

Project # PD-43: H₂ Permeability and Integrity of Steel Welds

Z. Feng, L. Anovitz, W. Zhang, and J. Wang; Oak Ridge National Laboratory

Brief Summary of Project

The objective of this project are to 1) quantify the effects of high-pressure hydrogen on property degradation of weld in pipeline steels; 2) develop the technical basis and guidelines for managing hydrogen, stresses and microstructure in the weld region to ensure the structural integrity and safety of H_2 pipeline; and 3) develop welding/joining technology to safely and cost-effectively construct new pipelines and/or retrofit existing pipelines for hydrogen delivery.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



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

• This project is extremely useful to the objectives of the DOE Hydrogen Program. It aims at analyzing the fracture behavior of welds in the presence of hydrogen.

Question 2: Approach to performing the research and development

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

• All four elements of the project's approach stated on slide #5 are important.

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

This project was rated 3.5 based on accomplishments.

- The project measured the permeability of the weld but it did not establish the diffusion coefficient of hydrogen through the weld at room temperature. This information is important because this is precisely the room temperature at which hydrogen embrittlement takes place.
- The team's baseline fracture tests with notched cylindrical bars of 4340 steel microstructures are good, but it is not clear how these tests and results help toward understanding the fracture response of the welds.
- The team's usage of the spiral notch torsion test (SNTT) for K_{th} measurement is an old test with questioned validity in particular with regard to mild and medium steel microstructures (yield strength less than 700MPa). The stress state locally in front of the notch is three dimensional despite the fact that an un-notched specimen experiences opening tension under macroscopic twist. Therefore, the mechanisms of fracture respond to all modes (opening, shearing, and tearing) and hence it is not correct to claim that the test isolates the mode I fracture response.

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

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

• The contributions of any of the partners listed on the opening slide were unclear.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

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

• With the exception of the K_{th} test with SNTT, the proposed work described on slide #19 is well thought out and important. In particular, the welding technology development and the management of the residual stresses in relation to the microstructure are both unique contributions. With regard to the K_{th} test with SNTT, it is an old technology and certainly does not isolate the opening mode of failure. The approach described in the ASTM standard E1681-03 is more precise and conclusive. In fact, there is doubt whether this SNTT test can yield any reliable information with regard to the proposed study of X52 welds (mentioned on slide #19). The X52 has a very mild microstructure and this makes it highly unlikely that conditions for pure mode I and small scale yielding are prevalent at the tip of the notch on the cylindrical bar subjected to macroscopic twist.

Strengths and weaknesses

Strengths

- The project's strength is in leadership and weldment expertise of Z. Feng.
- ORNL's capabilities in welding technology are project strength.

Weaknesses

• The project team's approach of analysis for fracture toughness of welds in the presence of hydrogen is a weakness.

Specific recommendations and additions or deletions to the work scope

- More emphasis should be put on conventional welding processes, as opposed to friction stir welding.
- The project team should focus on the project strengths that are the weld microstructure, namely identify the type of the microstructure that is most compatible with hydrogen. The K_{th} analysis is inferior when compared with the one recommended by the ASTM Standard E1681-03. It is suggested that the ASTM standard be adopted.

Project # PD-44: Composite Pd and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process Intensification

Yi Hua Ma; Worcester Polytechnic Institute

Brief Summary of Project

The objectives of the project include; 1) synthesis of composite palladium (Pd) and Pd alloy porous Inconel membranes for water-gas shift (WGS) reactors with longterm thermal, chemical and mechanical stability with special emphasis on the stability of hydrogen flux and selectivity; 2) demonstration of the effectiveness and longterm stability of the WGS membrane shift reactor for the production of fuel cell quality hydrogen; 3) research and development of advanced gas clean-up technologies for sulfur removal to reduce the sulfur compounds to less than 2 ppm; and 4) development of a systematic framework towards process intensification to achieve higher efficiencies and enhanced performance at a lower cost.



Question 1: Relevance to overall DOE objectives

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

- Barriers related to the Hydrogen Program are addressed in this project. This project also focuses on research on developing advanced gas clean up system.
- This is an important and comprehensive project on development and testing of composite Pd-based alloys and Inconel membranes, highly relevant to DOE's hydrogen and fuel cell technologies. The researchers have excellent and methodic approaches for membrane development and testing. The presented results for FY08-09 indicate substantial progress in determining the effects of a number of contaminants and H₂-flux. The H₂-flux rates obtained from the developed membranes are significantly higher than DOE's targets for 2010 and 2015.
- A membrane of this type has the potential to enable several important applications.
- Addressing the membrane R&D needs for purification from coal-to-hydrogen process is relevant to DOE objectives.
- Typically when pressure swing adsorption (PSA) is used, no preferential oxidation and sometimes no low-temperature shift (LTS) is used (just a note on slide 4).

Question 2: Approach to performing the research and development

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

- The project team's approach is to fabricate Pd and Pd-alloy (Pd-Au) membranes on porous stainless steel tubes and test the membrane performance. It is unclear what was done to develop advanced sulfur clean up. Slide #4 showed the schematic approach of this project that included the advance sulfur cleaning unit but there was nothing about it in the rest of the presentation. Also, the adsorption work is unclear. Is this project trying to develop improved PSA system?
- Approaches used in this program are sound and carefully implemented. Nearly all aspects of the membrane productions and testing have been considered and evaluated. Modeling simulations of Methane Steam Reforming (MSR) have provided useful information. Effects of pressure, temperature and compositions have been predicted.
- Sequential characterization and testing activities are appropriate in this project.
- Regarding the tubular membrane: while it is useful to test the membrane with synthetic mixed gas stream, the project team needs to test with actual syngas from a gasifier.

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

This project was rated 2.8 based on accomplishments.

- It is claimed the membrane system had very high selectivity (nearly infinite selectivity for hydrogen). The detection limit of the gas analysis unit for CO, CO₂, and other species should be presented. No data was presented on the structural stability of the membranes under cycling conditions. Was there any interaction between the Pd membrane and the interface oxide layer?
- The project has shown very good progress regarding synthesis, fabrication and testing of Pd and Pd alloy composites membranes for applications in WGS reactors. Results of the tests are satisfactory and promising. Reported test results of the membranes, using simplified gas mixtures, indicate very good long-term H₂ selectivity and stability. However these tests should be extended to gas mixtures that are more realistic and similar in compositions with syngas.
- The data reported shows good progress toward the project's flux goals.
- Given the length of the project to date, there needs to be testing with real syngas from a gasifier.
- Regarding long term testing (slide 8), what are the concentrations of the gases entering the membrane (62%H₂, 37%CO₂, 1.2%CO).
- The project team needs to address the impurities and their levels in the product hydrogen stream and compare them to California Fuel Cell Partnership Hydrogen purity specifications.
- Presentation overall lacks cohesiveness and difficult to follow by the team.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.5 for technology transfer and collaboration.

- Collaboration is seen with Adsorption Research, Inc., in the area of adsorption study but the objective of this collaborative work is not clear. Is it to develop an advanced PSA system or to develop advanced sulfur removal technology?
- It appears there is some collaboration with Adsorption Research, Inc. for production and testing of sulfur removal sorbents and for building and testing of the Pressure Swing Adsorption systems.
- Outside testing with Shell's reformer is useful for program validation.
- The project does not have significant collaborations with other institutions. The project team should work with other DOE sponsored projects to leverage any synergies.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- The project team has decided to continue the Pd-Au alloy membrane to improve the flux. Both Pd and Au are very expensive. Is there a plan to look into less expensive alternate membrane materials? How is the mass transfer resistance overcome in a very thin membrane?
- The project team's future work will include additional alloying studies for improving H₂ flux. Modeling studies will extend to a broader range of conditions and alloy types, including Pd-Au alloys. In addition to planned tolerance tests for CO and sulfur, poisoning effects of other major syngas contaminants should also be tested and evaluated. Major contaminants in a "typical" syngas, including halogens and nitrogen oxides, should be added to test mixtures and their poisoning effects should be evaluated and quantified.
- The project team should provide the connectivity to the baseline information that informed this project.
- The project team should also describe why this project is innovative in more detail then the general information provided. The concern about IP is understood but a credible examination of the claims of performance relies on some understanding of the mechanization.
- The project should compare the product against current hydrogen purity specs.

Strengths and weaknesses

Strengths

- The project team has significant experience with Pd membrane. The availability of graduate students and postdoctorate students to carry out the experiments and test new theories/hypothesis is beneficial. Professor Ed Ma is well respected in this field.
- The project applies sound and well-planned procedures for selection, fabrication and testing of the Pdcomposite membranes. The experimental testing methods are adequate and carefully performed. The modeling simulations are very useful for predicting the performance of the membrane in a broad range of conditions.
- The testing regime is thorough in this project.

Weaknesses

- The lack of knowing the detection limits for CO, CO₂ is a weakness. The selectivity numbers reported in this project are questionable (due to lack of detection limits for other gases). Nothing about an advanced sulfur cleaning unit was presented.
- No major weaknesses were identified.
- It is curious that no embrittlement has been reported by the project team. The representation that this simply does not occur is not credible without support.

- The project team should perform an economic analysis for the Pd-Au alloy membrane. Will it meet the DOE cost target? How about sulfur poisoning of Pd membranes?
- The potential poisoning of all major syngas contaminants, particularly nitrogen and halogen compounds, should be tested and evaluated by the team.
- The analytical detection limits for H₂, CO and other relevant species should be carefully established and considered in error assessments of the data.
- No changes are recommended.

Project # PD-45: Development of Robust Metal Membranes for Hydrogen Separation

Brian D. Morreale; National Energy Technology Laboratory

Brief Summary of Project

Studies suggest that incorporating separation membranes into coal conversion processes can reduce costs. The overall goal of this project is the development of robust dense metal, hydrogen separation membranes for integration into coal conversion processes. A test protocol has been developed that allows technological progression and comparisons for application to coal conversion processes. Several alloy compositions have been fabricated and screened for performance, and some alloys have shown potential for S-tolerance.



<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

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

- This project is pertinent to industrial applications.
- This project addresses the membrane R&D need for purification from coal-to-hydrogen process.

Question 2: Approach to performing the research and development

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

- The project team's idea of intentionally degrading the system is interesting.
- It is unclear if using Pd alloy membranes is the best approach for separating hydrogen from coal-derived syngas The syngas contains more contaminants (to the membrane) as compared to a cleaner reformate stream from a steam methane reformer. Research on Pd and Pd alloy membranes integrated with a reformer has been done for many years and the technology has not been applied commercially. This project's application potentially can be more challenging for the membrane.

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

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

- More analysis is necessary in this project to contrast the performance of a degraded system vs. a non-degraded system.
- The project team has had good progress towards addressing the three main tasks of the project and addressing the barriers.

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

This project was rated 3.0 for technology transfer and collaboration.

• This project has good collaborations with various institutions.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.5 for proposed future work.

- The project's Pd/Cu alloys have been used extensively in hydrogen work and it would be useful to have some connectivity to the baseline information that informed this project.
- It would be useful to describe why this is innovative in more detail then the general information provided. The concern about IP is understandable but a credible examination of the claims of performance relies on some understanding of the mechanization.
- The project team should consider developing a list of selection criteria in trying to optimize a membrane development.
- The project team should consider testing water-gas shift membrane reactor (WGSMR) with real syngas from gasifier.
- The project team needs to determine impurities and their levels in product hydrogen stream.

Strengths and weaknesses

Strengths

• The project's focus on durability is important to adaptation.

Weaknesses

• A degraded system has limitations that were not fully presented.

Specific recommendations and additions or deletions to the work scope

• None recommended.

Project # PD-46: Scale-up of Hydrogen Transport Membranes for IGCC and FutureGen Plants *Doug S. Jack; Eltron Research & Development Inc.*

Brief Summary of Project

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

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

Overall Project Score: 2.4 (4 Reviews Received)

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

- The objective of this project is to develop an H₂/CO₂ separation system that retains CO₂ at coal gasifier pressures, operates near water-gas shift conditions, tolerates reasonably achievable levels of coal derived impurities, delivers pure H₂ for use in fuel cells, gas turbines, and hydrocarbon processing, is cost effective compared to alternative technologies for carbon capture. Therefore this project supports DOE's Hydrogen from Coal Program.
- The development of practical and inexpensive membranes for hydrogen separation/purification for use in fuel cells is highly relevant to DOE's Hydrogen Program. However, most relevant and critical information necessary for evaluations of this project was not provided to reviewers. In the absence of such critical information it is difficult to evaluate the project, informatively and fairly, on its progress and soundness of future work.
- If this project is successful, this work would be highly relevant to DOE objectives.

Question 2: Approach to performing the research and development

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

- The project team's approach involves materials development, performance screening, mechanical design, process design and economics, and scale-up steps. The membrane and catalyst compositions are not disclosed; therefore it is difficult to determine whether the approach taken is right or wrong.
- The team's approaches utilized in this project are good and are now standard for development and testing of the separation membranes.
- The integrity of the welded seals mentioned might be sensitive to differences in hydrogen expansion. Welding has only been tested on disks so far.
- There seems to be an issue with the catalyst layer being affected by intermetallic diffusion in this project. Even at lower temperatures, this might become an issue over longer time periods.

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

This project was rated 2.0 based on accomplishments.

• The project's flux numbers are very impressive but they are measured under ideal conditions. The flux numbers should be reported using truly mixed-gas streams similar to a gasifier gas stream. What is the hydrogen recovery in experiments where fluxes over 350 SCFH/f² are obtained? Important information like gas flow rates, hydrogen recovery, and selectivity were not presented. It is difficult to evaluate the technical

accomplishments without knowing more about the membrane material and the catalyst used. This presentation appeared as if it was made by a representative from the Chamber of Commerce (to promote a business) rather than a scientific presentation for a peer review.

- No information was provided on the nature of the membranes used for testing. It is unclear if the project team has or will overcome the barriers for large scale and/or long term usage of the tested membranes. For example, if copper is a major component, based on several independent studies, exposure to sulfur will most likely rapidly destroy the membrane.
- The presented data indicates that the membrane material performance in this project will meet DOE's goals.
- The project's progress is hard to judge in this case. There was insufficient information provided to make a credible determination.
- Given that scaling up of the technology is the goal, the presented quantitative data on the basic problems (see above) do not address this goal. Maybe they are and the results are not made available to the reviewers?

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

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

- None of the project team's collaborators were disclosed. Partners include four membrane manufacturers and two industrial chemical producers.
- Information on collaborators in this project was not provided by the presenter.
- More information on collaborators would help address issues/uncertainties that the project can stand firmly on its merits.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

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

- It is stated (slide 6) that one alloy composition was down-selected for future testing and test results show the performance is meeting the targets. If this is the case, why will the team perform life testing on new materials? What is wrong with the already down-selected material?
- It is not possible to rate this project's proposed future work, when required information is not presented. For example, if the alloys to be tested contain Cu, a number of other recent studies have already reported various difficulties and performance problems with such alloys. Therefore, if this project intends to test copper containing alloys, it should present a convincing reasoning for repeating such studies.
- It would be useful to have some connectivity to the baseline information that informed this project.
- Also, it would be useful to describe in more detail why this is more innovative than the general information provided. The concern about IP is understood, but a credible examination of the claims of performance relies on some understanding of the mechanization.
- It might be too early for this project to scale up.

Strengths and weaknesses

Strengths

- The flux numbers in this project are impressive. Many years of experience on membranes is seen. The project team's ability to get new partners whenever needed is good (unfortunately no long-term partners).
- Developing and testing inexpensive, effective and durable H₂-separation membranes are of high priority for H₂ technology. Contributions of this project can be valuable to DOE's mission in advancing H₂ technology.
- This project has high potential if successful.

Weaknesses

- The PI was not able to disclose the material.
- Due to the lack of adequate quantitative data and information on composition of membranes developed and testing in this project, it is difficult to fairly assess the weaknesses or strength of this project.
- There is little attempt by the project team to actually describe the membrane or the methodology of testing the membrane.

- There was little effort to present any information other than unsupported claims in this project.
- No proof was provided that fundamental problems are sufficiently addressed in this project. It is too early for the team to focus on scaling up. Critical technology seems to be outsourced to subcontractors.

- The project team should address commercial scalability of the Eltron membrane and catalyst. They should study the stability of the membrane and catalyst under cycling of temperature and gas composition.
- Additional testing by the team for the membranes is needed before moving to the production stage. Particularly, in addition to sulfur and CO poisoning, effects of chlorine and nitrogen oxides should be tested and quantified.

Project # PD-47: High Permeability Ternary Palladium Alloy Membranes with Improved Sulfur and Halide Tolerance

Kent Coulter, Ph.D.; Southwest Research Institute

Brief Summary of Project

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



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

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

• The objectives of this project are to develop and test Pd-based membrane that has improved tolerance to corrosive contaminants in syngas. The objectives of this project are in support of DOE's hydrogen and syngas technologies and results will help to achieving DOE goals

Question 2: Approach to performing the research and development

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

- The experimental and computational modeling approaches employed in this project are generally well planned and effective. However, the density functional theory (DFT) computational modeling efforts need improvement. Modeling procedures can be calibrated and verified by comparing modeling predictions for properties of certain alloys with experimental results for the alloy with same composition.
- The sealing can be improved in this project as well as the bottleneck on method.

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

This project was rated 3.3 based on accomplishments.

- The project team has reported significant progress towards objectives of the project.
- Eventual large scale applications of very thin membranes foils and disks for syngas-H₂ purifications is not likely due to a large number of technical difficulties in fabrication and using such foils and films. However, test results derived from this and similar projects are very useful in understanding chemical and physical properties of various alloys relevant to hydrogen purification and fuel cells.
- Results of this study on hydrogen permeability for various alloys and different temperatures are very valuable in assessing the preferred alloys for hydrogen purification.
- Data presented by the team was lucid, clear, and thorough.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- The project team is working with a number of very capable groups, with complementary expertise, and is collaborating to achieve the objectives of this project.
- The project team performed all aspects of the studies, including design, modeling, fabrication, and testing of membrane.
- The project team can add work done by Lovvik et al, to incorporate in the theoretical model.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- The planned future work is generally sound and will help to achieve the stated goals of the project.
- It is recommended that more emphasis be given to improving and validating the modeling procedures for predicting hydrogen permeability of various alloys under different temperature and pressure conditions. If successful, modeling predictions should help in screening of a very large number of alloy compositions considered for testing. In the long run, using the modeling predictions for better selecting alloy compositions will lower the cost and shorten the time needed to achieve the objectives of the project.
- The goal of ultra thin membranes is constructive to integration and retrofit scenarios for several applications.
- Again, this project will encounter sealing barriers.

Strengths and weaknesses

Strengths

- This is a multi-approach and well-planned project. Collaborations among a number of expert groups with complementary capabilities have had past success and will help in achieving the future objectives of the project.
- The project represents a valid effort with 70 units fabricated.
- This project provides a powerful tool to make any alloy composition with high precision. This is highly valuable for the industry.

Weaknesses

- The computational modeling efforts are not well coordinated with laboratory studies. Hydrogen permeability for a large number of alloys has been determined experimentally and through modeling. However, alloy compositions used in modeling do not compare with those used in experimental studies. Consequently, direct comparison of the modeling and experimental results are not possible and experimental results cannot be used to calibrate the computational procedures.
- As test results from this work show, very thin membrane films are not likely to be durable for long-term applications. Alternative approaches, such as supporting of membrane on a durable base, should be considered.
- It would be useful to have some connectivity to the baseline information that informed this project.
- Sealing issues in this project are a weakness.

- It is recommended that more emphasis be given for improving the modeling procedures for predicting hydrogen permeability of various alloys under different temperature and pressure conditions. If successful, DFT modeling predictions should help in screening a very large number of alloy compositions considered for testing. And in the long run using the modeling predictions will lower the cost and shorten the time needed to achieve the objectives of the project.
- Continuing the testing of very thin membrane films should be replaced with other method(s) that provide more membrane durability.
- The Cu content of alloys may be responsible for rapid degradation and rupture of the membrane films.
- No changes are recommended.

