2015 — Hydrogen Storage
Summary of Annual Merit Review of the Hydrogen Storage Sub-Program

Summary of Reviewer Comments on the Hydrogen Storage Sub-Program:

In fiscal year (FY) 2015, the Hydrogen Storage sub-program portfolio continued its focus on onboard automotive applications as well as increased its emphasis on new materials and novel concepts to meet performance requirements. Reviewers commented that the sub-program is well managed and has effectively engaged partners in industry, academia, and national laboratories. The reviewers also commented positively on the use of results from the Hydrogen Storage Engineering Center of Excellence (HSECoE) to help direct and focus materials development efforts. Because FY 2015 marked the final year of the HSECoE, the researchers were encouraged to disseminate the lessons learned from this multiyear effort to the hydrogen storage community. The U.S. Department of Energy (DOE) Materials-based Hydrogen Storage Summit was cited as a good example of bringing the research and development (R&D) community together to disseminate results and exchange ideas. Reviewers remarked that the sub-program has evolved to include a more balanced portfolio of near- and long-term approaches than it did in previous years. Overall, reviewers recommended increasing the focus on longer-term, "higher payoff" technologies that could provide breakthroughs in performance. They noted, however, that these activities should include both basic and applied R&D efforts—ideally through a well-coordinated, collaborative approach.

Hydrogen Storage Funding:

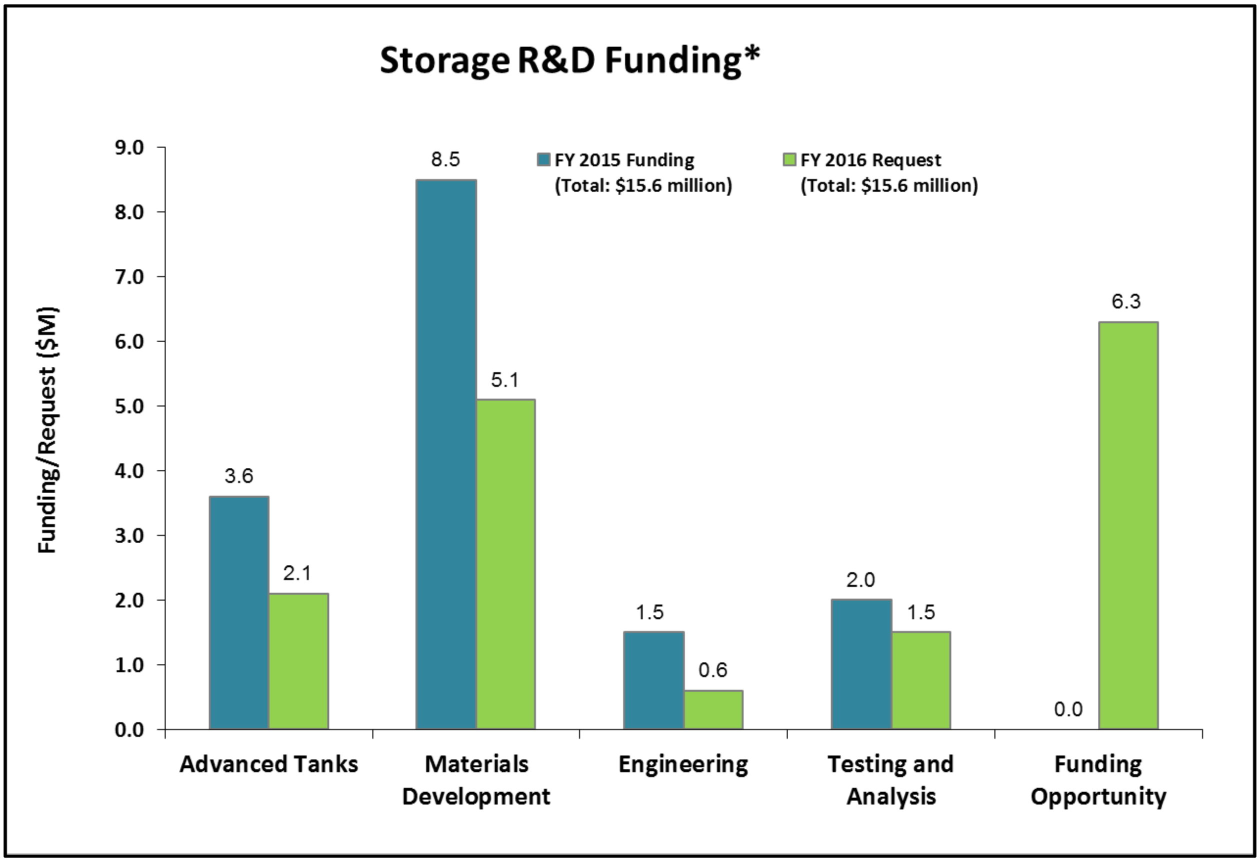
The chart on the following page illustrates the appropriated funding planned in FY 2015 and the FY 2016 request for each major activity. The sub-program received $15.6 million in funding in FY 2015, and it has a budget request of $15.6 million for FY 2016. In FY 2015, the HSECoE entered the final phase of its multiyear effort, which focused on validating systems models previously developed in earlier phases. HSECoE models are now posted online and available for use by the scientific community. Additional efforts aimed at advancing conformable compressed hydrogen storage systems were initiated in FY 2015. Work on hydrogen storage materials development remains an important part of the portfolio, with four new projects initiated in FY 2015. New efforts in materials-based storage technologies are planned in FY 2016.

Majority of Reviewer Comments and Recommendations:

The Hydrogen Storage portfolio was represented by 21 oral and 12 poster presentations in FY 2015. A total of 19 projects—via oral presentations—were reviewed. In general, the reviewers' scores for the storage projects were good, with scores of 3.5, 2.7, and 3.2 for the highest, lowest, and average scores, respectively.

Advanced Tanks: Six projects on advanced tanks were reviewed, with a high score of 3.3, a low score of 2.9, and an average score of 3.1. Reviewers considered the work to identify lower-cost precursors for high-strength carbon fiber manufacturing and efforts to demonstrate pathways to lower-cost advanced tanks to be highly relevant efforts that may have a significant impact. For the tank cost reduction projects, reviewers commented favorably on current efforts aimed to validate modeled predictions on cost-reduction pathways through fabrication and testing of real systems that include alternative fiber and resin as well as low-cost balance-of-plant components. Reviewers also noted the potential increase in hydrogen capacity offered by cold/cryo-compressed technologies, but they also emphasized the need for continued temperature/pressure cycling as well as additional emphasis on the vacuum jacket insulation and related hydrogen dormancy. In general, reviewers recommended more detailed and validated technoeconomic assessments. Overall, the reviewers thought the efforts could have a significant impact on the industry.

Materials Development: Four materials-based hydrogen storage projects were reviewed, with a high score of 3.0, a low score of 2.7, and an average score of 2.9. Generally, reviewers commented on the high quality of the scientific work and capabilities of the research teams. However, they also commented that many of the materials currently under investigation would not be able to meet the full set of DOE targets for automotive onboard storage of hydrogen. However, for nonautomotive applications, which are the focus of several of the projects, they noted that significant impacts may be realized. Materials projects will continue in FY 2015, subject to appropriations, and new projects will be initiated. These projects will emphasize a stronger link and feedback route between the



* Subject to appropriations, project go/no-go decisions, and competitive selections. Exact amounts will be determined based on research and development progress in each area and the relative merit and applicability of projects competitively selected through planned funding opportunity announcements.

experimental and theoretical efforts, as well as place more emphasis on meeting projected material-level property requirements to meet the system-level targets.

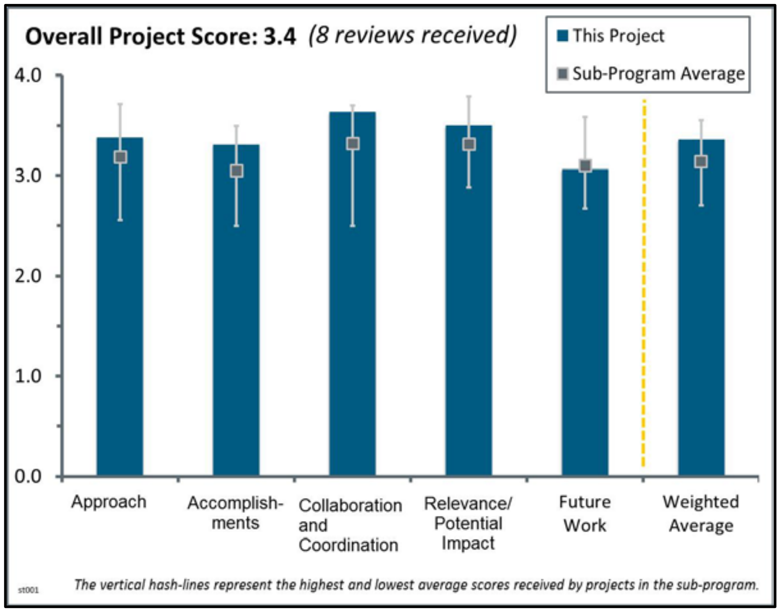
Engineering: Seven projects were reviewed on hydrogen storage engineering, with a high score of 3.5, a low score of 3.1, and an average score of 3.3. Reviewers stated that the HSECoE has made significant progress in the past year and features strong management, providing for good coordination and clear collaboration among the partners. The reviewers commented favorably on the development and use of integrated models on projecting system performance, especially for the relevant and important role in determining the material-level properties required to achieve the DOE storage targets. In general, the reviewers considered the individual HSECoE partner projects to be well thought-out and well executed. The reviewers commended the HSECoE for its use of detailed milestones for tracking progress. The reviewers also appreciated the HSECoE providing the lessons learned for use by future collaborative efforts. The reviewers recommended that the researchers place more emphasis on improving the system performance for targets furthest from being met. Overall, reviewers thought the HSECoE and its partners are making good progress in evaluating materials-based storage systems and making decisions to meet DOE performance targets.

Testing and Analysis: Two projects related to testing and analysis were reviewed, and both received a score of 3.4. Reviewers stated that these projects are very relevant in assisting DOE's R&D portfolio evaluation. Reviewers commended the project team's strong expertise in modeling thermodynamic, kinetic, and heat transfer phenomena, as well as its development of a comprehensive and rigorous set of tools and methodologies that enable detailed predictions of materials and system performance. Reviewers also commended the project team for developing an understanding of data from a multiplicity of R&D efforts and integrating that data into cogent analyses from a wide spectrum of technical areas. Reviewers recommended the continued use of experimental data, whenever available, to test and benchmark models. Reviewers also commended the project's strong and close collaboration with national laboratories, original equipment manufacturers, and tank manufacturers. Reviewers noted that the projects have done a good job in identifying major contributors to overall costs and pathways for cost reduction. However, reviewers noted the need to provide cost uncertainties in general, as well as to include a range of possible costs for systems analyzed. Overall, reviewers praised the thorough analyses performed by a strong team and emphasized the importance of these projects in improving the quality of research in the Hydrogen Storage sub-program and providing clear insight to guide future research.

Project # ST-001: System-Level Analysis of Hydrogen Storage Options

Rajesh Ahluwalia; Argonne National Laboratory

Brief Summary of Project:



The main objective of this project is to develop and use models to analyze the onboard and off-board performance of physical and material-based automotive hydrogen storage systems. Specific goals include (1) conducting independent systems analysis for the U.S. Department of Energy (DOE) to gauge the performance of hydrogen storage systems, (2) providing results to materials developers for assessment against system performance targets and goals and to help them focus on areas requiring improvement, (3) providing inputs for independent analysis of costs of onboard systems, (4) identifying interface issues and opportunities and data needs for technology development, and (5) performing reverse engineering to define the material properties needed to meet the system-level targets.

Question 1: Approach to performing the work

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

- The approach in 2015 follows from the efforts in previous years to use thermodynamic and kinetic models to assess the performance of materials-based storage approaches and to explore system-level issues. In addition, finite element analysis approaches were used to identify and quantify the relationship between liner properties and liner failures in cryo/cold hydrogen storage tanks. The approaches are providing useful information needed to understand performance limits and to guide the evolution of improved system designs. The approaches complement those adopted in the Hydrogen Storage Engineering Center of Excellence (HSECoE), and the project directly supports activities being conducted in the HSECoE and in independent studies of compressed tank designs and performance.
- The presenter discussed progress on the development of models to analyze onboard and off-board performance of physical and material-based automotive hydrogen storage systems using a reverse engineering approach to provide the material property needs to meet the system-level targets. This approach and insight is extremely valuable for materials developers.
- The plan aligned with DOE Hydrogen and Fuel Cells Program (the Program) goals. The value of this project is in informing research and development (R&D) work, helping researchers determine which materials and systems to pursue and which to stop. This project provided valuable support to the Centers of Excellence, but as those efforts wind down, what is next is not clear. Reverse engineering has provided useful input, but it is clear that new materials are required to meet targets. Additional system-level analysis or reverse engineering may be overkill at this stage.
- The approach for ST-001 was very good. This project is trying to address onboard and off-board targets, which is appreciated.
- This team consistently performs at a very high level and collaborates across the Program very well. The team members are always open to suggestions. There is one area in which there could be improvement: they could provide more concrete guidance to the materials development communities.
- Overall, the approach is very sound. Historically, this team has strong expertise in modeling thermodynamic, kinetic, and heat transfer phenomena. Extension of the effort to mechanical properties

modeling is being pursued for Type IV liners. It is unclear whether the team has the necessary expertise to conduct this work.

- It was good to document some of the specific results, but it appears that the overall results from the cold gas storage options were fairly obvious. The approach for off-board chemicals took into account only the thermodynamics of some of the materials. While this approach did provide a general range for acceptable material properties, it is not specific enough for actual materials, especially those that are kinetically limited.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- Important new results concerning the relationships between high-density polyethylene (HDPE) liner properties and liner failure in Type IV tanks at cryo temperatures were obtained. Specifically, predicting the internal pressures needed to prevent or mitigate liner separation at low temperatures and understanding stresses at critical interfaces in the tanks will be critical to the design of safe, high-performance cold gas tanks.
    - A careful analysis of cold tank performance characteristics, including well-to-tank (WTT) efficiency, fuel cost penalty, and overall system cost, provides DOE and the hydrogen storage community with solid benchmarks for deployment of cryo/cold tank storage systems.
    - A system analysis, based on a reverse engineering approach, and sensitivity analyses of a chemical hydrogen storage system provided a useful set of metrics for a high-efficiency–high-capacity chemical storage system compatible with current fuel cell operating parameters.
- There has been nice progress in modeling liner behavior at low temperature with preliminary validation from Hexagon Lincoln tanks. However, it is not clear where to go from here—perhaps making recommendations for redesign. There is nice progress with the cold gas storage analysis, which clearly shows challenges associated with meeting the volumetric target. Regarding chemical hydrogen storage, much of this seems similar to what was presented in previous years; it is not clear what was done in 2014. Conclusions are not revealing anything that is not already known (enthalpy change, ΔH = 20–40 kJ/mol and decomposition temperature, T_d = 60°C–80°C). The materials community is already actively looking in this area.
- Progress and results in the area of the tank liner interactions are very well communicated, as in all the areas in which the team is asked to provide in-depth energy and efficiency analyses to provide guidance to ongoing programs and to inform DOE program managers. This project is crucial to achieving the overall DOE goals in the area of hydrogen storage. One area that could be improved is the presentation of off-board regeneration issues; because the prior work in that area for all types of off-board materials was laser-focused not on energy efficiency but rather on proof of principle, the analysis of off-board WTT efficiency and the resulting message about the lower efficiency of off-board materials may discourage future R&D idea generation in this area. In other words, there may not be enough, or any, reliable data on what the real potential of off-board regeneration is, and so the analysis effort appears to paint perhaps too dismal a picture.
- The project showed progress toward estimating both onboard and off-board efficiency for different materials. It would be useful to see a side-by-side materials comparison with three columns: (i) onboard efficiency; (ii) off-board efficiency; (iii) off-board X onboard. The last column provides an overall view, assuming that off-board and onboard efficiency are equally weighted. Fuel cost is approximately 5% higher than the baseline, but onboard system cost is approximately 20% lower. It is not clear what the best way is to compare this trade-off. For example, perhaps the onboard system cost is a one-time cost, whereas the fuel cost is paid for each fill. Obviously, there are initial savings, but it is not clear whether the 5% added fuel costs “catch up” with those savings.
- This project has made a lot of progress since fiscal year 2014. The activities in reverse engineering to determine chemical storage properties will be very valuable.
- The energy efficiency calculations are based on the thermodynamic properties of the material, which seems narrow and does not take into account other losses; i.e., the regeneration of materials is highly specific and

dependent on the recycling process. In the future, it would be advisable to account for this to offer appropriate guidance in materials selection and design.
- There has been good progress, but the results—especially with respect to the chemical hydride work—are very general and may not apply to specific materials.

Question 3: Collaboration and coordination with other institutions

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

- Excellent collaborations with numerous organizations are in place, and they serve to support the overall goals of the project. Collaboration with Pacific Northwest National Laboratory (PNNL) on cryo-tank properties and validation of model predictions was especially fruitful in 2014/2015. The work directly supports multiple efforts within the HSECoE; solid cooperation and good coordination among those activities is apparent.
- There is excellent-to-outstanding collaboration with national laboratory researchers and the HSECoE, among others who rely on the analytical guidance from this effort to focus their own R&D efforts. This team works diligently to develop an understanding of the data that are derived from a multiplicity of R&D efforts and integrates them into cogent analyses from a wide spectrum of technical areas.
- The project has close, timely, and appropriate collaboration with other institutions; partners are full participants and well coordinated.
- It appeared that the collaboration with all of the partners was very close and well-coordinated.
- The team appears to be maintaining good collaborations with other groups within the Program.
- There are a number of collaborations with national laboratories and Strategic Analysis, Inc. Other than PNNL, it was not clear how close these collaborations are. Close collaborations, in which there are regular discussions with the tank or materials developers, are crucial.
- Collaboration exists between other stakeholders.
- Work is published and reviewed with the Storage Systems Analysis Working Group and others.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.5** for its relevance/potential impact.

- The independent systems analyses performed in this project directly support the goals of the Program by providing relevant and timely information concerning the performance of onboard and off-board hydrogen storage and regeneration approaches. Likewise, the models and predictive capabilities developed on this project are key enabling elements for future storage technology development.
- The project’s relevance to and impact on the overall Hydrogen Storage sub-program are excellent to outstanding. One area of improvement would be to communicate more explicitly the clear guidance that the analyses provide to the materials development communities. Often, this guidance is not heard well by the materials developers, and so the community continues to flounder with materials that have little or no chance of achieving technical success.
- The analysis for onboard and off-board will be very valuable for materials developers and system integrators.
- There is excellent independent analysis support.
- The project strives to offer guidance in the selection of materials, which is helpful in future materials selection and design efforts.
- Clear issues were identified with the liner at low temperature, but it is not clear what impact this work is having on tank design. Regarding cold gas storage, there has been no progress toward meeting the volumetric target, and there are similar problems with the cost target. It is not clear what the plan is. Continuing this has little value without a plan to meet these other targets. Regarding chemical hydrides, the project has identified a narrow band of free energy change and decomposition temperatures that should be pursued. These values are similar to back-of-the-envelope calculations that have been around for many years. Other than confirming what is already known, it is not clear how much value there is here.

- The work on reverse engineering of chemical storage materials was perhaps too general to have a substantial impact on current programs.

Question 5: Proposed future work

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

- The proposed future work is a straightforward and sensible extension of the prior work on this project. Emphasis is placed on both physical storage and materials-based storage. It will be important for the principal investigator (PI) and his team to consult with the DOE program manager to determine the levels of effort that should be allocated to different tasks and sub-tasks in the future. For example, given the current emphasis of the overall Hydrogen Storage sub-program on adsorbents and physical storage systems, it is not clear whether much additional work on chemical storage materials (e.g., AlH_3 and Ammonia Borane [AB] slurries) and metal hydrides is needed. These are important decisions and priorities that should be made in consultation with the Fuel Cell Technologies Office (FCTO).
- Plans build on past progress and generally address overcoming barriers. It is great that there are plans to provide system-level support to new projects.
- The proposed work for physical storage seems reasonable: working with partners to validate models and providing guidance for next-generation design. However, with the HSECoE winding down, it is not clear how much of this type of support is needed. Materials-based storage work seems less impactful. It is not clear what more analysis of decomposition behavior provides. It is not clear what is meant by "determine favorable properties of unstable room-temperature metal hydrides." In general, what these properties should be is known. There is little value in confirming what is already known. A key challenge here is regeneration. Guidelines for regeneration would be useful.
- Realizing that most of the future work in this area is dependent on FCTO guidance, there is one area that seems to have not yet been analyzed in detail, and that is the area of the complex metal hydrides. This appears to be an area of need because much of the ongoing materials R&D work in storage is focused on complex metal hydrides.
- The effort to reduce the cost of carbon-fiber-wound tanks will be valuable; however, it is uncertain how much value there is in validating AlH_3.
- Validating models from other national laboratories and the HSECoE is good, but more emphasis should be placed on developing new system models.
- For the future planned analysis on the tanks, it is necessary that created models are thorough and not oversimplified (e.g., for the AlH_3 slurry).

Project strengths:

- Overall, the project shows nice progress in evaluating tank design and the energy cost associated with cold fill. Previous results on metal and chemical hydrides have provided useful insights into WTT efficiencies and the energy cost associated with regeneration.
- This project provides important and valuable information to DOE concerning the performance characteristics and limits of physical and materials-based storage systems. The PI and his colleagues are acknowledged experts in systems analysis relevant to assessment of hydrogen storage systems. They have developed a comprehensive and rigorous set of tools and methodologies that enable detailed predictions of materials and system performance.
- Strengths include the team members' high technical competence and ability to effectively collaborate with the various R&D activities across the spectrum of storage activities.
- The project gets formal feedback at least two times a year, once from the technical team and once from the DOE Hydrogen and Fuel Cells Program Annual Merit Review (AMR), and the project team is very responsive to constructive suggestions. The timely feedback from a variety of experts in the community helps the team members stay focused and provide a more complete analysis. Each time they present their work, they get constructive feedback from reviewers. The AMR probably provides the best opportunity because the reviewers have time to read through the presentation prior to the AMR meeting.

- Overall, this project was very strong and well presented. No major weaknesses were seen. It will be good to see the progress through this year.
- The physical storage work using ABAQUS is a project strength.

Project weaknesses:

- No major weaknesses are apparent in this project.
- It is unlikely that important new information will be derived from further studies of chemical and metal hydride storage systems. Additional tweaking of existing assessments is probably not cost effective. It seems that additional work in those areas should be conducted only after materials discovery projects have identified more compelling candidates capable of meeting (or at least approaching) DOE targets. Experimental validation of the analyses conducted in this project is an important area that needs more emphasis.
- Work on chemical hydrides provides little new insight. Clearly more work needs to be done on the materials side. Additional analysis of hydrogen release rates from AB or alane is missing the point—cost/regeneration is the critical target for these materials, and all the focus should be on identifying energy-efficient regeneration strategies and working with the chemical hydride community to implement them. Similarly, additional work on cold gas storage seems unnecessary unless the volumetric limitations can be addressed.
- The energy efficiency calculations are very useful in down-selecting materials and tank designs; however, the reliance of the Gibbs function is useful only for qualitative, non-comparative-type analyses.
- The reverse engineering approach appears to be too general.

Recommendations for additions/deletions to project scope:

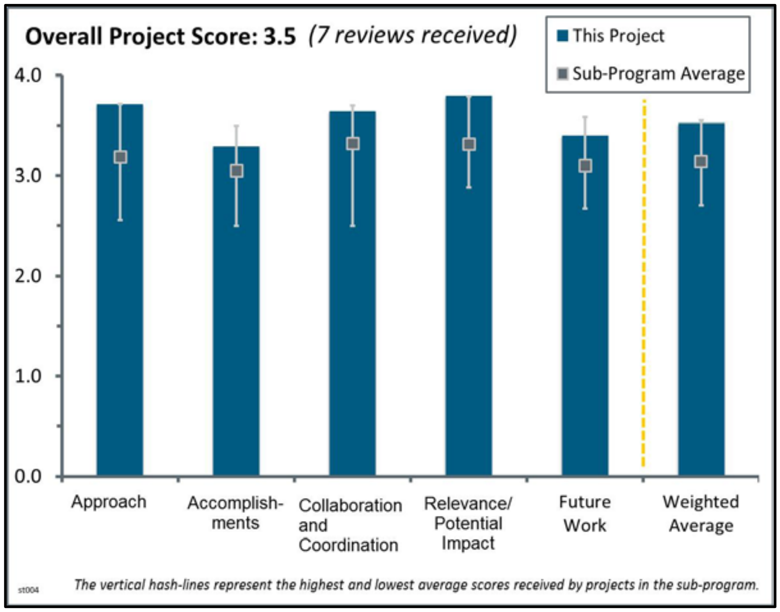
- The project should do the following:
  - Keep publishing results in a timely manner in appropriate peer-reviewed journals.
  - Continue to use experimental data whenever available to test and benchmark models.
  - Provide references (in backup slides) for experimental values used (e.g., changes in enthalpy and entropy for reverse engineering analysis).
- From this team's deep experience and technical excellence, a broader, more comprehensive examination of the bounding conditions for materials R&D would be very valuable. This team has developed important conclusions; some of its conclusions have an impact on *all* materials, not just the one material class this project examines. This appears to be lost on much of the materials development community.
- Physical storage and methods to reduce carbon fiber material and cost should be emphasized over validating HSECoE models that most likely will not be implemented.
- It is not clear whether this project will continue indefinitely or whether the project will be completed in the near future. Apparently, DOE makes decisions annually about continuation of the project (slide 2 in presentation). It would be helpful to understand what drives those decisions and how priorities for research directions are established.
- It is necessary that the assumptions included in these models are stated and that the models created are thorough and are not oversimplified.
- The project should probably be scaled back. The best hope of meeting targets lies with new materials discoveries. This work has provided significant benefit to the materials and engineering efforts, but there is little value in continuing at this level until new materials or engineering designs are developed.

Project # ST-004: Hydrogen Storage Engineering Center of Excellence

Don Anton; Savannah River National Laboratory

Brief Summary of Project:

Using systems engineering concepts, this project's goal is to design innovative materials-based hydrogen storage system architectures with the potential to meet U.S. Department of Energy (DOE) performance and cost targets. Savannah River National Laboratory (SRNL) will develop and validate system, engineering, and design models that lend insight into overall fuel cycle efficiency. All relevant materials data for candidate storage media will be compiled and required materials properties defined to meet the technical targets. SRNL will also design, build, and evaluate subscale prototype systems to assess the innovative storage devices and subsystem design concepts, validate models, and improve both component design and predictive capability.