Project # PD-48: Experimental Demonstration of Advanced Palladium Membrane Separators for Central High-Purity Hydrogen Production

S.C. Emerson, J.T. Costello, Z. Dardas, T. Hale, R.R. Hebert, G.C. Marigliani, S.M. Opalka, Y. She, R. Willigan, and T.H. Vanderspurt; United Technologies Research Center

Brief Summary of Project

The objectives of this project are to; 1) confirm the high stability and resistance of a PdCu trimetallic alloy to carbon and carbide formation and, in addition, resistance to sulfur, halides and ammonia; 2) develop a sulfur, halide and ammonia resistant alloy membrane with a projected hydrogen permeance of 25 m³m⁻²atm^{-0.5}h⁻¹ at 400°C and capable of operating at pressures of 12.1 MPa; and 3) construct and experimentally validate the performance of 0.1 kg/day H₂ PdCu trimetallic alloy membrane separators at feed pressures of 2 MPa in the presence of H₂S, NH₃ and HCl.



Question 1: Relevance to overall DOE objectives

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

- The objective of this project is to develop a sulfur, halide, and ammonia resistant alloy membrane for hydrogen separation and construct and experimentally validate the performance of 0.1 kg/day H₂PdCu trimetallic alloy membrane separators at feed pressures of 2 MPa (290 psia) in the presence of H₂S, NH₃, and HCl. This project supports the hydrogen from coal program (centralized hydrogen production).
- Objectives of this project include fabrications and testing of palladium-copper and tri-metallic membranes for hydrogen purification that are resistant to poisoning by syngas contaminants. Overall project objectives and technical plan may result in development of low-cost membranes for hydrogen production. This project is in line with DOE's cost goals.
- Currently, a H₂-flux of about 60 scfh/ft² with a 100 psi back pressure has been achieved. This flux is considerably less than the DOE 2010 target flux of 200 scfh/ft². Significant advancements by this team in membrane durability and H₂-permeation need to be made to achieve the DOE target. Also, tested membranes show inadequate lifetime and durability. Tests at higher backpressures have caused rapid membrane failures. Fundamental reasons for such failures need to be understood.
- It is very likely that significant amounts of copper content in Pd-Cu alloy react with sulfur and initiate failure of this class of membranes. Such failures have been reported in a number of independent studies.
- If this project is successful, this will be a very high-flux membrane.

<u>Ouestion 2: Approach to performing the research and development</u>

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

- The team's approach is to use advanced membrane property simulations by atomistic and thermodynamic modeling and experimentally verify the performance of hydrogen separator membranes made using the results of the modeling work. Unfortunately, all the membranes leaked and therefore the results are inconclusive.
- This project employs multiple testing procedures for designing and examining durability of Pd-Cu-based membranes. The approaches are sound. The durability tests indicate failure of the membranes after relatively short operating times. In addition to examining the physical reasons for failures, chemical effects of contaminant on the membrane, such as sulfur reactions with copper, should also be studied.

- In this study, a larger number of contaminants in the tests gases have been used, making the test results more realistic in comparison to several studies that have over-simplified the test gas mixtures.
- The project team has a good approach with proper tools.

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

This project was rated 2.5 based on accomplishments.

- The project team has evaluated the performance of fcc PdCu separators; quantified the effect of H₂S, CO, CO₂, N₂, and H₂O on H₂ permeability; demonstrated sulfur resistance of PdCu alloy; produced five (5) separators with United Technologies Research Center (UTRC) ternary composition; and has formed a secondary phase barrier on outer surface of membrane. There is a wide variation in flux for some membrane systems tested at nearly similar conditions but the reasons are unknown. Almost all the membranes leaked and there are defects in membrane tubes.
- Significant progress is being made in testing four separate Pd-Cu alloy membranes. Three of these membranes have failed. The Milestone Schedule indicated the project is near completion. However, several unresolved issues regarding the performance and durability of these groups of membranes still remain. The H₂ permeation needs to be substantially improved and reason(s) for relatively fast rupture of membranes should be established.
- The publication of information is important for this project.

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

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

- The project team collaborated with Power+Energy to manufacture the hydrogen separators and fabricate the UTRC alloys. Fundamental experiments on hydrogen solubility and experimental measurements of alloy systems for thermodynamic phase modeling were done in collaboration with Metal Hydride Technologies.
- This project is a collaborative team effort, involving four experienced groups.
- The University of Vermont and the Colorado School of Mines are valid collaborators in this project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The performance of a few more ternary alloys will be tested in 2009. The durability of membrane separators will also be studied. This project is scheduled to end in June 2009 and therefore no plans for future were given. Will there be a follow-up to this project?
- It is projected that two additional ternary Pd-Cu-based membranes will be manufactured and tested. In order to resolve the remaining issues with Pd-Cu ternary membranes a larger number of alloy types and performance tests need to be performed.
- Reason(s) for failure should be established and remedied in this project.
- The effort to connect with the 50kw fuel cell using logistics fuel for the Navy was interesting. A more thorough explanation of this effort would have been helpful.

Strengths and weaknesses

Strengths

- Collaboration with Power+Energy and Metal Hydride Technologies are a strength to this team.
- The project attempts to develop relatively inexpensive and durable membranes for hydrogen separations. A number of well-planned approaches have been utilized. Particularly the poisoning tests in this study are more realistic than those in a number of similar projects.
- Despite some shortcomings, results obtained from this project are valuable in better understanding of the factors affecting the performance of hydrogen separation membranes.
- The PI gave a frank presentation on this project.
- A high-flux membrane, from this project, would be enabling for many applications.

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• Encountered hurdles by the project team are well addressed.

Weaknesses

- In this project, all the membranes leaked and there is no apparent plan to address this issue. There is wide variation in flux for soae membrane system tested at nearly identical conditions, i.e., there is no reproducibility. There are no plans to control the defects in membrane tubes.
- The membrane manufactured and tested in this project has not performed as desired. Significant improvements are needed in the hydrogen permeation rate and durability of the Pd-Cu-based alloys.
- It would be useful to have some connectivity to the baseline information that informed this project.

- Due to its weaknesses, this project should not be considered for continuation/renewal when the current term expires in June 2009.
- A larger number of alloy Pd-Cu-based alloy compositions, fabrication methods, permeation, poisoning and durability tests should be performed.
- Systematic variations in the composition may help identify the reason(s) for failures of Pd-Cu membranes in this project.

Project # PD-49: Integration of a Structural Water Gas Shift Catalyst with a Vanadium Alloy Hydrogen Transport Device

Tom Barton; Western Research Institute Morris Argyle; University of Wyoming

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

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

- The objective of this project for the current year is to build a modular WGS/membrane integrated device capable of producing 10,000 liters/day of hydrogen from coal-derived syngas. WGS catalyst and hydrogen separation membrane module development are key parts of this project.
- Objectives of this project include development and testing of WGS catalysts capable of operating at high pressures and manufacturing an integrated WGS membrane system to produce 10,000 liters/day of hydrogen from coal derived syngas. This is an excellent project with clear relevance to DOE's mission in coal and/or biomass conversion into syngas and subsequently hydrogen. The WGS catalysts-membrane process design and integration used in this project should allow for better efficiency and greater flexibility.
- The project's approach has very good potential to be scaled up for commercial applications.
- This project has practical goals.

Question 2: Approach to performing the research and development

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

- There are four tasks in this project; 1) to develop WGS catalyst; 2) scale up the integrated devices catalyst plus membrane; 3) test the integrated module in a fluidized bed coal gasifier; and 4) perform economic analysis. The project's approach to develop a catalyst is good. The catalyst development was the objective for FY2006 and this objective was met in 2008. However, there is nothing in the approach that addresses how to overcome the membrane's oxidation problem.
- This is an excellent project relevant to DOE's objectives. A number of WGS catalysts have been developed and tested. Catalysts with Al and Ce show higher activity than other tested catalysts (vanadium-based).
- The process design and approaches used by the team can be utilized for large-scale operations. Two integrated WGS devices have been built and tested. The target rate of 10,000 liters/day at 600 psi for hydrogen production has been reported.
- The project's integrated system allows for using different membrane materials with the WGS catalyst.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 3.0 based on accomplishments.

- The structural WGS catalyst developed with Al and Ce shows higher activity and is more appropriate for the integrated WGS -membrane device than the commercial catalyst. The two scale-up designs for the membrane modules are carried out (one with Chart Engineering and the other with REB Research, Inc.). Two integrated devices were constructed that met the 10,000 liters/day hydrogen goal at 600 psig and 400°C in coal derived syngas. One device was constructed to incorporate anyone's best membrane material. The vanadium alloy membranes are challenging to manufacture.
- The project is near completion. Fabrication and testing of the integrated WGS units have been completed and testing is 90% complete. Overall, the technical accomplishments for this project have been very good.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- This project involves collaboration with University of Wyoming, Chart Energy and Chemicals, REB Research and Consulting, U.S. DOE Ames Laboratory. The roles played by the collaborators are clearly described in the presentation.
- The project team has good collaboration between the team members from academics, industry, national lab and small business consulting. Team members' responsibilities and their work and part in the team clearly described.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- The commercialization of the WGS catalyst monolith will be pursued with the assistance of a catalyst manufacturer. Completion of the testing of the two-scaled integrated devices will be followed by the design and fabrication of the 10x assembly based on the economic and performance data for testing under coal gasification conditions. The flux for the vanadium alloy membrane is low. Are there any plans to improve its flux and are there any plans to look into other membranes?
- Upon completion of testing of two more WGS integrated devices, the project has plans of commercializing the WGS units. Collaborations with large scale catalyst manufacturers will be required. The team's plans build on progress and address the barriers for commercialization of the WGS devices.
- The PI gave a frank presentation of the project.

Strengths and weaknesses

Strengths

- The project's strength is shown in developing a new catalyst and methods to incorporate the catalyst on membrane structural units. The researcher at REB Research, Inc. has strong background in membranes area. Chart is well known in developing engineering components for energy applications.
- Practical, efficient and durable catalysts-membrane combinations have been developed, tested and utilized in this project. The return for investment on this project is very good.

Weaknesses

- The project team should focus on vanadium alloy membrane especially if it cannot meet the 2010 flux target. It is very difficult to make vanadium alloy. There is no focus to avoid the problems with vanadium system. And there is no attempt to look into other candidate materials.
- The poisoning and durability tests have not used more realistic syngas compositions. The project's potential contaminants such as trace heavy metals or halogens may affect the performance and durability of the catalysts and membrane.
- The team should have some connectivity to the baseline information that informed this project.
- Also, the focus on vanadium should have been contrasted with other candidate materials more clearly.

- The project team should drop the vanadium alloy work and try to incorporate the catalyst onto a more practical membrane system.
- The performance tests for the WGS catalysts and membranes should be extended to conditions that better mimic more realistic syngas compositions.

Project # PD-50: Hydrogen Delivery in Steel Pipelines

Doug Stalheim; Secat, Inc.

Brief Summary of Project

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

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>



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

- This project is dealing with material microstructures that are hydrogen compatible. The main investigator, D. Stalheim, is an authority in the field of steel microstructure as it relates to mechanical properties. The proposed four steel-microstructures, namely A, B, C, and D are promising micro-alloyed steels we can manufacture today for hydrogen compatibility.
- Success in identifying/developing embrittlement-free and corrosion-free alloys and welds would have significant effects on building hydrogen pipelines. This would also be the most cost-effective means for delivering hydrogen from central production areas to hydrogen refueling stations. This project aligns with DOE's goals.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- The project's focus on the effects of steel structures on hydrogen sulfide stress cracking is well known and may be applied directly to loss of ductility due to high-pressure gaseous hydrogen charging.
- The project has analyzed the microstructure of four promising steels (A, B, C, and D) and established their grain morphology. The project has also studied the hydrogen effect on the uni-axial tension response of these steels. In particular, the project established the hydrogen effect on the yield and ultimate strength and the reduction in area as a function of hydrogen pressure.
- The microstructural analysis results of this project are very important since they will help in the analysis of the hydrogen-induced fractures. Therefore the project's approach to ascertain the steel microstructures in relation to the mechanisms of fracture is extremely important. The uni-axial tension results though are not important as they do not correlate with material fracture toughness.
- The evaluation matrix is well established for the project. This project relies on the existing pipeline materials and lacks novelty.

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

This project was rated 2.0 based on accomplishments.

- The effect of strain rate on tensile testing steels in high-pressure hydrogen needs to be evaluated, in order to fully interpret the project results to date.
- The proposed steel microstructures and their microstructural characterization is an important development. In fact, the project should focus on further developing and analyzing potential microstructures that are hydrogen compatible. To do this, the project should proceed with the fracture toughness assessment of the steel microstructures termed as A, B, C, and D, and establish what new advances in the material microstructures are needed to improve fracture resistance. As explained below, the project has already planned for these fracture assessment experiments. Therefore, the project is on the right trajectory.
- The project has very limited accomplishments and progress has been made, but these are proportional to the project schedule and DOE's funding.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- The team's collaboration between SECAT, DGS Metallurgical Solutions, and Sandia National Laboratories is outstanding. It sets the project on the proper trajectory toward achieving its goals.
- There is a good team structure involving a national laboratory and other companies. The majority of accomplishments presented were made by ORNL, and contributions from other team members are unclear.

<u>Question 5: Approach to and relevance of proposed future research</u>

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

- It is unclear what new insights the proposed validation of select reduction in area values of alloys B, C, and D in hydrogen will bring about in this project. As was mentioned above, uni-axial tension tests offer negligible information on the relationship between microstructure response and hydrogen embrittlement.
- Future work for this project is listed in detail. Economic analysis will be very helpful to determine the viable approach.

Strengths and weaknesses

Strengths

- The identification, development and analysis of promising modern low-carbon steel microstructures are a strength of this project.
- The participation of Mr. D. Stalheim is a strength of this project.
- This project has low risk of utilizing existing commercial products.

Weaknesses

- This project has no fracture assessment of the microstructures as of yet. However, the proposed collaboration with Sandia National Laboratories aims to do exactly that.
- This project is scheduled to be completed by 2011. It is unclear if this project meets the time frame of DOE's "go/no-go" decision milestones.

- Study of the uni-axial tension characteristics offers negligible information on the material resistance to hydrogen-induced fracture. This is a well-documented fact in the hydrogen literature. The project team should focus on fracture toughness assessment. They should redirect and work toward microstructural development, alloy modification and improvement, perhaps through thermo-mechanical or chemical treatment, after input is received from Sandia on the fracture behavior. In other words, capitalize on the project's personnel strengths that lie on alloy development.
- The project team needs to evaluate impurity effects on steel, especially for impure gases like moisture and trace of H₂S.

Project # PDP-01: Development and Optimization of Cost Effective Material Systems for Photoelectrochemical Hydrogen Production

Eric McFarland; University of California, Santa Barbara

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

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

- The project's development of a viable form of iron oxide for PEC water splitting is extremely relevant to Hydrogen Program goals.
- The team's long-term renewable hydrogen production supports Hydrogen Program objectives.
- Yes, this project is relevant to DOE's overall objectives.
- This project uses a greater than 2.2 eV band edge criteria for "go/no-go" decision screening.
- This project uses a 10% conversion "go/no go" decision screening.
- This project uses >8% solar H₂ production efficiency as "go/no-go" decision screening.
- This project uses <\$5/kg of H₂ criteria for the "go/no-go" decision screening.
- The materials development piece of this project is impressive and important to the goal of efficient PEC-based water splitting. The new modifications to Fe₂O₃ appear encouraging in lowering band gap of the metal oxide photo-electrodes.

Question 2: Approach to performing the research and development

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

- The project has done a good job of integrating state-of-the-art theory, synthesis and characterization approaches to tackle the difficult job of refining oxide materials and interfaces for PEC water splitting. Further emphasis on this integrated approach is strongly encouraged; both in continued research into hematite-based systems, and in the discovery of new material systems, such as the delafossites.
- The project team's approach is directly addressing key efficiency, durability, and cost.
- Focusing on cheap & abundant material is a logical approach by the project team.
- The PI has shown steady progress toward understanding of the chemical mechanisms that limit materials synthesis. This is not an easy problem to tackle.
- McFarland has a good grasp of materials issues and his approach to combine combinational synthesis with theory has a good chance of achieve many of the project's objectives.
- It is important for the PI to remain focused on the big picture. And as such, via tasks #6 to #9, must begin evaluating the conceptual reactor designs and ultimately, an estimation of the hydrogen production costs both with and without sacrificial reagents (e.g. municipal waste water, etc.).

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

This project was rated 2.7 based on accomplishments.

- The project team's integrated approach has yielded impressive results, particularly in the demonstration of record levels of unbiased PEC water splitting in modified hematite materials. Though these levels are below DOE targets, the results are encouraging and represent a significant step forward. Integrated multi-junction configurations might be of interest using the current forms of this material. Preliminary results from the delafossites are less auspicious, but the successful implementation of integrated theory/synthesis/characterization approach in the research of this "new" material class represents a good accomplishment.
- The projects use of iron oxide is not promising. More focus on other more promising materials is needed by this team. Significant improvement in incident photon conversion efficiency (IPCE) is still needed.
- No progress has been made on an actual reactor design and H2A cost analysis in this project.
- The high-temperature electrolysis (HTE) of Al doped hematite was identified 0.3-0.5% as optimal, and IPCE increased it 4-5 times over control samples.
- The PI's group has synthesized new CuMO₂ delafossites, M=Cr, Fe, Ga, La, as well as new oxides (CuCr₂O₄), sulfides (SnS, CuGaS₂), & selenides (WSe₂, CuInSe₂, CuGaSe₂). This project has had very good progress.
- The project team's fluorine surface modification was able to shift conduction band-edge of Ti-doped hematite producing zero bias (two electrode) efficiency for hematite ~ 1% at 450 nm.
- The project has had four times improvement on the performance of NiFe electro-catalysts.
- The PI's have shown that biomass analogues can be photo decomposed with increased performance (15 times or higher than NaOH). This is not surprising. It has merit for near-term applications of the technology but may not help with the ultimate objective of water splitting. It is unclear even if biomass assisted PEC hydrogen production will be economical and/or meet DOE's near- and long-term hydrogen production cost goals. The H2A analysis of this approach is in order.
- At this point in the team's research (5th year and 90% completion), the long-term catalyst stability data is still lacking in order to draw solid conclusions.
- McFarland and his group have made good progress in identifying potential materials for splitting water.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- The team's collaborations with the DOE PEC Working group, including efforts in theory, synthesis, characterization and techno-economics analysis have been exemplary.
- The project team has had good collaborations with NREL and various universities.
- A moderate number of publications and presentations have been done by the project team all in good archival journals. The PI's interactions with PEC community and others are noteworthy.

Question 5: Approach to and relevance of proposed future research

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

- The team's future work is well laid out and is consistent with meeting the fundamental needs of PEC materials discovery and development.
- More focus on other more promising materials is needed by the project team. Significant improvement in ICPE is needed.
- The project needs multiple miracles to happen to overcome the barriers.
- The PI has made good progress in addressing issues related to catalyst stability and conversion efficiency.
- Future plans for the project are reasonable if additional DOE funding can be made available. This should be predicated upon a system-level cost analysis using H2A platform to better define the cost-efficiency goals for the prospective catalysts and photo-reactors.

Strengths and weaknesses

Strengths

- This project has had good Progress, excellent collaborations and has a clear vision of research needs for future successful implementation of PEC hydrogen production.
- The project team's combinatorial materials synthesis is a strength.
- This project has a highly skilled group in material synthesis and characterization.

Weaknesses

- The team's scope of work is somewhat over-ambitious within the limits of current funding levels. There are still some fundamental 'mysteries' regarding performance of different hematite materials that should be pursued more aggressively. Perhaps using collaborative partners in characterization would be a benefit.
- No progress has been made on an actual photo-reactor design and H2A cost analysis in this project.
- No material with good long-term stability and photon to hydrogen conversion efficiency has been found yet.
- The use of biomass or other organic analogous present distraction to this DOE-EERE funded project.

- This project should have a continued expansion of collaborative efforts, especially in future work related to advanced material characterization and screening, but also in theoretically guided materials modification experiments.
- The project team should perform H2A analysis as they go along.

Project # PDP-02: Semiconductor Materials for Photoelectrolysis

John A. Turner, Todd G. Deutsch, and Huyen Dinh; National Renewable Energy Laboratory

Brief Summary of Project

The objective of this project is to discover and characterize a semiconductor material set or device configuration that 1) splits water into hydrogen and oxygen spontaneously upon illumination; 2) has a solar-to-hydrogen efficiency of at least 5% with a clear pathway to a 10% water splitting system; 3) exhibits the possibility of 1,000 hours stability under solar conditions; and 4) can be adapted to volume-manufacturing techniques. The main objective for the past year has been to develop and optimize state-of-the-art materials that we have identified as promising for meeting the DOE's near-term efficiency and durability targets.



Question 1: Relevance to overall DOE objectives

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

- The PEC fits the long-term renewable hydrogen production goal.
- This project has a very broad and long-term approach to address PEC production.
- The project's development of a viable form of high-performance III-V material for PEC water splitting is extremely relevant to Hydrogen Program goals, and investigating other important material classes is of high relevance.
- The project's discovery and characterization of materials that have the potential water splitting application to produce "green" hydrogen, if successful, is very relevant to the Hydrogen Program goal.

Question 2: Approach to performing the research and development

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

- This project uses cheap, durable and efficient materials for photoelectrode and is the key enabler for PEC success.
- The project team's approach is sharply focused on the "big three" challenges. By breaking down the very large set of possible materials into two general categories, it makes the progress more tangible to non-experts.
- The project has done a good job focusing on important material classes meeting some (though not all) of the critical requirements for practical PEC hydrogen production. Stabilization of the III-V materials class appears to be of central focus, but other important classes remain under investigation. Further emphasis on collaborative approaches integrating theory, synthesis and characterization are strongly encouraged; both in continued research into stable, lower-cost III-V semiconductor systems, and in the discovery and development of new material systems.
- This project has been on going for a long time. The team's approach appears too much trail-and-error. They need a more systematic approach to selecting and/or eliminating materials.
- The project team needs to include cost as one of main criteria (material and synthesis/manufacturing method).

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

This project was rated 2.8 based on accomplishments.

- The project's milestones were met on time.
- More durability data is needed from the team. What is the pathway to 10 % efficiency?
- There was clear progress in the synthesis and characterization of InGaN-based materials, though the presentation could have better pulled-together the key results on performance and stability, especially in relation to future directions for the research. There was also progress in the evaluation of CGS, a-SiN_X and copper spinel materials developed at NREL. Again, the presentation could have done a better job in tying together the results with synergetic activities within the DOE PEC working group, and the implications for future work. The work in this project is an important part of the validation process of new approaches integrating materials theory, synthesis and characterization, and this validation process should be strongly emphasized, especially at NREL (which is ideally suited for a leadership role in this area).
- The project team still has had no significant step change in improving combination of efficiency and durability.

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

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

- The project team has had good collaboration with members of the PEC working group.
- The project team should have more industry collaborations.
- There was an impressive list of collaborators, particularly within NREL and with international participants in the research. Collaborations with the DOE PEC Working Group were also implicit, though better integration of synergistic activities and results could have been demonstrated in the presentation.
- The team had strong collaborations with institutions doing similar researches.

Question 5: Approach to and relevance of proposed future research

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

- The project's durability testing is not explicitly mentioned in the future work.
- Future work on this project is somewhat open-ended, though well laid out in the presentation. Future work needs to focus strongly both on improving the stability and reducing the cost of the III-V focus materials, and this project needs to implement all available tools in materials theory, synthesis and characterization toward this end.
- The team needs to clearly show how to achieve incremental improvement in efficiency, instead of just continuing on with trail-and-error approach.

Strengths and weaknesses

Strengths

- Technical capabilities of the people involved in this project are a strength.
- Progress was made on several fronts in the development of PEC materials for solar hydrogen production in this project. Good synthesis and characterization results have been achieved.

Weaknesses

- This project has taken a long time to mature.
- The presentation could have better represented collaborations, synergies, and motivations for future work critical to the success of renewable PEC hydrogen production.

Specific recommendations and additions or deletions to the work scope

• Continued expansion of collaborative efforts, especially in future work related to advanced material characterization and screening is needed, but also in theoretically guided materials modification experiments. Pathways toward low-cost synthesis of III-V materials should be a stronger focus for the project team.

Project # PDP-03: PEC Materials: Theory and Modeling

Yanfa Yan, Muhammad Huda, Aron Walsh, Su-Huai Wei, Mowafak Al-Jassim, and John Turner; National Renewable Energy Laboratory

Brief Summary of Project

The main focus of the project is to 1) understand the performance of current photoelectrochemical (PEC) materials; 2) provide guidance and solution for performance improvement; 3) design and discover new materials; and 4) provide theoretical basis for "go/no-go" decisions to DOE PEC H₂ programs.

<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

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

• The PEC is relevant to long-term renewable hydrogen production. The project's modeling shall be a key enable:



- project's modeling shall be a key enabler to PEC materials search.
- It is uncertain why this project needs to be independent. This should be part of any PEC project. How this project adds value in addition to other on-going PEC projects is not apparent. Why does DOE need a separate project to study why certain materials work and do not work? Should this be the task of the PI's of the PEC projects?

Question 2: Approach to performing the research and development

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

- The density functional theory (DFT) is the right approach to perform material discoveries in this project.
- The team has had good coordination between theory and experiments.
- The team has a good effective use of modeling to understand materials performance

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

This project was rated 3.0 based on accomplishments.

- Project milestones have been met in time. Continuous search for new materials is still a part of this project but there is some delay due to fabrication of materials.
- Good progress is shown in working with other PEC projects to understand materials performance and issues.

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

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

- The PEC team has outstanding coordination within their group.
- More industry collaborations would be good for this project.
- This project has good collaborations and is in support of other PEC projects.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.7 for proposed future work.

- The project team has a good approach to iterate between models and experiments.
- The project team should consider merging the work with other PEC projects (if funding is available).

Strengths and weaknesses

Strengths

• The team has the right approach for problem solving. Their combination of theory and experimental work is a strength.

Weaknesses

• This project has taken a long time to mature.

Specific recommendations and additions or deletions to the work scope

• The project team should consider not doing this project on its own. The task of understanding materials performance should be done by all of the PIs of the PEC projects.

Project # PDP-04: Progress in the Study of Amorphous Silicon Carbide (a-SiC) as a Photoelectrode in Photoelectrochemical (PEC) Cells

Arun Madan; MVSystems, Inc.

Brief Summary of Project

The objective of the project is by September 2009, to fabricate the hybrid a-Si tandem solar cell/a-SiC photoelectrode (PV/a-SiC) device, which exhibits a photocurrent greater than or equal to 4 mA/cm², and durability in the electrolyte of greater than or equal to 200 hrs. In the past year, this project has 1) fabricated an integrated hybrid PEC device containing a-Si tandem solar cell and a-SiC photoelectrode; 2) investigated the effect of surface oxide (SiOx) on the photocurrent; and 3) improved the PV performance of a-Si tandem solar cell used in the hybrid PEC device.



Question 1: Relevance to overall DOE objectives

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

- This project addresses the program objectives related to PEC Hydrogen efficiency and durability.
- This project is in line with hydrogen project objective to produce low-cost, renewable hydrogen.
- This project has efforts to utilize full solar spectrum to raise efficiency, which is relevant to DOE's objectives.

Question 2: Approach to performing the research and development

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

- This project would benefit from a cost assessment to ensure their technology is on the path to achieving overall hydrogen production cost targets.
- The project team's approach to improving efficiency and durability seems logical.
- Tailoring the bandgap with deposition control and multilayer films is a good strategy for capturing solar spectrum.

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

This project was rated 3.0 based on accomplishments.

- The project team's corrosion resistance data looks good and at least some hydrogen was evolved during testing last year. More work is needed to generate hydrogen at the required rate.
- Major technical barriers still exist in this project to demonstrate the necessary current, but there appears to be a path to achieving the desired results.
- There were a very large number of publications listed for this project, but many of them were written before this project started. Listed publications should be those that derived directly from this research project.
- This project has had good progress in materials development and testing.
- The project's efficiency improvement is still minimal.
- Test data on corrosion after 150 hours is promising in this project.

- The project's multi-layer films appear to have good efficiency and corrosion resistance. The STH efficiency lagging is well below target.
- The project's HF etch study gave good results

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

This project was rated 2.7 for technology transfer and collaboration.

- It was unclear how well coordinated this project is with the listed partners. More collaboration may be beneficial.
- The project had good collaborations with various institutions.
- The project had collaborations with NREL.

Question 5: Approach to and relevance of proposed future research

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

- The project's list of future work looks appropriate, but there may not be enough time and funding to achieve the project goals.
- The team needs to focus on longer term testing (>150 hrs) to investigation corrosion issue, while addressing efficiency improvement.
- It is not totally clear on how >10% STH efficiency can be achieved.
- The project has a good listing of potential improvement mechanisms.
- Are the project's criteria for "go/no go" decision set? If so, what are they?

Strengths and weaknesses

Strengths

- The project's corrosion resistance looks good and at least some hydrogen was evolved during testing last year.
- There appears to be a path to overcoming the major technical barriers and achieving the desired results in this project.
- Good expertise in film production/characterization/testing can be seen in this project.

Weaknesses

- This project would benefit from a cost assessment to ensure the technology that is on the path to achieving overall hydrogen production cost targets.
- More work is needed to generate hydrogen at the required rate in this project.
- Listed publications should be those that derived directly from this research project.
- It was unclear how well coordinated this project is with the listed partners. More collaboration may be beneficial.

Specific recommendations and additions or deletions to the work scope

• The list of future work looks appropriate, but there may not be enough time and funding to achieve the project goals.

Project # PDP-05: Progress in the Study of Tungsten Oxide Compounds as Photoelectrodes in Photoelectrochemical Cells

Nicolas Gaillard; University of Hawaii

Brief Summary of Project

In the past year, this project has 1) continued WO₃ bulk modification using ion incorporation with synthesis of new alloys and theoretical analysis on band-gap reduction; 2) investigated the WO₃-based bilayer concept with fabrication of new devices, surface electronic properties analysis and crystallographic and structural analysis; and 3) evaluated RuO₂ nanoparticle deposition for catalytic treatment with deposition of thick (1 micron) films, characterization of RuO₂ film's oxygen evolution rate vs. that of Pt foil and the first evaluation of RuO₂ nano-particle onto WO₃ film.



Question 1: Relevance to overall DOE objectives

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

- The project team's work is relevant in establishing the next steps for photoelectrochemical hydrogen production (PEC) electrode structures.
- The project's photoelectrochemical hydrogen production is within the DOE Hydrogen Program plan.
- The project's use of WO₃ is shown to be a promising material.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated 3.7 on its approach.

- The team had a very methodical approach that evaluates the individual layers of the PEC electrode. Overall improvement in performance is obtained by the improvement in one or more PEC electrode layers in this project.
- The team's work on tailoring band gap/band-edge is good.
- The team has a good use of theory.

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

This project was rated 3.0 based on accomplishments.

- A continuous improvement in WO₃-based PEC electrode performance has been demonstrated via new materials/fabrication techniques in this project.
- The team has demonstrated an increase in photocurrent using new bilayer structures.
- The project's further improvement in SiC & WO₃ PEC electrodes are required to meet the STH efficiency target of ~5%.
- The project team has made reasonable progress towards goals. The 3D growth of catalyst particles is promising.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 3.7 for technology transfer and collaboration.

- The project is a well rounded team effort between institutions covering the theory, synthesis, and characterization R&D effort. The knowledge gained appears useful to all partners involved.
- Collaborations in this project were okay.

Question 5: Approach to and relevance of proposed future research

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

- New materials and fabrication techniques have been identified to further improve PEC performance in this project.
- Are the criteria for "go/no-go" decision in this project set? If so, what are they?

Strengths and weaknesses

Strengths

• There has been good collaboration between partners and DOE PEC working group.

Weaknesses

• The low current densities will result in relatively large systems for hydrogen production, which is a weakness of this project.

Specific recommendations and additions or deletions to the work scope

• This may be too early to say but the project team should complete an economic analysis of a PEC system to demonstrate feasibility of this technology for hydrogen-production.

Project # PDP-06: Photoelectremical Hydrogen Production

Jess Kaneshiro; University of Hawaii at Manoa

Brief Summary of Project

The objective of this project is to develop copper chalcopyrite materials for incorporation into a hybrid photoelectrode (HPE) device capable of splitting water for hydrogen production when immersed in a suitable electrolyte and illuminated by sunlight. Material development objectives are to 1) identify methods of increasing the bandgap of copper chalcopyrite films; 2) make thinner copper chalcopyrite films; and 3) make surface modifications. Device development objectives are to 1) use material development to synergize different components of HPE; 2) identify suitable underlying photovoltaic (PV) cells, possibly also copper chalcopyrite-based; and 3) identify suitable photoelectrochemical-PV interfaces.



Question 1: Relevance to overall DOE objectives

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

- The PEC is relevant to DOE's goal of renewable hydrogen production.
- The project's link to pdp_02_turner is unclear? It is assumed that it is shown in the collaboration with NREL.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated 3.3 on its approach.

- The project's investigation of copper chalcopyrite is a good as these materials are cheaper and durable.
- The project team's focus towards reducing voltage bias is the right approach.
- The project team has good use of theory to guide experimental work.

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

This project was rated 3.0 based on accomplishments.

- The team has demonstrated some progress in reducing the voltage bias via sulfur incorporation in the materials.
- The project team needs to have a crisp milestone plan.
- High currents are achieved in this project.
- The team has made not much progress on stability, but issues are being addressed.
- The team's look into the device's efficiency has not yet started.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- The PEC team has outstanding coordination.
- Are there other possibilities for industry collaborations in this project?
- The team has had good work with theorists and co-investigators.

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Question 5: Approach to and relevance of proposed future research

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

- The project team has continued to focus on the reduction of voltage bias through looking at new and/or different materials.
- Are the criteria for "go/no-go" decision set? If so, what are they?

Strengths and weaknesses

Strengths

• This team has had good technical background and coordination.

Weaknesses

• This project has taken a long time to mature.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PDP-07: Critical Research for Cost-Effective Photoelectrochemical Production of Hydrogen

Liwei Xu; Midwest Optoelectronics, LLC Anke Abken; Xunlight Corporation William B. Ingler, Jr.; University of Toledo

Brief Summary of Project

The objectives of this project are to 1) develop critical technologies required for cost-effective production of hydrogen from sunlight and water using thin film (tf)-Sibased photoelectrodes; and 2) develop and demonstrate at the end of the three-year project, tf-Si-based photoelectrochemical photoelectrodes and device designs with the potential to achieve systems with 10% solarto-hydrogen efficiency with a durability of 5,000 hours by 2018.

Question 1: Relevance to overall DOE objectives

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

- Overall Project Score: 2.5 (3 Reviews Received)
- The project is well aligned with the program goals, in particular finding low-cost PEC technology and materials.
- The work in this project has general relevance to the broad Hydrogen Program, although only a small fraction of the tasks are directly relevant to the goals of PEC hydrogen production, as outlined in the DOE MYPP.

Question 2: Approach to performing the research and development

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

- The team's approach appears to be reasonable given the early stage of R&D.
- Of the tasks presented, Task 1 is completely outside the scope of hydrogen production; Task 2 is more suited to research funding under PV and/or electrolysis systems; Task 3 has relevance to renewable hydrogen production using PEC solar water-splitting; and Task 4, based on waste-water treatment, is interesting, but outside the scope of renewable PEC hydrogen production from sunlight and water..

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

This project was rated 2.7 based on accomplishments.

- The project shows some good potential, but significant technical barriers still exist.
- Progress was made in the different tasks presented, though much was unrelated to progress in the development of PEC water-splitting materials and devices. The critical issue in PEC is the development of new efficient and cost-effective materials and interfaces to better utilize the solar spectrum in photoelectrochemical processes for splitting water, and only Task 3 attempts to address these issues. Unfortunately, the scope of work within Task 3 is limited, and does not incorporate research approaches and progress from within the DOE PEC Working Group.

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

This project was rated 2.7 for technology transfer and collaboration.

- The project's collaboration appears to be sufficient.
- The role of collaboration in this project was not made clear within the presentation, though there appears to be some collaborative results.

Question 5: Approach to and relevance of proposed future research

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

- There may not be enough time and funding to achieve the project goals.
- The future work outlined for Task 3 is somewhat limited in its scope and definition. Better integration of the materials R&D efforts with the broader efforts in the DOE PEC Working Group is strongly encouraged.

Strengths and weaknesses

Strengths

- The project is well aligned with the program goals, in particular finding low-cost PEC technology and/or materials.
- The team's approach appears to be reasonable given the early stage of R&D.
- The project team's collaboration appears to be sufficient.
- Progress was made in several different directions in this project, though few of these were directly tied to the advancement of PEC water splitting for solar hydrogen production.

Weaknesses

- Significant technical barriers still exist in this project.
- Too much work unrelated to PEC hydrogen production was presented by the team. Other funding sources would have been better suited to this project. Collaborative efforts need to be strengthened. The incorrect poster ID was listed on the first panel (pdp 24), indicating perhaps that some of the information may be from an outdated source.

- There may not be enough time and funding to achieve the project goals.
- The project team should find alternative funding venues for Tasks 1, 2 and 4. They also need to strengthen the materials R&D directions within Task 3.

Project # PDP-10: Composite Bulk Amorphous Hydrogen Purification Membranes

T. Adams, K. Brinkman, S. Garrison, and P. Korinko; Savannah River National Laboratory

Brief Summary of Project

Metallic glass materials offer the potential for excellent membrane function at a fraction of the cost of Pd-based alloys. The objectives of this project are to 1) examine novel Pd free membranes for hydrogen separation; 2) address the potential challenge of crystallization during operation at elevated temperature; 3) quantify hydrogen permeation properties of commercially available metallic glass membranes; 4) evaluate and understand crystallization and hydrogen flux behavior in metallic glass membranes; and 5) integrate permeation, crystallization behavior and modeling effort on materials chemistry to guide synthesis and characterization of novel metallic glass materials for hydrogen separation.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.6 for its relevance to DOE objectives.

- The project fits in to DOE's hydrogen separation R&D objectives. However, the work provides little support to DOE's hydrogen separation technology R&D intended results. This is because the DOE 2010 membrane flux performance target is 200 SCFH/ft² at 340-400°C and 100 psig trans-membrane ΔP.
- The project's concept is not novel; glass membranes have been studied before, generally with not much potential. The separation conditions are not synergistic with upstream process operating conditions and the separation flux is order of magnitude lower than would be required to process the throughputs of WGS reactors. It is doubtful the material can achieve DOE 2010 flux and other performance targets.
- The research is attempting to develop novel membranes to produce high-purity hydrogen. The researchers are aware of the need to develop effective hydrogen separation membranes and are aware of the DOE goals and targets (slide #3). This is a high-risk approach that would likely be much longer term than the DOE target timeframe. It is unlikely that any of the DOE targets will be met, but the work may provide some fundamental information on alternative membranes.
- This project meets some aspects of DOE goals.
- The project's hydrogen purification is a necessary step after onsite reforming or within the station to satisfy fuel cell purity requirements. Work in using low-cost metallic glass instead of high-cost palladium is absolutely in line with DOE programmatic goals.
- A cost effective membrane hydrogen separation system has the potential to lower the cost of several hydrogen production methods. Although some success has been obtained with palladium-based membrane systems, there are still some issues with this project's approach. Metallic glass membranes are an interesting alternative approach to explore.

Question 2: Approach to performing the research and development

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

- The work conducted thus far in this project is of academic value. The hydrogen separation mechanism is not clear. The work is in its fundamental stages and the success potential of the glass membrane, if any, is difficult to predict.
- The team's approach is reasonably novel and gets away from the use of high-cost precious metal membranes. The work is attempting to build on hydrogen separation using micro-porous glass membranes, which has shown some success for hydrogen separation. This is a high-risk approach, which is appropriate for a basic research laboratory like SRNL. The project is beginning to look at supported thin films, which would be the next logical step in the development of this type of membrane system. The work involves a high level of fundamental characterization and modeling which is acceptable for a project of this type operating on a minimal budget.
- The concept of using isomorphous alloys is intriguing and potentially a method to make cheaper membranes. Avoiding crystallization of the alloy is a key to the success of this method.
- Work towards understanding metallic glass hydrogen permeation is important in this project. The use of alloying to control glass transition temperature looks promising, as does use of thin film systems. The project team should continue to work on both increased flux but also hydrogen recovery.
- The approach being taken is to first look at the key issue of potential re-crystallization at elevated temperatures needed for use as well as to measure the hydrogen flux rate. This is a good first step for the project team.
- Computational molecular modeling is also being used to try to determine which glass metal alloys should have the best hydrogen permeability.