Question 1: Approach to performing the work

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

- The overall approach taken by the Hydrogen Storage Engineering Center of Excellence (HSECoE) is excellent, combining material exploration with practical engineering solutions for onboard materials-based hydrogen storage systems. Although ammonia borane (AB) is not considered a viable candidate material, the engineering work carried out by the HSECoE is applicable to a future, yet-to-be-identified chemical hydrogen storage material. Likewise, while metal-organic framework 5 (MOF-5) is not the sorbent material that will meet DOE targets, the tremendous amount of work invested in developing, analyzing, building, and testing prototypes is most valuable for a future sorbent system. Material property guidelines were developed for the overall system to meet the DOE performance targets.
- The project is progressing according to the plan and will likely fulfill the goals of developing and testing prototype storage tanks. Overall, this is an extremely productive and successful research project. A huge number of materials have been considered previously for hydrogen storage, but evaluation of the available physical and chemical data for practical applications is far from straightforward, and modification toward relevant technological system targets is even more challenging. This task has been conducted extremely successfully within the HSECoE.
- A well-formulated, phased approach to identifying system needs, design and development of engineering concepts, and prototype development and testing has been adopted. Timely go/no-go decisions were implemented. This allowed the team to converge on the most reasonable prototype systems based on the best materials candidates available to date. The time sequencing of the tasks and subtasks on this complex project is logical, and the highly collaborative nature of the project ensures that problems are addressed in a rigorous and effective way. By carefully addressing the "white spaces" in the spider charts, the team was able to focus on the critical issues that ultimately affect achievement of DOE targets.
- The project has a good-to-excellent organizational/engineering approach to delegating tasks and marrying engineering with research efforts to address the "white space" issues of the various materials classes and resulting storage systems. Toward the end of the HSECoE's efforts, the team demonstrated the substantial benefits of the "Center Approach" to a technically and organizationally complex area of research and

development (R&D) to drive the field forward at a higher pace than could be done by a collection of individual efforts.
- The overall approach to looking at completely different systems—applying a rigorous down-selection process and touching all the most important factors for future automobile applications—is highly commendable for other projects. In a very good functioning team of several partners, a very interdisciplinary approach—from basic research to technology development, from experimental to computational exploration of those systems—has been applied. Different alternatives were/are evaluated and compared in an extraordinarily professional way. In the case of those alternatives that are currently not competitive, the basic needs and demands were determined and clearly stated.
- This project's approach is excellent. It serves as the coordinating effort of the HSECoE, the most thorough and important Center of Excellence thus far in the DOE storage effort. It is an operational over-structure that is well planned and executed. The approach covers all the important system barriers, candidate materials data compilations, and a prototype demonstration.
- The approach was very good, and the HSECoE has provided a lot of beneficial work.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- A large amount of progress has been made during the nearly six years the HSECoE has been in place. This includes models, reactor design, heat transfer enhancement, risk analysis, practical data collection, information dissemination, and many other engineering areas. Both adsorbent and chemical hydrogen material model systems have been studied in major detail, and many practical innovations have been made. There have been some technical difficulties encountered with the final prototype. Given the large number of experts involved in this project, it may be argued that the problem (polymeric cryogenic seals) could have been anticipated better, or at least solved more quickly. Although a temporary flanged system has been applied to complete the prototype testing, this part of the project is incomplete as the project approaches its end this month. It is disappointingly clear that no current solid-state material is capable of reaching DOE goals, by far, but of course this was not the HSECoE's aim. The web/share sites have nicely disseminated results and models to the public. There have been a number of publications and conference participations.
- Through extensive analysis and modeling efforts, the project team developed an easily communicated set of spider charts that clearly indicated where various materials systems had advantageous properties, as well as where these systems were challenged to meet the current targets. The HSECoE overall was able to then focus on and communicate potential solutions to some of these "white space" issues. This is an important contribution to future materials development efforts. The use of failure mode and effects analysis helped the team establish a catalogue of issues and rank them in priority such that the issues that were most likely to be important were addressed first.
- The down-selection process has been applied strictly and in the right and correct way. The storage alternatives that are currently most promising have been identified. For all the others, it has been clearly stated what has to be done or achieved to fulfill the DOE goals. For the most promising alternatives, subscale prototypes have been assembled and several technical problems have been solved.
- The progress is outstanding.
- Testing for both Modular Adsorption Tank Insert (MATI) and hexagonal honeycomb heat exchanger (hexcell) systems was behind schedule. Testing of the pressure vessel was delayed because of leakage in the cryogenic seal of the pressure vessel and a funding transfer delay. A six-month extension is requested to complete the tests. The milestone for demonstrating dormancy and refueling time in a full-scale, 5.6 kg hydrogen tank appears to be in jeopardy. The HSECoE continues to make great progress in system modeling, having added more models to the website and making them available to end users. The models are extremely useful to system analysts for evaluating candidate hydrogen storage materials. The HSECoE can add significant value to the website if key experimental data are also included.
- Less progress was made in this final year of the project compared to prior years. Considerable effort and time were devoted to addressing problems with leaks in the cryogenic tank system(s). This detracted significantly from the overall technical progress. It is surprising (or perhaps unfortunate) that so many

problems associated with cryo-tank leakage became evident at this late stage in the project, given the close involvement of a partner with extensive tank expertise (Hexagon Lincoln) in the overall project. Likewise, internal bureaucratic problems associated with directing funds in a timely way to the University of Quebec severely limited the important work on adsorbent performance analysis by that partner.
- The delays, such as shipping the system from Oregon State University and the sealing issues of the tank from Hexagon Lincoln, were a little disappointing. Also, it would have been good to see lessons learned for all material classes.

Question 3: Collaboration and coordination with other institutions

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

- According to the presentations given by Don Anton and the other subproject leaders of the HSECoE, as well as further knowledge about the work of the HSECoE, it seems the project partners had excellent knowledge about what was done by the other partners. They seem to have worked together in an outstanding and intense manner.
- Overall, this is a very innovative and productive research center led by a very experienced and professional director, D. L. Anton. It is very likely that prototanks will be fully constructed and tested, which is a huge step forward for hydrogen storage for mobile applications. All partners are very well integrated in the project.
- Apart from the problems with transferring funds to the University of Quebec, collaboration and cooperation among partners was excellent. Over the years, this has been a hallmark of this project. This is a complex project comprising multiple interactive tasks and subtasks. The principal investigator and all team members have done a fine job to ensure that the technical efforts are coordinated and that information concerning results, progress, and future work is communicated effectively among all participants.
- There was top-notch collaboration among all team members. Don Anton has done an outstanding job coordinating the myriad activities in the HSECoE.
- The many partners within the HSECoE have cooperated very well together. There seems to be good synergy. There have been many communications and face-to-face meetings among the participants.
- In the end, the HSECoE developed into a fairly tight set of collaborators. It is unclear whether this was driven by the HSECoE director or was simply the force of will of the collected researchers and engineers from across the various institutions that participated in the HSECoE.
- Some of the delays were unnecessary and could have been managed better (e.g., the damage to the system from improper shipping).

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.8** for its relevance/potential impact.

- This project is directly relevant to the objectives and needs of the DOE Hydrogen and Fuel Cells Program (the Program). The project was burdened with the problem that no single material had hydrogen sorption performance characteristics that even approached DOE system targets. Nonetheless, the project provided system solutions that will undoubtedly be relevant when (or if) an adequate material or combination of materials is ultimately identified.
- Several alternatives for hydrogen storage in mobile applications have been evaluated. A subscale prototype has been developed for the most promising alternatives. Through this, a real alternative to (only) compressed gas tanks has been demonstrated that has a real chance to become competitive with compressed gas tanks.
- The work carried out by the HSECoE is directly relevant to the Program goals for onboard hydrogen storage. The HSECoE employs two surrogate materials (AB and MOF-5) to address the onboard engineering issues and develop sets of material requirements to meet the DOE targets.
- The project has had high relevance to and potential impact on the Program goals. The project is an example of a successful DOE Center of Excellence. Unfortunately, the overall results suggest considerable doubt

that DOE system targets can be met in the foreseeable future with either adsorption or chemical hydrogen storage materials. Compressed hydrogen storage seems to be the only practical solution for some time.
- The "Center Approach" to this highly complex area of developing the guiding engineering principles for storage systems and storage materials is critical and highly relevant to Program goals.
- The HSECoE is very relevant and the work that has been completed is good.

Question 5: Proposed future work

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

- Subscale prototype tests should be completed as planned. Outcomes should be put online as planned. The overall outcome of the work should be summarized in a book written by/with contributions from the core partners. The HSECoE should be continued in a network of the core partners that monitors scientific discoveries and technological achievements that could change the competitiveness of the different alternatives.
- The remaining tasks are consistent with the program plan and revised schedule.
- "Proposed future work" is not applicable, because the project is ending. A focus on providing detailed documentation of the approach, results, and conclusions is imperative.
- "Proposed future work" is not applicable, other than to figure out how to maintain the legacy of the HSECoE's output using enduring National Renewable Energy Laboratory support.
- This project has ended. It would have been preferable for the models that were completed to be useful externally instead of focused on SRNL only.
- The project officially ends this month.

Project strengths:

- This is a very well-organized and productive project. The project's aim is highly relevant. There is a strong network and strong collaboration between the partners in the project. The team members have developed completely new types of hydrogen storage tanks based on physisorption of hydrogen, as well as implemented Internet-based systems for the exchange of information and modeling of storage systems. Overall, this is a very innovative and productive research center led by a very experienced and professional director, D. L. Anton. It is very likely that prototanks will be fully constructed and tested, which is a huge step forward for hydrogen storage for mobile applications.
- A well-coordinated project team with expertise in all areas relevant to hydrogen storage system development has been assembled to conduct this project. In many ways, this project should serve as a model for DOE to use in the future to address complex and challenging system issues. The project is well managed and focused, as well as highly interactive and collaborative.
- The HSECoE was highly focused on the defined goals. It was managed extraordinarily well and in an organized manner. Collaboration was exceptionally good. The scientific/technological excellence of partners was extremely good.
- The project has great leadership and strong management. The HSECoE is successful thanks to its highly qualified and experienced researchers.
- The strength of the HSECoE was collaborating with the necessary teams in the industry to accomplish many tasks that will continue to be useful in the industry.
- This is an excellent and well-executed Center of Excellence.
- It took a while, but the HSECoE eventually gelled and became a highly functional team.

Project weaknesses:

- There are no weaknesses.
- The final year of the project has been plagued with both bureaucratic (fund transfer) and technical (cryo-tank leak) problems. This clearly inhibited the overall momentum of the project as it nears its conclusion. Although it is not the fault of this project, since its inception, the most noteworthy weakness of the overall effort continues to be the lack of a material that meets DOE requirements. It is unfortunate that so much

time, effort, and funds have been expended without the realization of a prototype system that meets DOE targets.

- The weaknesses were the lack of lessons learned for all material classes, the delays from shipping and sealing issues, and the models' not being for external use.
- Weaknesses are the difficult targets and very limited choices of adequately promising storage materials.
- It is not clear what is coming after the HSECoE. It has to be made sure that the gained knowledge is not lost.
- Test data may be hard to find years down the road if they are not documented, organized, and kept systematically on the website (similar to the efforts devoted to system models).

Recommendations for additions/deletions to project scope:

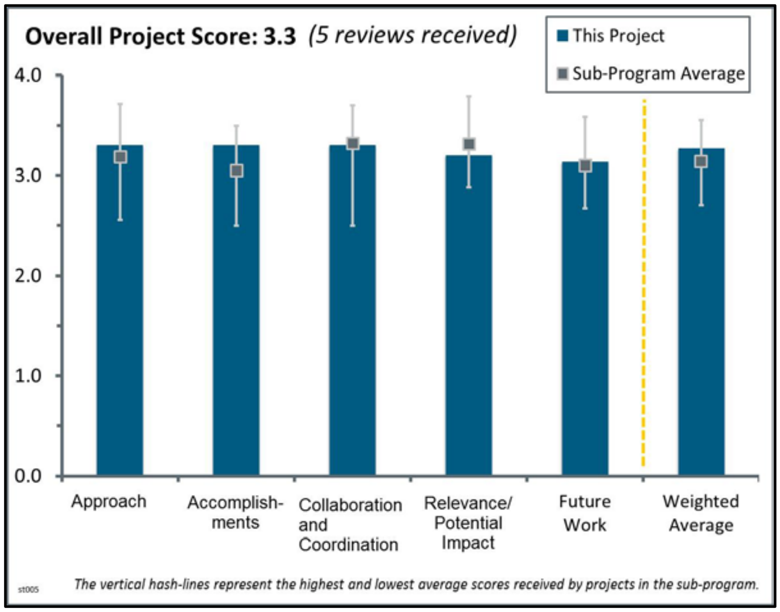
- It is important to maintain the gained knowledge. Because the HSECoE members are the best experts in their field, they should summarize the gained knowledge as completely as possible in a book. After the end of the HSECoE, a network of the most important partners/core partners should be established or maintained to monitor further developments and discoveries and to update/alter the outcome of this evaluation.
- Careful documentation of all aspects of the approach, results, and conclusions reached in this project is essential! Unacceptable loss of "institutional knowledge" is at stake here. Ensuring a positive impact of the project on the development of future systems depends on this.
- The results from this project are very promising and call for further R&D in this field. Allocation of resources to keep the software and databases up to date and to make the extreme amount of useful data generated within the project available for future projects in this field would be very valuable.
- It is hoped that the prototype can be finished and fully tested. It is also hoped that the models/designs/data can be continued via the HSECoE website for many years to come for future generations to use if and when a materials breakthrough is made. (The project leader indicated this will very likely be the case.)
- The project should consider adding experimental data to the Internet access.

Project # ST-005: Systems Engineering of Chemical Hydrogen, Pressure Vessel, and Balance of Plant for Onboard Hydrogen Storage

Kriston Brooks; Pacific Northwest National Laboratory

Brief Summary of Project:

The objectives of this project are to develop hydrogen storage systems that meet U.S. Department of Energy (DOE) 2020 targets for light-duty vehicles based on adsorbents and chemical hydrogen storage materials; develop engineering solutions to overcome deficiencies of materials from the Materials Centers of Excellence; identify, develop, and validate critical components for performance, mass, volume, or cost; and develop models and simulation tools to predict the performance of materials that would be acceptable in engineered hydrogen storage systems for light-duty vehicles.



Question 1: Approach to performing the work

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

- The project has taken a very effective approach, on which it thoroughly performed, which includes the following:
  - Developing and validating a liquid-nitrogen (LN_2)-cooled wall tank.
  - Conducting cost estimations.
  - Validating a balance-of-plant (BOP) redesign.
  - Reporting on findings and progress.
  - Producing a chemical hydrogen storage system model.

  Combined usage of experimental and computational experiments has been extremely well done. Strategic Analysis, Inc. (SA) and the Hydrogen Storage Engineering Center of Excellence (HSECoE) conducted independent cost analyses, which were very useful for verifying the results.
- The overall project appears to be well executed and logical in its design. The project is mostly wrapping up, so the work presented here is in its final stages and refers to specific tasks for cryo-absorbents and chemical hydrogen storage systems.
- There is a logical progression of tasks throughout the lifetime of the HSECoE to develop feasibility and/or cost assessments across several systems platforms. Crucial proof-of-principle validations should be provided when appropriate. The strength of the approach was the attempt to provide experimental validation of sub-models being developed in parallel with other members of the HSECoE.
- The project has a solid engineering approach.
- The project is reasonably well focused on relevant barriers: charging rate, BOP, cost (adsorption), and reducing the loss of hydrogen on the fill (replacing with LN_2). It is not clear what is being done to address the dormancy, which is another critical issue resulting in loss of hydrogen. New engineering solutions to help mitigate materials issues would be great, but it is difficult to see how the proposed tank designs will ameliorate these issues in any significant way.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- A very detailed and thoroughly analysis and improvement of the BOP has been performed. Test of fatigue at these low temperatures is extremely important and was successful. Prototype design and testing with different thermocouples is very important (although there seemed to be no simulation results). Correct conclusions were drawn (directing LN_2 flow). Consolidation of the valve block with extraordinary reduction of mass and volume, number of fittings, and cost is a special accomplishment to be praised. The evaluation of different polymer materials for seals, pistons, seats, and tanks/pipes was a very necessary part of the work and has been done very thoroughly. Tests performed are showing that the mechanical properties of these materials should be not affected by the hydrogen.
- Results from the LN_2-cooled tank show nice promise. This work addresses one of the key issues with these tanks: the loss of usable hydrogen.
  - Predictions on material fatigue are also very useful. Although it is likely beyond the scope of this project, it would be nice to have more experimental data in this area to develop life estimates for these tanks. Tank costs should be normalized by life for a true comparison.
  - It is not really clear what state the chemical hydrogen system model is in at this point. Perhaps this is a simple user-friendly toolkit.
  - The analysis of metal-organic framework tanks (Modular Adsorption Tank Insert [MATI] and Hexagonal heat exchanger [hexcell]) seems a little redundant with SA’s work.
- Regarding the LN_2-cooled wall tank tests, some type of experimental demonstration was needed. The accomplishments appear to be a broad exercise to explore and predict the cooling within the tank and to validate the model predictions via 2 L tank tests. Scaling up projections to a 120 L tank is a good idea and shows the kilograms of LN_2 necessary for cooling. However, there were limited other “lessons learned” from the testing. Cost validation with outside sources is a good idea. The project cost analysis is sound and comprehensive. The consolidated valve block is a good idea in theory, but it is quite complex. Further consideration of the thermal losses associated with the valve should be considered. The degree of industry input into the feasibility of the integrated valve is not clear. Polymer compatibility testing was worthwhile and useful despite not leading to significant variance from expectations. Posting the chemical hydrogen storage model to the Internet is a significant step toward analysis transparency and dissemination.
- Progress has been good to excellent on providing proof-of-principle demonstrations for specific components or approaches, such as cooling of the tank walls and others identified as crucial for the further development of systems models and for model integration, often in collaboration with other HSECoE members. The project collaborated well with SA on MATI/hexcell system cost estimations. Finishing off the chemical hydrogen storage systems model and having it posted on the HSECoE’s model page is a good-to-excellent accomplishment. Improvements in BOP componentry (e.g., the consolidated valve block) may result in cost and volume/mass savings.
- All objectives for the prototype LN_2-cooled wall tank have been met.

Question 3: Collaboration and coordination with other institutions

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

- The approach taken to— independently perform cost analysis and afterward compare the results—is very good and persuasive. The collaborations as listed on slide 23 is persuasive.
- Collaborations across the HSECoE and with SA are good to excellent.
- There are active collaborations internal and external to the HSECoE.
- There continues to be good coordination within the HSECoE and Storage Systems Analysis Working Group, and good outside collaboration with SA. That is good. However, there does not appear to be much other outside/non-laboratory collaboration. Discussion with BOP component manufacturers or seal vendors might be useful.
- There is excellent collaboration within the HSECoE but little beyond this group.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.2** for its relevance/potential impact.

- The Pacific Northwest National Laboratory (PNNL) team worked on disparate areas in which engineering demonstrations at the proof-of-principle level were required to provide feedback to model development. This is a highly impactful and relevant area to the HSECoE's efforts in support of the broader goals of the DOE Hydrogen and Fuel Cells Program (the Program). Development of models accessible by the public is absolutely an element critical to the HSECoE's success, and PNNL's team had a substantial impact on that program element.
- This project of the HSECoE is an important part of the Center. The demonstration of potential cost savings due to the consolidated valve block shows one way costs could be reduced.
- Comprehensive analyses such as this significantly contribute to the overall achievement of Program goals by conducting a deep dive in component technologies and issues.
- This project addressed a potentially significant engineering challenge for absorbent-based hydrogen storage for automotive applications.
- Work on LN_2-cooled tanks has clearly led to an increase in the fill rate. However, it is unclear what the impact is on the "loss of usable hydrogen." In the spider charts presented by other HSECoE members, this metric is one of the furthest from being met. Replacing liquid hydrogen (LH_2) with LN_2 will certainly reduce wasted hydrogen, but there is still a cost associated with LN_2. Overall, the challenge remains that significant cryogens are required to fill the tank. These costs should be worked out. The metric "loss of usable hydrogen" may need to be made more general, or a second metric may need to be added—"fill cost" or "cryogen cost."

Question 5: Proposed future work

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

- Completing the analysis and scale results of the LN_2-cooled wall tank prototype, finalizing the PNNL contribution report, improving the chemical hydrogen storage model, supporting material developers in using the framework, and documenting the results in reports and journal articles are very important tasks. Nevertheless, the results of the HSECoE should also be summarized in a book, and the results of this work should be summarized in one chapter of that book as well.
- The project is wrapping up, so future tasks are appropriately centered on documentation and ease of project information dissemination to the public.
- It is not clear that there are any plans to deal with the loss of hydrogen associated with dormancy. Mechanical testing at low temperature would be useful to better understand fatigue and tank life. It is probably beyond the scope of this project, but tank cost should really be normalized by life. A user-friendly toolkit for the chemical hydrogen storage system model (as proposed) would be useful. It may be valuable to consult with the chemical hydrogen storage materials community to get the right parameters.
- "Proposed future work" is not applicable, because the project is ending.

Project strengths:

- There is extensive collaboration with industrial and scientific partners within the HSECoE. The project is combining both evaluation of system components and modification/redesign to improve system costs. This is very good, systematic, and successful work. Congratulations to the project team.
- There are clear improvements in fill rate. Use of LN_2 will likely reduce cost (although this is still a little unclear because both LH_2 and LN_2 could be captured and reused). A user-friendly chemical hydrogen storage system model would be useful to help guide the materials work. Component integration (e.g., consolidated valve block) seems to be paying off.
- Strengths include the comprehensive analysis of engineering and cost aspects of adsorbent and chemical hydrogen storage systems.

- Project strengths include experimental validation at the proof-of-principle level in support of model development.
- PNNL has outstanding engineering capabilities.

Project weaknesses:

- No weaknesses were detected.
- Cost models for the hexcell and MATI prototype tanks are useful, but the overlap with SA work seems unnecessary. Certainly there is some value in comparing the two analyses and resolving discrepancies, but the limited funds may have been better spent targeting other key issues. The cost of cryogens is still unclear. Replacing LH_2 with LN_2 may be a good start, but it would be useful to get a comparison (perhaps "loss of hydrogen equivalent"). It is not clear how much LN_2 is needed and what the estimated cost is for a single fill (the best-case scenario would be capturing all LN_2).

Recommendations for additions/deletions to project scope:

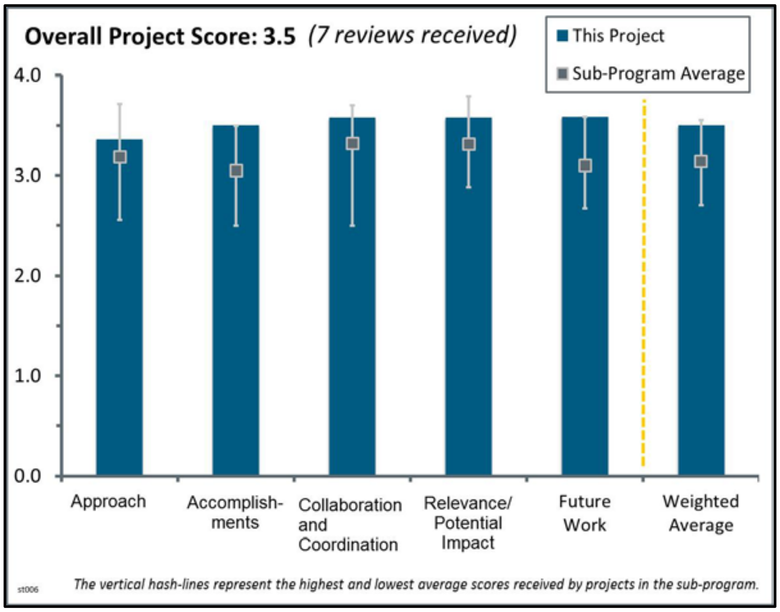
- The project should contribute to a book about the results of the HSECoE.

Project # ST-006: Advancement of Systems Designs and Key Engineering Technologies for Materials-Based Hydrogen Storage

Bart van Hassel; United Technologies Research Center

Brief Summary of Project:

The goal of this project, as part of the Hydrogen Storage Engineering Center of Excellence, is to design materials-based vehicular hydrogen storage systems that will allow for fast refueling and a driving range of greater than 300 miles. The major objectives of this project in fiscal year 2015 are to (1) develop Integrated Power Plant Storage System Modeling to compare hydrogen storage systems on a common basis, support storage system model integration, and develop a graphical user interface (GUI) for models on the Internet (www.hsecoe.org); (2) ensure hydrogen quality through particulate filter right-sizing; and (3) share results through publication.



Question 1: Approach to performing the work

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

- United Technologies Research Center (UTRC) clearly identified what had to be done in the relevant tasks of the Hydrogen Storage Engineering Center of Excellence (HSECoE) (e.g., the influence of compaction on the materials and the overall system's behavior). UTRC played an important role within the HSECoE without the early constriction of too narrow a focus on special details. In the end, this is very beneficial for the overall HSECoE initiative because UTRC could identify and react to various materials or system problems that were discovered in the progress of the HSECoE projects.
- This is a logical engineering approach to addressing the assigned tasks in collaboration with the HSECoE's partners. Experimental validation at the proof-of-principle level in support of sub-model development contributes significantly to the HSECoE's goals.
- The project is well focused on critical barriers and technologies necessary to contribute to the HSECoE. The project's contribution dovetails very well.
- The work is very thorough and well done.
- The overall approach was good; however, the cost analysis for the filter was lacking. The cost seemed very high and more work could have been done on that analysis.
- How barriers are being addressed needs to be better outlined in the work approach.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- Excellent progress has been made in modeling and in developing a GUI (Simulink). Models and appropriate data selections have been put on the HSECoE website. Progress has been made toward the modeling of various candidate systems: physical storage (compressed gas), metal hydride, chemical hydrogen storage, and adsorbents. Physical storage has apparently been included for comparison purposes relative to the HSECoE's material-based storage systems. The key contribution is the development of a common base for comparing various competing systems. There has been useful feedback from the public.

A side effort on the filtration of adsorbents (metal-organic framework 5 [MOF-5]) was completed. Especially useful was the generation of filter pressure drops at service flow rates. These important data suggest this potential problem can be adequately handled. A good spectrum of publications and presentations has been authored.

- UTRC accomplished many small-to-large achievements, rather than one very large achievement, within the time frame of the project. These achievements included using pellets to improve material properties, finding the right and proper method to guarantee high-purity hydrogen, and implementing software tools to describe whole systems. The models were made available on the Internet and can help both materials developers and systems engineers to evaluate new materials and technology achievements. UTRC's work, accomplishments, and progress are very important and necessary parts of the HSECoE.
- The system modeling and system integration work that has resulted in what may be a user-friendly Internet-based application for public access supports a key set of goals within the HSECoE. Demonstration of an effective particulate filter to validate the feasibility of the approach was good to excellent as well.
- The GUI and beta tests were good, and the storage model integration for the public was very strong. The requirements for the hydrogen filter can be used throughout the industry.
- The presentation was excellent and clearly highlighted progress toward project goals.
- The modeling effort is useful for technology development and selection, thereby addressing barriers. The specific technology development efforts need clearer ties to barrier reduction outcomes.

Question 3: Collaboration and coordination with other institutions

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

- UTRC demonstrates that it has collaborated effectively and intensively with the other HSECoE partners. On top of that, UTRC has communicated the results internationally via conferences and the International Energy Agency.
- Collaboration within and beyond the HSECoE has been excellent. Such collaborations are important in developing a broadly meaningful model. A good spectrum of publications and presentations has been authored.
- The project encompasses academia, laboratories, and industry, with reasonable participation across the project members.
- Collaboration is good to excellent with all HSECoE partners. Participation in Task 32 is good.
- There was no great need for collaboration on this project, but it seemed that UTRC was able to get all of the necessary information from the project partners.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.6** for its relevance/potential impact.

- In the years from 2009 to 2015, UTRC has made many important contributions (both experimental and computational) to the HSECoE in different fields: (1) metal hydrides, (2) chemical hydrogen storage, (3) adsorption, and (4) the Simulink framework. From 2014 to 2015, the main focuses were hydrogen quality (looking for efficient adsorbent particulate filtration), the general comparison of hydrogen storage systems on a common basis, the integration of storage system models in a framework, and GUI development for the Simulink framework. All of these are important tasks for the HSECoE, and thus they are highly relevant.
- The development of publicly available models of storage system interactions is a highly relevant and impactful contribution from this team. Sub-model validation via experiment also has a high impact in demonstrating model fidelity.
- Clearly, the work is important to sorbent storage systems. The most challenging aspect of the sorbents, besides their low capacity, is the liquid nitrogen cooling.
- The project clearly supports the HSECoE and thus contributes to progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan.