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

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

- The project's flux data is much lower than the immediate DOE 2010 target. Membrane separation performance varies with temperature exponentially and the separation mechanism is unclear. High-temperature membrane operating conditions may not be compatible with upstream gas clean up or water gas shift reactor conditions. The separation flux is an order of magnitude lower than DOE targets. Some knowledge applicable to advanced materials development may evolve.
- Unfortunately, the project has little technical success. Flux rates are very low and the project lacks a clear path to improve on these is proposed. The differential scanning calorimetry (DSC), X-ray diffraction (XRD), X-ray photoelectron spectra (XPS) and permeations studies are scientifically interesting but do not appear to be providing any valuable information for future material development. However, the researchers are to be commended for attempting a new and innovative approach. For a fundamental and novel approach, the results are considered reasonable, appropriate and acceptable.
- The project team's experimental work appears to be solid and well focused. Primarily screening different alloys for susceptibility to crystallization.
- Adding a computational modeling effort is a good idea to lead to possible other combinations of alloy components in this project.
- Experiments involving realistic feed gases are lacking in this project. All that is seen are experiments on just H₂ or Ar/H₂. What might be the effect of other compounds (H₂O, CO₂, etc.) on membrane stability?
- Especially considering a lack of funding in 2009, the project made substantial progress. Work towards understanding crystallization mechanisms looks good and promising in the future. The project team's work looks very promising to develop an excellent replacement for Pd membrane materials.
- The project team successfully used calorimetry to determine crystallization temperatures of metallic glasses. The team found that some crystallization can occur in the temperature range of interest depending on the metallic glass used.
- The project team measured hydrogen flux rates and compared them with palladium. Crystallization did decrease the hydrogen flux rate as expected and the rates were generally an order of magnitude below those of palladium. The team's work is now in progress to generate thing films of the metallic glass to improve hydrogen flux rates.
- The project team's computational modeling is in progress to help define the alloy compositions that should have enhanced properties for hydrogen separations.
- A lot of progress has been made in a short time with very modest funding for this project.
- The project team should include work to ensure a high selectivity separation of hydrogen from a mixture of gasses can be obtained with these metallic glasses.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- Some industry partnership has been reported in this project.
- Outside collaboration (based on slide #2) appears reasonable in this project. However, with the exception of MetGlas who provided samples) it is not clear what the involvement of the other partners actually entails. It is valuable that the investigators are actively seeking outside industrial participation. In addition, with the limited budget (\$200K), it is likely difficult to interest outside industrial involvement.
- It is unclear how effective the list of consulting partners were or if they were even used. Partners could have perhaps provided some of the metals?
- Partnership with manufacturers is good, but not discussed in the presentation. Do partners provide anything other than samples?
- There appears to be good collaboration with private sector companies working on metallic glasses.

Question 5: Approach to and relevance of proposed future research

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

- The project has not been funded in FY09 and future funding is not known. The project PI has listed some future work, at the fundamental level, which does not include selectivity and flux measurements, or integration potential with WGS reactors of Integrated Gasification Combined Cycle (IGCC)-Carbon Capture and Sequestration (CCS) plants.
- Scoping projects such as these, especially at low budget levels, are valuable to the Hydrogen Program. Without new, innovative ideas being developed, significant advancements are not possible. Although only minimal results have been obtained, it would be useful to consider funding this work for an additional year to allow the researchers to examine other materials of this class for hydrogen separation/purification. The planned future work is generally just a continuation of the ongoing effort, but should be considered a reasonable extension of the original fundamental effort. Additional funding, at the same level, would be appropriate.
- This work deserves consideration for future funding. The combination of experimental and computational modeling is good.
- Future work on integrating modeling with experimental work is an excellent next step. Initial work looks promising there, and a continuation of that work is important for additional materials development. This project has had excellent progress considering its funding.
- The project's future plan is well thought through. It includes work to generate and measure flux rates in thin films, additional modeling work, and testing of alloys suggested by the modeling work.
- This project needs clear milestones and a "go/no-go" decision built into the future work.

Strengths and weaknesses

Strengths

- The project is a good alternative and has a novel approach for development of hydrogen separation/purification membranes without the use of high-cost precious metals. Considering preparation of supported thin films this early in the work is a plus and could provide early cost information on producing larger scale units and also identify technical problems in scale-up/production of larger size membranes.
- The Savannah River group appears to be competent.
- The project team's combination of theoretical and experimental work is good. Their use of multiple analytical techniques to better understand metallic glass diffusivity with hydrogen. This project directly addresses DOE programmatic goals of reduced cost and hydrogen purity.
- A cost effective membrane hydrogen separation system has the potential to lower the cost of several hydrogen production methods. Although some success has been obtained with palladium-based membrane systems, there are still some issues with this approach. Metallic glass membranes are an interesting alternative approach for the project team to explore.
- Computational molecular modeling is being used to try to determine which glass metal alloys should have the best hydrogen permeability by the project team.

- This project has made a lot of progress in a short amount of time with very modest funding.
- The future plan for this project is well thought through. It includes work to generate and measure flux rates in thin films, additional modeling work, and testing of alloys suggested by the modeling work.

Weaknesses

- This project had no clear weaknesses for a fundamental membrane materials scoping project.
- This project has a fairly academically focused at this point.
- The collaboration in this project is a weakness.
- The project team should include work to ensure a high selectivity separation of hydrogen from a mixture of gasses can be obtained with these metallic glasses.
- The project needs to have clear milestones and a "go/no-go" decision built into the future work.

- This project is worth considering continuation with the current/future work scope at the same funding level.
- This project includes realistic gas feeds to test membrane stability.
Project # PDP-12: Catalytic Solubilization and Conversion of Lignocellulosic Feedstocks

T.A. Semelsberger, Kevin C. Ott, Rod L. Borup, and Roshan Shrestha; Los Alamos National Laboratory

Brief Summary of Project

The objective of this project is to develop novel low-temperature chemical routes and catalysts to produce hydrogen/syngas from lignocellulosic feedstocks. The most abundant constituent of biomass is lignocellulosic (~80%). Discovering new chemistries and catalysts that can convert lignocellulosic into hydrogen/syngas will be critical if biomass is to be used as a feedstock for hydrogen or other alternative fuels. The target for this project is to, by 2012, reduce the cost of hydrogen produced from biomass gasification to \$1.60/gget at the plant gate (<\$3.30/gge delivered). The target for 2017 is to reduce the cost of hydrogen produced from biomass gasification to \$1.10/ggeat the plant gate (\$2.10/gge delivered).



Question 1: Relevance to overall DOE objectives

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

- This project is a really good idea where it explores catalytic approaches to directly treat cellulose and lignin.
- The project's focus on biomass sourced from non-food/feed crops is an excellent feedstock for the production of hydrogen. It is plentiful and can be developed to be even more plentiful. The production cycle of plant growth through hydrogen production is near zero in GHG emissions and can reduce GHG air concentrations if the GHG generated in the production process is sequestered. Aqueous Phase Reforming (APR) of sugars and other compounds derived from biomass is a low-temperature and low-cost process to produce hydrogen. If the cost of the feedstock (sugars, etc.) could be reduced, it could be a very low-cost green approach to hydrogen production that could exceed the DOE hydrogen cost targets. This project is targeted at finding lower cost processing and digestion of biomass to produce sugars or other compounds that can be used in APR.
- This project's process uses a very abundant feedstock for H₂ production. This route can have a very favorable central and semi-distributed production economics.
- Based on the project team's presentation materials, their appeared to be good relevance toward the development of biofuels pathways toward the DOE's hydrogen goals.

Question 2: Approach to performing the research and development

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

- A crisp rationalization for the approach or the investigation that could lead to a preferred approach is not apparent.
- The team's approach that has been taken is to perform screening experiments with an array of potential catalysts using solid biomass and potential biomass digestion products to look for evidence of biomass breakdown to APR processable intermediates. APR catalysts were used in conjunction with other catalysts in some experiments to seek evidence of combined biomass digestion and APR in one pot. Several different analytical techniques were used to identify the products produced. The screening approach allowed examination of a wide array of catalyst options.

- It appears the team's entire effort went into screening experiments. It would have been better to identify some of the more encouraging catalysts earlier and done more extensive experiments to try to improve on the results achieved with them.
- LANL is applying the right tools for developing understanding of this difficult chemistry environment. The process can also have offshoot technology applications and side products that improve the economics of the process.
- The team's approach was laid out clearly in the presentation.

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

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

- Objectives for current fiscal year are not well detailed in this project. Funding is practically close to nothing. It is not clear what has been done recently by this team.
- The screening experiments in this project resulted in some encouraging results including: the demonstration of catalyzed hydrolysis of cellobiose to glucose, conversion of cellobiose to syngas but only to 5%, demonstrated catalytically enhanced decarboxylation of lignin and low-temperature catalyzed gasification of lignin.
- It appears that the entire team's effort went into screening experiments. It would have been better to identify some of the more encouraging catalysts earlier and done more extensive experiments to try to improve on the results achieved.
- In many cases, the analysis of the products, particularly the gas phase products was incomplete.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 1.3 for technology transfer and collaboration.

- There were no apparent collaborations in this project.
- LANL has had no collaborators on this project. There has been a great deal of research over the past 20 years on the digestion of biomass to sugars and other compounds. Much of this work was based on enzymes and thus the reason for this project. However, some work has been done on thermochemical breakdown of biomass and those in the field of enzymatic biomass digestion could have brought some valuable insights to this project. NREL and PNNL have been working on biomass digestion for decades. Many universities have also been in this field for a long time. In addition, Virent has pioneered APR and PNNL has recently been studying it as well. Thus there is a long list of potential collaborators that could help in this effort.
- This project can be leveraged a lot more. For example similar consortium can be applied as the one for PEC.
- Not applicable. It would have been helpful to involve a commercialization partner in some aspect of the project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- Project plans are not written in way that can give confidence, The PI has any specific ideas to explore.
- The future project plan includes both additional screening experiments and some focused work on lignin, which has proven to be the most difficult part of the biomass to digest. This project has shown some degree of success in converting cellulose to APR processable sugars and oligomers. If low-cost catalytic digestion of biomass to lignin and APR processable products could be developed, this could be a major success. The lignin could be used to generate power and the rest of the biomass could be a low-cost feedstock for APR generation of hydrogen. Research on this approach should also be a part of the future work plan.
- The project's work scope needs to be in line with other work happening outside LANL, in order to improve the general technology development.
- The "future work" pathway looks like an expanded investigation work similar to what has already been done. No pathway to commercialization clearly identified in this project.

Strengths and weaknesses

Strengths

- The biomass sourced from non-food/feed crops is an excellent feedstock for the production of hydrogen is a strength. It is plentiful and can be developed to be even more plentiful. The production cycle of plant growth through hydrogen production is near-zero in GHG emissions and can reduce GHG air concentrations if the GHG generated in the production process is sequestered. Aqueous Phase Reforming (APR) of sugars and other compounds derived from biomass is a low-temperature and low-cost process to produce hydrogen. If the cost of the feedstock (sugars, etc.) could be reduced, it could be a very low-cost green approach to hydrogen production that could exceed the DOE hydrogen cost targets. This project is targeted at finding lower cost processing and digestion of biomass to produce sugars or other compounds that can be used in APR.
- The project team has taken an approach to perform screening experiments with an array of potential catalysts using solid biomass and potential biomass digestion products to look for evidence of biomass breakdown to APR processable intermediates. APR catalysts were used in conjunction with other catalysts in some experiments to seek evidence of combined biomass digestion and APR in one pot. Several different analytical techniques were used to identify the products produced. The screening approach allowed examination of a wide array of catalyst options.
- The project's screening experiments resulted in some encouraging results including: the demonstration of catalyzed hydrolysis of cellobiose to glucose, conversion of cellobiose to syngas but only to 5%, demonstrated catalytically enhanced decarboxylation of lignin and low-temperature catalyzed gasification of lignin.
- The project team has provided strong technical detail.

Weaknesses

- It appears the entire effort went into screening experiments in this project. It would have been better to identify some of the more encouraging catalysts earlier and done more extensive experiments to try to improve on the results achieved.
- LANL had no collaborators on this project. There is a long list of potential collaborators that could help in this effort.
- Partnering and commercialization efforts in this project are weak.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PDP-13: Novel Low-Temperature Proton Transport Membranes

Andrew Payzant; Oak Ridge National Laboratory

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.6** for its relevance to DOE objectives.

- The team's work provides little support to DOE's hydrogen separation technology R&D efforts. This is because the DOE 2010 membrane flux performance target is 200 SCFH/ft² at 340°-400°C and 100 psig trans-membrane ΔP.
- The project's proposed proton transport membrane flux performance, although above the above leak level, is orders of magnitude lower than the immediate-term target.
- The membrane looked interesting, perhaps as a hydrogen purification membrane, perhaps only as a solid oxide fuel cell material, perhaps neither. Either objective would be worthwhile; however, it would be nice to know which it is at this stage. The project has been defunded, so cannot expect too much from the researchers.
- This is a novel and high-risk approach to develop materials and membranes for hydrogen separation. The investigators are well aware of the DOE targets and goals and are striving to meet these goals and targets while still conducting a fundamental development project (at minimum cost). Although not successful, their efforts are to be commended.
- A reliable, cost effective, stable hydrogen separation membrane that could operate below 500°C could be a key enabler for the Hydrogen Program. It could reduce the cost of thermochemical hydrogen production in general and for reforming of natural gas and biofuels in particular. The Pd membranes are beginning to be commercialized but an alternative that might have some advantages could be very useful.

Question 2: Approach to performing the research and development

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

- The proton transport membrane (PTM) R&D work has been going on and off for several years with no significant progress and the findings presented are not new. All of the DOE 2010 membrane performance parameters need to be studied and satisfied; this is not expected to happen. The team's work is at a very fundamental level and may be of some academic value.
- The researchers made a membrane and presented data on transport at low pressures, but did not examine the effect of pressure. The project team examined the effects of temperature, but the results were quite aberrant,

suggesting high-flux solid-state transfer with almost no activation energy and 100% selectivity. No analysis was done as to why transport properties were this way.

- This is a good approach for basic development of new separation ceramic materials that may operate at reduced temperatures. The compositions are based on materials that have shown some promise and further examination is warranted for this project.
- The project team understands and has defined all the key properties needed for a hydrogen membrane to be useful. It is testing the novel LAMOX-based material for these properties, as well as developing improved LAMOX-based materials where the properties are deficient.
- This project includes a fundamental approach by obtaining crystal structures and other fundamental properties and using atomistic computer modeling to identify potential improved ceramic materials.
- The first LAMOX material to be identified as promising has a H₂ flux rate 5-6 orders of magnitude, which is too low. The researchers have identified plausible approaches to solve this fundamental problem including: generating a thin membrane, use of higher pressure across the membrane, increase the proton conductivity by using dopants to alter the crystal chemistry, and increase the H₂ proton dissociation rate with a surface catalyst.
- The project's diffusion of impurities should be evaluated in this system. The project's 100% hydrogen is an optimistic assumption. The project's CO₂, CO, and H₂O need to be accounted for in purity measurements at the least.

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

This project was rated **2.4** based on accomplishments.

- As of now, the membrane separation performance is not of any significance to this project. The flux improvement strategies, based on known theories, are speculative and may not apply to this membrane. It is not even guaranteed the material is truly transporting protons. Besides, even the desired low operating temperature is not compatible with upstream process conditions.
- This project was defunded a year ago, so not much progress can be expected with only carry-over funds. The project team's graduate student has left. The data that was taken looks very interesting except for the holes that suggest something odd is going on behind the scenes.
- Unfortunately the project's technical progress is limited. The overall flux is still very low and it is unclear how this can be improved. The development of low temperature ceramic materials for hydrogen/proton is a difficult problem and the investigators have made a good attempt to improve on past materials.
- The project has successfully synthesized 10 micron films on Y-stabilized zirconia.
- The project has demonstrated that LAMOX is stable in H_2 at 500°C and CO₂ at 800°C.
- The project's crystal structure of the LAMOX material has been determined with XRD.
- This project has had very good progress for the funding level. The diffusion rate appears to be very low, or the diffusion gradient is not there. If dilute hydrogen is used, the concentration on the purified side at ambient pressure would predict no diffusion. The project team should show pressure differential effects. The team should also describe the bulk proton transport mechanism that they are hypothesizing.

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

This project was rated 2.4 for technology transfer and collaboration.

- Collaborations in this project include ORNL, the University of Cincinnati (hydrogen permeation tests), and the Imperial College.
- Project work is being done at different groups, but there was no effort to combine the results from the different groups.
- External collaborations are limited to academics and national laboratories in this project; however; this is appropriate for this type or research.
- The project is collaborating with the University of Cincinnati for permeation measurements, Imperial College, London for impedance spectroscopy, and other scientists at ORNL for NMR to identify H₂ bonding.
- There is a lot of excellent work being done at several universities and national labs on ion and proton conducting membranes. It seems that collaboration with some these efforts would be very helpful in this project.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.2 for proposed future work.

- The project has not been funded in FY09 and future funding is unknown.
- The team researcher hopes to keep carrying on with this project. This is heroic given that the project was defunded a year ago.
- The additional slides for reviewers only indicate that this project is being terminated. However, this reviewer would strongly suggest that DOE continue to allow this project to continue at a moderate level. The Hydrogen Program needs some need ideas and direction and this work is providing this approach. The work may not be successful, but it may provide data and information for future research direction.
- There is no future work-plan presented by this team. The researchers appear to be assuming that this project will not receive additional funding.

Strengths and weaknesses

Strengths

- At first glance, the project has a miracle material, and a durable, solid-state transport membrane that has 100% selectivity, and very low activation energy for transport. This could be used as a low-temperature separation membrane, or as a low-temperature solid oxide fuel cell.
- A reliable, cost effective, stable hydrogen separation membrane that could operate below 500°C could be a key enabler for the Hydrogen Program. It could reduce the cost of thermochemical hydrogen production in general and for reforming of natural gas and biofuels in particular. The Pd membranes are beginning to be commercialized but an alternative that might have some advantages could be very useful.
- The project understands and has defined all the key properties needed for a hydrogen membrane to be useful. It is testing the novel LAMOX-based material for these properties and developing improved LAMOX-based materials where the properties are deficient.
- The project includes a fundamental approach by obtaining crystal structures and other fundamental properties and using atomistic computer modeling to identify potential improved ceramic materials.
- The first LAMOX material to be identified as promising has an H₂ flux rate 5-6 orders of magnitude which is too low. The researchers have identified plausible approaches to solve this fundamental problem including: generating a thin membrane, use of higher pressure across the membrane, increase the proton conductivity by using dopants to alter the crystal chemistry, and increase the H₂ proton dissociation rate with a surface catalyst.
- The project has successfully synthesized 10 micron films on Y-stabilized zirconia.

Weaknesses

- What was transferred in this project, O, H, or both, is not apparent. We do not know how it was transported nor why there activation energy with 100% selectivity is lacking.
- The hydrogen flux rate needs to be improved by 5-6 orders of magnitude in this project.
- There is a lot of excellent work being done at other several universities and national labs on ion and proton conducting membranes. It seems that collaboration with some these efforts would be very helpful.
- There is no future work-plan presented by the project team.

Specific recommendations and additions or deletions to the work scope

- This project should be re-funded. The team researcher should measure H₂ transport using a simple, Sievert transport apparatus at different pressures and different gases so we know if O, O₂, H, H₂, or some combination is being transported. The team should also conduct either nuclear magnetic resonance (NMR) or infrared (IR) work to understand how atoms are moving.
- The project team should continue at a moderate level. Fundamental material development is a necessary part of an overall program and could have a longer-term payoff.

Project # PDP-14: Ultra-thin Proton Conduction Membranes for H₂ **Stream Purification with Protective Getter Coatings**

Dr. Margaret E. Welk, Dr. Robert Grubbs, and Dr. Andrea Ambrosini; Sandia National Laboratories

Brief Summary of Project

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

Question 1: Relevance to overall DOE objectives

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



- This project will develop a hydrogen purification membrane technology that incorporates sulfur getter-ing to address DOE hydrogen production targets for impurities, flux, durability, and hydrogen selectivity.
- This project aims to extend the life of oxide membranes by coating them with ZnO to protect against H₂S poisoning. The project team has achieved the desired protection, however, they do not have selectivity. This project was defunded. Ideally, the team should try to work with some other project where they produce membrane with selectivity, but short life in H₂S.
- The PCM is relevant to renewable hydrogen production goals. It is not clear if this is the right time to look at H₂ separation membranes
- The project team's approach is interesting, but is unlikely to be able to compete with cheap guard bed based on solid ZnO-based sorbents.

Question 2: Approach to performing the research and development

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

- The project's approach integrates sulfur getter and H₂ separation into a multifunctional membrane. Their use of ALD for materials deposition for both getter and proton conducting material should allow thin film deposition on surfaces of support and fine control of film properties.
- The work done by the team is nothing spectacular, but it worked to the extent that work was done. The team coated with ZnO, got H₂S protection. They, however, still do not have the flux and selectivity problem solved.
- A high-cost membrane is not a good solution for H₂ separation. The PCM themselves have a cost barrier to overcome and this makes the task all the more challenging.
- The project team has performed good work on deposition and stabilization on ZnO thin film.
- The project team should show how this would be scaled up in a manufacturable scale. Large areas of this material would appear to be fragile and challenging for handling. Is tube arrangement the geometry of choice?

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

This project was rated 2.4 based on accomplishments.

- Initial attempts to deposit SrTiO₃ using ALD were not successful, but had never been previously demonstrated. The project team's effort has transitioned to a new Sr precursor identified in a recent literature report. There has been good success in demonstrating uniform deposition of ZnO getter in Al₂O₃ substrate, and initial results indicate this material can be cycled and fully utilized to purify a gas stream containing H₂S. The estimated performance of an S-getter was based on this technology and assumed full utilization, but did not compare to existing S-getter technologies to baseline pros/cons of this approach.
- The project team has had good progress in the area worked on. The project was defunded; therefore only carryover funds were used. The team should have a better membrane underneath in terms of flux and selectivity.
- Not much progress has been made since the last time, possibly due to lack of funding for this project.
- The project team has done good work to solve problems in depositing uniform films.
- The project's 70 days operation is very short for a complex and expensive film like this.

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

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

- The project team identified other partners, but did not pursue further after a decision made to end this project.
- The team should collaborate with someone that has a better membrane, and try coating it with their ZnO. The lack of funding is hindering, but still would expect that there are other people who would like to piggyback on the work.
- The PECM team has good coordination within themselves.
- This project team has done okay considering funding was cut.
- This project could leverage a lot of participants. BASF, for example, has extensive interest and experience in similar filtration systems.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.4 for proposed future work.

- The project team will determine whether appropriate $SrTiO_3$ stoichiometry can be achieved, and if so, then they will measure H_2 flux of films. The project team will also determine the rate of sulfur uptake.
- No particular future work is planned for this project.
- The project's lack of funding from DOE would be a major obstacle.
- The project team needs a realistic estimate of reactor cost and comparison with sacrificial ZnO guard bed.

Strengths and weaknesses

Strengths

- The project team's integrated/monolithic approach to S gettering/H₂ purification should provide a simplified system design and good robustness.
- This is a nice part of a membrane durability project.
- None.

Weaknesses

- The project team needs to baseline component (getter and H₂ membrane) performance by comparing with existing technologies/approaches.
- The team needs to work better with others so that this part does not stand alone, but becomes part of a viable membrane.
- This project is an outside focus area for PCM research. Firstly, the right PEC materials should be obtained and then the team should focus on H₂ separation/purification.
- This project has questionable economics.

Specific recommendations and additions or deletions to the work scope

• The project team should get a good oxide membrane substrate, coat it, and repeat tests comparing it to the uncoated oxide membrane in terms of flux, selectivity, and life.

Project # PDP-15: Distributed Bio-Oil Reforming

S. Czernik, R. French, and M.M. Penev; National Renewable Energy Laboratory J. Marda and A.M. Dean; Colorado School of Mines

Brief Summary of Project

The overall objective of this project is to develop the necessary understanding of the process chemistry, compositional effects, catalyst chemistry, deactivation and regeneration strategy as a basis for process definition for automated distributed reforming. The fiscal year 2009 objectives are to 1) improve bio-oil atomization with less MeOH addition; 2) demonstrate noncatalytic partial oxidation of bio-oil at the bench scale; 3) demonstrate catalytic conversion of bio-oil to syngas at the bench scale; and 4) provide mass balance data for H2A.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

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

- This project is going to develop distributed bio-reforming capabilities that directly address H₂ production targets for fuel feedstock issues, operation and maintenance, and control and safety.
- Bio-oil is a low-cost, renewable fuel, far cheaper than hydrogen. In this project, it is being reformed to H₂ and other gases that can be used in a fuel cell or for other power applications. This is a good and simple project. The work is straightforward and relevant to the hydrogen goals. The team's results are also good results; however, more work is needed.
- While this project meets the scope of direction and supports DOE objectives, converting biomass to hydrogen may not be the smartest thing to do.
- This project broadly supports objective of producing hydrogen from renewable sources. The project's cost potential is low; however, this low-cost potential comes at a price.
- This project has a fatal flaw in that it requires distribution of very dirty pyrolysis oil to forecourt locations. The distribution chain can't be made tolerant of dirty, unstable liquids; these bio-oils will need to be substantially upgraded before they can be distributed and stored for forecourt use; and these steps will add exactly the cost that this project seeks to avoid.
- This project presents a good analysis of a hydrogen production pathway that is not getting a lot of attention.

Question 2: Approach to performing the research and development

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

- The project team's approach addresses key individual processes, as well as overall system considerations. The team has a good understanding of how its research must feed into the overall system to achieve DOE's targets. It also has a good balance of fundamental experiments and practical system considerations.
- This project's experimental apparatus appears straightforward. The team has good experiments as well as analysis and has done good work. It would be better if the team looked at a lower-cost catalyst.
- This project has had a sound process path during period of performance that is consistently seen year to year. The team is well focused on the challenges and it is challenging to find how they can improve on their processes. This project team has done outstanding work in all aspects.

- This project's barriers are mischaracterized. The team's use of a dirty feed (pyrolysis oil) addresses the barrier of feed cost, by substituting a lower cost feed (than ethanol for example). Framed this way, a key issue is whether these cost advantages are outweighed by logistical (distribution) disadvantages.
- The boundary limits in this project need to be widened to include pyrolysis oil manufacture, distribution, and storage. In this project, it appears that oil handling distribution and storage are the most important barriers.
- This project has a good approach and the misting reactor is non-standard. The investigator needs to carry out studies using traditional reactors under a variety of conditions and compare results to ultrasonic nozzle reactor to establish its advantages and justify its use. The reactor has made interpretation of results difficult because temperatures are not well defined.
- The project team needs to look at steel reactors to explore higher pressures.

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

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

- This project team has had significant progress in testing a range of feedstocks and conditions using the benchtop reactor both developed and built previously. The quantitative results for providing good insight for optimizing the overall reaction process from bio-oil to syngas. The initial results indicate that either a system that operates on a range of feedstocks could be developed or that the individual components could be developed to enable optimized systems in distributed locations for the primary feedstock in that location.
- This group is developing a technology that could be used in current or near-future fuel cells. The catalyst is still expensive and it would be better if Pt-Ni were used in the project instead. Also, the data should be presented in terms of turn-over numbers, and other, more normal, terms. Still, this project shows good solid work.
- While one may question the value of the objectives, the project clearly achieves steady technical accomplishments during the period of performance. The team's ultra-sonic nozzle development might prove to be very interesting, and beneficial. This is an outstanding performance by the project team.
- The project's objectives are well detailed for 2009, and are mostly accomplished despite minimal support.
- The team's reactor appears to generate consistent results. The team has also achieved good conversions of biomass and shown the effect of oxygen partial pressure.
- The project team has not made it clear that material balances are closed.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- This project has strong collaboration with key partners that provide complimentary expertise and capabilities.
- This project has a good collection of distributed work, plus various students and collaborators. More input from catalyst researchers and a commercial catalyst supplier is recommended.
- The project team has met the requirements of collaboration with other institutions.
- This project has a little more than a catalyst supplier relationship with Lanny Schmidt and a funding relationship with Chevron.
- This project has collaborators listed, but no elaboration of how they contributed to program.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The team's proposed future work builds on prior results and is focused on an ultimate system design concept and demonstration.
- This project seemed to be winding down. The team also seems open to looking at other catalysts, but had no particular plans to test them. They have no plan to feed into FCs, or to reorganize the data either.
- The project team has clear plans to address "what's next." It is also clear that future plans capitalize on progressto-date and that past progress supports future.

- This project needs to consider the whole "life cycle" of oil creation, storage, transportation, storage, and conversion.
- The project team needs to collaborate more. More industrial collaborations are suggested to better understand data needs for scale-up and consider improving reactor design.

Strengths and weaknesses

Strengths

- This project is a good idea. Making hydrogen from renewable cellulosic materials has allowed for good results.
- This is a very well thought out project and has a nice progress of getting from point A to point B.

Weaknesses

- This project should be continued, however it should look at less-expensive catalysts. Would like to see different data presentation, and more next-generation planning.
- The hydrogen cost chart seems to raise as many questions as it answers. The project team might want to make this chart clearer.
- The project team needs a better reactor design so that the temperature is controlled and measured.

Specific recommendations and additions or deletions to the work scope

- The project team should feed gas to current or near-future fuel cells. It would be nice to see results in terms of residence time vs. extent of reaction. Also, the catalyst is still expensive and it would be better if Pt-Ni were tested instead of Rh.
- The project team needs to consider the whole "life cycle" of oil creation, storage, transportation, storage, and conversion.
- The project team should improve the reactor design. The team should look at pyoil from a variety of pyrolosis conditions and determine optimum conditions for process.

Project # PDP-16: Pressurized Steam Reforming of Bio-Derived Liquids for Distributed Hydrogen Production

Sheldon H.D. Lee, Dennis Papadias, and Shabbir Ahmed; Argonne National Laboratory

Brief Summary of Project

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



<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

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

- This project supports the DOE Hydrogen Program objectives.
- Based on slide 3, the researchers are aware of the DOE goals and targets. The work is attempting to address the target of efficiency. However, there appears to be little consideration about the cost. In particular, increasing reactor pressures in a membrane reactor will likely require more robust materials and seals (which will increase the cost). Coupled with the need for a turbo-compressor, reaching the cost target may not be realistic. The work, overall, does not address any cost issues.
- This program provides a key understanding of relative merits of the key reforming and separation routes (membrane vs. PSA) for H₂ manufacture. This is a small but very important point, as projects will emerge that purport advantages via one route or the other.
- The distributed reforming of bio-based liquids such as ethanol is a promising near-zero GHG emissions route for the production of hydrogen if the capital costs can be reduced and selectivity improved. The DOE Hydrogen Program is funding several projects in this area. This project is trying to achieve cost reduction by operating at higher pressures and employing an *in situ* palladium hydrogen membrane. This can reduce capital costs to a degree but does not have the potential of more significant cost reductions of other options being researched.
- This technology has a potential of reducing the already low-cost steam methane reforming (SMR) hydrogen production. The process has relevance in both long-term biogas applications, as well as today's refinery SMR applications.

Question 2: Approach to performing the research and development

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

- The rationale behind the technical approach in this project is unclear.
- The team's energy and cost analysis data should substantiate the claim why it is cheaper to pressurize an incompressible fluid (fuel and water) compared to hydrogen, a compressible fluid. It is well known that compressing hydrogen is energy intensive. A Google search shows that to compress hydrogen from 100 psi to 700 psi, the energy need is 2.6-3.6 kWhe/kg. Energy needs to compress liquid fuel and water is necessary for comparison.
- The project team has idealized assumptions on membrane performance without identifying a membrane operating at 650°C and achieving DOE 2015 performance targets.

- The recovery of a non-permeate streams' temperature and pressure energy into shaft work is not a new idea. The availability of appropriate capacity turbo-machinery for distributed production scenario is not discussed in this project.
- If a reactor operates at 800°C and 80 atm, it is unclear which membrane is available to separate the hydrogen at DOE's 2015 flux target. It is also not explained why it is so cost-effective and operationally simple to operate a SMR/membrane integrated reactor at 800°C and 80 atm.
- The project's engineering design and plant operation of the proposed approach may not be practical.
- The overall approach to evaluate/model a high-pressure reaction on the reaction side of the membrane does not appear to make sense. Increased pressure may increase flux (due to a higher partial pressure differential) but the product pressure will not be affected.
- This may have benefit for a conventional SMR reaction but increased pressure for SMR has already been examined in detail in many studies in the past. In addition, this appears to be a pure modeling effort with little experimental results to back up the modeling results. There needs to be a better balance in the approach of this project. Slide 9 simply uses the DOE target. This is not a reasonable approach. The actual flux rates (with mixed gas) need to be incorporated for realistic model results. This work also needs some independent verification.
- The project's model approach is perfect for this program.
- The team's approach to this effort over the past year consisted solely of modeling several options for distributed ethanol reforming including the high-pressure *in situ* membrane approach being taken by this project and the more conventional approach using lower pressures and PSA technology. Although modeling can be very useful, this modeling work only included performance (energy efficiency) without any analysis of costs which is the issue for ethanol reforming.
- There was no experimentation done to verify the modeling effort or to further the development of the approach being researched by the team.
- There was no collaboration mentioned with the other DOE Hydrogen Program funded projects working on ethanol reforming. Collaboration with these efforts would be very beneficial to this effort as well as the other projects.
- This team has demonstrated outstanding systems engineering and optimization of its technology. This process can be used to evaluate the performance of other similar applications of hydrogen separation. It would be worthwhile to benchmark the various technologies of this flavor in this fashion.

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

This project was rated 2.4 based on accomplishments.

- The team's studies and reports have areas where analysis is based on ideal assumptions. The project team has not analyzed if the technical strategy is practical, nor has analyzed or substantiated some of the technical claims.
- The team's summary statement of higher efficiency at 10,000 psi delivery pressure is made with ideal assumptions. The DOE target is 100 psi trans-membrane ΔP. The project team needs to say what feed pressure they recommend to achieve the delivery pressure to exceed the efficiency of a conventional, proven, SMR-PSA system.
- The project's results are minimal for the funding provided. There has been very little advancement since last year. The work has changed to look at ethanol, which should be easier to reform; however, few results are actually provided. Efficiencies are still not reaching the targets and increasing efficiency by even a few points is a difficult problem with systems such as these. The only potential result appears to be that addition of a turbo-compressor may add some benefit to the efficiency. The cost of it may cause this benefit to be impractical.
- The team's objectives are poorly expressed in the poster for the specific piece of work that was executed and described. However, the project accomplishments are very good.
- The team's modeling work performed is quite good and does help to understand the potential performance (energy efficiency) leverage of the approach to ethanol reforming being researched. However, there is no cost analysis work being done to quantify the potential benefits of this approach. Cost is the key issue.
- The future plan from last year's merit review presentation included exploring O₂ and CO₂ membranes. There was no work done on this.
- The team has done good systems analysis work. More results from material performance and properties were expected and this technology may need to be demonstrated in scaled up reactor.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **1.6** for technology transfer and collaboration.

- The project team is working with REB Research and Consulting, but the extent of their collaboration is not discussed.
- Outside collaboration appears minimal to none in this project. Some interaction appears to be with REB; however, the REB membrane is used for a small scale system and has minimal flux at moderate conditions. They are neither considering nor addressing conditions that would be used in a larger scale process. All other project work is being done within Argonne. In order for this work to be credible both industry input and collaboration is necessary. The models need some independent verification outside the lab to have any meaning of value.
- There are not a lot of collaborations in current phase nor do there need to be.
- The only collaboration mentioned by the team is within ANL and with REB who supplied the palladium membrane. There are several other excellent ethanol reforming projects being funded by the DOE Hydrogen Program. Collaboration with these efforts would be very beneficial to this effort as well as the other projects.
- The modeling work performed by the team is quite good and does help to understand the potential performance (energy efficiency) leverage of the approach to ethanol reforming being researched.
- This project can benefit itself and other projects by collaborating. This can especially benefit others with issues such as systems engineering capabilities and practices.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.2 for proposed future work.

- This section is missing from the project.
- This is a project that should be considered for termination. Few results have been obtained and the results thus far do not suggest continuing the project. The future plans are standard and vague and still appear to focus on modeling with little experimental verification. There is considerable other work in the suggested areas that is being conducted by other researchers. The team's work is not providing any new or novel insight that could not be obtained elsewhere.
- The team should complete the economics due to being the highest priority of the several items identified.
- The project's future plan includes cost analysis, which is good. However, it should have been part of this project from the beginning.
- The team's future plan appears to include experimentation work with other biofuels based on the proposed approach which would be useful.
- The future work for this team includes evaluating systems based on CO₂ removal. It is unclear if this approach could significantly reduce the cost of biofuels reforming. A very simple analysis might determine this.

Strengths and weaknesses

Strengths

- No clear strengths are identified in this project.
- Distributed reforming of bio-based liquids such as ethanol is a promising near-zero GHG emissions route for the production of hydrogen if the capital costs can be reduced and selectivity improved which is a strength.

Weaknesses

- Minimal results have been shown for an estimated investment of \$750K. The work is not achieving the DOE efficiency target and cost has not been clearly considered at all. There are no clear targets or milestones for this work and seems to be simply continuing on a random path to provide some basic, minimal results.
- The DOE Hydrogen Program is funding several projects in this area. This project is trying to achieve cost reduction by operating at higher pressures and employing an in-situ palladium hydrogen membrane. This can reduce capital costs to a degree but does not have the potential of more significant cost reductions of other options being researched.

- The approach to this effort over the past year consisted solely of modeling several options for distributed ethanol reforming including the high-pressure *in situ* membrane approach being taken by this project and the more conventional approach using lower pressures and PSA technology. Although modeling can be very useful, this modeling work only included performance (energy efficiency) without any analysis of costs which is the issue for ethanol reforming.
- There was no experimentation done to verify the modeling effort or to further the development of the approach being researched by the team.
- There was no collaboration mentioned with the other DOE Hydrogen Program funded projects working on ethanol reforming. Collaboration with these efforts would be very beneficial to this effort as well as the other projects.

Specific recommendations and additions or deletions to the work scope

- Many assumptions realistic for engineering development.
- This project should be considered for termination. No additional funding should be obligated.

Project # PDP-17: Renewable Electrolysis Integrated System Development and Testing

Kevin W. Harrison, Greg Martin, Todd Ramsden, and Genevieve Saur; National Renewable Energy Laboratory

Brief Summary of Project

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



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

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

- This project addressed a highly relevant topic. There will be significant payoff if project is successful. This could be highly significant for industry, military, and individual consumers.
- The project team broadly supports renewable energy to fuel hydrogen.
- The project's wind to H₂ project fully supports the DOE Hydrogen Program.
- The project's focus on the need for "as close to direct coupling" of renewable sources to electrolyzers is important and relevant. This is because, in the end (when fossil sources get prohibitively expensive), renewable electricity would be the only logical power for electrolysis of water to produce hydrogen.
- The project's hydrogen-oxygen redox couple is not convincing especially regarding the claim that it is the best couple for renewable energy storage. This exercise is useful in developing the groundwork for understanding the rate-limiting challenges in this source especially load coupling.
- The project supports critical analyses of renewable hydrogen production systems.
- This is an important project that helps to assess the capability of hydrogen to serve as a storage medium and to maximize the use of intermittent renewable resources.

Question 2: Approach to performing the research and development

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

- Barriers appear to be accurately identified in this project.
- The team's approach clearly addresses barriers, but this is a very expensive, pre-commercial scale activity. It is possible that this work was done too soon before there was adequate commercial interest to take the findings into commercialization.
- With the push to get renewable energy onto the grid, the assumption of a dedicated solar or wind facility for hydrogen generation seems unlikely in near future. If the benefit of the advanced power electronics is in elimination of the turbine's power electronics (which is what the cost analysis shows), then this part of the project should be deferred until closer to when it is likely that a wind turbine that is dedicated to hydrogen production would occur. Doing this research does not seem effective since it is likely that turbines and electrolyzers of the future (when the power electronics are needed) will be substantially different requiring the power electronics to be re-developed. In addition, the power electronics seem to be turbine type specific,

therefore power electronics for each manufacturer and model of turbine would be required. It is hard to see how the power electronics will be used in the time frame the team envisions.

- The barriers addressed by the project team (capital cost, system efficiency, and renewables integration) do not include the design, construction and commissioning of a fuel cell vehicle filling station. This should not be part of this project, but it should be in Tech Validation. The Production and Delivery budget is too small to maintain a filling station. Resources from Production and Delivery should not have been spent on the filling station. This portion of the project should be given to Tech Validation.
- The team should have spent more effort on getting long-term on-wind or on-solar hydrogen production generation. Showing a limited number of hours on-sun or on-wind hydrogen generation is not impressive considering the very large budget of the project and the length the project has been in place.
- The team's approach is solid and reasonable but efficiencies developed here tend to be individual component efficiencies rather than a "quantum leap" in system-integrated efficiencies.
- Numerous barriers are being addressed in a well-integrated project.
- The team's approach for research and development seems generally good, but it would help to have a more specific approach to meeting technical barriers such as overall system efficiency, auxiliary power losses, etc.