- The project is very relevant, and there will be a strong benefit to the industry from this project.
- The modeling effort has clear utility. It is not as clear that the contribution toward reaching targets is attributable to filter work.

Question 5: Proposed future work

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

- The project is about to be completed very successfully through development of an Internet-based GUI for programs. Furthermore, experimental studies of particle-free release of hydrogen were conducted very successfully. The aim and outcome of this project is highly relevant.
- The project ends this month, along with the HSECoE. The only remaining work is the final report and publication preparations and submissions.
- The project is nearly complete, and the remaining work is reasonably defined.
- The project is scheduled to be completed in June, so other than submitting final reports, there is no future work.
- Future work comprises the remaining tasks necessary for the project.
- This question is not really relevant to this work because the project ends in June.
- This is not applicable, because the project is wrapping up.

Project strengths:

- The project contributes to the design of materials-based vehicular hydrogen storage systems that will allow for fast refueling and long driving range—in particular, development of approaches to compare hydrogen storage systems on a common basis (i.e., by Internet-based GUI programs for modeling and a very user-friendly Internet-based simulating [Simulink] framework). The results from the project are very valuable for future research and development (R&D) in the field. Furthermore, experimental R&D is conducted with a focus on hydrogen quality and gas filtration regarding particle-free release of gas, which is also highly relevant. Thus, the project combines experimental work, both within this project and using results from other partners, with modeling. This project is well integrated in a larger research consortium. In conclusion, this is a very well-organized and productive project led by a very experienced and professional principal investigator (PI). The project is highly relevant, well organized, and integrated in a larger consortium. The project has progressed according to the plan and will likely fulfill the goals and soon be finalized very successfully.
- Overall, this project was very strong. The focus of the project remained on enabling customers to fill their vehicles quickly and provide a range greater than 300 miles.
- The project strength, and indeed the strength of UTRC’s contribution, seems to be the in-house experience in various engineering disciplines. In accordance with that expertise, the UTRC project has yielded many important contributions in various fields.
- The team members provided high-quality work throughout the project. Their openness and generosity in sharing what they were doing and learning is appreciated by the hydrogen storage community. They did not appear to withhold information that might help out someone outside of their project.
- Model integration and sub-model experimental validation are strengths.
- Modeling and container engineering contributions were the main strengths.
- The model development is a valuable tool.

Project weaknesses:

- No weaknesses are observed.
- No weaknesses are detected.
- No weaknesses can be seen in the 2015 work. In the 2014 work, the carbon used in the filtration materials studied for ammonia scrubbing was custom-made, and the procedure for making it is not something that an average laboratory can do. In work that is supposed to be for commercialization, the PIs should stick to materials that are available to the public at reasonable cost.

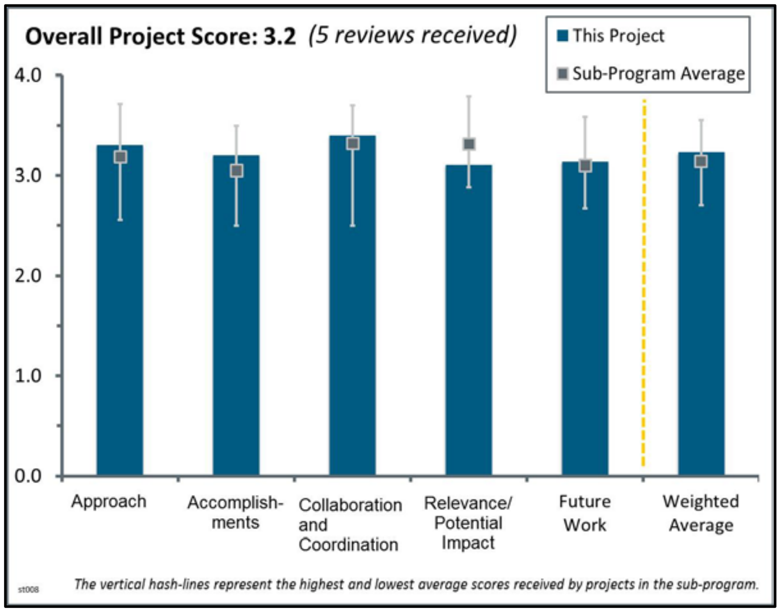
- The only weakness was the cost of the filter. The cost seemed high, and there could have been more focus on understanding why it was so high.
- Better relationships need to be identified between DOE goals and specific technology development efforts.

Recommendations for additions/deletions to project scope:

- The results from this project are very promising and call for further R&D in this field. Allocation of resources to keep the software and databases up to date is very useful for future projects in this field.
- It would be useful if low-level, online model support could be continued in the future.

Project # ST-008: System Design, Analysis, and Modeling for Hydrogen Storage Systems

Matthew Thornton; National Renewable Energy Laboratory



Brief Summary of Project:

The objectives of this project are to manage Hydrogen Storage Engineering Center of Excellence (HSECoE) vehicle performance, cost, and energy analysis technology areas; lead an effort to make models developed by the HSECoE available to other researchers via an Internet-based portal; and develop and apply the model for evaluating hydrogen storage requirements, operation, and performance trade-offs at the vehicle system level.

Question 1: Approach to performing the work

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

- System-level modeling and correlation of vehicle performance with hydrogen storage requirements and characteristics are useful for the design and development of optimized storage systems. The approach adopted in this project for model development and creation of an improved graphical user interface (GUI) is logical and straightforward. Development of a user-friendly operating environment is a valuable feature embodied in the overall approach. The principal investigator (PI) and his team should be commended on their efforts to incorporate reviewer suggestions (especially the need for a more robust model validation effort) into the approach for the 2015 work.
- The approach to getting the finalized models onto the Internet in a publicly available, documented, user-friendly format is without flaw. The approach to collaborating with other HSECoE partners in developing the integrated storage, fuel cell, and vehicle performance model is very solid.
- The project is highly relevant, and the National Renewable Energy Laboratory (NREL) is very well suited to integrate the vehicle, fuel cell, and storage models.
- The approach is appropriate and well defined. The user-friendly modeling framework is very useful for system analysts to evaluate a candidate storage system.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- The coordination and migration of the modeling framework and Internet posting of system models developed in the project were important and valuable accomplishments in 2015. In addition, solid progress was achieved regarding developing protocols for conducting simulation performance checks (e.g., power failure caused by storage system or speed trace misses). Also, for a project of this kind, extensive model documentation is critical. The PI and his team have done an excellent job to ensure the documentation is available and updated.
- Dealing with the multiplicity of issues surrounding the Internet publication of models that have come from a variety of sources on a variety of platforms and are being used by the public on a variety of platforms is a great accomplishment. It is hoped that this accomplishment will endure to maintain the usability of the models, which is the key legacy of the HSECoE.

- The vehicle system-level model of hydrogen storage systems that was created, which is also available to the public, is very useful for researchers developing hydrogen storage materials.
- The researchers have achieved modest improvements/upgrades to the modeling framework that lead to significant enhancement in usability. Incorporation of system diagrams is a big help and greatly enhances clarity. System-level modeling performance checks are a very good addition to the project, given the complexity and integrated operation of the models. There appears to be a significant (+25%) over-estimation of fuel consumption between the model and U.S. Environmental Protection Agency data on the city drive cycle. This needs to be explored further.
- Not much progress was made in this past year because the HSECoE is winding down in its final year. The page views per session and average session duration declined by about one third compared to last year's report.

Question 3: Collaboration and coordination with other institutions

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

- The solid collaborations with multiple HSECoE partners have been important and valuable features of this project since the inception of the HSECoE. The project features especially noteworthy collaborations with Pacific Northwest National Laboratory and Savannah River National Laboratory on model development, with the United Technologies Research Center on GUI development and model integration, and with multiple HSECoE partners on model documentation.
- The project leveraged excellent-to-outstanding collaboration to publish the integrated models on the Internet. It also collaborated highly effectively with the other key HSECoE partners involved in each of the models in developing the integrated models and in providing documentation for the public domain.
- The team appears to be working well and in a collaborative fashion with the many groups within the HSECoE.
- The PI interacts well with all members of the HSECoE to coordinate the model posting.
- Collaboration seems to exist with other institutes.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.1** for its relevance/potential impact.

- The HSECoE's efforts address many aspects of the storage system. This task integrates the design and expected performance into an integrated model to assess overall performance. Such a holistic view is essential to both understanding and achieving DOE's goals and objectives.
- This project is relevant to the Hydrogen and Fuel Cells Program (the Program) and supports critical Program goals. System-level modeling and correlation of storage characteristics and requirements with vehicle performance provide a valuable framework for quantifying system trade-offs and optimizing system design.
- Getting the integrated system—fuel cell—vehicle models onto the Internet and in working condition is a highly significant and visible milestone for the HSECoE. This is also an area of high impact because this effort provides for the enduring legacy of the HSECoE and is available to the public.
- This project is essential in keeping all of the developed models in one place and making them available to end users. The benefits go beyond the end of the lifetime of the HSECoE. It is to be hoped that DOE will continue to fund some minimum effort for maintaining the website. The potential impact can be enhanced if the HSECoE will consider including test data on the website in support of the models.
- The models are indeed useful to get a "feel" of how the materials may perform onboard a vehicle; however, they are likely not representative of a real system.

Question 5: Proposed future work

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

- The project is ending soon; one anticipates the remaining work on the adsorbent model will be just as good as the work on the other system technologies.
- This question is not applicable—the project is ending. A focus on model validation and completion of system documentation are important tasks to be conducted prior to project completion.
- The remaining tasks are consistent with the project plan.
- The future work is limited but appropriate for a project that is winding down.
- The project is almost complete.

Project strengths:

- This project is being conducted by a well-qualified team that leverages extensive and valuable collaborations with other HSECoE partners. The project provides a vital link between vehicle performance and hydrogen storage and fuel cell system operating characteristics and requirements.
- The ability to use the models generated by the HSECoE and integrate them into a vehicle system-level model helps the researchers get a good idea of how the materials would perform in a fully integrated system.
- A strength of the project is the collaboration to achieve an Internet-friendly documented set of integrated models for public access.
- NREL has done a nice job of integrating many aspects into an overall system assessment.

Project weaknesses:

- No weaknesses were detected.
- The main weakness in the project in prior years has been an insufficient emphasis on model validation. The PI and his team have recognized this issue, and they made significant progress on this important area in 2015.
- The main weakness of this project is that the vehicle system models do not allow for flexibility in integrating other tank models beyond those generated by the HSECoE. These may not be representative of the tank systems onboard a vehicle, and therefore the performance obtained is not representative.
- Model validation continues to be an area with opportunity for improvement.

Recommendations for additions/deletions to project scope:

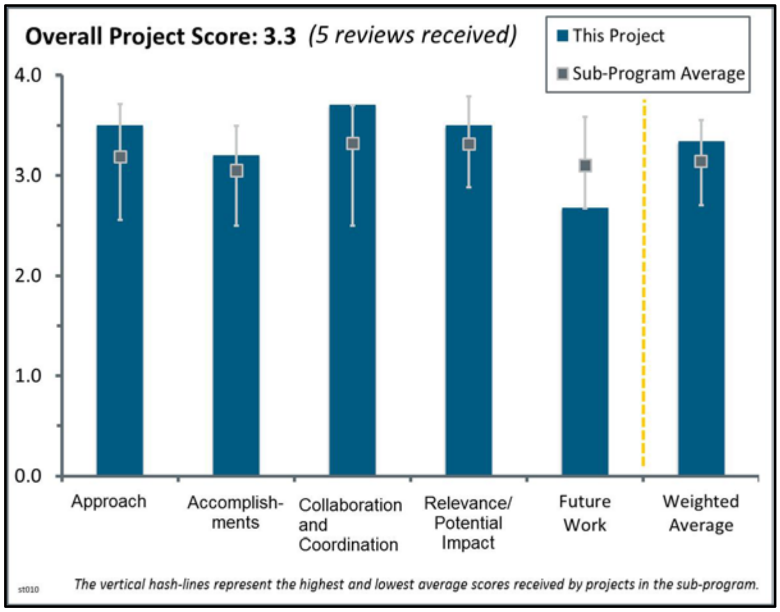
- There are no recommendations to make—the project is ending. Completion of model validation work and updating documentation are important focus areas as the project draws to a close.
- The research team should consider adding experimental data to the Internet portal.
- This question is not applicable.

Project # ST-010: Ford/BASF-SE/UM Activities in Support of the Hydrogen Storage Engineering Center of Excellence

Mike Veenstra; Ford Motor Company

Brief Summary of Project:

This project, led by Ford, is focused on material-based hydrogen storage systems that offer potential advantages, such as volumetric efficiency, over conventional physical-based hydrogen storage systems. This project has three goals that contribute to the overall Hydrogen Storage Engineering Center of Excellence mission: (1) to develop a dynamic vehicle parameter model that interfaces with diverse material-based hydrogen storage system concepts, (2) to develop robust cost projections for these storage system concepts, and (3) to devise and develop system-focused strategies for processing and packing framework-based sorbent hydrogen storage media.



Question 1: Approach to performing the work

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

- The project has clear goals and provides extensible inputs for modeling to account for variations in potential adsorbent materials such as metal–organic frameworks (MOFs), should they become available. The team has overcome barriers and challenges and made progress beyond the specific, measurable, attainable, realistic, and timely (SMART) goals in ways that help other partners in the Hydrogen Storage Engineering Center of Excellence (HSECoE).
- This project focuses sharply on practical properties and adsorbent barriers from the very important point of view of an original equipment manufacturer (OEM) (automobile and adsorbent manufacturers). This view is critically integrated with the overall HSECoE. Cost analysis is an important component. The project is responsible for the very important determination of gaseous impurity effects on the potential deactivation of adsorbents (particularly MOF-5). It serves as the major manufacturing entity for HSECoE adsorbents and cost studies.
- The approach in 2015 focused on evaluating MOF-5 performance characteristics, including potential degradation modes, failure mode and effects analysis (FMEA) for MOF-5 in both Hexcell and modular adsorbent tank insert (MATI) operating environments, and continued work on development of a robust cryo-adsorbent system model. The approach addressed important issues related to the use of MOF-5 (and related adsorbents) in a high-performance cryo-adsorbent system. Especially important was the focus on evaluating impurity effects, identifying and mitigating potential system failures, and maximizing MOF-5 properties by compaction and enhancement in thermal conductivity.
- The overall efforts of the HSECoE were excellent. It would have been good to see a summary of how the researchers purified the MOF-5 sample. MOF-5 performance is very dependent on the amount of residual solvent remaining in the sample. Also, with both tetrahedral and octahedral Zn sites for adsorption, the manner in which one degases can significantly affect the results. As the project moves forward, a summary in the final report for the HSECoE would be helpful. Also, the description of the effect of pellet processing and compaction on slide 20 was interesting. However, a more complete explanation of the extent of solvent remaining and how a better “sweet spot” could be found would have been helpful.
- The approach is good, but it can be improved.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- The project team has made a significant amount of very useful progress. The comparisons among two MOF-5 systems and state-of-the-art compressed gas systems (slide 7) are especially useful. The cost, volumetric, and gravimetric calculations show potential competitive possibilities of MOFs relative to compressed hydrogen. The main disadvantage of an adsorbent approach, relative to compressed hydrogen, is the need for a more complex cryogenic system. Contractors have made impressive progress in understanding MOF manufacture, impurity effects, failure modes, compaction, thermal conductivity, and modeling. All of these are encouraging and are of immediate practical value to the HSECoE. The selection of the optimum tank design from the OEM point of view (i.e., Hexcell versus MATI) cannot be made at this time. The presenter indicated a little more testing is needed.
- The project team achieved all of the SMART milestones and additional goals. MOF-5 cycling is complete, and robustness has been illustrated. The FMEA is robust. Exploring the robustness of puck formation and particle size was reasonable. The new layered puck and aluminum pins seem like positive advancements.
- This question earns a "Satisfactory" rating. The cost comparison should be corrected by estimating the cost per 1% of gas storage. In such a case, the high-pressure system is more cost-effective than those developed during the project. There is no evidence that the graphene used is really graphene and not a nano-graphite; a Raman spectrum could provide such evidence. The role of the residual solvent requires clarification because it is removed during cycling (if there is no role, the team should explain that).
- While it would have been helpful to have a more in-depth study on some aspects of the thermal conductivity properties of various sorbent materials, it is understood that the scope, as defined by DOE, did limit some other initial studies on "new" sorbent-based materials.
- Progress in 2015 was less significant than in prior years (especially 2014). It is not apparent that noteworthy new results were obtained in 2015 on maximization of MOF-5 material properties. Likewise, only minor advancements to prior work (2014) on MOF-5 robustness to hydrogen impurities and FMEA analyses were made during this reporting period.

Question 3: Collaboration and coordination with other institutions

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

- Excellent collaborations and coordination with other HSECoE partners are readily apparent. The OEM perspective provided by this project is a critical component of the overall HSECoE effort.
- The HSECoE, by design, was an excellent illustration of a successful collaboration between industry, academia, and national laboratories.
- Subcontractors BASF and the University of Michigan provide outstanding expertise and contributions. This project has integrated very well into the HSECoE.
- The interactions seem to be strong, well handled, and proactive.
- The project features good collaborations.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.5** for its relevance/potential impact.

- The project is well designed, integrated with the HSECoE, and well implemented. Moving forward in parameterizing the laboratory-to-OEM production and implementation of a chemisorption-based solution seems possible from this contribution to the HSECoE. It is clear that many of the obstacles and solutions generated in this project will have an impact on any storage solution.

- This project provides an essential OEM perspective to the HSECoE on important issues and problems relevant to achieving DOE storage system targets. The project is directly relevant to DOE research, development, and demonstration (RD&D) goals.
- This project is particularly relevant to the Program because it provides practical OEM input to the HSECoE. Its impact has been measurably valuable toward meeting goals and targets.
- The project is aligned with the Program's and DOE's RD&D objectives.
- As next-generation materials are developed, the groundwork laid by the completion of this project within the HSECoE will be important. It would have been good for an OEM to take a stance on which tank design is most relevant to its current thoughts on hydrogen storage systems.

Question 5: Proposed future work

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

- The team should prove that the obtained results are transferable onto other absorbents—for example, activated carbon.
- The project formally ends this month with the overarching HSECoE. There are some work completions and reporting planned to follow. The end story will be very useful to the future of adsorbent research and development (R&D).
- This question is not applicable—the project is ending this year. Comprehensive documentation of project results and conclusions is essential.
- There is not much left to do, and time is running out. The future plans might be seen as excessive, given the short remaining time.
- The project ends in June 2015. Therefore, the future work is limited to a final report.

Project strengths:

- Since the start of the HSECoE, this project has been an essential element of the overall technical effort in the Center. Involvement of a principal investigator with deep knowledge of OEM needs and requirements is a great benefit. The project team is well organized and highly coordinated, and it has consistently maintained a keen focus on the critical issues that need to be addressed in this project.
- The interaction between the partners is a strength of this project. The extent of the questions that were answered over the previous years is another strength. This HSECoE was unique in the level of accomplishments achieved.
- The project is meeting goals, demonstrating positive aspects of absorbents, and contributing to the HSECoE's use of MATI pucks. In addition, it had enough time to do extra analysis and measurements.
- Collaborations and interactions within the HSECoE are an area of strength.
- The project features excellent practical OEM perspectives and R&D approaches.

Project weaknesses:

- There are no real weaknesses other than the inherent challenges with adsorbents, especially the need for cryogenic containment.
- Weaknesses include MOF-5 as being a model system only, lack of sufficient cost estimates, and that some materials characterization issues are possible (the nature of graphene additives).
- Weaknesses include the limitation of the work scope and the inability to look at some newer materials at the end of the project. However, it is recognized that the logistics of such were almost impossible.
- This has been a consistently strong project, and it has no major or notable deficiencies. However, the progress in 2015 was less significant/noteworthy than in prior years.

Recommendations for additions/deletions to project scope:

- There is a critical need for the HSECoE to develop a comprehensive final report that includes the results and conclusions from this project as essential elements. The need for a detailed report of this work cannot be overstated. Future work on advanced system development employing new/improved materials will build on the findings from this work. Unless the results are clearly and comprehensively presented, unnecessary and costly duplications in the technical effort will result.

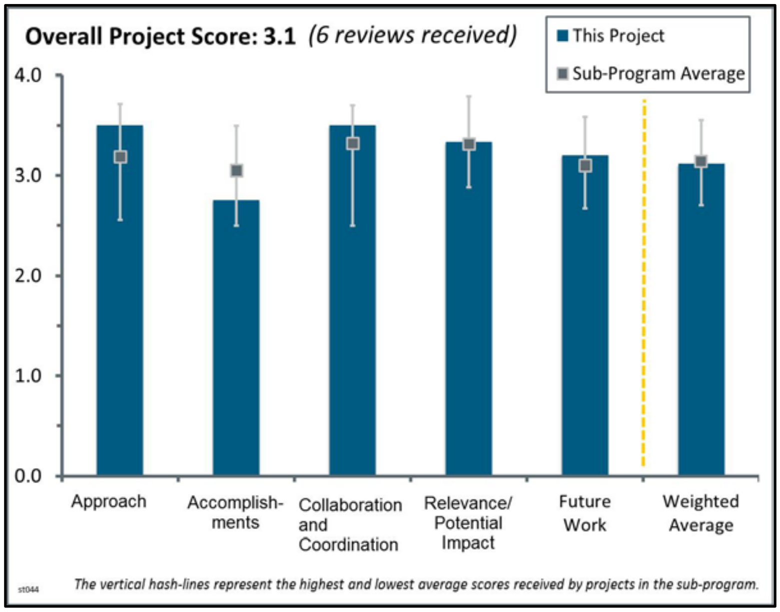
- The project should add spot-testing of selected results on the system with a different hydrogen absorbent(s)—for example, using activated carbon or a different MOF.
- The project should finish its work as planned.
- This question is not applicable.

Project # ST-044: Savannah River National Laboratory Technical Work Scope for the Hydrogen Storage Engineering Center of Excellence: Design and Testing of Adsorbent Storage

Bruce Hardy; Savannah River National Laboratory

Brief Summary of Project:

Objectives of the current phase of this project include (1) designing, fabricating, testing, and decommissioning the subscale prototype systems for adsorbent storage materials; (2) validating the detailed system model predictions against the subscale prototype system to improve model accuracy and predictive capabilities; and (3) developing and demonstrating the acceptability envelope for adsorbents.



Question 1: Approach to performing the work

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

- The focus in 2015 was to develop a subscale prototype for adsorbent storage materials and to validate model predictions with experimental results in order to assess the predictive capability of the models. The team employed a straightforward and reasonable approach based on (1) demonstration and evaluation of the modular adsorbent tank insert (MATI) type and hexcell type of heat exchangers and (2) use of the results to update the cryo-system performance models. The approach enabled useful information about heat exchanger properties and performance to be acquired in a timely way. Additionally, a well-formulated approach was used to identify and quantify the coupled adsorbent and storage system properties needed to meet performance goals.
- The design and fabrication of prototype systems with validation of modeling to contribute toward the predictive capabilities is well executed. Progress has been made in completing the test facility. Modeling and system properties are strongly integrated and well aligned across the Hydrogen Storage Engineering Center of Excellence (HSECoE).
- The project appears to be well aligned with key barriers. It seeks to design, fabricate, and test adsorbent systems; compare the results with predictions; and provide acceptability envelopes.
- The overall approach is logical and reasonable. Small-scale prototypes of the MATI and hexcell are built and tested to gather data for model (kinetics and thermal) validation.
- The approach is sharply focused and difficult to improve significantly. The same approach can be used to evaluate/analyze similar systems. However, it is not quite obvious that the results of this work are directly transferable to other gas storage systems. This should be experimentally proven before the project is completed.
- The project features a well-defined approach for comparison of tank construction. However, it was surprising to see alumina utilized for the system tests. It would have been better to use a standard that consisted of a composite of a material with a thermal conductivity similar to metal–organic framework (MOF)-5 and the same amount of expanded natural graphite or graphene added.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- The team obtained important new information concerning MATI and hexcell heat exchanger performance characteristics. Unfortunately, progress was limited by the need to address persistent leak problems in the cryo-systems. While this inhibited overall progress on the technical effort, the leaks occurred in a fully instrumented testing apparatus, so this issue should be less problematic in a final, fully welded system that does not require feed-throughs and ancillary connections for system testing. Useful information was obtained on adsorbent acceptability envelopes that determine whether current adsorbents can meet targets and provide the coupled range of required properties for new adsorbents. It would be helpful if a trade-off analysis of the hexcell and MATI heat exchanger approaches could be made available to the research and development community. A considerable amount of development and engineering work has been conducted on these systems. A comparison of these two different heat exchange approaches is needed to assist original equipment manufacturers (OEMs) in selecting the optimum system embodiment for a specific application. Testing and validation data are needed.
- The team has made nice progress with the development and testing of MOF tanks (hexcell and MATI). The models show good agreement with tank evaluations. Progress on the adsorbent acceptability envelope has identified some concerns:
    - Meeting the 700 bar tank target will require a substantial increase in the number of adsorption sites.
    - The inverse correlation between gravimetric and volumetric adsorbent acceptability is a concern (but not too surprising). Predicted capacities are below compressed gas (700 bar) under most scenarios.
- The results will help to solve multiple issues; however, it is unfortunate that the project is not going to conclude in a system that can be used in real applications. Therefore, this question deserves a “Good” rating.
- The lack of multiple cycle testing overshadows the other significant accomplishments.
- The team made relatively little progress this year, with the major items being the implementation of the test system and hexcell manufacturing and implementation. Simple calculations to describe the characteristics of the ideal adsorbate were performed.
- Progress was slow this past year. The project was listed as 95% complete (as of 4/10/15), but there remains quite a bit of testing to be done with both the MATI and the hexcell. Model validation will then follow after testing is complete.

Question 3: Collaboration and coordination with other institutions

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

- Close collaboration is needed and well executed with partners in this project. Significant progress is made through the combination of design, testing, and modeling in the different institutions with added perspective coming from external collaborations.
- The collaboration between Savannah River National Laboratory (SRNL) and other HSECoE members, especially Oregon State University (OSU) and Université du Québec à Trois-Rivières (UQTR), was strong and fruitful.
- Solid and valuable collaborations among partners are evident and have continued to contribute to the overall success of the project.
- The project features very good collaborations; partners participate and are well coordinated.
- It was good to see Richard Chahine included in the HSECoE.
- Overall, the HSECoE partners appear to be working together very well. It was difficult to differentiate the level of effort from each institution for any one task. The icons at the bottom of the slide are helpful, but they do not really describe the level of effort. External collaborations were less clear.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.3** for its relevance/potential impact.

- The hexcell manufacture is useful, along with the limited theory for adsorbate. The testing facility should be the most useful element of the project and deliver meaningful results to direct the future of the Hydrogen and Fuel Cells Program (the Program).
- The project is important to the overall success of the HSECoE effort and, by extension, to meeting the overall Program goals.
- Testing of MOF-5 in both the MATI and hexcell provides crucial data for model validation. The test data covers a wide array of engineering issues—such as heat management and balance-of-plant requirements—that must be integrated in an onboard system so that the system can meet the DOE targets in weight, volume, and refueling time simultaneously.
- This project has made nice progress, and the results are clearly having an impact on the community. At this stage, there appear to be a couple of key outstanding issues related to MOF tanks (e.g., loss of usable hydrogen and gravimetric/volumetric capacity trade-off) that must be addressed by the materials community.
- The project supports advances toward the Program's goals and DOE research, development, and demonstration objectives. However, there is little chance to meet those goals, owing to the limitations of the adsorbents (MOF-5).
- A decision and/or recommendation needs to be made about which tank design is most applicable to which types of hydrogen storage materials.

Question 5: Proposed future work

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

- Determining low-temperature mechanical properties and life cycling would be useful. It is unclear how much damage occurs to the pucks after 1 cycle and 10 cycles, whether cracked pucks matter, and whether there is a buildup of impurities. Results indicate that system targets require a material with at least 160 adsorption sites; this suggests future work should focus on materials development rather than on tank design and analysis.
- The proposed future work is reasonable. The team may want to add another task (e.g., experimental validation of the project's results using other types of adsorbents, such as activated carbon).
- This question is not applicable—the project is ending. It is essential that the approach, results, and conclusions are carefully documented.
- The project is ending, and the remaining tasks are needed to complete the testing program and model validation.
- The team is so close to getting this done. It is not clear whether there will be time to actually analyze any data that comes from the testing.
- The project is ending.

Project strengths:

- A well-thought-out approach comprising modeling, experimental development, testing, and evaluation elements has been adopted. A highly coordinated team with expertise in all relevant project areas is conducting a highly focused technical effort. The results from the project are key enablers to development of a prototype test system.
- Strengths include the integration across the HSECoE, smart choices taken in deciding the path forward, and step-wise monitoring of tank properties, etc.
- The results provide useful feedback to the materials community.
- Project strengths include the approach and collaborations.
- The collaborators are a strength of this project.

Project weaknesses:

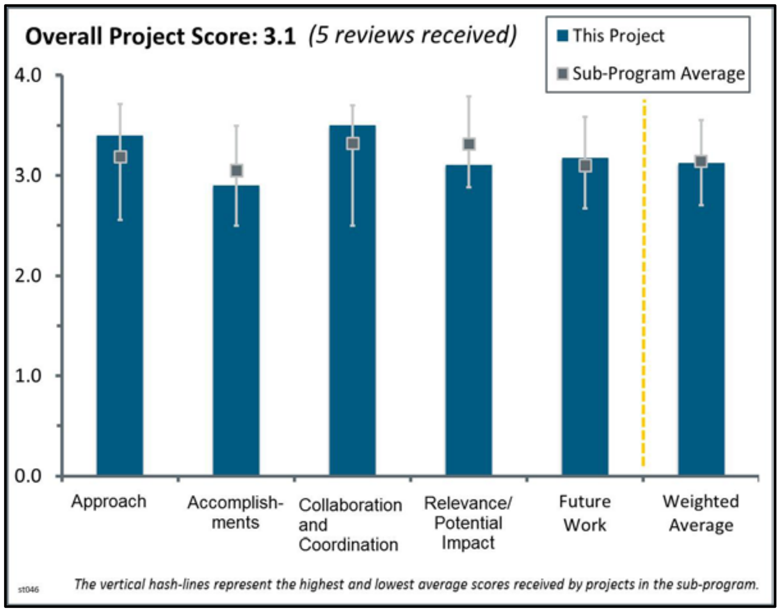
- Determining low-temperature mechanical properties and effects of thermal cycling would be useful. Tank life is probably outside the scope of this project, but it needs to be considered. There are no clear plans to deal with the “loss of useable hydrogen.” Using liquid nitrogen to cool the tank may help, but this scenario will still require considerable cryogens. The cost estimate per fill is unclear. It is also unclear whether there are any plans to deal with dormancy issues.
- Progress was limited by the need to address persistent leak problems in the heat exchanger systems. It is surprising these problems only became apparent near the end of the project. It is unfortunate that the partner(s) responsible for the tank development (possibly Hexagon-Lincoln/SRNL) was unable to address the problems in a more timely and effective way.
- There is little chance the project will meet DOE goals, owing to the limitations of the adsorbents (MOF-5).
- The project has been quite expensive, and progress seems to be particularly slow.
- The lack of multiple cycle testing is a weakness.

Recommendations for additions/deletions to project scope:

- A comprehensive final report is needed. Future efforts on system development should not be forced to “reinvent the wheel.” The report should include a trade-off analysis of hexcell and MATI heat exchanger approaches for specific OEM applications.
- This project has made nice progress and identified clear challenges for the materials community. Given the limited resources, it is probably best to refocus on addressing the materials challenges.
- The team should add another task (e.g., experimental validation of the project’s results using other types of adsorbents, such as activated carbon).
- This question is not applicable.

Project # ST-046: Microscale Enhancement of Heat and Mass Transfer for Hydrogen Energy Storage

Kevin Drost; Oregon State University



Brief Summary of Project:

As part of the Hydrogen Storage Engineering Center of Excellence, the objective of this project is to use the enhanced heat and mass transfer available from arrayed microchannel processing technology to design, fabricate, and test a modular adsorption tank insert (MATI) prototype to address the weight, volume, and charge/discharge rate challenges commonly associated with adsorbent-based hydrogen storage systems. The specific objectives of this project for Phase III are to demonstrate fundamental technical feasibility and validate simulations through subscale system evaluations.

Question 1: Approach to performing the work

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

- A MATI utilizing enhanced thermal and mass transfer is the centerpiece of one of the two principal heat exchanger concepts adopted by the Hydrogen Storage Engineering Center of Excellence (HSECoE) for a prototype cryo-adsorption storage system. A solid approach based on results obtained previously by the project team has been formulated and adopted in 2015 for assembly and testing of the device and validation of a thermal model that simulates the device performance. The novel concept and approach address important storage system needs.
- The design and fabrication of prototype systems with validation of modeling to contribute toward the predictive capabilities is well executed. Step-wise approaches to the scale-up of the MATI system have been taken. Modeling and cooling plate development have been performed.
- This project nicely addresses the barriers associated with heat and mass transfer of a practical adsorption-based system (i.e., size, weight, and charge/discharge rates). It is nicely integrated into the HSECoE.
- The approach is well designed for the remaining work scope.
- It is surprising that with all of the efforts at Ford, the thermal conductivity and hydrogen permeability data were missing. Even the mechanical stability of a puck should have been a straightforward evaluation within any engineering department. A before-and-after evaluation of the pucks after multiple cycles would have added to the long-term properties of the metal–organic framework (MOF)-5 samples. The engineering issues the principal investigator (PI) discussed (i.e., thermocouple leak-through at elevated pressures and cryogenic temperatures) should have been self-evident. Slide 20 appears to show there is still considerable heterogeneity in thermal distribution within the pucks; this will not be solved with the pins.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.9** for its accomplishments and progress.

- Good progress was achieved on assembly and testing of three MATI prototypes, enhanced puck design and fabrication, and first steps toward model validation. A fully instrumented test system was developed to

experimentally characterize the thermal performance of the device. Unfortunately, persistent leaks at various locations in the MATI assembly during cryo-temperature cycling precluded complete and timely testing of the device. Important new results were obtained related to improvements in MOF thermal conductivity in the MATI assembly (e.g., Al pins and expanded natural graphite enhancement in MATI pucks) and development of a modeling protocol for simulating gas fluid flow and heat transfer.
- The project's MATI adsorption system design has been largely developed, built, modeled, and tested. The pressed pucks have been tested for mass flow and heat transfer using a highly instrumented testbed. There have been some serious problems with cryogenic leaks that put the project well behind schedule. The project formally ends this month and is only 95% complete. A temporary (stopgap) flanged container was developed to at least complete the prototype system. It is not completely clear that this project's MATI design is superior to the alternate hexcell design.
- Project objectives are being met, but it is not clear how these objectives relate to DOE goals.
- The team has made limited progress since last year. There is an almost one-year slip in the specific, measurable, assignable, realistic, time-related (SMART) goals for Phase III because issues developed during cooling. Some aspects have moved forward, and pressure testing has begun on the larger test system. Modeling has been extended, and new pucks with pins have been designed. It is not clear the team can finish the project in time.
- Accomplishments were limited by engineering issues.

Question 3: Collaboration and coordination with other institutions

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

- Valuable collaborations with HSECoE partners are evident. The interactions with the University of Michigan/Ford on puck design and with SRNL on prototype development and device simulation are especially noteworthy.
- The collaboration and coordination within the HSECoE seem excellent.
- The project worked well with SRNL.
- Collaborators are involved in project planning and execution.
- This project has to connect with several other groups in the HSECoE to be successful. It does this in several ways—relying on partners for MOF pucks, delivering prototype systems to SRNL for testing, and providing data for simulations. However, the year's efforts seem to be less collaborative and more divided, with little effort by some partners.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.1** for its relevance/potential impact.

- The heat exchange technology developed in this project is an important element of the approach adopted by the HSECoE for a cryo-adsorbent storage system. The approach is innovative and addresses issues of cryo-system weight and size and charging time. The project is relevant to the goals and objectives of the Hydrogen and Fuel Cells Program (the Program), and the level of effort is appropriate to meet those goals.
- Except for some degree of incompleteness, the project has made clear advances toward the Program's goals and objectives delineated in the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan in terms of its participation in the HSECoE.
- The system focus of the project is geared toward DOE goals and will have some impact if the design and modeling are all extensible.
- With the end of the project near, the impact of the work is muted and incomplete. Significant progress was made, but more answers should have been forthcoming.
- It could be made clearer how improvements in volumetric density and heat transfer contribute to better meeting DOE targets. Additionally, improvements do not come without cost, and the impact is not well presented.

Question 5: Proposed future work

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

- This question is not applicable—the project is ending. Careful and comprehensive documentation of the Oregon State University (OSU) work in the final report is essential. If possible, the work to validate the heat and fluid flow model should be completed.
- The project formally ends this month. The proposed future work is fine, but it is not clear how it will be accomplished after the end of the contract.
- The future work is clearly defined. With most of the funding spent, it appears there is more work to complete than funds available.
- This should be the end of the project, but it is not finished, and there will be no time to analyze any testing data.
- The project is sunsetting.

Project strengths:

- This is an innovative project that addresses important technical issues in the successful deployment of a practical cryo-adsorbent hydrogen storage system. The project team and the collaborators have expertise in all areas relevant to successful prototype system development. Throughout the project, the PI and his team have been responsive to reviewers' suggestions and recommendations. This project is a critical component in the overall HSECoE effort.
- The project has made good, practical heat/mass transfer contributions to the HSECoE.
- Collaborations among the partners are an area of strength.
- Development of a MATI system is a strength.

Project weaknesses:

- The overall pace of the effort in this reporting period was not consistent with the pace in prior years. The progress in 2015 was clearly limited by problems with leaks in the instrumented MATI subsystem. It is unfortunate that given the involvement of Hexagon-Lincoln (tank expertise) in this project, and in the HSECoE as a whole, so many problems with cryo-tank leakage plagued the important later stages of this effort.
- Clear connections need to be made between technical goals and accomplishments and progress toward achieving (or approaching) DOE targets.
- Project weaknesses include the slow final year and high expenses for the current deliverables.
- The incomplete evaluation is an area of weakness.
- There are tank design problems relative to cryogen containment.

Recommendations for additions/deletions to project scope:

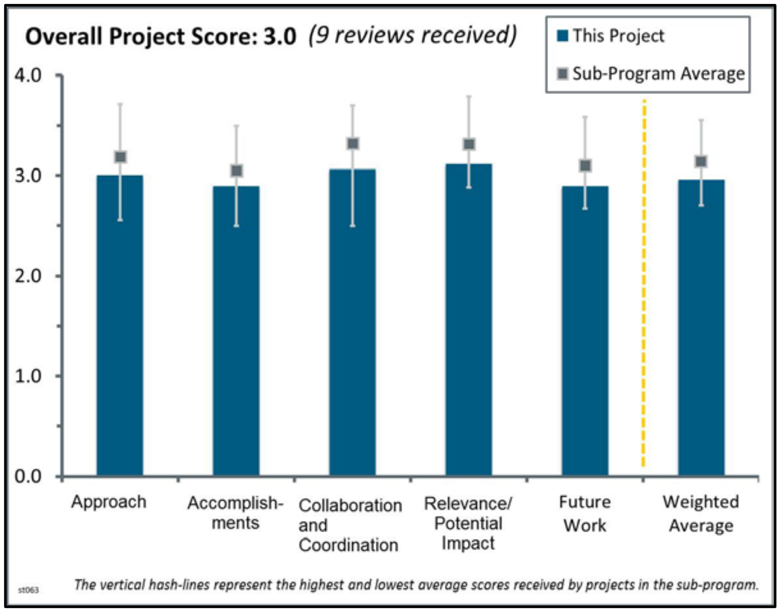
- This question is not applicable—the project is ending.
- This question is not applicable.

Project # ST-063: Reversible Formation of Alane

Ragaiy Zidan; Savannah River National Laboratory

Brief Summary of Project:

The overall goal of this project is to develop a low-cost rechargeable hydrogen storage material with cyclic stability, favorable thermodynamics, and kinetics to meet U.S. Department of Energy (DOE) onboard hydrogen transportation goals. Specific objectives include (1) development of cheaper techniques to synthesize alane (AlH_3) that avoids the chemical reaction route that leads to the formation of alkali halide salts such as LiCl or NaCl, (2) utilization of efficient electrolytic methods to form AlH_3, and (3) development of crystallization methods to produce alane of the appropriate phase, crystal size, and stability.



Question 1: Approach to performing the work

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

- Past work has focused on improving the electrochemical efficiency of AlH_3 production from $LiAlH_4$ and Al electrodes (made by compressing spent alane). This year, the focus appeared to be more on methods to crystalize the AlH_3 from the ether adduct.
- The relevant barriers addressed are intrinsic to the project design. Alane as a material has properties close to meeting many automotive targets, and the project can do no better than this. The electrochemical regeneration proposed is a relatively efficient process, and therefore, the project focus should be on attaining the highest efficiencies and yields.
- This alane project is unique within DOE. Barriers for small and medium storage applications are well addressed. (The project is not applicable to DOE vehicle targets.) The project is very well designed, feasible, and integrated with at least one commercial effort. The project is based on an elaborate, but novel, electrolytic/adduct method of AlH_3 manufacture.
- Electrochemical synthesis is very efficient, and the follow-on procedures to remove the solvent also provide control of particle size and polymorph of alane formed.
- The approach is effective at the laboratory scale and contributes to overcoming most barriers. Its efficiency should be proven while it is scaled up.
- The electrochemical generation of the alane adduct is the right approach to regenerating the material.
- This work is all empirical. It is lacking any features of experimental design. At this point, this should not be scouting work anymore, as the chemistry of alanes is well established. If there is only 80% regeneration for one step, then after three steps, less than 50% will be generated from the starting material, which is unacceptable for use in any sector. The flashpoint of ether is not stated. It is not clear that this process can be used for any real industrial processes. The team members do not understand thermodynamics. They do not understand Lewis acid-base interactions and how they work. It makes little sense that a pure solid material can have different amounts of hydrogen in different phases. There must be impurities, so nothing can be compared. It is not clear how the team will control crystallization. The project needs a physical model and does not have one. Crystallization needs to be controlled over a very narrow temperature range for success, so the whole concept is not likely to be feasible. It would be good to have examples of an industrial process in which crystal morphology is controlled and size is controlled. How the project will control dendrite formation is unclear.

- The approach, i.e., electrochemical synthesis of AlH_3 in $LiAlH_4$-based electrolyte, is relatively well established. The work seems to be focused on crystallization of alane adduct from the solution and on preparing adduct-free alane in correct polymorphic form, i.e., alpha- alane. The following remain to be addressed:
  - The achievable rate of the electrochemical synthesis of AlH_3 (perhaps per unit area of Al electrode) is unclear, and it is uncertain whether this rate is high enough for potential commercialization.
  - Concentration on preparation of adduct-free alane seems a bit out of scope. Etherated alane adducts and their desolvation have been relatively well studied in the past.
  - It is unclear how critical the concentration on recycling of spent aluminum is. Cost estimates indicate that aluminum represents the bulk of the cost; however, the cost analysis does not account for expense in collecting, necessary pre-processing, and transportation of spent aluminum.
- The stated approach is to develop a low-cost route to the synthesis/regeneration of alane consistent with onboard vehicle applications. However, as stated on slide 4 of this presentation, this is anything but low-cost, as the estimate for large-scale production of alane is stated as $100/kg, inferring $1000/kg hydrogen—orders of magnitude away from the fuel cost target. This presentation would be improved if the presenter acknowledged this fact and that the stated focus of the work is on medium-power or niche-type applications in which fuel cost may be less sensitive to success. Whereas the regeneration costs are likely unimportant for certain military applications, the first fill costs are still important if those costs are substantially greater than the rest of the system that the fuel supplies. *[DOE note: neither the presentation nor the principal investigator (PI) stated the project is aimed at vehicular application; in fact, it was indicated that the project partner, Ardica, is developing man-portable, low-power systems that use AlH_3 as the hydrogen storage technology.*]

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.9** for its accomplishments and progress.

- The contractor has made excellent progress during the duration of the project, especially during the last year. Much progress has been made with the electrolytic approach and the important crystallization of the optimum alane final product from intermediate adducts. The production of AlH_3 from recycled Al and H-depleted AlH_3 (Al powder) has shown significant cost reductions approaching DOE small and medium power storage targets. In particular, the potential to recycle alane has been demonstrated. The work has been pioneering, with many publications generated. Some practical problems remain, but this DOE project has clearly shown the potential for a solid state storage for special applications. As indicated by the PI, as well as the Ardica presentation (ST-116), alane has nearly zero probability of ever meeting DOE cost targets for light-duty vehicles; thus, these projects are focused on low-power applications.
- There is good progress in the project, with a focus on avoiding formation of dendrites of alanates during formation of alane.
- Outstanding accomplishments were achieved (80% yield).
- The basic results are very interesting, and there have been many improvements during the last years.
- It was not clear how much was accomplished over the past year. The cost analysis was the same as the previous year. The project reports a near-80% regeneration efficiency for $LiAlH_4$ in fiscal year (FY) 2015 that compares well to the regeneration efficiency of $NaAlH_4$ for FY 2014. The PI discussed two areas of progress: (1) reducing dendrite formation by using a reverse pulse technique during reduction and (2) approaches to crystallize the alane adduct to produce the optimum size and phase of alane. It is unclear whether the cost analysis changes if the reaction needs to be run in reverse pulse mode. It seems like it would affect cost, so it is not clear whether the team is suggesting this as a solution or believes other approaches are necessary. The elimination of dendrite formation is suggested in future work, but no details were provided.
- Accomplishments presented are mainly the reduction of dendrites, a demonstration of 80% yield for one step, and a demonstration of crystallization of the alpha phase. The dendrite slide shows a before and after comparison, but the other results are shown without context, and it is difficult of assess how much progress has been made in the current year. The results are generally one-off comparisons; in the crystallization

study, for example, it would have been preferable to see something like a results-based phase diagram that showed how changing the conditions led to various phases and/or crystal sizes. Such information would be more valuable for the community (and partners) than a “here’s a good result” slide.
- Progress seems to have stalled, as there were no substantial experimental results reported in this year vs. previous years. The crucial problem areas still reside in the electrochemical area, and it appears that these problems may be beyond what this team can solve quickly. Last year, an area of criticism was that the kinetics of the regeneration process were miserable; there was no evidence that this was addressed this year. One area in which there was progress was in the reduction of dendrite production, which can be very problematic for large-scale production. Progress was shown in reducing the formation of dendrites by using a pulsed electrochemical approach. This approach, however, reduces the duty cycle by perhaps 30%, thus decreasing the space-time yield of alane by probably 30% in any continuous process, and likely increasing the cost of alane even more; this is counter to the stated project goal. It was also unclear from the presentation and from the question-and-answer session whether the 80% yield of alanate regeneration resulted in 20% material that could be recycled in a second pass, or if that material was “waste”—which would be an absolute “must” to resolve. The purity of the hydrogen gas was also questioned, and while a residual gas analyzer (RGA) might be somewhat useful in looking for impurities, a long-path-length infrared cell and/or gas chromatography–mass spectrometry to look for adducts, adduct fragments, etc. might be a more appropriate and powerful set of analytical tools to judge hydrogen purity. However, this should not be a priority; solving the remaining electrochemical problems should be the priority if this project goes forward.
- The work is empirical only, without experimental design. The regeneration percentage is poor. The project team needs to be careful of the energy associated with electrochemistry. The team needs to count electrons as well. It is very hard to tell what was really accomplished. How crystallization is controlled was not well described. The cost is very high. It is not clear that the electrochemistry cost is viable in industry for large-scale production. No data were provided to indicate the nature of the catalyzed and activated Al for regeneration. Basic science is needed for what is essentially an engineering application—control of crystal structure, size, and morphology. The project does not have it. The team is still scoping the process, not working toward an industrial application. No real progress was observed.
- Accomplishments during the last year are not quite clear. There were no new publications or presentations after the 2014 Hydrogen and Fuel Cells Program (the Program) Annual Merit Review.

Question 3: Collaboration and coordination with other institutions

This project was rated **3.1** for its collaboration and coordination.

- There are excellent working collaborations with Ardica (a commercial cooperative research and development agreement) and SRI International.
- Having twice-weekly discussions demonstrates an intense collaboration between SRNL, Ardica, and SRI International.
- The collaboration with SRI International and Ardica appears to be good to excellent.
- Judging from the information given, there appears to be a good collaboration within the project.
- There are good communications and collaborations with partners, although there were signs of duplication with the sister project led by Ardica. The projects seemed to share some future work (dendrites, conductivity), and concentrating on the strengths in each project could be more effective.
- It would be useful to see an independent cost analysis from Argonne National Laboratory or Strategic Analysis, Inc., to compare with the preliminary cost analysis provided by Savannah River National Laboratory (SRNL).
- The internal group collaboration is acceptable, but the project has no outside collaborations and needs them.
- Collaborations could be expanded to other partners with relevant expertise.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.1** for its relevance/potential impact.

- Development of a low-cost rechargeable hydrogen storage material with favorable thermodynamics and kinetics, fulfilling the DOE onboard hydrogen transportation goals, is highly relevant. The utilization of alane is already demonstrated by the U.S. Army. Although the method regenerates the storage material "off-board," the approach is still highly relevant and efficient.
- Alane is one of the few current metal hydrides showing the potential to meet 2020 DOE onboard system targets.
  - SRNL is world-leading in this field.
  - The project is very important and being performed by the right team.
- The project is critical to the Program and has potential to significantly advance progress toward DOE research, development, and demonstration goals and objectives.
- The project is clearly focused on addressing barriers for regenerating alane and doing this in a cost-effective and efficient manner. It therefore has strong potential to make progress toward meeting DOE goals.
- This project has demonstrated clear advances and progress toward the Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan for small and medium off-board storage applications.
- The potential for impact is excellent, as alane can be used in a variety of applications.
- Regeneration of off-board materials is highly relevant to the Program goals, and reducing the costs of fuel from off-board regenerable systems might have a significant impact, were the effort to be successful. However, this is likely not the materials system of choice on which to expend effort to provide low-cost fuel for vehicular applications. This topical area has more impact and relevance to lower-power niche applications in which the sensitivity to fuel cost is less.
- The current and proposed work will have no impact. The cost is too high. The regeneration percentage is too low for a single step. The team members have to deal with the issue of ether vapor in an industrial setting. They have not shown that the work is practical in terms of controlling crystal size, purity, or morphology at the small scale, much less at a larger industrial scale. They are not addressing or meeting DOE needs.
- DOE has recently appeared to indicate that off-board regeneration is not of interest, so it is more difficult to justify off-board electrochemical regeneration of alane.

Question 5: Proposed future work

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

- The project is progressing according to the plan. The future focus on reduction of dendrite formation is very relevant. Developing cheaper techniques to synthesize alane that avoids the formation of alkali halide salts such as LiCl or NaCl is extremely useful.
- Critical barriers are tackled: increase the rate of production, eliminate dendrite formation, and optimize crystallization for large-scale production.
- Future work is good. The project may need some additional unexpected work to enable the scale-up of the process.
- The plan for future work is well crafted and expressed. The project should proceed as planned.
- Aside from the possible duplication of effort with the Ardica project, the proposed work is directed at overcoming the challenges identified. However, the proposed work is vague in some cases, e.g., "develop efficient method for…", "explore additives to …", "develop techniques for the crystallization…". A little more detail is needed to assess whether these approaches are likely to result in substantial progress.
- It would be prudent to measure the efficiency of removing the tetrahydrofuran (THF) from the THF-AlH_3 adduct on an authentic sample before too much effort was expended on the electrochemistry in THF. If reaction conditions are not found that minimize decomposition of alane, then this may not be a viable

direction. If alane slurry is used, it is not clear how the presence of the slurry material will affect the process. The team proposes exploring additives to increase conductivity, but no details were provided. It was believed that the project had done this in the past, e.g., with LiCl.

- Several points are unclear:
  - Which additives could be used to increase conductivity
- Whether they will affect formation of alane
  - Whether alane will be formed if sufficient conductivity is reached
  - What reducing the distance between the electrodes is going to accomplish, even if dendrite formation can be prevented
  - How much alane formation can be accelerated as a result
- The project is focusing on the wrong issues. The team is not addressing the low conversion percentage. The project needs a proposed work plan to understand the physical processes that need to be controlled, and the project does not have such a plan. The approach is too Edisonian.
- Little specific detail was expressed as to the guiding scientific principles of how the electrode and electrolyte conductivity problems were to be resolved. The "what" is obvious, but regarding the "how," it is not apparent what the specific experiments to implement the approach might be. There were no comments this year about whether any improvements in kinetics have been achieved.

Project strengths:

- This is a very well-organized and productive project led by a very experienced and professional principal investigator. The project aim is highly relevant. There has been good progress in improving preparation techniques. The project is progressing according to the plan and will likely fulfill the goals and soon finalize very successfully.
- Materials that are being used are of great safety concern, i.e., extremely volatile and highly flammable solvents, as well as unstable phases of alane. The SRNL research team members appreciate the need to be extremely careful in their operations and might do more to communicate this to their new partner, Ardica.
- The project is focused on a material that advances toward DOE targets and is investigating efficient methods for regeneration. Regeneration has been a frequent stumbling block for many promising materials.
- The project is built around a simple hydride clearly capable of approaching DOE goals for special small and medium storage applications.
- The correct approach is being taken by the correct team.
- This is a small company collaboration that has a real application in mind.
- This is good basic research.
- The project aims at cost-effective preparation of alane.
- The only strength is that alane is an interesting material. There are no others.

Project weaknesses:

- No weaknesses are observed.
- It is unfortunate that high alane cost will preclude light vehicle applications.
- It is not clear that the idea about the temperature window is 100% correct. Good crystals of the pure alane were obtained in boiling toluene and higher-boiling solvents.
- Results are frequently presented without a more systematic exploration that would assist commercial partners and others. Given that DOE is funding an associated scale-up or pilot commercialization project, the current project should concentrate on providing understanding and knowledge that would guide this. The project appears to treat each step in isolation. While this is suitable for providing the understanding, at some stage the project should address the overall electrochemical regeneration to understand what efficiencies can be achieved in a full pass from spent alane to regenerated alane. Regeneration of 80% for one of the steps will rapidly result in loss of material, and the yields and efficiencies need to be known when the whole process is strung together, preferably in multiple cycles (this may improve yields if some of the material is simply dissolved in solutions that will be reused).
- Electrochemical efficiency is strongly correlated with conductivity. Unfortunately, the optimum reaction conditions that favor formation of an adduct that can crystallize to the alpha-phase of alane are counter to the optimum reaction conditions to optimize increased conductivity. There is little information about the

cost analysis of regeneration of the consumable electrolyte ($LiAlH_4$). The presentation shares that yields >80% are achieved, starting with LiH, but the source of the LiH was not clear—perhaps it is the $LiAlH_4$ formation from Al. It is not clear whether the process will be viable if recycling of $LiAlH_4$ is not much more than 80%.