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

This project was rated 3.2 based on accomplishments.

- The project team's stack size reductions are commendable. The whole process to make a more-durable, more size-economic system could be well received.
- Overall, the team's accomplishments are great, but presentation does not identify what was actually planned or executed in 2008 or 2009, and a lot of this material has been around for a while.
- This project started in FY06 and has been very well funded (\$4.625M), but has produced relatively little on-sun or on-wind data. One would expect long term (days at a minimum, preferably weeks or months) worth of data to show how the system operates over a wide variety of conditions. The hydrogen does not necessitate the need to be captured for this operation, it could be vented or consumed (they have a generator).
- DOE provided the 2008 AMR presentation. In that presentation, the PI said that they were validating their cost/performance models that NREL was developing. The results of the validation were not presented. It is unclear where these results have been presented.
- Seeing new wind to hydrogen data from the team was good.
- The power electronics improvements from generation 2 to generation 3 did not seem extremely significant; however, power electronics improvements are difficult to achieve.
- Since the power electronics are a major focus of this project, a more detailed explanation on why the 3rd generation did not achieve the anticipated improvements would be useful.
- The team's cost analysis assumes that the wind turbine would be used exclusively for hydrogen production. This is not a realistic assumption in the current rush to put renewables on the grid. The cost analysis should be done again, with the assumption that the wind turbine will be used primarily for electricity generation and then curtailed wind will be used for hydrogen generation. This is a more realistic scenario.
- The team's development of standardized testing protocols is an important accomplishment.
- The project team accomplished straight-forward experiments and well-presented results (e.g., the direct coupling for PV-PEM.)
- The team produced good, reasonable, conclusions related to criticality of power electronics (command and control), need for greater standardization of interconnects and components, and need to define redundancies.
- The findings and lessons learned document shows strong progress in the team overcoming barriers.
- Several significant improvements have been developed and implemented by the project team.

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

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

- A significant number of partner activities are involved in the program.
- There seems to be good collaboration with other institutions including international collaborations in this project.

- It is unclear how the team is sharing and offering feed back regarding its information and what information on the electrolyzer is being fed back to electrolyzer manufacturers. Are the electrolyzer companies interested in using the power electronics? Who will manufacture the power electronics? Since it is unlikely that the electrolyzer companies will manufacture power electronics, have they talked with power electronics companies?
- A large component of this project is integration with wind and solar. Collaborations with wind and solar companies are not apparent.
- The team's collaborations are solid because of the equipment supplied by the many players.
- There are several partners that are well integrated into this project.

Question 5: Approach to and relevance of proposed future research

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

- A compelling argument to do any of this is not apparent.
- The team has been working on the system upgrades for unattended operation for at least two years without being able to begin unattended operation.
- What is the purpose of the higher-pressure storage? Is an renewables to electrolyzer project? Should storage be part of a storage project or tech validation project?
- The team has well developed plans for future work should continue progress in addressing the specified barriers.
- The team could use more specific plan.

Strengths and weaknesses

Strengths

- The project addresses a technology that could be beneficial to a great number of users.
- The team has a good relationship with electrolyzer manufacturers and utilities.
- The team is providing a necessary and needed independent testing facility to the DOE to validate the electrolyzer projects results.
- The team has been very involved in the international community and given many presentations and published many reports.
- This project is somewhat unimaginative project but well-executed and presented.
- The team's conclusions are good (and expected) however no major revelations or show-stoppers are seen (other than system costs.)
- Strong technical integration is widely evident in this project.
- The team addresses a key area of hydrogen use with renewables.
- The team has a good combination of analysis and experimental results.

Weaknesses

- The team has been working on the system upgrades for unattended operation for at least two years. If it is that difficult to design a system for unattended operation, is this technology viable?
- The team needs to talk with wind and solar companies to get their "buy-in" on dedicated renewables for hydrogen.
- The project's progress seems slow, especially for the amount of resources they have received.
- It seems that the team has gotten side tracked. For example, the team worked on electrolyzer cost modeling for a few years and then stopped, but the outcome has not been presented. The team is putting in a fueling station and high-pressure storage, but it has not produced any long-term wind-to-hydrogen results. The compressor studies were interesting, but it is unclear why these studies were not done under Hydrogen Delivery element funding?
- There are no apparent weaknesses because this project's objective is to explore system interactions.
- The team should develop more specific technical targets.

Specific recommendations and additions or deletions to the work scope

- Because of the design differences between more-traditional fuel cell stack and tube-like systems, one could suspect that the team's system's ability to manage freeze conditions is a significant advantage over traditional stacks as water can more efficiently drain off.
- The project should focus on getting renewables-to-hydrogen data, especially long-term data.
- The power electronics development should be deferred until closer to when large central production facilities are necessary.
- The project should turn the fueling station to the Technology Validation Subprogram.
- The project should turn the compressor testing to the Hydrogen Delivery element.
- The project should work closer with electrolyzer companies on helping the companies understand the impact of renewables on the electrolyzers. However, this cannot be done until they have long term data is available.
- The team should continue the work but figure out an open portal for spiral integration of new technologies. They should explore more close-coupling (direct-coupling) projects.

Project # PDP-18: Hydrogen from Water in a Novel Recombinant Oxygen-Tolerant Cyanobacterial System

Qing Xu; J. Craig Venter Institute Pin-Ching Maness; National Renewable Energy Laboratory

Brief Summary of Project

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

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>



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

- Biological hydrogen supports the Hydrogen Program's RD&D objectives.
- This project aligns with the need for a renewable hydrogen production technology.
- Several approaches are being taken to add oxygen tolerant hydrogenases to cyanobacterial systems. This is key as the only real source of electrons is water and therefore oxygen will always be present.

Question 2: Approach to performing the research and development

This project was rated 3.5 on its approach.

- The approach is very systematic and well thought out.
- The project team has good focus on one key barrier: oxygen tolerance; however, it is unclear whether the final objective is to demonstrate an approach or an enzyme that can be manipulated into other more attractive organisms. It is unclear whether this organism would be stable. This is excellent science. There is not an obvious plan to incorporate other barriers for this type of technology.
- The project team is combining metagenomic searches for oxygen tolerant hydrogenases with expression in T. roseopersicina. The team is also taking a known oxygen tolerant hydrogenase gene from Rubrivivax gelatinosus CBS and expressing it in the cyanobacterium SynechocystisPCC6803. The metagenetic approach in particular has great promise.

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

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

- The team is achieving difficult milestones.
- The PI clearly identifies accomplishments and contributions of partner.
- Although NREL has received similar funding, they seem to be lagging behind J. Craig Venter Institute (JCVI).
- The project team has made excellent accomplishments in transferring genes and expressing a better oxygen tolerant hydrogenase.
- The project team is observing some hydrogenase activity from hydrogenase genes found and expressed in T. roseopersicina. The team has been trying to transfer the system into Synechococcus and can do this with the native hydrogenase from T. roseopersicina. NREL is having problems with the expression in synechocystis of

an oxygen tolerant hydrogenase from Rubrivivax gelatinosus CBS in terms of activity of the enzyme, though some subunits are present. They have demonstrated protein expression of the catalytic subunit in E. coli.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- The project team has good collaborations with other institutions and they clearly identify partner contributions.
- There is a good collaboration with NREL, but no mention of Vanderbilt University or University of Szeged, Hungary. It is unclear whether any of this work is linked to the Office of Science and if so what type of collaboration there may be.
- This appears to be a strong collaborative effort between JCVI and NREL.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- Continuing analysis does not seem very specific. More description in future work would be nice.
- More characterization and transfer is planned; however, nothing is mentioned about the stability of the hydrogenase through a number of generations. The work should at least validate the new gene sequences will remain active before additional bacteria systems are tested.
- In both JCVI and NREL, the proposed work is largely to continue optimizing the expression and activity of the hydrogenases in cyanobacteria.

Strengths and weaknesses

Strengths

- The team has a vast library to examine and the tools to examine it.
- The team is strong and they are communicating well.
- This is a good research team.
- The team has a well thought out plan for an oxygen tolerant hydrogenase.
- The strong capability in metagenomics of JCVI is the biggest strength. This, combined with the ability to identify and express the various components of the oxygen tolerant hydrogenases that they find, is potentially very powerful.

Weaknesses

- Contingency plans need to be developed.
- Understanding of the outcome is limited beyond the funding of good science. Does this work have any practical use in a real production system?
- The project is still at a point where it is very hard to extrapolate to commercial value or scale.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PDP-19: Use of Biological Materials and Biologically Inspired Materials for H₂ Catalysis John W. Peters, Trevor Douglas, and Mark Young; Montana State University

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

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

- The project consists of two parts: hydrogenase studies and biomimetic devices. The former aligns very well with the Hydrogen Program's objectives, although the latter seems to be too basic to be funded by EERE.
- The project goals are well-aligned with DOE program targets for improving both stability of hydrogen production and rate of electron transfer
- The focus on the hydrogenase of the purple sulfur bacterium is relevant since it is one of the most stable one reported thus far.
- Encapsulation of the hydrogenase will eventually improve stability, coupling that with a photosensitizer will improve the efficiency of solar hydrogen production.
- The project aligns well with DOE's objectives for biological hydrogen production.

Question 2: Approach to performing the research and development

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

- The approaches are good, although it would probably be better for the PIs to focus in a fewer approaches in the future.
- Good approach and synergy between biochemistry and material science
- Hydrogenase from Thiocapsa is a good model to determine protein structure and the possibility of uncovering underlying mechanism conferring overall stability
- The use of carbon nanotube, sol gels, photosensitizer, and polyethylene glycol may improve overall protein stability and rate of electron transfer while harnessing solar energy for hydrogen production. The team is also developing various materials for light capturing properties to harness solar energy.
- Approaches are logical. Focus on encapsulation of active hydrogenases in gels is good.

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

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

• The accomplishments are good and exciting, particularly in the area of hydrogenase studies. The accomplishments regarding the Thiocapsa roseopersicina hydrogenase's C-terminal and its possible relationship

to high O_2 tolerance are very promising in terms of future molecular engineering and biotechnology approaches to modify other hydrogenases.

- The progress toward goals was good.
- Protein alignment suggested the extra amino acids in the C terminus of the hydrogenase small subunit may confer stability, although no biochemical data supporting this hypothesis yet.
- The EM pictures revealing supermolecular structures of Thiocapsa hydrogenase is an important achievement
- Hydrogenase activity was demonstrated when it was entrapped in silica gel and was further enhanced when carbon nanotube is added.
- Low but obvious hydrogen production was observed in the nanotube in the absence of methyl viologen
- The finding of enhancement by polyethylene glycol (PEG) is novel, suggesting improvement in mass transfer is the contributing factor.
- The project team determined the photocurrent with hematite and methyl viologen (MV). Hydrogen production is to be expected with reduced MV, although the data was not shown.
- Good progress has been made. 100% recovery of hydrogenase activity encapsulated in Sol-Gel was achieved and gel encapsulation may be used to stabilize Fe-Fe hydrogenases. Identification of the C-termini end that contributes to the stability of Thiocapsa hydrogenases is interesting.

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

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

- Both PIs belong to the same institution and there are no outside collaborators. The two projects (hydrogenases and biomimetics) could be better coordinated.
- The collaboration is among the team members of this project: a multidisciplinary team comprising of biochemists and material scientists.
- This project is not yet ready for technology transfer.
- Good collaboration was demonstrated.

Question 5: Approach to and relevance of proposed future research

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

- Plans are good.
- A clear plan is laid out for device testing and evaluate hydrogen production efficiency
- Device optimization is underway
- Proposed future work is appropriate. The plan to establish benchmarks for hydrogen production efficiency is good.

Strengths and weaknesses

Strengths

- The PIs are knowledgeable in their respective areas of research and the institution is well-positioned to address the proposed research plans.
- This multidisciplinary team comprises expertise in hydrogenase biochemistry, crystallization, and material sciences.
- The investigators have demonstrated progress toward meeting well-defined goals.
- The biochemistry side of the research is strong, with the PI being a leader in the field of crystallography of difficult hydrogenase protein.
- This research may lead to identification of protein structure conferring its overall stability. This knowledge can serve as a model to study other hydrogenase and to improve their stability.
- The material sciences part of the team can generate materials with properties for improving electron transfer, mass transfer, and light capturing.
- The investigator is an expert in structures and structure-function relationship of NiFe-hydrogenases and Fe-Fehydrogenases.

Weaknesses

- The is a lack of coordination between the different projects.
- It is unclear as to a final choice between hydrogenase and platinum/palladium as the hydrogen-producing catalyst.
- Similarly, it is not clear as to whether ferritin or Ru(bpy)³ is preferred as the photosensitizer. There should be a more logical plan to include or eliminate and focus on the more promising materials.
- Ferritin needs ethanol as the sacrificial electron donor, but this may or may not be practical.
- The project's goal is not specific and there are no benchmarks for hydrogen production.

Specific recommendations and additions or deletions to the work scope

• The project team should focus more on down-selecting different configurations for the biomimetic device, at this point.

Project # PDP-20: Hydrogen Embrittlement of Structural Steels

Brian Somerday; Sandia National Laboratories

Brief Summary of Project

The objectives of this project are to 1) enable application of structural integrity models to steel hydrogen pipelines; and 2) enable development of micromechanics models of hydrogen embrittlement in pipeline steels. Models can demonstrate that hydrogen embrittlement can be accommodated and pipeline safety margins can be quantified. Micromechanics model are essential for understanding the fundamentals of hydrogen transport and embrittlement in steels.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>



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

- The project team should address how embrittlement rates compare to other forms of degradation.
- The acceptable performance target for these materials is unclear.
- This subject is important but in the overall list of items is probably ranked in lower quartile. The multiplier effect would have been to tie in this project with infrastructure validation programs fro end-of-life analysis.
- Knowledge of metal behavior in hydrogen service is important to delivery scenarios.
- Hydrogen pipelines may or may not be critical to the long-term success of fuel cells and the Hydrogen Program.
- It is unclear what the current hydrogen pipeline materials lack in properties.
- Knowledge of embrittlement required for use of steel in pipe and parts of hydrogen systems.

Question 2: Approach to performing the research and development

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

- The round robin approach will improve confidence in the data. It is unclear whether the different lab equipment/tests been calibrated.
- The sampling preparation and the hydrogen leakage were difficult issues and affected the program. The sampling issue could have been resolved by connecting this program with ongoing infrastructure validation projects to get field data and samples.
- It is not clear why the particular steels were chosen for evaluation.
- Evaluating the samples by ASME procedures is technically sound.
- This project measures material properties for use in hydrogen pipelines. Existing materials are evaluated for their use with hydrogen. It is unclear if the current material properties lack sufficient properties or not.
- Materials testing in support of ASME B31.12

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 2.7 based on accomplishments.

- Some test apparatus issues still remain.
- Good progress has been made considering no funds were made available this year.
- This is not reflective of the PI's work but the organizational and budgeting issues.

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- Low funding for FY09 has hindered progress.
- Some data have been generated in round robin tests. Conclusions are weak. Metal behavior as a function of composition should be addressed to validate the original reasons for choosing the candidate metals.
- This project received no funding in FY09, thus accomplishments for FY09 were minimal. It is not fair to evaluate a project which was not funded in the current fiscal year.
- The project team should duplicate testing to demonstrate reproducibility.
- This project needs continued funding!

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- This is not a criticism of the PIs but rather an indication of lack of coordination between the ongoing and parallel programs within the entire hydrogen effort. While as is, this project provided good data, but it could have had a higher potential to be a very useful and practical project.
- The problem that beset this project could have been worked out if the program was coordinated with the ongoing infrastructure projects for sample recovery.
- Participation of DOE Pipeline Working Group is positive but there seems to be weak participation of steel and pipe supplier companies.
- Work with the Pipeline Working Group is good.
- It seems as though there should be emphasis on industry: energy and industrial gas companies, as they have working hydrogen pipelines.
- Work with the DOE Pipeline Working Group is an excellent example of collaboration.
- Round robin testing is being conducted.

Question 5: Approach to and relevance of proposed future research

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

- The reliability of the testing methods is still outstanding. This should be first on the agenda.
- As the program appears to be at an end, there is no significant work planned.
- DOE funding is in question.
- Future work at some point should include an analysis of metal properties and behavior as functions of composition.
- No additional work is planned in FY09 due to lack of funding

Strengths and weaknesses

Strengths

- Embrittlement is an important issue with hydrogen.
- Round robin testing is a good approach.
- Useful concept with wide industrial application.

Weaknesses

- Issues with testing methods should have been resolved earlier.
- There has been a lack of coordination.
- This project has had limited budget.
- The experimental set up and procedure were weaknesses.

Specific recommendations and additions or deletions to the work scope

- It is unclear what other materials are being proposed for these pipelines.
- It is unclear whether the round robin partners have calibrated their tests with a known/standard material.

- The slide on critical assumptions discusses the issues, but there is no resolution for these. For example, it is unclear whether this program can work in conjunction with the infrastructure validation program to analyze the on-site steel storage tanks that have been through multiple cycles at pressures up to about 6000 psi.
- It appears a highly useful and practical program but it is handicapped by lack of adequate planning and interprogram connections and collaboration.
- The budgeting cycle could have been timed better to coincide with the end of the other programs for sample recovery.

Project # PDP-21: Oil-Free Rotor-Bearings for Hydrogen Transportation & Delivery

Hooshang Heshmat, Ph.D.; Mohawk Innovative Technology, Inc.

Brief Summary of Project

The objectives of this project are to 1) assess the feasibility of centrifugal compressors for hydrogen transmission and delivery; 2) demonstrate full-scale oil-free foil bearings in a compressor simulator rig; and 3) test candidate bearing/shaft materials and coatings. The hydrogen centrifugal compressor operated at very high speeds and required oil-free compliant foil bearings. Multi-stage, high-speed centrifugal compressors operating in series are necessary and feasible as demonstrated by low friction and long wear life of Korolonä.



Question 1: Relevance to overall DOE objectives

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

- Research in any new modes of efficient compression for bulk hydrogen handling is an important subject with wide reaching application.
- This project is a Phase II SBIR project aimed at the development of foil bearings (journal and thrust) for hydrogen pipeline compressors. This project directly addresses hydrogen compression targets and barriers.

Question 2: Approach to performing the research and development

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

- The project is segmented in different parts and funded separately. It was somewhat difficult to grasp the entire approach without knowing the entire scopes of the work. Apparently this project was just the preliminary modeling and scoping phase.
- The project team has a good approach based on foil bearing technology developed for air and gas turbine applications. Phases I and II of the project are focused on development and testing of bearings in non-conventional gases that simulate hydrogen e.g., use He to simulate lightweight properties of hydrogen. He tests appear to validate models, which can then be used to predict lift-off speeds and rotor dynamics in hydrogen.

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

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

- Based on the materials and the objectives, the project has made steady progress and is on its way to the next proto-type setup and testing.
- One of the problems is reducing environment with hydrogen. This project could have benefited if it had a closer collaboration with the other project (ANL, PDP-25) on coating tests.
- Good progress on modeling rotor dynamics and lift-off conditions for He. In final stage, project started to address seals and appears to settle on dynamic compliant foil seals.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

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

- This is partly because of the PI issues and proprietary nature of the work. It would have been useful if the PIs would allow ANL to test their coating. It is understood the reducing hydrogen environment can rapidly affect the coating performance.
- There was limited collaboration with outside firms. Mitsubishi Heavy Industries (MHI) interaction was noted, but no details were given on the interaction. It would be nice to know details of MHI interaction and if MHI intends to be involved in testing/demonstration of prototype compressor, and if prototype will be designed for hydrogen or natural gas.

Question 5: Approach to and relevance of proposed future research

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

• Future activities on this specific project will focus on final report of overall project and dynamic seal tests at high pressures, speeds, and temperature.

Strengths and weaknesses

Strengths

- This is an innovative concept with wide ranging application.
- The design of foil bearing seal technology can enable significant design improvements in centrifugal compressors.

Weaknesses

- There has been a lack of collaboration.
- Reliability and durability of bearing and seal materials in hydrogen environments does not appear to be considered in test plans. It is unclear whether the proposed materials and coatings survive in hydrogen environments.