- There are many weaknesses. The team members have a poor choice of complexing agent, ether, which could be dangerous to use at the temperature needed for crystallization. They need to use experimental design tools. They need to get a real physical understanding to minimize the Edisonian approach. There is no guarantee that they can control crystal size, morphology, and level of impurities. They have no explicit go/no-go decision points.
- The team may have reached the asymptote of the remaining available improvements to make in cost. The team members may need to add some electrochemistry expertise if they hope to make additional progress at a more rapid rate.
- The electrolyte is expensive. Currents are very low, and resulting yields are low. Side reactions, e.g., formation of Li_3AlH_6, are unknown.

Recommendations for additions/deletions to project scope:

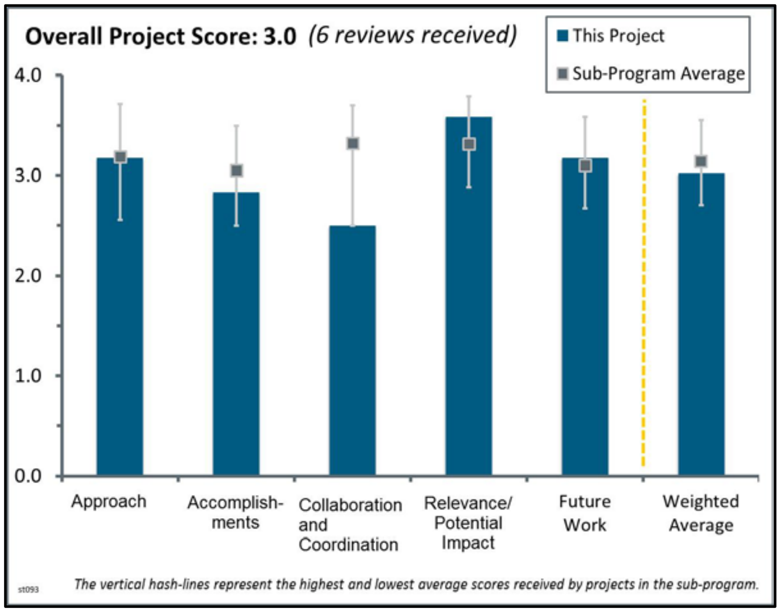
- The project should continue.
- The results from this project are very promising and call for further research and development in this field. Alane remain one of the most promising hydrogen storage materials, with very high capacity.
- The project should focus more on the electrochemical regeneration and less on the recrystallization. The project has a little over a year to run, and the best value will be achieved by overcoming the barriers to efficient regeneration of the alane adduct. The main disadvantage of poor crystallization is instability of the resulting alane; this should not inhibit multiple cycles since it needs to be dehydrogenated anyway. There is little point in perfecting the crystallization if the adduct cannot be formed with high yield and efficiency from spent material (with $LiAlH_4$ and LiH produced in situ as indicated) through multiple cycles.
- The project should (1) use experimental design, (2) focus on getting to 100% in regeneration, (3) focus on understanding what controls crystal morphology and size and get away from an empirical-only approach, and (4) deal with the impurity issue.
- The team needs to pay attention to the overall rate of throughput, e.g., kinetics, even for military applications in which fuel cost may not be that critical. If it is too slow, the reactors get too big, and the costs might then exceed even the military's ability to pay.
- The project should focus on the fundamentals of electrochemical preparation of alane rather than on solving minor issues related to scale-up. (Ardica has a separate project to do just that.)

Project # ST-093: Melt-Processable PAN Precursor for High-Strength, Low-Cost Carbon Fibers

Felix Paulauskas; Oak Ridge National Laboratory

Brief Summary of Project:

The objective of this project is to significantly reduce the manufacturing cost (>25%) of high-strength carbon fibers (CFs) by (1) introducing high-quality polyacrylonitrile (PAN) precursor melt-spinning techniques; (2) developing alternative formulations for advanced precursors capable of being melt spun in high volumes; (3) developing and demonstrating appropriate conventional and/or advanced CF conversion technologies; and (4) advancing properties, scaling, and overall economics to meet high-pressure storage targets.



Question 1: Approach to performing the work

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

- The overall approach of the project is good because it pursues melt-spun processing as an alternative to the solution processing. It is excellent that the project is focused on PAN-methyl acrylate (MA) to attempt the targeted performance rather than the vinyl acetate (VA). The basic steps of the project are appropriate and include precursor chemistry, melt spinning, and hot fiber drawing.
- The project’s approach of building on the past patents is very sound. Appropriate actions have been taken to address the equipment deficiencies experienced last year.
- This work directly addressed cost barriers for the use of CFs. The approach of trying to modify the process covered under BASF patents is straightforward.
- This project aims to prepare PAN-MA precursors and use melt spinning, which is expected to result in lower production costs by simplifying the production process.
- The approach of using melt spinning to replace wet spinning the CF precursors could have a tremendous impact; however, this project still seems to have problems progressing to make long tows for evaluation.
- The overall approach was good; however, it would have been good to see stronger support from Virginia Tech (VT).

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- Proof of concept was completed; i.e., the project demonstrated the ability to melt the precursor prior to crosslinking, resulting in an acceptable strength of the fibers. However, the project has been experiencing delays due to the engineering challenge with filament production.
- The project is finally on the verge of making significant progress with the new hot fiber drawing machine, but it is also on the verge of missing many critical milestones, and it seems as though the VT partner should be reevaluated. If DOE really wants progress made in this area, more funding to build specialized equipment will be required; however, this is probably outside the scope of the Hydrogen Storage sub-program and more of a manufacturing issue.

- The principal investigator (PI) reports difficulty with the process scale-up work, and this has caused slips in schedule. The explanation offered—that detailed direction on the process was not provided in the BASF patent information, and the nature of the engineering effort involved complications, including a combined flow, control of a complex chemical process, and a mechanical process that varies with scale—is believable. However, DOE should monitor the effort, in case assistance to the PI or project is warranted. Success may pay big "dividends."
- The equipment improvements are the most notable progress for the year. However, the improvements could have been made faster and with better collaboration on the part of the university and its resources. The resultant properties of the CFs from the switch to MA are needed.
- The project has experienced significant delays due to engineering issues associated with the spinning scale-up at VT. It is unclear what approaches are being taken to resolve these issues. A systematic approach to problem resolution would be recommended, along with a consideration of external assistance.
- Per the presentation, all fiscal year (FY) 2015 milestones have slipped. It is questionable that the roadblocks with VT will be eliminated.

Question 3: Collaboration and coordination with other institutions

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

- The collaboration on this project appears to be good, but it could be improved by including other partners to assist in the process engineering, because it appears that much of the delays are due to VT. It was encouraging that the Oak Ridge National Laboratory (ORNL) PI has made contact with the engineers at BASF who previously developed this melt-spun PAN precursor.
- The drive and collaborative effort on the part of the PI are excellent. However, with the unfortunate change in resources at VT, a similarly driven proponent within VT is very much needed. This is valuable and important research that needs to be a high priority for all parties.
- While the combined acumen of institutional partners should be adequate, it seems that additional experience is required in this effort. The PI has taken the initiative to find experience associated with the original BASF effort. The short-term outcome of this interaction should be monitored for effectiveness.
- It seems that discussion has been initiated with companies such as BASF. However, CF manufacturers should be involved to assess these engineering issues.
- The collaboration with VT seems to be strained at the moment, so other possibilities should be evaluated. The addition of Izumi International and ReMaxCo to address the equipment is a move in the right direction.
- It does not seem like there is strong collaboration with VT, and it does not seem like it will get better in the future.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.6** for its relevance/potential impact.

- The project is highly relevant because it is focused on the main cost factor (i.e., precursor) associated with the CF, which is clearly the highest cost driver in the compressed hydrogen tank system. The potential cost savings of 31%–33% would have a notable impact on reducing the cost of the tank system and fuel cell electric vehicles.
- Melt-spun precursor has the potential to make a significant impact on the cost of the CFs used in hydrogen storage, as well as on the rest of the high-performance composites industry. This research needs to become a priority with DOE, and resources should be expanded as needed, or the true potential may never be realized or even identified. The timing to bring in other sponsors or collaboration parties, such as a CF producer, is right to expand the resources provided to this project. Equipment vendors also represent a key element that is not currently being leveraged.
- Melt spinning, rather than wet spinning, the CF precursor could have a great impact on the price of tanks and could have further-reaching impacts into decreasing the costs for high-strength fiber that could be used for vehicle body parts.

- The overall relevance of the project was very good, and the technology has the opportunity to increase the throughput of the PAN precursor.
- If realized, the potential impact would be outstanding.

Question 5: Proposed future work

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

- The future plans are well developed and show a good path to success. However, a critical juncture is being reached where further resources are required to keep the project on schedule and allow the team to complete the future work plans.
- The refinement and scale-up of the process will be very beneficial to this project, which has the potential to have a positive impact on the industry.
- The proposed future work includes the necessary steps to prove-out the melt-spun scale-up. The team needs to consider contingency plans for the engineering issues to avoid further delays.
- The work plan seems reasonable, but the team should initiate communications with CF manufacturers.
- The milestones seem to be slipping, so Milestone 6, which is due on 12/31/15, will be critical. If the project hits that point, then it should be well on its way to meeting Milestone 10. However, it seems both of these will depend on the partnership with VT and the team's ability to produce lengths of tow that can be further processed and tested.

Project strengths:

- The team is very competent and knowledgeable with the precursor chemistries. The use of the melt-spinning process may simplify the production process and reduce costs of the CF, pending the economic model planned in the future.
- The PI and the approach both represent strengths of this project. With these strengths, the real potential of melt-spun precursor should be able to be identified, and further efforts should be able to be planned for commercialization.
- The key strength is the ORNL team's background and expertise in CF. In addition, the project has high importance because it could significantly reduce the CF cost.
- The overall work in this project was very strong, and it will be good to see the results in FY 2015.
- The success in this project's approach would address cost issues at a fundamental level.

Project weaknesses:

- The project is based on a cost improvement, but the economic model has not been updated for many years. The benefit of the melt-spun techniques should be quantified with a current cost model. There have been several delays, and a plan needs to be developed to ensure the project can meet the future milestones without additional delays.
- Where good progress was realized early in the year, the passing of the key leader at VT has left a deep void. This has now become a weakness that urgently needs to be addressed to keep momentum. The lack of a CF supplier and a key equipment supplier as part of the team also represents a weakness.
- There seem to be engineering challenges associated with the production and upscale of the filaments so that they could be ultimately used in tanks. There also seem to be several delays due to unforeseeable technical challenges.
- Success requires control of a number of engineering parameters that may be "art" as much as "engineering."
- There were major roadblocks with VT and ORNL, and it is questionable that they will be overcome in the near future.

Recommendations for additions/deletions to project scope:

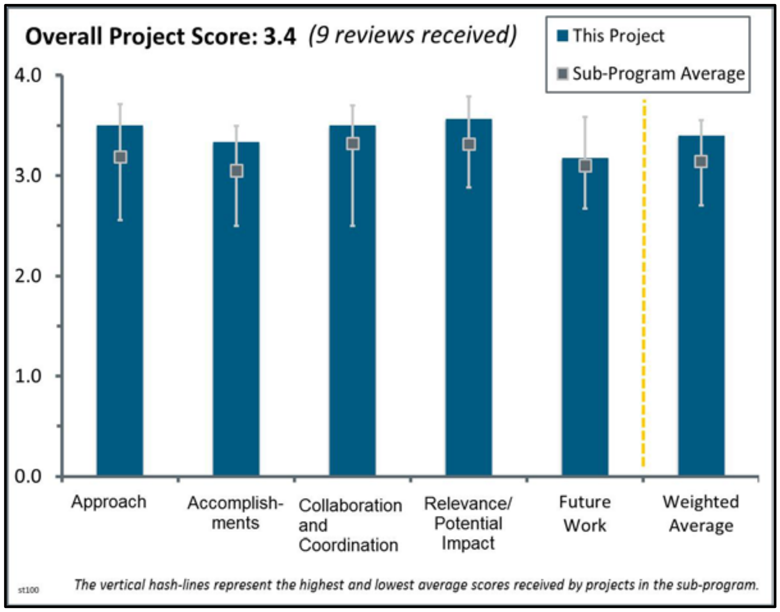
- The project should consider evaluating the composite properties in addition to the fiber properties. The team should also accelerate the economic model update to help understand the process cost drivers and influence the project earlier, rather than later, in the timing. The researchers should provide information to Strategic Analysis, Inc., to complete a cost analysis. In addition, the team should consider additional funding and/or partnerships to improve the timing and accelerate solutions to the engineering problems.

- It is highly recommended that CF producers are involved in this project to help overcome the engineering challenges and to provide cost estimates related to upscaling the processes proposed.
- The project team should redefine the priority of this project at VT and identify the key investigator, as well as consider adding a CF producer and a melt-spinning equipment vendor to the collaboration effort.
- Additional time may be needed to complete the engineering goals.

Project # ST-100: Hydrogen Storage Cost Analysis

Brian James; Strategic Analysis, Inc.

Brief Summary of Project:



The goals of this project are to (1) conduct independent Design for Manufacture and Assembly (DFMA)® cost analysis for multiple onboard hydrogen storage systems, including 700 bar pressure vessel systems, adsorbent systems (Hexcell and modular adsorption tank insert [MATI] concepts), chemical systems (alane and ammonia-borane [AB]), and metal hydride for forklift applications (Hawaii Hydrogen Carriers); (2) assess/evaluate cost reduction strategies; and (3) identify pathways to reduce the cost of onboard hydrogen storage systems by 15% compared to the U.S. Department of Energy's (DOE's) 2013 record and meet the DOE 2020 target of $10/kWh for onboard hydrogen storage for light-duty fuel cell electric vehicles (FCEVs).

Question 1: Approach to performing the work

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

- This project focuses very well on very important cost barriers via design optimization of onboard storage systems. By the end of the contract, all DOE candidate systems will be cost-quantified: 700 bar pressure vessels, adsorbent systems, chemical systems (alane and AB), and conventional metal hydrides for forklift applications. The project should provide at least preliminary answers to the long-open questions on comparative system costs. The project is well integrated with other DOE projects, including the Hydrogen Storage Engineering Center of Excellence (HSECoE). The target of 15% cost reduction of compressed hydrogen (CH2) systems under the 2013 DOE base is reasonable.
- The approach for this project was very strong. It appears that the cost analyses will be valuable for those in the industry.
- The project focused on translating technology developments into cost, which provides useful guidance to engineering teams to meet cost targets. The project seems to be well integrated.
- The approach is thorough for gathering information and putting it in a usable cost model. The one area of improvement would be the incorporation of more "what if" scenarios in those models. An example would be "what if" production volumes were significantly different from the 500,000 assumed. Another example would be "what if" 15% weaker carbon fiber (CF) were used but at a 25% cost savings on the price of the fiber.
- The project utilized DFMA cost analysis to directly compare 700 bar, Hexcell, and MATI sorption concepts.
- The project used DFMA analysis to develop estimates.
- The approach is generally good. However, there are other projects within Fuel Cell Technologies Office (the Office) initiatives that are producing data that could be relevant to the cost analysis. It seems like only partner projects are being considered in data input.
- The approach is generally effective but certainly can be improved. The cost analysis is based on single-tank, and some assumptions are very optimistic. The $/kWh should include uncertainty.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- Thus far, 700 bar CF tanks (from Oak Ridge National Laboratory CF) and two HSECoE systems (Hexcell and MATI) have been optimized and cost-quantified. Potential cost reductions have been identified, both in the tanks and balance of plant (BOP) components. The 15% reduced cost target for 700 bar CH2 has been essentially met. The three analyzed systems seem to be roughly competitive in price. For the two adsorption systems, the operational disadvantage of cryogenic operation seems to add complexities and possible lifetime restrictions. The presenter indicated there are more uncertainties in the adsorbent cryogenic systems, but the best estimates have been made based on 500,000 annual production. Work has begun on the other storage systems (e.g., the forklift tanks). It is not certain whether there will be time to complete them by the time the contract ends next year. Perhaps this important effort should be extended a few years.
- It is good that Strategic Analysis, Inc. (SA) is looking into component and system integration of the low-pressure system for the BOP. If SA is able to reduce the number of fittings used in the system, it will make the BOP much more robust and cost-effective.
- The results generated are very useful because they integrate tank designs obtained from the HSECoE.
- Considerable cost reduction was estimated from integrated design and low-cost CF—approaching DOE goals. There has been nice progress with the adsorption system. Cost estimates (~$2,500) are comparable (on an energy basis) to 700 bar CF. It is not clear that tank life has been considered in cost estimates. It seems a true cost would be normalized by life expectancy. No accomplishments were listed for chemical hydrides (alane and AB), so it is not clear whether any progress has been made in this area.
- Progress has been excellent in identifying specific targets for cost reduction, particularly through proposed integrated pressure regulators and valves, which reduces the overall complexity and risk of the systems. However, what is not clear is whether there is buy-in for fabrication of these integrated structures, and thus the question remains as to whether the identified cost savings can truly be realized.
- This is excellent analysis and work but lacking the "what if" evaluation that would allow DOE to take the results and formulate research plans. Especially critical is that the sensitivity to different production volumes be conducted and presented, possibly as a series of curves.
- For the cost comparison of Hexcell and MATI systems, the assumption should be clearly stated. The cost-per-kilowatt-hour difference between these two systems is within 5%. It is not certain that this is real and not just noise.

Question 3: Collaboration and coordination with other institutions

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

- The project has close, timely, and appropriate collaboration with other institutions; partners are full participants and well-coordinated. The project is working with the National Renewable Energy Laboratory and Argonne National Laboratory to provide complementary analysis.
- There have been numerous outstanding collaborations in this project. This includes the HSECoE, manufacturers, and national laboratories. They have been critical to the success of this project.
- It appeared that the project had strong and close collaboration between laboratories, original equipment manufacturers (OEMs), and manufacturers.
- The team engaged the tank manufacturer and OEM early on. They were able to obtain input from experts in different fields of expertise.
- There are a number of active collaborations (Pacific Northwest National Laboratory, Hexagon Lincoln, and Ford, with some input from HSECoE for cost analysis).
- Visible collaboration exists with other partners.
- Coordination with the identified partners has been excellent. However, there are a number of other ongoing Office-funded projects that could offer contributions to the cost analysis. It does not seem like there has been an effort to seek out or include these projects.

- The researchers do an excellent job of gathering the data from researchers and suppliers. The one gap is in referencing or bringing in other cost models.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.6** for its relevance/potential impact.

- The project sheds light on costs of future tanks and gives valuable information on potential paths to minimize cost. For example, the finding that the metal–organic framework (MOF)-5 tanks have costs similar to the 700 bar tanks, despite the much lower pressure, is very important and unexpected.
- The cost analysis has done a good job of identifying targets with significant potential for further cost reduction through the fabrication of integrated pressure regulators and valve systems. It remains to be seen whether resources will be allocated for these activities so that the cost savings can truly be realized.
- This is very important. If more scenarios for production volumes are included and comparisons to other cost models are made, the output of this project can be better used to guide future decisions.
- This project has given, and is giving, excellent support to DOE goals to quantify and reduce hydrogen storage system costs.
- The cost analyses that SA is completing are very relevant, and the work that is ongoing for the low-pressure system will provide a great benefit for the industry.
- This project has critical value to the DOE Hydrogen and Fuel Cells Program.
- Analysis of MOF tanks (Hexcell and MATI) seems redundant with HSECoE. Certainly, there is some value in comparing the two analyses and resolving discrepancies, but considerable funding was consumed in the process, which might have been better spent targeting key issues (such as volumetric capacity or loss of usable hydrogen).

Question 5: Proposed future work

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

- It will be interesting to learn the results for endothermic and exothermic chemical hydrogen storage carriers. An independent analysis of the electrochemical regeneration of alane would be useful.
- The plan addresses future potential paths to reduce costs of high-pressure tanks and other materials-based tanks, which is helpful in future materials selection.
- The work progression from year to year is right on track.
- The project should continue as outlined.
- Some further exploration of the benefits of integration seems reasonable. As HSECoE winds down, it is not clear what the source will be for the new input, required for these analyses. Projected MOF tank cost is similar to CF, but there are considerable outstanding issues with the MOF system (loss of usable hydrogen, volumetric capacity, etc.). More systems analysis may not be worth considering. A cost analysis of a chemical hydride, volume displacement tank may be worthwhile. However, it is probably not worthwhile to evaluate multiple chemical hydride tank designs at this stage. The key challenge with the chemical hydrides is the cost of regeneration, and this should be addressed first.
- The proposed work seems to fit nicely within the scope of that already planned. It would be nice to see inclusion (or at least mention) of other projects that might be generating data that could contribute to the overall big picture of the analysis.
- The initial estimates for the MATI and Hexcell costs are nearly identical. Given the uncertainties present in any projection, it may be better/safer to state this interpretation rather than state that the "Hexcell is cheaper" (as was done in the slides). When the MATI analysis is complete, it will be helpful if the team presents the total uncertainties (i.e., range of possible costs) for both systems back-to-back. Perhaps refueling costs over the lifetime of the Hexcell and MATI systems can be included in the analysis.
- With more OEMs announcing their hydrogen FCEV programs, there will be more and more 700 bar hydrogen tanks in the market. The future work should include some cost validation using real hydrogen tanks rather than compressed natural gas tanks.

- The reviewer looks forward to component integration and alternative materials but is a little skeptical of the relevance of the chemical storage work.

Project strengths:

- Overall, this is a strong project. Costs of MOF tanks are complex, and this type of analysis is essential.
- This is a very broad cost analysis that attempts to address all areas contributing to the cost of hydrogen storage, both in the near term and long term. The team has done a reasonable job of identifying the major contributors to overall cost and has identified a few pathways for significant cost reduction.
- Overall, this project was extremely valuable, and no major weaknesses were seen. The reviewer looks forward to seeing the progress in fiscal year 2015.
- Using DFMA, the project sheds light on costs of future tanks and gives valuable information on a potential path to minimize cost.
- The project team is very appropriate and well qualified—excellent work.
- This is an extremely important cost analysis for all important candidate systems.
- The project has excellent collaboration with different organizations.
- The project team is responsive to DOE and Technical Team suggestions and directions.

Project weaknesses:

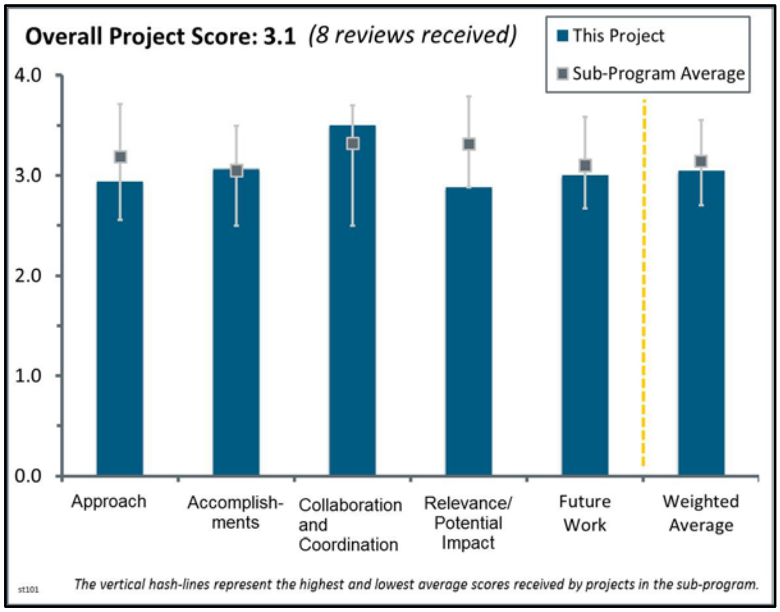
- There is only one weakness—the relevance of the chemical storage work—and it is not a major weakness.
- Three items need attention:
    - 1. Projections for different production volumes
    - 2. Projections for various cost/performance ratios for CF.
    - 3. Cross-references of existing cost models, when available.
- It would be useful to clarify the underlying assumptions of using the DFMA tools to avoid incorrect estimates, especially for materials-based tanks.
- The MOF tank analysis is redundant with HSECoE. Detailed cost analyses on chemical hydride or metal hydride tanks are probably a little premature because there are no materials that come close to meeting targets.
- Cost modeling does not necessarily cover unexpected problems and all service life considerations.
- Because the project is so broad in nature, potentially useful contributing data may have been overlooked.
- The cost uncertainty in this analysis is not clearly stated.

Recommendations for additions/deletions to project scope:

- The project is appropriately scoped.
- The duration of this important project should be extended.
- The project should get the cost-per-liter value for different hydrogen storage tank options.

Project # ST-101: Enhanced Materials and Design Parameters for Reducing the Cost of Hydrogen Storage Tanks

David Gotthold; Pacific Northwest National Laboratory



Brief Summary of Project:

The primary goal of this project is to reduce pressure vessel cost, mass, and volume in hydrogen storage systems through efficient use of carbon fiber (CF) in engineered materials for storage tanks. The project tasks focus on improving the individual constituents of materials, design, and cold gas operating conditions to synergistically enhance tank performance and reduce cost.

Question 1: Approach to performing the work

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

- The project's approach represents a sound approach to meeting the objectives. This is much improved over last year and has finally provided some real learning for the team. After working to understand the effects of wind patterns, wind process parameters, and key CF aspects, the team has been able to now focus on a portion of the original project that may yield real, commercial results: the resin system. However, the relationship of fiber, resin, and process beyond only burst strength is a key element that is not being addressed by the approach. The absence of this understanding (e.g., impact and cycle) may lead to a retraction of the learning to date and may force a new look into the winding process and/or fiber reinforcement.
- This is a good, systematic approach. The one missing factor was that a switch was made with the CF from 24,000 fibers per tow to 12,000 fibers per tow when switching from epoxy to vinyl ester, but the team did not account for the additional cost of the smaller tow.
- This project attempted to improve overall Type IV tank costs by changing alternative resin materials and investigating additives, while retaining sufficient strength to provide sufficient safety margins. The team members examined various formulations and process variables. They fabricated a number of tanks and destructively tested them to detect whether any improvements were achieved. The project team chose to store hydrogen at approximately 200 K to allow a lower tank mass. Fiber-resin properties were evaluated primarily using test specimens rather than actual vessels. In summary, a rather straightforward methodology was followed to search for better combinations.
- The approach entails the pursuit of three ideas; success in any of these three will lead to a cost reduction, and together they could be synergistic. The number of potential variables is large, but as a "scoping" study, the results will be useful. It is not clear how this work relates to the low-temperature evaluation of composite overwrapped pressure vessels to be conducted by Lawrence Livermore National Laboratory.
- The project employs a multipronged approach to reduce the tank cost by 30%. The most significant method is the use of cold gas storage. The main challenge is to maintain the vacuum in the vacuum insulation throughout the life of the tank. This challenge and the associated maintenance costs are not addressed by the project.
- Using alternate resins and alternate fibers could potentially offer improved hydrogen storage densities and reduce the cost of high-pressure hydrogen tanks.
- There may be too many trade-offs for the vinyl-ester resin, which may result in no net gain.
- More detail is needed in the Approach section, particularly with regard to decision points.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.1** for its accomplishments and progress.

- The team made significant progress last year, having built and burst tested 60 tanks. The test results for low-cost resin alternatives were excellent. The projected $0.5/kWh savings appears to be on target. The projected $0.8/kWh savings for the alternate winding pattern is now eliminated, based on the test results. The savings projected for cold gas storage was revised up from $3.5/kWh last year to $4.2/kWh. There was no explanation (analysis or data) to support the upward revision.
- The team has finally delivered on some real test bottle production and has gathered some good learning from this experience. The progress made this last year is the first notable progress and data achieved by the team. The burst results show a much improved failure mode, and efforts to understand this ideal failure mode should have been further identified or, if known, shared during the presentations. The failure mode experienced from these test specimens and the knowledge of how to produce such a pressure vessel laminate are learnings that could be shared throughout the industry.
- The project made good progress: building 60 tanks to evaluate the actual performance improvements.
- Burst tests were conducted using real tanks to demonstrate the properties of the resin proposed and to show reduction of the tank's mass. However, using alternate fibers was not as successful because of the increased shear strain.
- The lower-cost resin substitution is going well, but the nanoparticle incorporation, while progressing, does not seem to be founded on a strong scientific principle. It is doubtful that putting particles in the resin will improve load translation because that is a function of the fiber/resin interfacial strength. It will likely stiffen the resin.
- While the accomplishments have been good overall, the results under constant operating conditions (i.e., temperature) have not shown a significant potential to reduce cost.
- The team made tangible progress with the fabrication of tanks; however, results are still pending.
- While the team examined a number of combinations of resins and fabrication options for the tanks, there was little indication that any significant improvements were being achieved to reduce the quantity of materials or lower costs. The team members were able to modify their simulations to improve correlations of burst test of tanks with modeling predictions. They identified some candidates for lower-temperature (i.e., approximately 200 K) resins, but evaluations were behind schedule. It appears the team will not reach its objectives, even with a no-cost extension of the project.

Question 3: Collaboration and coordination with other institutions

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

- There was strong collaboration among all team members. The monthly call with team members; Strategic Analysis, Inc. (SA); and Argonne National Laboratory was very useful in helping SA with its cost analysis.
- Multiple collaborators across a spectrum of skills/experience appear to be contributing in useful ways.
- The collaboration on this project appears to be excellent. In particular, Hexagon Lincoln's openness and willingness to wind so many test bottles should be noted. However, the presentation did not show the fiber supplier's level of involvement—a switch from 24,000 to 12,000 fibers per tow and only the comparison of two commercially available sizings does not lend itself to optimizing the fiber surface characteristics for use with these resin systems.
- The interactions and distribution of effort are generally strong. The production and characterization of resins appear to be well handled by the partners, from the formulation stage through burst testing and modeling efforts. The only potential exception is that the specific contributions from Toray were not clear.
- There was strong collaboration with the project partners.
- The researchers have assembled an excellent team.
- The current collaborations with tank manufacturers are useful.
- The collaboration appears to be working.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **2.9** for its relevance/potential impact.

- The work is directly relevant to the DOE objective of bringing the system cost down to $10/kWh by 2020.
- All of the project goals directly support hydrogen storage objectives.
- Reduction of the hydrogen tank mass and cost may be enabled with the proposed designs.
- The primary focus of this project has been to substantially reduce the cost of the most expensive component of the Type IV hydrogen storage vessels, while still retaining adequate safety margins and the durability of these tanks. Although a number of alternatives were examined, there do not appear to be any resin formulations developed to significantly impact the cost of ambient temperature vessels. Furthermore, variations in winding geometries were not found to improve vessel properties. While the development of a 200 K storage vessel will potentially reduce system mass, volume, and cost, issues related to mechanical behavior over the desired operating conditions and identification of suitable effective insulation materials have not yet been clarified.
- The work on developing a new resin system is notable and could improve the prospects for hydrogen storage. However, this aspect alone will not advance the project to achieve its goal. Based on last year's comments, the change to a 500 bar storage vessel may have much merit, and if this is truly believed within the Hydrogen Storage sub-program, then the specifications and targets for the hydrogen storage efforts should appropriately reflect this result. The decision on whether to proceed with a 700 bar or 500 bar system should be made. This decision could then have a significant impact on the overall goal of the Hydrogen and Fuel Cells Program.
- The project is certainly relevant. Aside from a change in operating conditions (to cold gas), there does not appear to be much potential to significantly change the cost of gaseous storage.
- The project is well aligned. The use of the lower-cost resin may provide some benefit, but the nanoparticle portion of the work has not shown much progress.
- It seems like the cost savings achieved with the vinyl ester and the cost increase due to the 12,000 tow may result in zero net gain.

Question 5: Proposed future work

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

- The proposed future work is appropriate for wrapping up this project.
- The proposed future work is sound and consistent with the work plan.
- The future work is well planned. However, the improved modulus of the laminates must be considered in more types of testing analysis than just burst strength. The 60 bottles that have been produced should be considered for additional test analysis using natural gas vehicle type test standards to determine the effects of impact, fatigue, and cycling. Cold testing and thermal cycling relationships using the modified vinyl-ester resin system need to be accelerated to understand whether this would be a barrier in the near future.
- The burst, fatigue, and impact testing will be very beneficial, but more work should be done to reduce the cost of the 12,000 tow and bring down the cost of the system.
- In the remaining months of this project (with a no-cost extension due to the lack of some key equipment), the team will primarily validate some of the unresolved postulates and complete burst and other tests. It is less clear how far the team will progress toward finalizing its full-scale cost models with updated experimental results. Completing the low-temperature characterization also seems to be in question.
- More detail should be provided concerning future testing of insulating materials' cost and performance.
- In addition to completing the initial test goals, the team should also pursue the proposed fatigue testing.

Project strengths:

- The five-member team brought diverse viewpoints and expertise to address the challenging issue of reducing costs of high-pressure hydrogen storage vessels. Another positive is the sequential approach of

forming and testing modified resins, fabricating prototype tanks with property testing, and conducting burst tests.
- Project strengths include that the team's original equipment manufacturers in both the tanks and resin areas have superior expertise.
- Strengths include the knowledgeable team and its appropriate expertise, as well as the project's unique concept.
- The teams involved must be considered a strength of this project because all of the companies have the necessary resources and expertise to complete this project.
- An excellent selection process was used for determining which lower-cost resin to use. The validation test plan is appropriate.
- Overall, the project was very strong. The vinyl-ester resin has potential, but further testing is required.
- The project's straightforward approach to investigation is a strength.

Project weaknesses:

- The project appears to be dancing around an optimized tank design with a target pressure lower than the original target. The decision needs to be made that savings will truly be achieved if the team is allowed to let the future work address the lower bottle properties, and that this work will fully show and prove these savings. Also, the lack of non-burst testing means the team has not completed the full picture on the performance of the fiber, resin, and process improvement combinations. Degradation in impact, fatigue, or other commercial specifications could negate any progress to date.
- The presentation did not include the expenditures to date, making it difficult to gauge progress relative to budget. The potential cost savings from resin modifications appear rather modest, at about 7%. The threshold for continued investigation of resins is unclear.
- The intended systematic feedback loop between materials development and mechanical strength did not seem particularly effective in producing fiber-resin combinations with greater mechanical strength and improved cryogenic properties. It was unclear how active the Toray partner was in this project.
- The lion's share of the projected cost reduction relies on the success of cold gas storage. There are many uncertainties and unknowns that have yet to be discovered. Therefore, the intrinsic risks are high, and there are no alternative pathways within the scope of this project to mitigate the risks.
- With the cost savings from vinyl ester and the cost increase for the 12,000 tow, the project may end up revealing zero net cost savings.
- It is necessary to further consider real-life operating conditions when these new systems are tested. For example, the effect of operating temperature needs to be considered under the right cycling conditions.
- The project appears ambitious, in that the effort could have been split into several projects. It may overlap with other DOE efforts.
- The nanoparticle work is unlikely to produce positive results.

Recommendations for additions/deletions to project scope:

- Rather that focus on developing a full-scale tank model, emphasis should be placed on completing as many characterization measurements at low temperatures as possible to correlate performance with predictions and subsequent final burst tests. A thorough documentation of these relationships would serve future studies on identifying robust and less expensive Type IV storage tanks.
- The practicality of a low-temperature gaseous system (including changes on the infrastructure side) is not clear. It would be good to know the potential failure modes and their effects on loss of thermal control/insulation.
- The team should complete the modeling effort to optimize the pressure rating and tank size for hydrogen storage. It should take very seriously the impact, cycle, and fatigue testing efforts to complete the picture on whether the new resin, fiber, and process combination produces a superior pressure vessel.
- It is necessary to further consider real-life operating conditions when these new systems are tested. For example, the effect of operating temperature needs to be considered under the right cycling condition.
- In light of the success of the low-cost resin tests, the principal investigator may want to consider testing tanks that use other low-cost resins that have even lower viscosity than XR-4079.

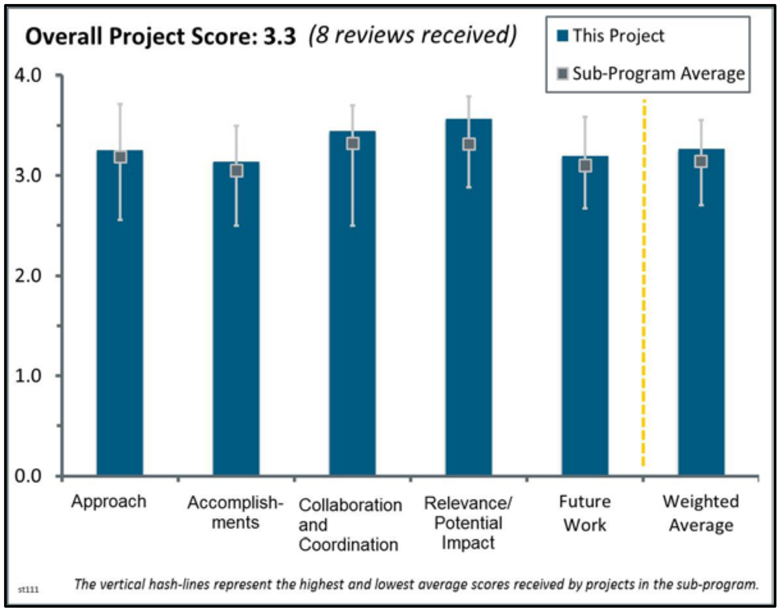
- The project team should delete the nanoparticle work and focus more heavily on validation of the lower-cost resin.
- There are no recommendations at this time.

Project # ST-111: Thermomechanical Cycling of Thin-Liner, High-Fiber-Fraction Cryogenic Pressure Vessels Rapidly Refueled by Liquid Hydrogen Pump to 700 bar

Salvador Aceves; Lawrence Livermore National Laboratory

Brief Summary of Project:

The objective of this project is to demonstrate the cryogenic durability of 12-inch thin liner hydrogen storage vessels cycled 1,500 times and able to achieve 50 gH_2/L_{sys} and 9 wt.% hydrogen. The project will also evaluate a liquid hydrogen cryo-pump that can rapidly and consistently refuel cryogenic onboard hydrogen storage to 700 bar, with the potential to exceed U.S. Department of Energy (DOE) weight and volume targets with substantial dormancy improvement for modest cost with ideal scalability.



Question 1: Approach to performing the work

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

- The project approach is well organized, with proper milestones. The strength of the approach is shown in the project's ability to reset priorities as obstacles are experienced and further understanding is gained. The focus on developing and implementing proper safety standards for fill systems is notable, and the project's ability to couple the development of these safety standards with proper fill and vehicle storage equipment should result in standards that will be established for this industry. In summary, the practical approach will be able to safely determine the effects of cycling through the filling process and lead to standards that may become industry standards.
- The approach addresses quantity barriers directly. Building and qualifying a facility capable of performing the necessary tests is important by itself.
- The work plans appear reasonable to achieve the goals of evaluating thermal cycling of small 700 bar tanks. It is especially positive that there is an allowance for testing a more "conventional"-looking system in the event that the more aggressive designs prove insufficient for the application.
- This project consists of two major tasks:
  - Design, fabricate, characterize, and pressure/temperature cycle prototype 5 kg-hydrogen capacity 700 bar cryo-compressed vessels that may meet ultimate DOE gravimetric and volumetric targets.
  - Establish a unique pressure cryogenic liquid hydrogen filling and testing facility to demonstrate critical operating behavior, integrity, and durability of the cryo-compressed vessels. This is an ambitious plan but has important objectives.
- The project addresses the critical barriers in hydrogen storage, such as volumetric capacity, gravimetric capacity, and possibly cost; however, dormancy can be a tremendous issue with this technology, and super multilayer vacuum insulation should be a focus for this project in the design of vessels. The focus on achieving 700 bar cryo-compressed operation is concerning because (1) this technology is not widespread, (2) it is uncertain that there has been a complete analysis of the energy and cost demands of this delivery technology, and (3) it is not clear that it will ever be available on a widespread commercial basis.
- The project approach is focused on 700 bar cryo-compressed operation, which is interesting, although it combines two difficult parameters (high pressure and extreme cold). The benefits of a 700 bar demonstration rather than using lower pressures should be clarified. The project should not reduce the

priority of the insulation. In fact, this effort should be increased because the insulation is the key feature that could enable or prevent this storage technology from being used onboard a vehicle.
- The approach is generally OK. However, there should be some safety and cost comparison of a traditional 700 bar compressed gas system versus a cryogenic compressed system.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.1** for its accomplishments and progress.

- The accomplishments realized to date (creation and practice of the safety standards for liquid hydrogen stations) are impressive. The development of a 12-inch diameter tank with its improved volumetric efficiency is also notable. It should also be noted that the team has postponed certain parts of the project to ensure safety without compromising the overall flow and targets of the project. The physical equipment installation is impressive.
- As of this reporting, progress is good. Hydrogen Safety Panel (HSP) participation drove consideration of a variety of factors, including a thicker-walled containment vessel, which has been incorporated. Progress toward completion of the facility alone is a substantial accomplishment.
- The demonstration system is quite impressive.
- Considering the bureaucratic challenges of safety and permitting a unique high-pressure cryogenic hydrogen facility, progress with installation and commissioning has been good. It would have been good to see more progress on completing the design and fabrication of the 12-inch cryo-tanks. It was not apparent how soon these prototypes will be available for evaluation and testing.
- Because of the need for facility design and safety approvals, it is difficult to tell how much progress has been made toward the goal of evaluating thermal cycling. However, this will likely be overcome before the next review, now that the necessary facilities and approvals for the thermomechanical cycling are in place.
- The vessel modeling and manufacturing are progressing toward the goals, but it seems like the station testing facility is falling somewhat behind schedule, which could have a major impact on the project’s ability to meet future milestones.
- The progress on the pump performance appears to have been delayed. The timing indicates the project is near the midpoint, and a significant amount of effort is needed to accomplish the deliverables.

Question 3: Collaboration and coordination with other institutions

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

- Coordination between partners on the facilities design side seems to have been very effective in getting things up and running. Production of the tanks needed for evaluation also seems to be proceeding well at this time.
- This team has been working with an original equipment manufacturer (OEM) and the expert in this area for a number of years. The team is well equipped for this kind of study.
- The partners are well known. Collaboration includes working with the HSP, which brought in wide-ranging safety acumen.
- There seem to be excellent interactions among all of the partners in this project. The level of communication appears high, with substantial cooperation on complementary capabilities.
- In the early phases of this project, Linde appears to have been a very important and cooperative partner. BMW and Spencer also show good involvement, but it is difficult to fully understand BMW’s influence and participation. The presentation of the project could be improved to better understand the depth of the partners’ involvement, because one could derive from the presentation that Lawrence Livermore National Laboratory (LLNL) is yielding very strong control over the project. Next year’s review should more clearly show the industrial partners’ influence and resource participation.
- The project involves collaborations with Linde, BMW, and Spencer Composites, which are very appropriate collaborations. It would be nice to see some of the other gas companies involved in order to demonstrate complete commercial market pull and support for the technology.

- The project appears to have the right mix of industry leaders. An improvement could be to add a domestic OEM and/or a series-production tank supplier.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.6** for its relevance/potential impact.

- This project directly addresses critical engineering issues with both the vessel design and construction and the filling of nominal 700 bar cryo-compressed hydrogen storage systems. It also examines lifetime behavior on the operating life of the cryogenic hydrogen pump and the pressure/temperature cycling of the tank. These results are important to establish whether cryo-compressed tanks are practical onboard storage systems for vehicles. LLNL is also breaking new ground toward safety regulations of future liquid hydrogen dispensing stations for commercial applications.
- This project is very relevant to the overall goals of the Hydrogen Storage sub-program. Though much of this work is based on developing safety standards and determining the effects of cycling, this is critically important to creating standards for commercialization. The provisional patent and records of invention need to show authorship and relevance to better understand whether this project is creating new, applicable technology or simply creating standards for the safe commercialization of hydrogen storage.
- Understanding both the effects of thermal cycling on the thin-walled cylinders and the effects of repeated 700 bar fueling on the pump system is critical for implementation of hydrogen as a fuel source for consumer vehicles.
- The project is highly relevant because cryo-compression is estimated to have high volumetric and gravimetric energy densities, but robustness testing is still required to increase confidence in the technology.
- Successful demonstration of composite overwrapped pressure vessels (COPVs) for cryogenic liquid hydrogen service at 700 bar would be a substantial technology coup and advance progress toward realizing DOE volumetric capacity goals.
- This technology can potentially have a key impact on the DOE Hydrogen and Fuel Cells Program (the Program).
- The project aligns very well with the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan and specifically, the goals of the Hydrogen Storage sub-program, but it is critical at this juncture to get support across all gas companies before continuing to invest in this technology.

Question 5: Proposed future work

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

- Overall, the future plans are good. It is agreed that the project should postpone fabrication and testing of the 163 L 700 bar vessel until Phase III of the project. Assessing the properties of the 65 L prototype is much more valuable. Completing construction and getting safety approvals for filling/testing the pressurized liquid hydrogen system looks very time consuming, and it will probably require considerable effort to achieve the goals specified for this project. Obtaining safety approval and licenses may need more time than estimated in the schedule.
- The future work is well organized and follows the original approach of the project. Completing the fill station and initiating the much-needed cycling work is very good. The thin liner technology includes a good plan, but the small number of candidates and small DOE investment do not appear to provide enough scope to optimize the tank design.
- The project, as currently envisioned, will go a long way toward addressing currently recognized technical barriers. However, the project will presumably identify additional barriers as it proceeds.
- The project team has a well-structured technical approach with go/no-go milestones.
- The future work represents a logical progression from current efforts.

- The cycle testing and station build-out are critical for this technology to move forward. The fact that the station's initial 700 bar operation is not scheduled until July 2015 does not give much room for error in meeting the 1,500-cycle go/no-go in December 2015.
- The future work is aligned with the deliverables. Further evaluating the vacuum insulation for robustness and durability could benefit the future work.

Project strengths:

- The project is pushing to demonstrate the performance and reliability of a 700 bar cryogenic hydrogen filling station for cryo-compressed storage vessels. Behavior of the prototype vessel is very important to ascertaining whether this would be a viable and safe solution for fuel cell vehicles. LLNL and BMW each have more than a decade of experience in the development and testing of cryo-compressed hydrogen vessels, while Linde is a commercial vendor of liquid hydrogen.
- The accomplishments in creating safety standards and in understanding safe pumping conditions and liquid hydrogen handling reflect the strength of the project. These are key areas critical to the commercialization of hydrogen as an effective alternative fuel. The design of a thin-liner pressure vessel will also prove to be a key technology in the future. The well-organized approach and the phased approach to achieving targets are also strengths.
- Data generated during the course of this project will contribute greatly toward optimizing designs for both 700 bar pressure vessels and for the associated fueling systems.
- The project provides a useful assessment of the cryo-compressed tanks in an extreme mode to evaluate fatigue with various tank designs.
- This team has been working in this area for many years and is well positioned to conduct this kind of study.
- This is a simple, direct approach to evaluating COPV technology for cryogenic hydrogen storage.

Project weaknesses:

- The effort is ambitious. It relies on the facility test system to perform challenging testing that involves numerous cycles and tests in parallel in a fashion that has not been demonstrated elsewhere.
- There are no obvious weaknesses at this time.
- This project may be too broad in scope in addressing handling, storing, and pumping as well as cycling influences from a newly designed tank. This project, though very relevant, could actually have been split into two projects. This larger scope appears to force LLNL to take a controlling stance and to segregate the industry partners, all of whom are focusing on their own influence but not learning from one another.
- Considerable resources and labor are required to fabricate and certify both the filling/cycling facility and the prototype and larger vessels. The important issues of the dormancy and thermal stability of the vessels may not be getting sufficient attention.
- The project is focused on too high a pressure and should consider additional work in the area of insulation robustness.
- The acceptable hydrogen boil-off rate at the fueling station, both from the regulation side and from the experimental validation side, is not clearly stated.

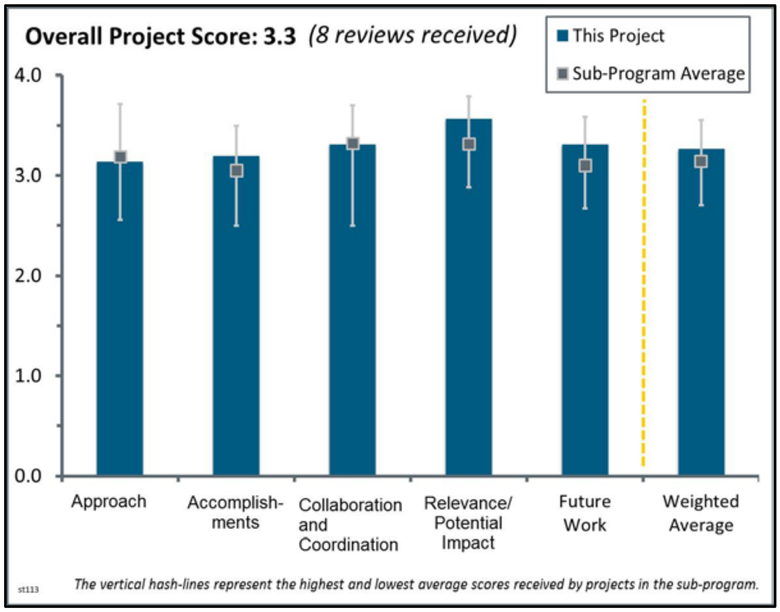
Recommendations for additions/deletions to project scope:

- There are no suggested changes in scope for the project at this time.
- None should be considered.
- This project needs to focus on closing the fill station phase, which will allow focus on the cycling phase to understand the filling and emptying influence on thin-walled tanks. More information on the liners would help explain why the number of candidates is so small.
- With so many years of effort spent in this area, there seems to be only little interest from the OEM side, other than one OEM that showed strong support. The team may consider contacting other OEMs and forming a steering committee for this project.
- The project could benefit by further evaluating the vacuum insulation for robustness and durability.

Project # ST-113: Innovative Development, Selection, and Testing to Reduce Cost and Weight of Materials for Balance-of-Plant Components

Chris San Marchi; Sandia National Laboratories

Brief Summary of Project:



The overall objective of this project is to identify an alternative to high-cost metals for high-pressure balance-of-plant (BOP) components for onboard hydrogen storage systems. The project goals are to (1) reduce weight by 50%, (2) reduce cost by 35%, and (3) expand the scope of materials of construction for BOP.

Question 1: Approach to performing the work

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

- This project aims nicely at the U.S. Department of Energy (DOE) barriers of system weight and cost via metallurgical optimization of austenitic stainless steels (especially lower Ni content and process strengthening) of the BOP components of hydrogen storage systems. This is a long-neglected, yet very important, area. Sandia National Laboratories (SNL) have world-renowned expertise in hydrogen materials interactions and safety. SNL will use fatigue testing in hydrogen environments, the most logical testing procedure for the purposes of the project.
- This project employs a two-pronged approach to identify low-cost, lightweight alternatives to annealed 316L stainless steel for use in BOP components. The computational effort complements the experimental testing program to identify new alloys.
- The approach of evaluating low-Ni steels (lower cost) on the basis of fatigue life and stacking fault energy (SFE) theory makes good sense. If a methodology can be validated, this would be an advance.
- Overall, the effort's approach is well-thought-out. The integration of the experimental and computational paths could be better defined in the approach section (details can be found in the future work section).
- It is always a good approach to have both sides (experiments and simulations) together in one project. However, there must be a strong coupling with experiments and simulations. Even if it is one project, it still has some characteristics of two different projects. The planned experimental work and the planned computational work have to be attuned to each other in a better way. If this is already happening, the presentation should emphasize it more. The experiments should give results that can be used or should be reproduced by the simulations and vice versa. In that way, a much deeper understanding could be gained.
- The approach is generally good, including both experimental and computational effort. However, there is no clear indication of how the experimental results will be used to validate the computational model.
- The alloys to be examined computationally are all compositionally complex (i.e., typically contain many components). It is unclear how this complexity will be addressed in a high-throughput-compatible fashion, given that large cell sizes may be required (an example cell with 400+ atoms is given as an example). In addition, the local chemical composition in the vicinity of the stacking fault could have a strong effect on the SFE; this ordering may differ from alloy to alloy. Sorting this effect out will also limit the throughput of the calculations. It is unclear whether the SFE alone is a good descriptor for the performance of these alloys in this application. This is mentioned in the presentation, and a literature search is proposed to address it. It is not clear what the fallback plan is if a good correlation is not possible. Related to this, calculating the SFE is a good starting point, but it is not clear why unstable stacking faults (i.e., barriers along the deformation path) or twinning energies are not part of the research plan.

- Evaluating lower existing Ni-containing alloys may or may not substantially reduce the overall BOP costs, especially at high volumes. The costs are higher at low volumes, but much of this work, especially developing new alloys from the computational effort proposed here, will take time and may not have much of an impact in the near term. A greater reduction on BOP costs may be gained from designs that eliminate valves, long tube lengths, etc., than from changing from one stainless steel material to another.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- The results obtained so far are very good (considering that the project was started only one year ago). The project has characterized 316L stainless steel as a reference system and found it to be very suitable for hydrogen applications. The team has tested ab initio calculations for Ni. The model is consistent with known literature. The computational effort for ternary Fe-Cr-Ni stainless steel alloys has been assessed. Everything is in line with the overall project and DOE goals.
- This is Year 1 of the project. The team has made very good progress toward the milestones. In the slide on relevance and objectives, the project goals are to reduce system weight by 50% and system cost by 35%. It should be clarified in next year’s presentation that the reductions are intended for BOP components only (not the system). BOP cost consists of materials cost, processing cost, and assembly cost. It is not clear whether the project goal is for a 35% reduction of the total BOP cost or just the materials cost.
- The project is less than a year old and is effectively still in the startup stage. However, much early progress has been made in planning, collaborations, and prior technology assessment. The contractor has been able to start some computational (density functional theory [DFT]) and cost reduction efforts on paper.
- The plan described is straightforward, and progress as stated follows the plan. Accomplishments thus far for the materials chosen for evaluation are proving out the approach.
- Given the fact that this project is new and only spent $300,000, the accomplishments and progress are reasonably good.
- Accomplishments to date are reasonable. About one quarter of the project period has passed, with about one eighth of the budget expended.
- This is a new project. Most of the effort thus far was to benchmark existing 316L stainless steel.