Specific recommendations and additions or deletions to the work scope

- It would have been useful to have the entire roadmap for the project. Also, it would have been useful to have the PI at the poster session.
- Project is in final stage and is transitioning to larger design project with MHI. Would like to see a trade-off design comparing overall performance of a centrifugal compressor using current off-the-shelf bearings and seals against foil bearings and seals. Comparison should include parasitic losses, leakage, and anticipated durability/reliability. The project team should look at how predicted leakage of foil seal technology compares to an optimized labyrinth seal. The team should examine how much is gained by using foil bearing technology over a well-designed/optimized compressor using conventional bearings and seals.

Project # PDP-22: Development of Highly Efficient Solid State Electrochemical Hydrogen Compressor (EHC) *Ludwig Lipp; FuelCell Energy, Inc.*

Brief Summary of Project

The objectives of this project are to 1) demonstrate feasibility of a solid-state hydrogen compressor cell capable of compressing hydrogen to 2,000 psi; 2) increase the cell performance (power consumption, compression efficiency) while lowering the cost compared to previous designs; and 3) study thermal and water management to increase system reliability and life. FuelCell Energy increased compression mode operation capability from 500 psi to 4,000 psi in a single state EHC cell and completed >100 pressure cycles from 100 to 3,000 psi without performance loss.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

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

- The project goals and development efforts aligned to delivery barriers on the development of high-pressure forecourt hydrogen compressors.
- The project supports a critical delivery objective within the Hydrogen Program.
- The project provides improved means of compressing hydrogen, which can facilitate refueling with highpressure hydrogen storage tanks on vehicles.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated 3.7 on its approach.

- The approach is well thought out and described. Specific goals/milestones and metrics (2000 psi/FY08, and 6000 psi/FY09) were identified. Plans to scale up capacity to 2 #/day are presented.
- The project is clearly focused on technical goals and objectives to enable future delivery targets.
- Technical barriers were well addressed. The project team should perform cost analysis to help establish design and capital cost goals. The project team should compare these goals with goals for PEM fuel cells and electrolysis on a cost per active area basis.

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

This project was rated 3.7 based on accomplishments.

- Good progress is being made. The ability to provide a 300:1 compression ratio is impressive. Durability studies (1000 cycles to 3000 psi) demonstrate good durability.
- The project team has made excellent progress within scope of an SBIR project.
- The project team has made very good progress for Phase I. This project is promising.

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

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

- Collaborations and coordination with FuelCell Energy are in place and offer a route to integrate there process with a fuel cell developer.
- Collaboration was noted but not detailed in presentation.

Question 5: Approach to and relevance of proposed future research

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

- Proposed future effort to 6,000 psi and 2 lb H₂/day are in line with the process. The project team still needs to make significant advances in capacity (kg/day) to make this work attractive.
- Plans for future work appear positioned to continue success of first two years.
- The project team should establish cost goals in addition to performance in order to focus future work.

Strengths and weaknesses

Strengths

- High compression ratio (300:1) and capability to reach pressures up to 6,000 psi.
- The project team uses a solid technical approach with good initial progress.

Weaknesses

- Low capacity is a weakness.
- The project team needs to identify how much scale-up will be required to make this technology commercially viable, and give an indication of the magnitude of development needed.
- The project team needs to establish commercial viability by assessing capital cost issues.

Specific recommendations and additions or deletions to the work scope

• The project team should discuss the potential to go to 100 to 1000 kg/day, and what barriers exist in terms of size/footprint, and size/pressure differential over membrane. The project team should provide estimates of (capacity * delta-P) verses power requirements for this concept as compared to other compressor technologies.

Project # PDP-24: Composite Technology for Hydrogen Pipelines

Barton Smith, Barbara Frame, and Lawrence Anovitz; Oak Ridge National Laboratory

Brief Summary of Project

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

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

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



- Nonmetallic pipeline could meet DOE's target cost
- This project meets a critical need for high quality, cost effective pipeline distribution of hydrogen.

Question 2: Approach to performing the research and development

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

- The project team is investigating the application of commercially available fiber-reinforced polymer (FRP) piping for hydrogen application, which could result in identifying a low-cost alternative to steel.
- The approach shows solid engineering work built upon a strong scientific base. Go/no-go decisions have been built into the plan.

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

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

- Joining technology is critical to the use of plastic piping.
- The researchers found unexpected success, (i.e., better results than they expected or could explain). Further investigations of possible explanations might lead to a short cut or a better cost model.

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

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

- There is a mix of industry and national labs, as well as a pipeline working group.
- The list of collaborators is impressive, but the presentation does not provide any information on the nature of the collaboration.

Question 5: Approach to and relevance of proposed future research

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

- Permeation and diffusion testing of liner materials would provide additional information of the suitability of FRP to hydrogen service.
- Future work should include consideration of codes and standards.

Strengths and weaknesses

<u>Strengths</u> No strengths were provided for this project.

<u>Weaknesses</u> No weaknesses were provided for this project.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PDP-25: Coatings for Centrifugal Compression

George Fenske, Robert Erck, and Osman Eryilmaz; Argonne National Laboratory

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

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

- The lubrication and coating issues in reducing environment such as pure hydrogen is very practical but critical work. This has wide implications and application industry-wide.
- Identification of suitable materials for use in compression in pipeline and forecourt service needed to utilize hydrogen as a motor fuel.
- Methane work is interesting, but not critical to the DOE program.
- This project is relevant only to central applications (compression <2000 psig for pipeline).
- Potentially, this research could benefit any compression applications (outside of hydrogen) to address reliability and operating costs.
- High-speed centrifugal compression critical component of delivery.
- This project supports delivery reliability goals.
- Understanding hydrogen effects on the tribological behavior of contacting surfaces is extremely important to the development of hydrogen compressors. Hydrogen effects on friction is an area totally unexplored and the current project aims at achieving exactly that: to shed light on the hydrogen effect on friction and assess the presence of surface coatings. In fact, to the best of my knowledge, this is the only project in the US exploring the interaction between hydrogen and friction. Another effort underway is in Japan, but it has not addressed coatings as of yet.
- This project seems somewhat general and needs more specific goals.
- As long as this work is transferable to higher pressure hydrogen systems, it could help reduce operating costs. The PI believes the work is transferable. If not transferable, then (in my opinion) this project only has a fair relevance to DOE objectives as large-scale centrifugal compressors seem unlikely to be deployed in hydrogen infrastructure for several years.

Question 2: Approach to performing the research and development

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

• The approach is sound. The testing is bench-scale simulating various parts in control environment. It would have been useful to broaden the scope to more than centrifugal compressor system.

- It also would have been useful to tie in this project with infrastructure technology validation for testing and consultation/collaboration.
- The project team is conducting tribological testing of materials used in critical compressor components.
- Approach to address reliability and H₂ embitterment related to critical components is logical.
- This project needs to have clear targets and decision criteria.
- It is not clear why there is a need to conduct tests on any gas other than hydrogen. Methane, air, and inerts WILL have different effects on compressor components.
- The project team has done good testing of materials and novel coatings.
- Scope appears to be fairly limited and focused. Materials and coatings characterization is being addressed. Future progress appears to be dependent on obtaining a new test device.
- The approach of the project is the right one. A great number of coatings are investigated at room temperature and coefficients of friction are determined. Magnitude comparisons between coefficients of friction in hydrogen and other gases are made. The effect of normal load and relative velocity (motor speed) between the contacting surfaces are addressed. The project is moving to address the effect of hydrogen on friction at high temperature. This will also be an important development, since compressor operation takes place at high temperature environments.
- The project team should focus on coatings, but needs to consider base materials as well. The team should look at whether hydrogen will diffuse through coating to base metal.
- The project team has a well thought out approach. For the amount of funding, the PI covers several topics and options.

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

This project was rated 3.0 based on accomplishments.

- Considering the budget issues, the program has been steadily progressing and yielding good data.
- The high-speed, hydrogen tribometer is now operational and the team is testing materials.
- The project team needs to have some real life test data on running on hydrogen.
- The project team's accomplishments have been good considering the lack of funding.
- Near-frictionless carbon (NFC) materials show great promise.
- Progress is being made in characterizing materials issues, but it is not clear that pathways to overcome barriers and meet goals are being developed.
- A great number of coatings have been investigated at room temperature and coefficients of friction have been determined. Magnitude comparisons between coefficients of friction in hydrogen and other gases have been made. The effect of normal load and relative velocity (motor speed) between the contacting surfaces has been addressed. The project has identified that in the absence of coatings hydrogen prevents oxide formation which serves as a friction reducing agent. In addition, hydrogen was found to increase wear between the contacting surfaces. An interesting result is that in some occasions (short duration tests) hydrogen was found to increase the coefficient of friction (e.g., MoS₂/Graphite) relative to air and decrease the coefficient of friction under long duration tests. Japanese researchers also reached a similar conclusion. These results are interesting and merit further study.
- Progress has been limited so far, which is understandable since the project is in early stages. Several coatings are identified for analysis.

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

This project was rated 2.7 for technology transfer and collaboration.

- There are many material failures in compressor and higher pressure mechanical devices that could have benefited from this work. This is not reflective of PI's work, but rather the potential that this work could have had if it were connected to the infrastructure program.
- This project has involved a good mix of national lab and industry.
- Collaboration with Mohawk Innovative Technologies Incorporated (MITI) is a plus. The project team should also consider working industrial gas companies and compressor companies.

- Partners are bearing and coating suppliers. The extent of collaborator involvement in the development of technology solutions is not evident.
- Collaboration with MITI on oil-free centrifugal compressors is a good one. Pursuing it further will give the project industrial relevance.
- Collaboration with the University of Illinois on carrying out focus ion beam (FIB) lift-out of material to investigate cracking and embrittlement of surfaces in contact will be a high impact one. This approach is truly novel and never has been undertaken before in this area of hydrogen effects on tribology.
- Not a lot of detail was offered on collaboration and roles of the project partners.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- The team's future plans include coating and testing of materials.
- The team should consider looking into addressing issues related to startup/shutdown issues, extreme cold ambient temperatures, and impurities in hydrogen stream (e.g., moisture and trace H₂S).
- It is not clear that pathways to overcome barriers and meet goals are being developed. Plans focus on characterization of materials issues, but need to state how that understanding can be translated into solutions.
- The proposed FIB work is outstanding. The proposed electron microscopy of wear is indeed the next level where the project ought to be heading.
- The high-temperature hydrogen tribometer is needed to study the temperature dependence of the hydrogen effect as it relates to the tribology of the contacting surfaces.
- The team's future work should include positive displacement compression and higher pressure applications.

Strengths and weaknesses

Strengths

- The team has used a very practical and useful approach to material failure in reducing environment
- Several promising coatings have been tested side-by-side, so that valid comparisons can be made.
- The systematic study of hydrogen interaction with various coatings is a strength. Another strength is the experimentally observed relationship between the friction coefficient and the relative velocity (motor speed) of the surfaces in contact. These studies provide a valuable collection of experimental data that can be used in the study of understanding the mechanisms underlying the hydrogen effect on friction coefficients. The proposed collaboration with the University of Illinois on TEM studies of the friction/hydrogen interaction is a strong development for the project.
- The project team has a good understanding of coating technology and approach to assessing their performance in hydrogen atmosphere.
- This is a good project for studying ways to minimize hydrogen embrittlement in high-temperature, high-pressure environments.

Weaknesses

- There is a lack of connection/collaboration with infrastructure VT for samples and networking.
- The study has not advanced to the level of understanding the mechanisms that underlie the hydrogen effect on friction. However, the proposed FIB work will help toward this direction. Also, the dependence of the coefficient of friction on the relative velocity (motor speed) between the contacting surfaces has not been explained.
- The project needs better definition of applications and comparison with existing materials.
- Centrifugal compressors may not be the correct application for study at this time. More focus may need to be focused on direct displacement compression?
- It would have been useful to have this project and team as a material testing resource to the infrastructure projects.
- In the future, the project should be focused on understanding the mechanisms by which hydrogen affects the tribological features of interfaces.
- The project team should add direct displacement compression in scope

Project # PDP-26: Purdue Hydrogen Systems Laboratory

J. Gore, J. Patterson, R. Kramer, L. Pelter, and E. Ting; Purdue University

Brief Summary of Project

The objectives of the project are to 1) increase the production of hydrogen from the anaerobic fermentation of organic waste; 2) develop methods and techniques to maximize hydrogen production for a modular energy system for local energy production; 3) develop methods to optimize the value of the produced hydrogen for use in a modular system for local energy production; 4) develop a solar thermal energy system to pre and post process associated waste streams thereby reducing ancillary energy requirements and reducing potential environmental contamination issues for the final product; and 5) identify methods to separate hydrogen from biogas and investigate feasibility of using catalysis



to produce a marketable chemical product from the produced carbon dioxide.

Question 1: Relevance to overall DOE objectives

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

- The project objectives are very broad. The project focuses on hydrogen production from the anaerobic fermentation of organic waste; optimizing the value of produced hydrogen for use in a modular system for hydrogen production; and developing a solar thermal energy system to pre- and post-process associated waste streams; and identify methods to separate hydrogen from biogas.
- Interesting low-capital expenditure and yet energy efficient approach producing bio-hydrogen.
- This project supports the Hydrogen Program plan to identify renewable sources for hydrogen production.
- The concept of this project is to produce hydrogen through anaerobic fermentation of organic waste. This approach has been looked at and researched in the past. Without dramatic genetic engineering of existing organisms or the discovery of new organisms it is extremely remote that this could be a cost effective way to produce hydrogen. Only a fraction of the fermentation products are hydrogen.
- The anaerobic hydrogen production part in this project is relevant to DOE's objectives for biological hydrogen production. The part of "using catalysis to produce a marketable chemical product from produced carbon dioxide" is not clearly relevant.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- Purdue's approach is divided into eight areas. The approach seems reasonable considering the broad objective of the project.
- Overall, the project team uses a simple but elegant approach to producing hydrogen albeit with some kinetic limitation.
- The approach to hydrogen production by anaerobic fermentation of waste is well designed. The concept of using solar heating to supply process heat and heat for waste drying may enable the development of distributed systems which is a plus.
- No theoretical or technical basis is apparent to justify approach.

- The only somewhat novel part of this project is to try to use solar energy to pre- and post-process the waste systems.
- There is no work planned on genetic engineering of existing organisms never mind the dramatic alterations required for these organisms to have far better hydrogen production selectivity. The only work proposed to improve the hydrogen fermentation is to optimize the temperature and pH. There is prior work on this approach to hydrogen production that went beyond the work proposed for this project relative to the fermentation productivity with little success.
- The objectives include using anaerobic fermentation of organic wastes for a modular hydrogen energy system. The approach states this includes developing designs for implementation of this concept. The only thing mentioned about this is an energy balance that has been done. This concept needs a complete process design and cost analysis as well as the design and cost of obtaining enough organic waste, storage of that waste and the cost and method if getting rid of the wastes from the fermentation.
- The approaches used to maximize hydrogen production are good.

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

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

- The modular system developed for local energy production is good. Research to maximize hydrogen production through the use of a statistical experimental design is ongoing. The team has designed, constructed, and tested a solar thermal system.
- The progress towards the objective of identification of ideal process parameters is significant. However, more progress towards a continuous process (vs. batch process) will be necessary.
- There has been fermentation experimentation to try to optimize the hydrogen yield based on varying pH, temperature, and water content. Most of this type of work on anaerobic fermentation of wastes has been done by other researchers in the past.
- There has been work done with a vacuum tube solar collector and control system to determine the temperatures that could be achieved for pre and post processing of the organic waste as well as experiments to ensure this approach eliminates methanogens in the feed material and pathogens in the end waste material.
- The project began in September 2006. It did not make the planned contacts with industrial advisers until November 2008 and has had only one additional meeting with them since then. All of the other milestones shown are for 2008 and 2009. It would seem appropriate that there should have been milestones earlier during the project and that some or parts of the 2008 and 2009 milestones should have been completed earlier.
- All of the work done has been fairly elementary rather than breakthrough state of the art research.
- Progress seems slow. Two types of feedstock (food waste and distiller's grain) have been investigated. Water contents of the feedstock had opposite effect on hydrogen production, indicating that optimal parameters for hydrogen production could vary dramatically when different feedstock is used.

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

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

- Periodic advisory board meetings are held to gain input from industry (Cargill, Griffith Laboratory, BP, Advanced Power Technologies, and Innovene). Collaborative efforts with researchers at the Calumet campus are to be continued. Unfortunately the poster presenter (the PI was not present at the poster session) could not explain the nature of their collaboration.
- The project has assembled a very good advisory team and a collaboration with NREL but it is unclear from the presentation how much guidance has been used to direct the experimental program.
- The project lists several partners including Cargill, NREL, BP, Advanced Power Technologies, and Innovene. This is an impressive list and these organizations could offer a great deal to the project. However, it is not clear how these collaborations worked and were made useful other than through two advisory board meetings.
- Some collaboration was demonstrated in the project.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **1.8** for proposed future work.

- The future plan is fair. The project team will continue their efforts in various areas. It would be good to have some quantitative numbers to their planned future accomplishments.
- The future work seems to be a simple continuation of the current effort. There are no decision points or alternate development pathways.
- The project team plans to continue to try to optimize the fermentation by varying operating conditions, look at other inoculum, and look at other waste materials. Based on prior work in this area, it is very doubtful this can result in an attractive, cost effective approach for the production of hydrogen and energy.
- There is no cost analysis planned.
- Proposed future work is general and not focused.

Strengths and weaknesses

Strengths

- Professors' expertise and the availability of graduate students and post-docs to carry out this broad range of research are strengths. Purdue's effort will produce future hydrogen technology scientists/researchers.
- The is a simple and elegant method for making hydrogen.
- This is potentially one of the lowest capex and cheaper raw materials for making hydrogen.
- This is a solid, somewhat simple, experimental approach. The project goals are in alignment with the DOE Hydrogen Program goals.
- The one somewhat novel part of this project is to try to use solar energy to pre and post process the waste systems. The project has done work with a vacuum tube solar collector and control system to determine the temperatures that could be achieved for pre and post processing of the organic waste as well as experiments to ensure this approach eliminates methanogens in the feed material and pathogens in the end waste material.
- The idea of generating hydrogen through the anaerobic fermentation of organic waste is good.

Weaknesses

- The focus is too broad.
- The bio approach generally suffers from low kinetics and scale-up. Roughly 30% yield hydrogen (and rest CO₂) at ambient pressure may have some separation challenges.
- There is no clearly described vision for taking this technology forward into a commercially viable, scaleable process.
- The concept of this project is to produce hydrogen through anaerobic fermentation of organic waste. This approach has been looked at and researched in the past. Without dramatic genetic engineering of existing organisms or the discovery of new organisms it is extremely remote that this could be a cost effective way to produce hydrogen. Only a fraction of the fermentation products are hydrogen.
- There is no work planned on genetic engineering of existing organisms never mind the dramatic alterations required for these organisms to have far better hydrogen production selectivity to make this approach attractive for hydrogen production. The only work proposed to improve the hydrogen fermentation is to optimize the temperature and pH. There is prior work on this approach to hydrogen production that went beyond the work proposed for this project relative to the fermentation productivity with little success.
- The objectives include using anaerobic fermentation of organic wastes for a modular hydrogen energy system. The approach states this includes developing designs for implementation of this concept. The only thing mentioned about this is an energy balance that has been done. This concept needs a complete process design and cost analysis as well as the design and cost of obtaining enough organic waste, storage of that waste and the cost and method if getting rid of the wastes from the fermentation.
- All of the work done has been fairly elementary rather than breakthrough state of the art research.
- There is no cost analysis planned.
- Project goals are too broad and not focused on specific barriers.
- DOE targets for hydrogen production yield are listed. But, the yield, baseline, and benchmark of anaerobic hydrogen production are not reported. This issue was raised in previous review, but was not addressed by the investigator in this report.
- There is no consideration of cost.

- The team should focus on increasing the hydrogen production by optimizing the anaerobic fermentation of organic waste. The team shouldn't spend effort on solar thermal energy system.
- It is recommended to have a preliminary scale-up analysis is performed and further analyze the economic potential of this approach.
- The project should focus on continuous, scaleable fermentation processes.
- Funds would be better spent elsewhere.
- This project should design a complete system including sourcing the organic waste feedstock and disposing of the remaining organic waste and do a cost estimate for the cost of the hydrogen produced and or the cost of the power produced.