Question 3: Collaboration and coordination with other institutions

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

- There are excellent collaborations with a fatigue testing organization, fitting manufacturer, and stainless steel producer.
- SNL has assembled a well-qualified team. The partners are instrumental in the success of this project.
- The project has good collaboration, with each party’s responsibilities well defined.
- Having a component manufacturer (Swagelok) and steel manufacturer (Carpenter Technology) on the team for advice and direction is good.
- Partners are all experienced, and the mix is appropriate. It is early in the effort, and the contributions of the partners are not yet clear.
- Collaborating institutions have good reputations.
- Collaborations exist with SNL, Hy-Performance Materials Testing, Swagelok, and Carpenter Technology. Internal collaboration (experiments and simulations) is essential for the project and should be deepened.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.6** for its relevance/potential impact.

- This project is highly relevant to DOE Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan. The project has a previously unexplored potential for BOP cost and weight reduction.
- Identifying suitable materials that result in cost reductions and communicating these results to materials and component manufacturers could help make appreciable progress toward DOE goals.
- This is a very important project and will have critical impact on the Hydrogen and Fuel Cells Program.
- This project could make a big impact on cost and weight associated with BOP.
- Hydrogen embrittlement is one major obstacle to the cost-efficient commercial usage of hydrogen technologies.
- The work is directly relevant to the DOE objective for bringing the system cost down to $10/kWh by the year 2020.
- If a methodology for identifying low-cost materials and evaluating necessary design data can be validated, the cost of BOP components could be reduced. Designers would have greater flexibility in identifying materials for use.
- This work should lead to a better understanding of the merits of various high-strength steels in hydrogen service. However, the risk is high that the project will not meet its short-term objectives of having an actual impact on near-term BOP costs simply by changing out materials for others with somewhat less Ni content in existing components.

Question 5: Proposed future work

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

- Both planned experimental and computational work is focused on critical barriers. The question as to whether a correlation exists between SFE and experimentally measured effects of hydrogen on mechanical properties is essential for this project and will be reviewed.
- The proposed future work is sound and consistent with the work plan. It should be noted that the Al-6061 alloy is increasingly being used in BOP components for hydrogen systems. Therefore, it is recommended that future work include a comparison of the results (cost and weight) with the Al-6061 alloy.
- This project has a well-scoped project plan with clearly defined go/no-go decision points.
- A decision point on whether modeling can be used to predict SFE and whether SFE can be correlated with other material properties should be accelerated.
- The integration of experimental and computational approaches is carried through the effort in a rational manner.
- Pursuit of the plan by examining candidate low-Ni alloy is logical.
- Future work is very appropriate.
- There are some concerns with the computational approach. The future experimental work seems sound.

Project strengths:

- The team is very experienced in this area and has done some similar work for others. The team can move quickly in this project by applying lessons learned from other projects.
- Team members are experienced and well qualified.
- This is a well-thought-out project with potential to materially reduce BOP component costs.
- Experimental and computational approaches are combined, which is very good.
- This is a metallurgical/mechanical properties look at containment and BOP components.
- The project has a straightforward approach that should be pursued as is.

- The experimental program to evaluate other potential lower-Ni-content steel for hydrogen service has potential.

Project weaknesses:

- This reviewer cannot identify any project weaknesses but is not a metallurgist.
- Modeling efforts need to be evaluated quickly to see whether they indeed have the potential to make a difference during this project. It appears that this is a longer-range research effort.
- It is not clear how the computational model will be validated.
- The project focuses only on austenitic stainless steels.

Recommendations for additions/deletions to project scope:

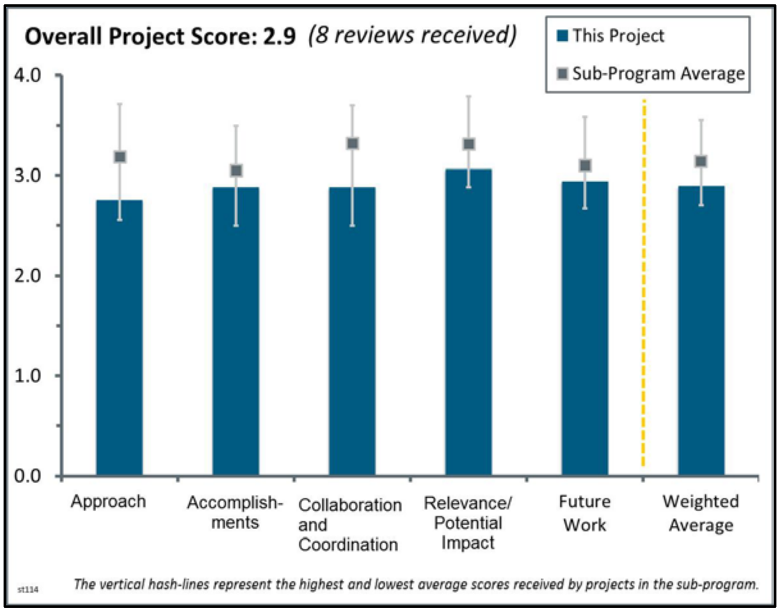
- Computationally derived alloy compositions may not be available commercially (or at all). The cost implications of uncommon alloys should be explored.
- The team members should try to work very tightly together; experimental and computational work should overlap significantly.
- The project should continue experimental work and decide whether modeling efforts should continue based on whether results can be provided in the proposed project time frame.
- The computational component has the potential to make a strong contribution to this project. However, for that to be the case, the relationship between the properties to be calculated and performance needs to be more clearly demonstrated. Fortunately, the project team seems to be well aware of this issue.
- Al-6061 should be included in the comparison of results/analysis.
- The team should consider including Al alloys in the study.

Project # ST-114: Next-Generation Hydrogen Storage Vessels Enabled by Carbon Fiber Infusion with a Low-Viscosity, High-Toughness Resin System

Brian Edgecombe; Materia

Brief Summary of Project:

The objective of this project is to develop and demonstrate a 700 bar, Type IV tank with (1) a reduction in carbon fiber (CF) composite volume by 35%; (2) a cost of composite materials of $6.5/kWh, which is an important element of the U.S. Department of Energy (DOE) 2017 system cost target of $12/kWh; and (3) maintained performance (burst strength of 1575 bar and 90,000 cycle life).



Question 1: Approach to performing the work

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

- The approach is to use a polyolefin-based resin that has low viscosity in an infusion process to make a Type IV composite overwrapped pressure vessel (COPV) to reach a cost of $6.5/kWh for the composite portion, demonstrate performance of 1.8 kWh/kg at 700 bar, and meet an overall cost of $12/kWh. The infusion process can drastically reduce voids, which will increase fracture toughness, and the lower viscosity should increase wetting to increase the overall tensile strength of the composite. If successful, this would have a large impact on the growth of fuel cell electric vehicles (FCEVs).
- The project offers new processing of CF wounds through vacuum infusion processing of the fiber wounds to reduce the voids content. Ultimately the project would like to use new winding patterns. Although the project strives to reduce the tank's cost, there exists no preliminary calculations that help predict extra costs that may be introduced through this additional processing
- The approach is OK in general, but there was a lack of manufacturing complexity comparison between the "dry" and "wet" process. When using a new resin for onboard application, the resin property comparison (slide 6) should also include the effect of temperature and hydrogen.
- This approach may or may not work out, but is worth pursuing. The proposed plan of attack makes sense.
- The approach generally seems to make sense. However, the lack of real data, particularly in comparison to conventional carbon/epoxy composites makes it very difficult to tell if the approach is truly viable to achieve the desired goal of such a huge reduction in CF content.
- The general approach of the project identifies a potential break-through technology, but does not adequately address the benefits and how it addresses the cost goals of the Hydrogen Storage sub-program. Critical cost to produce items such as winding efficiencies, resin cost, cycle time, etc. are not addressed and thus, leave this project with little focus. However, the resin technology is excellent, and the effect of reduced void content is valid technology.
- The work is based on an assumption that lowering void content in the resin will allow for substantially improving the composite material properties. Void content affects resin's dominated properties. Pressure vessels are designed to minimize the impact of resin properties and maximize the use of the fiber properties. Therefore, minimizing void content further is unlikely to have a big impact. The approach is primarily a vacuum assisted resin transfer molding (VARTM) process. Flat plaques were produced, and the void content was measured, but no data was given. This has been done many times by many researchers. The team does not have a baseline of what void content is in current tanks, so it does not know how much it should improve.

- The approach is based on the premise that tank wall thickness can be reduced by eliminating voids, improving fatigue properties of the resin, and developing dry-winding patterns. The linkage from these improvement tasks to the reduction in wall thickness for a current state-of-the-art 700 bar tank was not established. In fact, the voids are low in current tanks and fatigue is not a design driver for Type IV tanks, so it is unclear if the approach will result in any improvement. The dry-winding approach is interesting, although further investigation is needed to ensure proper wetting of the fiber and to confirm a lower cost including the additional process steps for the vacuum infusion.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.9** for its accomplishments and progress.

- Considering this is a new project and for $350,000, the team has achieved a lot.
- The team has initiated the winding process through vacuum infusion of a filament wound and investigated the presence of voids. This effort is coupled finite element analysis (FEA) modeling to understand the effects of voids on the mechanical properties and explore new resins
- Accomplishments suggest that the project should continue.
- The principal investigator has down-selected the resin based on panel tests from a triaxial wound fiber. Performance has been demonstrated in previous projects at the panel level, but the projects could not get the performance to translate to the tank, primarily because of winding conditions.
- Additional information could have been provided regarding the resin selection including material and process cost. The consideration of the baseline epoxy properties and selection process of alternative resins would have enhanced the accomplishment. It was unclear that how the infusion of the thick panel fabric related to a reduced thickness dry-braided tank. More effort is required to demonstrate the feasibility of a 35% CF reduction.
- The ability to infuse low void content panels using the Materia resin system was already well known. The efforts to make a thick, flat laminate are notable, but not necessarily new or applicable to this project. The effect of this resin in a pressure vessel are not yet known and key to achieving a tank with 35% less fiber content. There does not appear to be any tangible, new progress as the resin system was, presumably, already known. Pressure vessel production should have been a higher priority and earlier accomplishment.
- The accomplishment of the proposed work seems just a little behind schedule, but because they did not establish a baseline from existing tanks, they do not really know what they are shooting for as far as final void content. No cost model projections or goals were given.
- The only things really demonstrated at this point are a very low-viscosity resin with high elongation, and the production of a very low void content in a thick panel. Neat resin properties that could be used in predictive models and composite data, particularly in comparison with the baseline system, were not available and probably should have been. Wall thickness of the baseline case tank was not specified—this will be where the reduction of fiber comes from. The fabric panel thickness of 32 mm is about 30% thinner than current wall thicknesses for 700 bar pressure vessels, but there was no modeling presented to support the contention that this is, in fact, possible. The bottom line is that some modeling based on constituent properties would have helped to provide evidence that this approach is feasible for reducing CF content by 35%. At this point, the evidence is not convincing.

Question 3: Collaboration and coordination with other institutions

This project was rated **2.9** for its collaboration and coordination.

- The partners appear to have clear roles and responsibilities. It was good to see the addition of Hypercomp Engineering and Powertech Labs. The project would benefit from having a series-production tank manufacturer either as a partner or in a consulting role.
- The collaboration with Montana State University (MSU) and Spencer Composites are appropriate and well defined.
- The team appears knowledgeable and experienced.

- It appears that there are decent collaborative relationships in place. However, the contributions of collaborators have been minimal at this point in the project (at least based on the material presented).
- The project has collected the right collaborative partners with each having distinct tasks. It remains to be seen if the partners will execute these tasks. It is not clear how the association with MSU and its efforts will impact the overall cost to produce a hydrogen tank, although modeling is an important technology.
- The team is working well together but lacks a tank manufacturer.
- There is some collaboration. For a project like this, the early involvement with a tank manufacturer and getting its input is very important.
- Collaboration with tank manufacturers is advised to expedite the progress of this project.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.1** for its relevance/potential impact.

- The project has high relevance because it is focused on the main cost factor of the compressed hydrogen tank system, which is the CF. The potential of a 35% CF reduction would have a notable impact on reducing the cost of the tank system and FCEV cost.
- The concept of developing a breakthrough technology using a high performance, unique resin system shows good relevance to optimizing hydrogen storage system. This project could lead to improved efficiency and cost, which may result in a satisfactory impact for the overall DOE Hydrogen and Fuel Cell Program (the Program).
- Showing a reduction in CF composite volume by 35% and cost of composite materials of $6.5/kWh addresses DOE 2017 system cost targets.
- If successful, this project has a potential big impact for the Program.
- This could have high impact if the project can successfully demonstrate a 35% reduction in composite cost. It would be interesting to compare the cost of the infusion process to the typical wet wound process to understand the total cost impacts on the COPV. This should be less costly as the infusion process would lead to less wastage and hopefully better incorporation of the resin in the composite.
- The use of dry winding and vacuum infusion for tank production is interesting and may improve throughput and tank performance. Without modeling or other data, however, it is really difficult to assess what the true impact will be.
- Costs associated with the process are not known at this point
- No cost model was provided nor were goals for tank fabrication speed. The only test data was on a flat plaque, and the jump to filling an entire tank mold using VARTM is highly challenging, but no plan for doing that was given other than using a less viscous resin.

Question 5: Proposed future work

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

- The testing through March of 2016 should really confirm the success of this project. The work proposed seems adequate to meet the goals and is on schedule.
- Proposed future work meets DOE targets.
- The proposed next steps are appropriate.
- The team had a reasonable work plan, but there are no clear defined go/no-go decision milestones.
- The plan going forward looks reasonable. It is suggest that the team consider fiber sizing effects for its matrix resin because it is very different in chemical structure from most resins that are traditionally used in composites. This could affect the ability to achieve a good fiber/matrix interface and could result in significant reductions in fiber property translation in the composites.
- The general steps to prove-out the infusion are good, but the key deliverable of the project is to demonstrate a cost savings. The team should develop a cost projection model that includes the vacuum infusion cycle time and capital. The project should review the cycle life requirement target for tanks since the proposed

future work suggest a 90,000 cycle target, which is greater than required by current standards (e.g., United Nations Global Technical Regulations, EC 79, or SAE International J2579).
- The future work to produce tanks and prove the infusion technology is adequate. The overall project needs to address all factors that affect the cost of producing a hydrogen tank. In addition, key performance characteristics such as cycle and impact testing need to be better identified and a focus of the project.

Project strengths:

- The project is strong in that it offers a novel approach to tank fabrication that, if successful, will result in higher quality composites and a potential reduction in the amount of CF required.
- The resin system and the expertise of the collaboration partners represents the strength of this project.
- The idea of using the composite processes and the thermoset resins to reduce the amount of CF is a project strength.
- The approach is unique and includes experimental validation and theoretical estimation.
- The project is focused on the key cost driver for compressed hydrogen tanks.
- The project takes advantage of known improvements in resins, processes, and winding techniques.
- The team’s understanding of resin chemistry is a project strength
- Using a less viscous resin and VARTM may reduce void concentration.

Project weaknesses:

- The major weakness of the project at this point is that modeling and/or data supporting the approach was not presented. Without access to the proposal for the project, the basis for the aggressive project goals are unclear. Some baseline property data—for neat resin, composites, or both—should have been acquired early and models constructed to illustrate where the project is going.
- There is no modeling work to direct the experimental setup. All the parameters used in the experimental work are not well explained.
- Costs associated with the process are not known at this point and collaboration with tank manufacturers seems necessary to justify the viability of the project. In addition, testing of the materials should be done based on real-life operation conditions of the tanks.
- The project needs to conduct further assessments of the baseline to evaluate the potential improvements of the approach. A review of the current tank design requirements, such as the cycle life target, is needed. The linkage of the proposed improvements to the 35% CF reduction is not shown.
- The lack of progress and the lack of overall cost impacts show a weakness in the approach. The back-up slide showing the cost targets of the Program are a good example of the overall project. This slide shows the work of others, but this project should already know and project its own cost model. The testing of flat panels also shows a technical weakness where pressure vessel mechanics and laminate failure modes are different than that found in flat panels. Progress is not being made in an adequate fashion.
- No correlation between void concentration and performance is given, except for resin-dominated properties that tanks are already designed to avoid. The project did not provide cost models or specific performance metrics relating to void content.

Recommendations for additions/deletions to project scope:

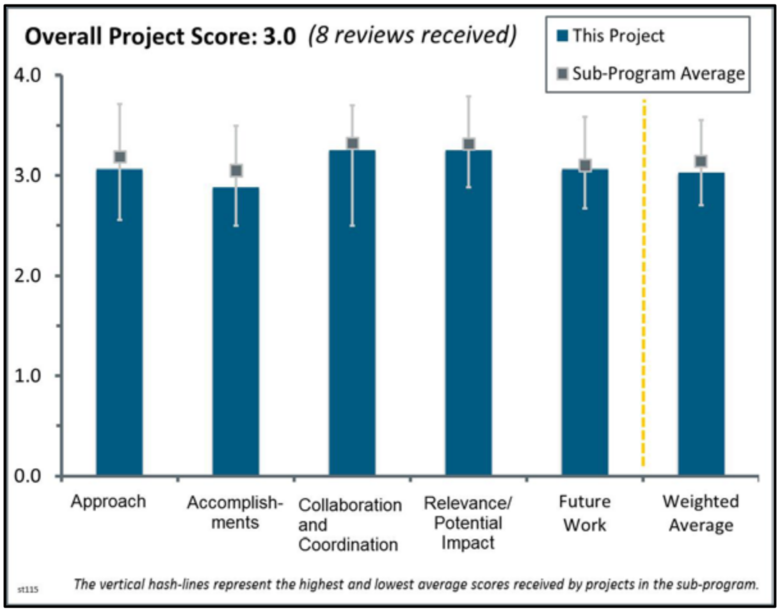
- The project should consider adding a tank manufacturer to the team.
- Costs associated with the process are not known at this point, so it suggested that these are evaluated in addition to considering collaborations with tank manufacturers.
- The project would benefit from having a series-production Type IV tank manufacturer either as a partner or in a consulting role. The project should reduce the emphasis on fatigue and evaluate other parameters that could influence the wall thickness, such as burst strength and impact.
- Focus efforts on infusing pressure vessels and begin testing. This includes cycle and impact testing. The efforts to test flat panels are not relevant and add unnecessary cost to the project. Understanding how the Materia resin performs in a pressure vessel needs to be understood, and comparing that performance to typical wet wound tanks is necessary. The resin is interesting enough that a pressure vessel wet wound with

the Materia resin would provide a good comparison in the tank production techniques (e.g., infusion versus wet wound). This would also provide data to show whether or not the Materia resin is superior to existing resin systems and would result in lower void content even using standard manufacturing techniques.

- The project is focusing on the wrong issues to reduce cost.

Project # ST-115: Achieving Hydrogen Storage Goals through High-Strength Fiber Glass

Hong Li; PPG Industries, Inc.



Brief Summary of Project:

The objective of this project is to develop a Type IV composite overwrapped pressure vessel (COPV) reinforced exclusively with glass fiber that has the composite strength to match that of the T700 carbon fiber (CF) composite. The new tank will lower the composite contribution to system cost by nearly 50%, with minimal impact on tank weight and capacity compared to tanks made with T700 CF.

Question 1: Approach to performing the work

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

- The project approach is well organized, with specific tasks for each participant clearly described. It is not clear what value adding the new test stand and the effort to optimize tabbing brings to the overall project. Testing and tabbing standards are well established and should be followed to ensure that the data can be directly correlated with previous attempts to produce a high-strength glass fiber and to compare results to existing S-glass and CFs.
- This project involving three partners is focused on one primary objective: reduce the cost of Type IV hydrogen storage vessels without significant consequences to mass and volume targets. The pathway is via use of presumably inexpensive glass fiber in lieu of aerospace-grade CF without a significant impact on the other properties. PPG Industries, Inc. will develop and produce the resins and glass fiber for structural characterizations at Pacific Northwest National Laboratory (PNNL) and prototype tank fabrication and testing at Hexagon Lincoln.
- The ability to replace T700 CF with high-strength glass offers the potential for significant cost reductions in the production of 700 bar COPV for onboard hydrogen storage applications.
- Achieving performance comparable to CF with glass fibers would pave the way for cost savings in the use of COPVs.
- The approach is generally well designed and involves the partners. Additional details regarding the challenges associated with pilot production of new fibers would be helpful. A project schedule in graphical form (e.g., a Gantt chart) would be helpful as well.
- Using high-strength glass fiber as an alternative to CF, if successful, may help reduce the tanks’ cost.
- The project has a good approach to looking at the possibility of developing a high-strength glass as a possible CF replacement. The glass development work is well thought-out and the approach is appropriate. The low-density resin and hybrid composite portions of the work seem to have been ignored.
- Using glass fiber to replace CF does reduce the cost at the tank level. However, this approach will incur the penalty of lower gravimetric- and volumetric-based energy density. The overall gain will need to be systematically analyzed.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.9** for its accomplishments and progress.

- This is a new project, but much work has been accomplished in a short period.
- The development of a new high-strength glass fiber is progressing very well.
- Initial results support pursuit of experimental goals.
- PPG reported that, so far, two fiber compositions have been produced with properties similar to baseline CF. Some characterization work has been completed, but there does not appear to be any prototype vessel yet fabricated. Hence, the project tasks appear to have slipped by three to six months, according the dates on slide 25. Substantial recovery seems unlikely, and significant de-scoping of objectives is more likely.
- The presentation suggests that chemistry has been developed with proper temperatures and binders to produce fibers that exceed T700 strengths. However, the box plots of the data show something completely different, with the new glass fiber chemistries showing S-glass type properties. The actual accomplishment is hard to rate because of this discrepancy. The value of the efforts expended on tabbing methods and test stand progress is not clearly shown.
- It seems like a number of problems must have been encountered early in the project, because significant slippage in the schedule is noted. To date, there have been no composite data presented, only filament-strength data, and no modeling was presented. The fact that the stress rupture testing is so significantly delayed and appears to drive a good number of the final fiber selections is a significant problem.
- The presentation of the fiber performance data should be done better and with scales. It is difficult to discern the relative merits of various results.
- The project is new, and the progress is limited at this point.

Question 3: Collaboration and coordination with other institutions

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

- The team showed good collaboration and, in particular, got the tank manufacturer’s input early in the project.
- The partners provide an appropriate range of expertise and appear to be engaged and participating.
- The companies involved are excellent, with very good expertise and reputations. The organization of tasks is well thought-out, with all participants fully aware of their level of effort and needed results. However, with each participant’s efforts so well defined, it is not obvious how much sharing of information or collaboration is actually taking place.
- Collaboration involves reputable organizations.
- Collaboration with other partners seems to be planned.
- Collaborations seem to be good, although it is not clear exactly why the stress rupture test fixture design seems to be so far behind where it is needed in the project.
- The partners on this project have well-delineated assignments that match their capabilities, and it appears that progress should have been OK. However, some issues in meeting joint targets are apparent, resulting in schedule slippage. There does not seem to be any involvement of other researchers or organizations.
- The team is working well together, but the development of stress rupture fixtures at PNNL seems inappropriate. National laboratories should already have those. PNNL seems to simply be acting as a test laboratory.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.3** for its relevance/potential impact.

- The development of a new fiber is outstanding. The application of a low-density resin and hybrid composite concept seem to have received little thought. If the fiber development is successful, a follow-on effort will be required to develop a hybrid tank using the fiber.
- The potential for significant cost savings in COPVs for hydrogen storage, even when making a partial substitution of T700 CF, is excellent.
- Replacing CF with glass fiber could ultimately reduce the tanks' cost.
- Glass-wrapped vessels could provide substantial cost savings.
- If successful, this will be a high-impact project for the DOE Hydrogen and Fuel Cells Program.
- This effort is very relevant to the overall goals of the Hydrogen Storage sub-program. The optimization, including hybrid development, of the fiber reinforcement is key to minimizing cost and creating value. However, this effort is not new; others have attempted to create high-strength glass fiber in the past. The novel chemistry is not clear at this early stage of the project. In addition, one of the partners is currently producing pressure vessels using a well-established hybrid fiber system. Again, it is not clear how the technology in this project is different from technologies already in place.
- The project has the potential to significantly decrease composite costs. The impact on weight and capacity in switching to glass fiber should be quantified.
- This project looks almost exclusively at reducing the cost of Type IV hydrogen storage vessels through substitution of glass fiber for T700 CF. However, slide 27 shows approximately 40% mass and approximately 10% volume penalties for about only a 30% cost benefit through use of just glass fiber alone. The team speculates that better performance may be possible by using additives, reducing safety factors, etc. However, still unresolved are possible degradation issues during pressure-temperature cycling of such tanks on vehicles.

Question 5: Proposed future work

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

- The future work is properly organized and addresses the important steps of producing test vessels and completing the testing. The focus on actual tank performance is very good. The efforts surrounding the tabbing and test frame do not appear relevant to project success. Strand and filament testing should follow current standards. The work surrounding the chemistry, thermal parameter optimization, and binders is good.
- The plan moving forward appears to be well thought-out and should provide necessary data for further recommendations. The speaker's comment regarding a preliminary down-select of fiber based on passing the highest planned stress level should help to bring the project closer to schedule. It is not certain that an E-glass reference tank is the best choice because the team is really trying to replace the T700 CF. Reference data using T700 fiber, at the coupon level at minimum, would go a long way toward making the case for replacement with high-strength glass fiber.
- The team proposed a well-structured work plan with a clearly defined go/no-go decision milestone.
- The future work is thoughtfully designed for the remaining decision points and efforts.
- The future work is appropriate.
- The proposed work specifies limited fabrication and testing of test vessels according to project plans.
- With the several months of schedule slip, as shown on slide 25, it would seem that greater effort should be made to accelerate glass fiber development and characterization, along with prototype bed fabrication and testing, rather than cost and performance modeling of marginal materials.

Project strengths:

- A strength of this project lies in the partners' capability and the conscious efforts to prove the new fibers in actual pressure vessels. The overall project organization and outcome by each participant is well organized; the outcome that each is expected to produce is clear. The other strength appears to be the science behind the chemistry and how it relates to the glass fiber's performance. The approach to go from pilot to production shows that the project understands the influence of processing parameters that can affect the cost of the fiber.
- The biggest project strengths are in the potential for cost savings through substitution of T700 fiber with high-strength glass. There is little doubt that the fiber production can be successfully scaled up at PPG.
- A good combination of organizations with experience and expertise should promote a balanced assessment of glass fibers for less expensive hydrogen storage vessels.
- The team has balanced technical expertise with a carefully scoped technical plan that outlines efforts from modeling to experiment.
- The project team is knowledgeable and in the business of producing fibers and tanks.
- The project has the potential to significantly decrease composite costs.
- This is excellent work in developing the new glass fiber.

Project weaknesses:

- The current weakness is the lack of composite data for either the glass-based composites or the control systems. Basic coupon data (or even calculated data) could have been used in (1) models to provide some validation of the approach's feasibility and (2) even some rudimentary projections of cost reduction that would arise from this effort. The schedule is currently a significant concern. A number of tasks appear to be four to six months behind schedule.
- Technical challenges with processing, such as the production of glass fiber at scale and limitations with the melting temperature, are recognized. However, there seems to be no countermeasure plan in place. In addition, economic estimates would need to be presented to justify the lower cost claims and demonstrate whether high costs could result from the processing itself.
- The report made at the Hydrogen and Fuel Cells Program Annual Merit Review sheds little insight into why the schedules for the fibers and components have slipped so far. Also, the fundamental limitations of glass fibers compared to high-strength CF may severely limit achieving large (i.e., >30%) cost savings without having an impact on both vessel weight and volume.
- Mass, volume, and cost targets are lacking. Hybrid design work is lacking.
- Even though the participants have great reputations and expertise, it is hard to determine whether any cross-team activities are leveraging the expertise in a way that could benefit the overall success of the project. The efforts of the tabbing and test frame do not appear to be adding value.
- The team should get some original equipment manufacturer input when comparing the glass fiber to the CF, because such a replacement will have an impact on the final onboard storage energy density.
- The schedule risk, from both existing slippage and potential production issues (e.g., existing furnace limits), is significant.