Project # PDP-27: Developing Improved Materials to Support the Hydrogen Economy

Michael Martin; Edison Materials Technology Center

Brief Summary of Project

The objectives of this project are to 1) demonstrate feasibility with job creation potential; 2) cross-cutting breakthrough materials technology; and 3) stimulate nearterm manufacturing-based commercialization. Edison Materials Technology Center manages a program with a DOE Cooperative agreement in Hydrogen, Fuel Cells & Infrastructure Technologies. The program features 37 individual, topically related projects. Each project targets at least one DOE technical barrier. Successful projects generate jobs and marketable products or processes.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.4 for its relevance to DOE objectives.

- The project seems to be a random collection of tasks with no clear orientation toward the goals of the Production and Delivery Subprogram. It is unclear how these tasks were selected. More direction is needed from DOE to align the project with much needed work.
- This mix of projects associated with DOE goals that have near term commercial viability.
- Most of the projects supported by Edison Materials Technology Center (EMTEC) support DOE Hydrogen Program objectives.
- The project develops hydrogen and fuel cell technology, but seems to be focusing on helping businesses over come the "valley of death."
- The investigators are funding the state of Ohio only, which is not consistent with the DOE's nation wide mandate.
- This project, compared with other earmarks, tries to address Hydrogen Program goals. They attempt to address programmatic goals with the projects they fund, but the programmatic goals would likely have been better addressed with competitively bid projects.

Question 2: Approach to performing the research and development

This project was rated **2.2** on its approach.

- Giving money to random institutions for performing work unrelated to the Production and Delivery Subprogram is the worst possible approach. No progress can result from this.
- The team solicited projects for funding for near-term commercialization.
- There is no coherent picture as to the approach of the various projects.
- EMTEC's approach is to run solicitations and fund outside work. This is generally effective, but it is not clear why they should be running the solicitations for federal money instead of DOE. If the state of Ohio wants them to do this for state funds that is fine; however, it would seem to be more responsible use of federal money to have the DOE run the solicitations which will be funded with federal money.
- The actual project DOE is funding is a nonprofit that funds research projects. The EMTEC does not do any of their own research, so therefore personally does not contribute to overcoming the barriers to hydrogen commercialization. Some of the programs they have funded are addressing interesting questions, but direct funding of the research organizations would be more cost-effective.

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

This project was rated 2.2 based on accomplishments.

- Some progress has been achieved, although the details are unclear from the presentation.
- R&D 100 award.
- No performance indicators are provided. A small number of the projects appear to be generating revenue which is a sign of technical success.
- Technical accomplishments seem to include starting two new projects- one for in-line PEM and electrolyzer monitoring and another for a multi-fuel SOFC.
- The PI reported progress from previous years as progress in the current year making it difficult to determine what has been done currently.
- The microballoon project should be ended. There are better technologies (metal and chemical hydrides) currently available.
- Their presentation only highlighted about 6 of their 38 projects. What are the other 30 projects on? What progress on the 6 projects was done in the last year? This was not clearly presented.

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

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

- There have been no collaborations outside the random institutions selected for conducting the work.
- Collaboration appears high.
- There appears to be no collaboration aside from direct support of partners.
- They seem to be working with a large number of partners.
- EMTEC brings various organizations together with their projects. They are actively pursuing commercialization of their work with industrial partners.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.8 for proposed future work.

- It seems that fortunately the project is over.
- This project is complete. There is no additional funding.
- This project is 95% complete.
- The future of this project is unclear.
- Since the program ends in the summer 2009, their next steps are writing the reports for DOE as required. This is reasonable. Also, their plans to continue working towards commercialization with a few of their projects is admirable, as is their plan to apply for the R&D 100 award.

Strengths and weaknesses

Strengths

- There are some good skills from subcontractors.
- Several of the projects appear to directly support DOE Hydrogen Program objectives.
- This project has been very well funded.
- This project has many partners.
- Their effort to commercialize the projects they have funded is good. Also, some of their technical work is interesting. Partnershiping is an important part of their work and an important DOE focus.

Weaknesses

- EMTEC has made a poor selection of irrelevant tasks
- There is no basis for determination of technical success and apparently no accountability for the money given to project partners.
- This seems redundant with the federal DOE program.
- Primary participants have been limited to the state of Ohio.
- There has been a limitation to only support research being done in Ohio.

- We need to rework processes to permit more substantial DOE direction in projects like this to enhance relevance to the program
- This project should be run by the DOE Fuel Cells Subprogram. Useful "partner" projects should be continued by DOE and other projects (like the hydrogen balloon) should be ended.

Project # PDP-28: Hydrogen Production and Fuel Cell Research

D. Yogi Goswami; University of South Florida

Brief Summary of Project

The objectives of this project are to 1) investigate the feasibility of the UT-3 thermochemical cycle theoretically and experimentally; 2) develop calcium oxide reactants with favorable characteristics and better performance; 3) conduct kinetic studies of gas-solid reactions to examine and improve cyclic stability and performance of solid reactants; and 4) lower hydrogen production cost by increasing hydrogen yield with an improved solid reactant.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>



This project earned a score of **2.3** for its relevance to DOE objectives.

- Task 1 is to investigate the feasibility of UT-3 thermochemical cycle. Task 2 is to investigate hydrogen production from biomass. Task 3 is on photoelectrochemical hydrogen production. Task 4 is on photo-catalytic hydrogen production. Task 5 on proton exchange membrane fuel cell (PEMFC) freeze degradation. Task 6 on the development of PEM electrolytes. The objectives are too broad.
- This project involves research exploring various hydrogen production paths (thermochemical, biomass, photoelectrochemical, and photocatalytic), in addition to research in PEM-based fuel cells.
- Particular research can give insight to which hydrogen-production processes are viable.
- Each of the six topics investigated have moderate relevance to DOE objectives.
- There is a total lack of focus. At this point, in its 5th year of funding, one would expect efforts having been focused on one particular and potentially promising technology. Instead, the University of South Florida (USF) group reports on a slew of technologies that include thermochemical H₂ Production, H₂ Production from Biomass, Photoelectrochemical H₂ Production, and Photocatalytic H₂ Production. These areas are obviously of relevance to DOE objectives. However, PIs contributions to-date have been meager, at best.
- For the hydrogen production part, it is not clear what they are doing. No answers to the questions given.
- This project has had no coordination with any of the DOE projects.

Question 2: Approach to performing the research and development

This project was rated **1.8** on its approach.

- UT-3 cycle has been studied for several decades. What is new here is not clear. The feasibility of the UT-3 process was done few years ago by researchers in three continents. It is not clear why are experiments are being performed to demonstrate feasibility. Are there any pitfalls in the earlier experiments? If so, the PI should explain what they were and clearly differentiate the present experiments from the past experiments. The other tasks for hydrogen production are going on in several institutions, and it is unclear how the USF approach is different from other on-going work.
- The approach is reasonable, focusing on some key gaps within each of the technologies addressed.
- The overall approach of having 6 separate research topics subdivides the efforts into small units and limits their capability to make significant progress.
- It is not clear why UT-3 cycle was selected for investigation. This cycle has been thoroughly studied in Japan and taken to the bench-scale closed loop demonstration stage. It is unclear what is it that they are doing

differently which is worth pursuing in the light of Japanese work (well over 30 papers going back to 1980). Thermal efficiency figures presented are questionable. No H2A cost analysis has been carried out for this or other hydrogen production methods investigated by the PIs.

- Again, no rationale has been given for the PIs' approach toward biomass-based hydrogen production via gasification in the presence of dolomite. The PIs reference the initial experimental studies that they carried out claiming significant improvement in hydrogen and overall gas yield in presence of sorbents. However, no gasifier data has been provided to support their claim. Information included in the poster is vague and superficial. The PIs seem to lack both understanding and knowledge required to tackle thermochemical conversion of biomass to hydrogen that is new or different than what has been done to-date or is not duplicative of already well-planed and executed effort funded by DOE.
- On photoelectrochemical (PEC) and photocatalytic water splitting the PIs present no rationale for their methods to improve performance. For example, their basis for nitrogen doping of titania for photocatalytic hydrogen production is unclear. N- and S- doping of TiO₂ (both rutile and anatase forms) have been investigated before. However, under visible light irradiation no hydrogen evolution occurs without the presence of electron donors or acceptors. Clearly, this not in accord with the DOE goal for direct water splitting using solar energy but without sacrificial reagents consumed.
- In general, the approach is still poorly defined and lacks sufficient detail. It is promising too much and unlikely to deliver.
- There is no clear project management organization.
- As noted above, most of the hydrogen production schemes attempted above have already been thoroughly studied.

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

This project was rated 1.8 based on accomplishments.

- There are six different tasks in this project. Technical accomplishments for each tasks is listed separately. It appears that this team has met their objectives.
- Task 1 (UT3 Thermocycle): Efficiency improvements are gained via heat recovery. However, it is not clear how thermal efficiencies are calculated. Hydrogen production must be about 284 kJ/mol. It is unclear what 593.5 kJ/mol refers to.
- Task 2 (hydrogen-production from biomass): No hydrogen yields, capital cost, or gasification efficiencies presented for this specific hydrogen-production process.
- Task 3 (photoelectrochemical hydrogen production): Improvement in window p-layer doping is stated but needs to relate Voc to efficiency.
- Task 4 (photo-catalytic hydrogen production): Optimum doping concentration profile is not given.
- Task 5 (PEMFC Freeze Degradation): The team needs repeat data on freeze/thaw testing to make a conclusion. The amount of water leading to degradation in PEM needs to be quantified during freeze/thaw cycling.
- Task 6 (Development of PEM Electrolytes): No conductivity vs. relative humidity data is given for membrane. This data is critical to make a reasonable comparison for membranes used in PEM-based fuel cells.
- Thermochemical H₂ Topic: UT-3 thermochemical cycle appears to be low efficiency and complex. One stated goal was to "improve the solid reactant's cyclic life, reaction rates and conversion". There is no evidence any of this was done just a lab experiment.
- Biomass Topic: Objectives are lengthy and grand, but actual work conducted appears basic and unremarkable.
- PEC Topic: Significance of achievements is not clear.
- Photocatalytic H2 Topic: Nitrogen dopant of TiO₂ appears to achieve a significant improvement in optical properties. Testing in an actual device should be conducted to quantify energy capture improvement.
- PEM Freeze Degradation Topic: Useful finding that blowing dry air over the membrane for 10 minutes prior to shutdown to remove water effectively allows low/no degradation freezing, but this finding has already been published by others.
- PEM electrolyte Topic: SPEEK membrane was prepared but not yet tested.
- The project team has very little to show after 5 years.
- The project team has made few publications.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.0 for technology transfer and collaboration.

- The nature of collaboration was not explained. The mandatory slide on collaboration is missing.
- The collaboration between partners is not clearly defined.
- Collaboration appears to be limited.
- There is no evidence of broad collaboration with other DOE funded projects.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.8 for proposed future work.

- Considering the broad scope of work, the plans for the future appear to be reasonable. It is impossible to judge the plans for the last two tasks (on PEM fuel cell).
- Future and current work needs to focus more on overcoming DOE barriers stated for each of the tasks.
- Some new avenues are planned on improving photocatalytic efficiencies.
- Improvement in photocatalytic efficiency of N-doped TiO₂ by Ag metal ion doping is not novel. The project team should check literature.
- The future plans lack of specificity, rationale, and detail to be compelling.
- This project is unlikely to meet DOE hydrogen production goals because very little has been accomplished as of 2005 start date.
- Statements about future activities were vague with no quantitative mileposts as to how the project will meet the DOE H₂ production targets and objectives.
- No H2A cost analysis of the production schemes has been mentioned.

Strengths and weaknesses

Strengths

- Knowledge and experience of the team members. Long list of publications/presentations.
- This project's strength is in involvement with several hydrogen production technologies.
- Each of the topics has worth, but having so many topics dilutes focus.
- None.

Weaknesses

- FY08 & FY09 funding numbers were not provided and therefore it is difficult to judge their accomplishments/performance. Nature of collaboration with partners is missing. The project focus is too broad.
- Discussion is needed on how DOE barriers are being overcome.
- The project team should interact with companies familiar with fuel cell testing and evaluation.
- The large number of mostly independent topics being investigated makes for an unwieldy presentation.
- There's no coherency and focus.
- Too many areas dilute the PIs' efforts and slow meaningful progress.
- Management and partnership have been very weak.
- The expertise of the PIs in all of these areas is highly suspect.

- The UT-3 process task can be dropped.
- It would be beneficial to make comparisons between the varying hydrogen production technologies (thermochemical, biomass, photoelectrochemical, photocatalytic), with respect to system efficiencies, capital and hydrogen production costs.
- The project team should focus efforts on a smaller number of topics to achieve more substantive progress.
- The budget for the actual activities being reported should be listed.

- The project team should narrow production scope to no more than one technology area that complements, rather than poorly duplicates other DOE funded activities.
- The project team should develop meaningful partnerships with experts in the field.
- The project team should let H2A cost analysis guide their hydrogen production R&D path and related decisions.
- Project management and coordination needs to be improved.
- The PIs should attend other PIs' presentations and network.

Project # PDP-29: Integrated Hydrogen Production, Purification and Compression System

Satish Tamhankar; Linde North America Inc. Tony Boyd and Ali Gulamhusein; MRT Mark Golben and David DaCosta; Ergenics Corp.

Brief Summary of Project

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



Question 1: Relevance to overall DOE objectives

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

- The overall objective of this project is to develop an integrated system that directly produces high-pressure, high-purity hydrogen from a single unit. This project is in its first phase. The objective of Phase I is to verify the feasibility of the concept, perform a detailed techno-economic analysis, and develop a test plan. Another objective of Phase I is to build and experimentally test a POC integrated membrane reformer/metal hydride compressor system.
- This project has very high relevance to DOE objectives.
- An integrated production, purification and compression system has the potential to provide an efficient systems solution.
- An integrated system for hydrogen purification and compression is relevant to the DOE program goals.
- This project is relevant to DOE's forecourt hydrogen production program goals.
- This project does not address the greenhouse gas footprint of the technology and as such only partially meets DOE's overarching objectives for clean and renewable hydrogen production.
- Hydrogen from natural gas or other hydrocarbons using a Pd membrane reactor integrated with a metal hydridebased thermal compression device is a novel idea and has relevance to DOE's near term (transitional) hydrogen production and delivery objectives.

Question 2: Approach to performing the research and development

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

- The approach is to combine the membrane reformer developed by Membrane Reactor technology with the hydride compressor developed by Ergenics in a single package. This approach reduces capital cost and increases efficiency compared to conventional fuel processors. The membrane reactor technology and the hydride compressor are shown to work in separate tests. This team is focusing on issues involved in integrating these two technologies.
- Experimental proof-of-concept module is well suited to this project.

- It is not clear whether the engineering problems are simpler (solvable) when the processes are separated. A slide providing data on the engineering on the individual components would have been helpful.
- The team has a good overall approach, including POC for both the purification and compression system components, as well as the H2A analysis for evaluating cost effectiveness.
- The approach is credible as it combines good engineering with pilot scale testing.
- The team used innovative engineering of the metal hydride thermal compressor.
- The team used a methodical approach to the complex integration of the membrane reactor and multi-stage metal hydride thermal compressor.
- The approach is guided by cost analysis to reduce system components and improve reliability.
- It appears that PIs may have moved too quickly from optimization of individual subsystems (i.e. membrane reformer and thermal compressor) to integrated stage. Results to date point to possible interface issues affecting the overall performance of the integrated system.

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

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

- Auto-thermal fluidized bed membrane reformer was tested. Membrane was operated at 550C and 25 bar. The team successfully tested a 15 micron thick membrane. Membrane foil quality diminished during testing. Hydrogen purity was an issue. After initial operation, leakage was observed in the metal hydride compressor.
- The project had moderate deficiencies in all areas:
 - Reactor: reduced catalyst activity, relatively low-methane conversion.
 - Membrane: permeance met expectations but leaks due to manufacturing quality led to low H₂ purity.
 - Compressor: leaks in tubing due to manufacturing defects led to substantially degraded performance.
- However, also had moderate successes:
 - Reactor: demonstrated tolerance to thermal cycling. Demonstrated production of high-purity gas.
 - Integration: demonstrated integration of reactor with compressor using waste heat to drive hydride compressor.
- The team has done solid work. The economics are promising but preliminary. More detailed information is needed for a real evaluation, but this is a good start.
- Progress has been on schedule, though unexpected problems in hydrogen leakage and performance degradation were encountered. The program appears to be adapting to the setbacks, and proposing reasonable paths forward to resolve the issues.
- Consider third party, unbiased testing and evaluation of the integrated system.
- Long-term verification testing needs to be conducted.
- There are no discussions with respect to operational safety issues, failure modes and consequences.
- What is the effect of impurities in the reformate/permeate on the metal hydrides used?
- No data have been presented for the factors influencing hydride bed operation and long-term stability. In other words, where is the weak link in the integrated chain of interconnected sub-systems and components? Can metal hydride beds be regenerated, if needed? If so, how?
- What is the effect of mercaptans and other sulfur organics on the long-term stability and conversion efficiency of the membrane reformer? Can landfill gas be used in this system? If so, what is the effect of silanes?
- PIs have shown continuous operation of a multi-stage, dual-line hydride bed heat exchanger successfully, albeit for a relatively short period of time. PIs report limited operational data to draw a solid conclusion as to the viability of this system, under extended operation.
- PIs need to address the issues related to Pd membrane stability, startups/shutdowns, and the ability to recover hydrogen from permeate and retentate steams to allow for 100 bar pure hydrogen delivery.

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

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

• MRT and Ergenics are key partners in this project. It is not clear what the other partners (University of British Columbia, National Research Council, and Noram Engineering) did for this project. The roles of partners were not presented.

- There appears to be very tight contact/collaboration between team members. The extent of collaboration with others in not known.
- It would be nice to see a formal university partner to ask questions around the periphery of the project and perhaps introduce a little more imagination.
- It is not entirely clear whether additional collaborations within industry or with academic institutions would be beneficial in helping to solve technical issues encountered.
- Good combination of industrial and university collaborators.
- There are no indications that the team has or has had interactions with other projects within this DOE program.
- Eventually need a third party, unbiased testing and evaluation of the integrated system performance and costs.

Question 5: Approach to and relevance of proposed future research

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

- Reduced catalyst activity, hydrogen purity, and MHC performance will be addressed during rest of FY09. Go/no-go decision will be reached by June 2009 (i.e. next month) regarding the next phase. Based on the information presented, to the team will probably not be in a position to make this decision.
- The future course of action is not well defined.
- A solid path forward was identified.
- The future work was well laid out for project continuation.
- The team presented clear future plans and go/no-go decision points.
- Go/no-go decision on next phase should also consider a safety audit of the system and detailed "what if" protocol.

Strengths and weaknesses

Strengths

- This is a strong team involving Linde, MRT, and Ergenics. The idea of combining membrane reactor with MHC is very good.
- The biggest project strength is its approach: experimental demonstration of an integrated reactor/membrane/hydride compressor is the appropriate course of action.
- Overall, and interesting approach to integration of hydrogen purification and compression; and an effective project for demonstrating the proposed system.
- Good transitional device for forecourt hydrogen production.
- Good collaborative work and mutually beneficial partnerships amongst participants.
- Innovative hydrogen compression engineering.

Weaknesses

- There is no clear plan to address the problem of reduced catalyst activity. It is unclear how they are going to improve the MHC performance? Membrane durability is an issue.
- Substantial problems in each of the major systems: catalyst activity, pin-hole free membranes, hydride leak-tightness.
- The cost analysis is weak. More needs to be done to support the cost projections.
- The problems encountered with hydrogen leakage and with unexpected performance degradation need to be better elaborated in terms of proposed solutions for future work
- Testing time is limited.
- System sensitivity to impurities is a weakness.
- Pd membrane and metal hydride materials stability and robustness are key to project success.
- The integrated system is more complicated.

- The team should have an independent third party look at the H2A results and try to use membranes made by Pall Corp.
- The hydride compressor is good in concept but, in additional to it leaking, seems to consume substantial energy thereby reducing the overall system efficiency. A careful examination of the hydride compressors net benefit to the system should be conducted. It should be compared to a well-understood/low-risk mechanical compressor to see if an advantage is really achieved.
- Cost analysis needs to be enhanced. My confidence in their estimates is low. The team should show much more detail/assumptions.
- The team should update H2A analysis with the most current estimates and clearly identify pathways to solving the encountered problems in leakage and reduced activity.
- The team should consider adding a safety audit of the system and detailed "what if" protocol.
- The team should identify sources, fate, and effect of all known and potentially present impurities in the feedstock on all subsystems in the hardware chain.