Recommendations for additions/deletions to project scope:

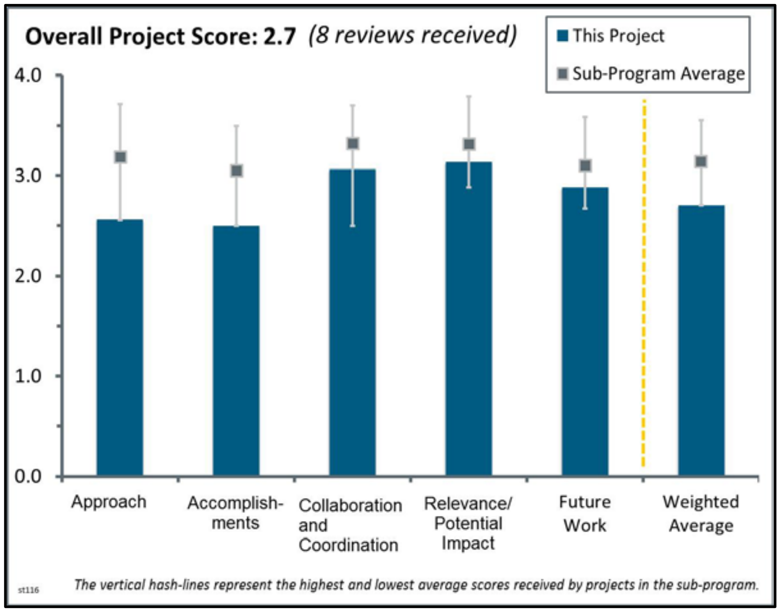
- Technical challenges with processing, such as production of fiberglass at scale and limitations with the melting temperature, are recognized. However, there seems to be no countermeasure plan in place, and this needs to be addressed. In addition, economic estimates would need to be presented to justify the lower cost claims and demonstrate whether high costs could result from the processing itself.
- A reference tank based on T700 CF should be used, rather than an E-glass control. Because the project is trying to replace T700 with the high-strength glass, the former would be a more valid comparison.
- With a little over a year left for this project, no further cost or design modeling is recommended. Instead, more effort should be made to develop and test glass fibers and resins with greater potential for high strength, along with fabrication and testing of prototype tanks.
- The project is early in its progress. The efforts and resources expended on behalf of the tabbing and testing portion should be reconsidered if they could be used to add more value in other areas of the project. Current

strand and filament testing standards should be used to keep the data relevant to understand the overall performance of the glass fibers.

- It is not clear whether the fiber translation loss is within the current project scope.
- The project should drop the low-viscosity resin idea and focus on the hybrid fiber design.

Project # ST-116: Low-Cost α-Alane for Hydrogen Storage

Richard Martin; Ardica



Brief Summary of Project:

The overall objectives of this project are to reduce the production cost of α-alane (AlH_3) to meet the DOE 2015 and 2020 hydrogen storage system cost targets for portable low- and medium-power applications. Results enable broader applications in military and consumer electronics (e.g., smartphones, tablets, and laptops), backup power, unmanned aerial vehicles, forklifts, and vehicles.

Question 1: Approach to performing the work

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

- The Office of Energy Efficiency and Renewable Energy reorganized, and the Fuel Cell Technologies Office (FCTO) now falls under sustainable transportation. There does not appear to be a path for alane for hydrogen storage for light-duty vehicles. Alane can be viable as a storage material for portable power, and it is encouraging that such a niche application is receiving research and development funding. It appears that the cost model for the economic analysis needs to be redone and verified by an independent organization, such as Strategic Analysis, Inc. The presentation shows insufficient details about the major assumptions that went into the economic analysis. The capital cost of electrochemical processes tends to scale with current density. The current density that was used for developing the capital cost estimate was not reported. How much progress was made toward an economically viable current density was also not reported. The researcher reported that the alane adduct was present at only a low molar concentration, which creates concerns about a possible high operating cost of the separation and crystallization steps (e.g., high solvent volumes). It will be important to report the alane cost as a function of the annual production capacity because it will take a while to reach the point where 4 million cartridges per year will each be filled with 80 grams of alane (i.e.., 320 metric tons/year).
- The project focuses on cost reduction of alane production and investigates scale-up of the synthesis process, both of which are indeed relevant.
- Conducting economic modeling prior to launching the experimental work is an excellent approach, provided a realistic cost estimate can be obtained. A complex fluidized bed is a risky approach to solving the electrochemical and economic problems with this system.
- The project has the right approach to an electrolysis process to reduce cost significantly.
- Employing more of an engineering approach to the electrochemical regeneration of alane is a useful addition to this topical area. The process and cost modeling area should help in setting research or development priorities for alane regeneration and help in making go/no-go decisions.
- This project intends to adapt the electrochemical synthesis process of AlH_3 that was conceived and demonstrated on a small laboratory scale at Savannah River National Laboratory (SRNL). The current effort focuses on improving the overall efficiency of producing the alane adduct from various sources of aluminum metal other than the expensive alanate compounds. The team has performed cost analyses of the chemical processes to produce alane and built small test reactors to assess the performance of the electrochemical method. However, the team provides only vague, general statements on the processes necessary to purify the electrochemical product into the desired alpha-AlH_3 phase or stabilize this material against ambient decomposition or violent reactions with air. There appear to be very few plans to characterize the compositions and purities of the products at different stages of the reaction. The project

milestone table on slide 21 is misleading because several tasks appear to be currently “underway” rather than 100% complete.

- The cost estimate and technological approach could use additional improvements:
    - According to slide 7, the economic modeling has been done “using standard chemical engineering methodology” whose details are not explained. Thus, it is safe to assume that the team used the cost of building and operating a standard explosion-proof chemical facility at its partner’s site. Because explosion-proof ratings exclude the presence of volatile solvents and sources of a potential discharge (sparks) or open flame in the same confined space, the “standard” approach cannot be used for electrolytic generation of pyrophoric materials (alane/activated aluminum-based by-products) in diethyl ether (the presented approach) or even THF (the approach proposed in the past).
    - Because of the process’ non-conventional nature and the high explosion risk at the facility, the qualification and number of employees required for safe operations—i.e., the cost of labor—would have to exceed those projected for standard air-sensitive operations at a traditional chemical plant.
    - Safety and security measures would also have to be enhanced; to localize potential disastrous events, the facility would have to be designed in a remote area with a very low moisture content in the air (e.g., in a desert), which will further increase the cost of operations.
    - Thus, it should be expected that for at least the first three to five years of operation, the alane production cost may easily exceed $350–$400/kg and remain higher than $250/kg, even after an exhaustive optimization of the process, versus the $87/kg projected by the team.
- Because cost analysis is a critical aspect of this work, the team should provide the reviewers (at least) with a more detailed description of the methodology and criteria used for determining the numbers that were presented. Justification for the numbers used is lacking. The presentation could have been clearer about each chemical step of the new route and how it compares to the chemical route used in the past.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- Cost reduction is clearly envisioned. More details about the economic modeling are desirable—not only because it has an influence on some of the milestones. Important milestones have been met.
- Initial experiments at the laboratory scale confirmed the initial SRNL results. However, the “moving bed” experiment shown at the Hydrogen and Fuel Cells Program Annual Merit Review cannot represent the “fluidized bed” approach. In the fluidized bed approach, the aluminum particles are dispersed in the organic solvent, which will cause their isolation from the source of electricity, while such contact is still maintained in the “moving bed” approach. Low concentrations and large solution volumes represent another challenge, which the team has not addressed.
- An economic analysis was performed that predicted that the costs for making alane can be substantially lowered by using Al metal from different sources in variations of the SRNL electrochemical process. Thus, alane should be economically suitable for various low- and medium-power devices, but it would still be far too expensive for most fuel-cell-powered vehicles. Preliminary studies at SRI International suggest that these reaction schemes may be viable; however, there does not seem to have been much characterization of the intermediate and product phases so far. Designs for improved electrochemical reactors have been described but not yet built or tested in the laboratory.
- Progress toward a continuous fluid bed process seems quite slow. The flowsheet used for process modeling seems quite sparse to generate what those skilled in the art might consider a reliable, realistic chemical engineering model of cost and energy, etc. The process entails a few key separation operations (e.g., adduct separation and extraction of the alane adduct) and a moderate-to-high-pressure operation (alanate regeneration). The presentation of the flowsheet is not nearly detailed enough for one to understand whether the team is adequately representing those and other key unit operations and whether the estimated costs are representative of reality. More detail in this portion of the discussion would improve the presentation. The scale of 372 mg of alane would seem to be quite a small step on the way to a large,

continuous process. The fluid bed process, while being discussed last year, seems to be still quite a way from practical realization with high conversions and high space-time yields.
- Detailed economic analysis was either not carried out or glossed over in the presentation. In addition to the electrochemical step, there are three other steps in this proposed method of alane synthesis. Analysis should have a breakdown of the costs associated with each step. The estimated cost of $87/kg seems very unrealistic. It is not clear how only 80% recovery of $LiAlH_4$ (or $NaAlH_4$) in each cycle can possibly meet cost targets. Raw yield rather than percentage yield information was given. It is not clear what the percentage yield of 4-ethylmorpholine adduct is or what percentage of 4-ethylmorpholine is recovered. It was stated during the question-and-answer session that 4-ethylmorpholine would not be used, but it is not clear what the alternative is.
- Alane does not provide a path toward meeting the onboard hydrogen storage targets. DOE has established some targets for portable power applications. The reported system-specific energy density of 466 Wh/kg and 577 Wh/L appears to be quite a bit lower than DOE's 2020 target of 1,000 Wh/kg and 1,300 Wh/L for a medium-power rechargeable system or 1,300 Wh/kg and 1700 Wh/L for a single-use system. The project reported that only 372 mg of the Alane adduct had been isolated from the electrochemical cell. It is not clear that such a small amount is sufficient for concluding that the 20% of the aluminum present in the alane shall originate from the aluminum electrode in the electrochemical process when implemented at a larger scale.
- It was not clear that the team really has achieved the 100% progress toward goals that was claimed. Perhaps this was just a reflection of how the team members presented their work. It is recommended that they improve the content of their slides for better clarity.
- The project follows the proposed plan.

Question 3: Collaboration and coordination with other institutions

This project was rated **3.1** for its collaboration and coordination.

- The project has a strong team. The first year of the project has been completed, but the amount of AlH_3 generated from the actual electrochemical process (372 mg of the adduct) appears to be low. It is not clear whether there is a means to accelerate the knowledge transfer from SRNL to Ardica Technologies and SRI International so that the electrochemical process development and the critical subsequent processing steps (e.g., crystallization and adduct removal) can be accelerated.
- Biweekly telephone conferences show an impressive coordination and collaboration.
- The interactions between Ardica and SRI International seem very closely coordinated; the latter organization is responsible for nearly all of the electrochemical work and characterization performed so far. A consultant from the University of California, Berkeley, is supporting the development of a fluidized reactor bed. It is less obvious what role SRNL and Albermale are playing in the current efforts. There does not seem to be independent assessment of the compositions or purity of the AlH_3 product or intermediate phases. This information from knowledgeable outside organizations would be helpful as a reality check.
- The collaboration with SRNL and SRI International appears effective.
- There is good collaboration between partners. No outside input was solicited in preparing cost estimates.
- It is hard to tell how closely the team works together based on the information presented. It is not clear how often the team meets in person—e.g., whether there are weekly or monthly reviews—or what the program management structure is.
- The information given seems to indicate that there is little collaboration between this project and another DOE project on alane, led by R. Zidan. It may be fruitful if the research results from the other project were better integrated in this project.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.1** for its relevance/potential impact.

- Alane has already been demonstrated as a useful hydrogen storage material by the U.S. Army for personal mobile energy storage units. A closed cycle for the elements is developed in which alane is rehydrogenated, which is very useful. Thus, this project is highly relevant.
- This area of research may be able to achieve the medium-power targets that are relevant to DOE Hydrogen and Fuel Cell Program (the Program) goals. This could enable some non-automotive technology applications of fuel cells, which is also relevant to DOE goals.
- The project is critical to the Program and has the potential to significantly advance progress toward DOE research, development, and demonstration goals and objectives.
- The cost reduction of alane is essential to enable commercial use in portable low- and medium-power applications.
- New materials research is critical to the success of DOE programs. Unfortunately, there are so few materials programs left, and the DOE scope has narrowed too much. It is interesting to use a military application to highlight project relevance to DOE.
- Large-scale-production AlH_3 at the costs being suggested by this project would make this hydride a very viable candidate for a wide range of small and intermediate fuel cell power systems. However, it is also very important that the AlH_3 is sufficiently pure (i.e., does not contain residual organics from synthesis or processing) and possesses good stability against decomposition during processing into devices and during a finite shelf life. This project does not seem to be addressing these issues very thoroughly.
- It has long been recognized that low-cost alane would open the door to major fuel cell applications in personal electronics. However, it not clear that alane can be made at a lower cost from the electrolysis of $LiAlH_4$/Al than it could through improved chemical methods.
- Alane does not provide a path toward meeting the onboard hydrogen storage targets. DOE has established some targets for portable power applications, but the reported system-specific energy density of 466 Wh/kg and 577 Wh/L appears to be lower than DOE’s 2020 targets of 1000 Wh/kg and 1300 Wh/L for a medium power rechargeable system or 1300 Wh/kg and 1700 Wh/L for a single use system. The portable power application appears to be more critical to the U.S. Department of Defense.

Question 5: Proposed future work

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

- The proposed future work contributes to overcoming most barriers.
- There is complete reviewer agreement with the plans to do extensive laboratory assessments of various electrochemical reactors and components to enhance production efficiency and demonstrate formation of high-purity alane. However, more complete characterization will be important to validate independently that appropriate phases of sufficient purity are produced. Step 6 on slide 18 has been attempted by many groups over the years and remains extremely challenging to resolve.
- The project is progressing according to the plan and will likely fulfill its milestones and goals. There is a good plan for future work, but work by the individual partners could be better integrated.
- The proposed future work is generally effective but could be improved. The necessary improvements may be more significant than anticipated.
- Perhaps Future Work Item 2 should be performed before Future Work Item 1. The loss of $LiAlH_4$ at the cathode was identified as a significant problem that may need to be addressed before adding the complication of a fluidized bed of particles at the anode. The discussion did not include how the lithium-conducting membrane material was going to be selected/developed or whether it is already available off the shelf for the operating conditions in the project’s electrochemical cell. There is no mention of the current density at which the electrochemical process appears to become economically feasible, or how the project team plans to achieve such current density.

- It appears the team members are going to spend significant effort on the desolvation step. It is not clear what is wrong with the desolvation step of the current chemical route. If the researchers are doing something different, then they should not show their process merging with the chemical route on slide 5. Given the amount of work needed to optimize the electrochemical process alone, perhaps it makes more sense to isolate the product as something that can feed right into an already established desolvation/crystallization process. The Achilles heel of both alane production routes is the desolvation/crystallization process.
- The discussion of future work would be improved by expanding on the technical basis for each task, beyond "optimize deposition." Rather, it would be good to know what the first key experiment is that one will employ to "optimize deposition." Without the details, it is difficult to assess the probability of success of any future approach. A more detailed discussion of what the work at the University of California, Berkeley, will entail to help to solve the moving bed reactor problems would be very nice.
- Bottlenecks in the production scheme and reasonable approaches to circumventing them have been identified. However, the practical value of this work is questionable in view of the shaky analysis of the economic viability of alane production through this method.

Project strengths:

- This project involves both a commercial organization and a research institute to address the challenges of adapting small-scale synthesis of research quantities of alane into a more cost-efficient manufacturing process for much larger production levels. The team is focusing on the important issue of generating the key intermediate (alane adduct) and looking at methods to scale up processing.
- The team has long-term experience with alane. The project has a materials focus. An economic method for preparing alane would be very beneficial for niche applications, given the purity of the gas stream.
- Scale-up of chemical reactions and cost assessment are challenging and extremely important. Thus, this project is highly relevant.
- The project started just one year ago. Nevertheless, good progress can be seen, and a very precise vision of where to go is given.
- The team has good collaborations and represents a small company with a potential market outlet for low-to-medium-power applications.
- The project has a strong team with SRI International, SRNL, and others.
- Team member SRI International has a great deal of experience in alane synthesis.
- A strength is the fundamental results collected by SRNL.

Project weaknesses:

- The following are project weaknesses:
  - The presentation did not show the details of the cost analysis.
  - For alane, the most critical barrier to scale-up is the desolvation/crystallization step. The electrochemical approach does little to affect this step. It is not clear why the team has not demonstrated scale-up above 20 g/batch yet in the crystallization step—a step that has been optimized for years by a number of groups.
  - Random switching between $NaAlH_4$ and $LiAlH_4$ as starting materials is confusing. There is a big difference in cost between the two; perhaps the team is claiming numbers for Na but using Li because of the solubility issue with Na.
  - The project did not provide details on the electrochemical reaction, such as concentration, alane adduct yield, how it is separated from LiH, what the purity of the final product is, or what else is in the final product besides alane (e.g., aluminum, $LiAlH_4$, or Li metal). It would be good if the team could show characterization data of as-prepared alane.
  - It is not clear where/how the morpholine was added in and the alane adduct was extracted.
  - Reaction scale appears really small for estimating production costs—laboratory scale rather than pilot scale.
  - It is not clear why slide 13 shows a different amine adduct.
  - The toluene extraction step to isolate the alane amine adduct is not shown on slide 5 in the scheme. It is not certain that this step was included in the cost analysis.

  - It is not clear why the team did not show an engineering diagram of the complete electrochemical process.
  - The fluidized bed seemed fluid only in the top 25% of the reaction flask. It seems that it would be more efficient if all the particles were moving uniformly across the reactor.
- The team is not sufficiently addressing the energy-intensive solvent management issues of converting the adduct into the final alane product that would be suitable for device application. There should be additional characterizations of the composition and purity of both the intermediate species and the alane product using various methods such as x-ray diffraction, electron microscopy, and nuclear magnetic resonance, for example. The researchers on this team have only very limited personal experience on the properties and handling of metal hydrides (especially alane).
- Performing a technical and economic analysis does not appear to be the strength of this team. More information may need to be shared about the assumptions, and those assumptions need to be validated. The project does not show how the Li-ion-conducting membrane material is going to be selected, if available. Validating the alternative cathode approach appears to be critical in order to avoid dendrite formation and the loss of $LiAlH_6$.
- Better integration of work by the individual partners could be fruitful.
- The project did not show details of the cost analysis.
- The project is guided by a shaky economic analysis.
- The approach and technical results to date are weaknesses.
- Progress appears slow.

Recommendations for additions/deletions to project scope:

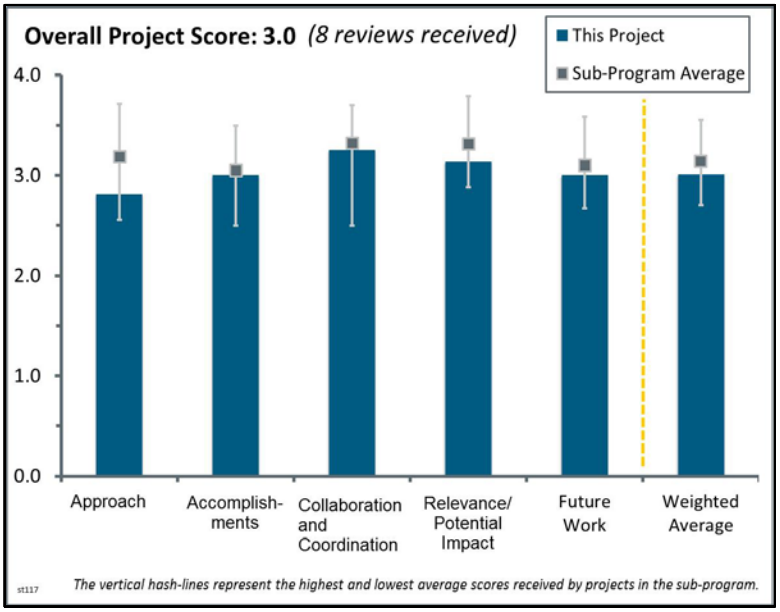
- The results from this project are very promising and relevant. More investigation on the choice of solvent may be needed to optimize the particle size of the obtained product, which is important for the performance of the alane hydrogen storage material.
- The scope of the project is okay, and the project should continue exploring methods to control reactions that occur within the electrochemical cell. The team should also devote more effort to optimizing the solvent removal and stabilizing the alane final product. Finally, the reviewer recommends that the team bring in some consultants with substantial experience and expertise in the properties, characterizations, and handling of metal hydrides (especially the various alane phases).
- An independent organization needs to perform a technical and economic analysis of the electrochemical process that Ardica, SRI International, and SRNL propose. More validation of the assumptions that form the basis for the economic analysis is needed. An activity should be added that will make the project move faster to demonstrating, for instance, a 10-gram scale of producing alane with the electrochemical process versus isolating the alane adduct at less than 1 gram.
- The project should expand the effort by adding alternative approaches to the electrochemistry and the traditional batch chemistry, which may increase project's chances for success.
- The applied cost model should be presented in a very detailed and comprehensible manner. Capital, maintenance, and labor costs seem to be rather low when compared to materials costs.
- A more detailed economic analysis should be carried out. There appears to be duplication of several of the tasks included in the companion SRNL project; these should be eliminated.
- A more complete process spreadsheet presentation might allay fears that some key unit operations have been overlooked in the process modeling activity.
- The project should describe the pathway for scaling up the chemistry from laboratory scale to pilot plant scale.

Project # ST-117: Boron-Based Hydrogen Storage: Ternary Borides and Beyond

John Vajo; HRL Laboratories, LLC

Brief Summary of Project:

Boron-based materials have been identified as a versatile and high-capacity option for hydrogen storage. The primary goal of this project is to improve kinetics in onboard hydrogen storage systems by (1) eliminating multiphase kinetic barriers in ternary borides/mixed-metal borohydrides that maintain single phases during cycling and (2) minimizing B-atom rearrangement with lithiated boranes that cycle, while preserving the B-B framework.



Question 1: Approach to performing the work

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

- The basic research proposed and carried out is interesting and may produce results that could not be obtained by previous researchers.
- The project utilizes an interesting approach that focuses on enhancing kinetics by attempting to minimize multiphase or multistep hydrogen release pathways. The two concepts are novel and, to a great extent, counterintuitive. The team uses computational screening to guide experimental design.
  - One approach attempts to form borides by mixing transition metal borohydrides with Mg borohydride and avoiding B-B bond formation. This will require the different borohydrides to react with one another to provide an alternate reaction pathway, instead of independently, to yield ternary boride products. If there is precedence for different borohydrides to react together to provide alternate reaction pathways, it would be helpful to share this with the reviewers. Additionally, it would be helpful to learn what precedence gives the research team confidence that the hydrogenation of the borides will not lead to phase separation of the regenerated borohydrides.
  - The other approach has potential for greater novelty in that "borohydrides" are proposed to react with lithium "hydrides" to form hydrogen and a lithiated borane. This sounds like a higher energy reaction pathway that will require formation of very unstable species. On the other hand if the Li-B species can be formed, it should be reversible. If this concept were to work, starting with a less "stable" metal hydride (Na or Mg) might provide some proof of concept of the novelty. Maybe the predicted enthalpies of reaction with the B framework with Na and Mg hydrides can be investigated to learn whether the enthalpy is not as large as with LiH.
- A lot of previous research has focused on the synthesis of new metal borohydrides, but with little focus on the dehydrogenated state. This project presents a new approach to focus on the design and preparation of the dehydrogenated state.
- The tandem exploration of both the hydrogenation of borides and the dehydrogenation of the corresponding borohydrides is an excellent approach. Prototype electrostatic ground states (PEGS) calculations seem to be a weak theoretical basis for launching an effort to synthesize and develop a new hydrogen storage material. Ball milling of LiH and neutral polyboranes will certainly produce Li salts of polyborane anions, not "lithiated boranes."
- Mg-transition metal borides may be a viable route toward complex borohydrides. Theoretical predictions are being verified. Li-B systems are difficult to assess for their viability as hydrogen storage materials at this time, but the idea is interesting.

- A focus is on ternary borides and lithiated boranes, and a focus is on kinetics of hydrogen release. The team uses computational methods to help guide the experiment, and it uses lithiated borons to control B-B bonding. It uses solid-state or mechanochemistry (ball milling) to synthesize new materials. It is not clear what is really new, compared to what has already been done in this area.
- The approach is designed to improve kinetics of hydrogen cycling in B-based materials, and therefore it addresses important barriers for U.S. Department of Energy (DOE) targets. It is somewhat speculative, and the chances of success are unclear. The mixed-metal borohydrides are still more likely to undergo release via polyborane anions, and there are limited acidic hydrogens in the polyboranes that may be replaced by Li.
- PEGS is not a viable approach for modeling systems of this type. The co-principal investigator (PI) stated during the question-and-answer (Q&A) session that the values were "not real" but that they can be used for comparison. This invalidated all of the assumptions made on the modeling. Diboranes will be a by-product; it appears some of the peaks ascribed to B-H interactions on slide 12 could in fact be diborane. Many other issues associated with entropy effects, kinetics, etc., need to be addressed in a more in-depth analysis of the results.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- This is a new project, and the researchers have gotten off to a good start. The presentation did not clearly identify the computational methods in use. PEGS is not reliable for energetics. The solid-state electronic structure calculations are good and of reasonable quality for the metal alloys. The PEGS calculations are not reliable for energies. The energy differences are very small and within the error limits of the methods, so there is no differentiation (slide 6). There are too many decimal places—the energies are not accurate to even ±10 kJ/mol (more like 20 kJ/mol). The researchers need to be careful in interpreting the calculations and their accuracy. They need to understand the computational limitations. None of the calculated energetics are reliable enough for the researchers to make the decisions they are making. They need to benchmark the computational methods—especially density functional theory (DFT) for the molecules—which are not particularly accurate for these B hydrides. The new synthesis of $Mn(BH_4)_2$ is good. The researchers need to be careful about confusing thermodynamics and kinetics, which was done in the presentation. The reaction on slide 10 makes no sense because there are 15 extra LiH. The researchers need to look at the B-Li bond dissociation (BDE) energy versus the B-H BDE versus the Li-H BDE. The Li_7B_6 alloy is interesting. It is not clear how much hydrogen is lost on polymerizing $B_{10}H_{14}$. The researchers' interpretation of their IR spectra could be improved by using results from the calculations. The synthesis work is quite nice.
- DFT and PEGS have provided significant guidance for the experimental work. It was not clear whether the goal was to cycle through a boride that remained a single phase to minimize the multiple phase kinetic limitations (e.g., Mg_3MnB_8 disproportionate to Mg_2MnB_6 and MgB_2). It is not clear whether this means this boride will be down-selected. Hydrogen uptake by the Li_7B_6 alloy was interesting, and formation of $LiBH_4$ is consistent with a report presented at the 4th Symposium "Hydrogen & Energy" (2010), although those results came at much higher temperatures.
- Some results, such as the preparation of phase-pure metal hydrides and understanding of their phase transformations, may be of substantial practical importance.
- A number of relevant compounds have been investigated and characterized by experimental methods. A number of higher boranes are suggested by theoretical methods.
- Accomplishments so far are commensurate with the fact that the project was only about nine months old when the report was submitted for this presentation.
- The project has delivered a good quantity of results in a relatively short time. However, progress toward DOE goals is limited, with only modest demonstration of reversible storage so far.
- While some progress has been made over previous years in materials synthesis, the interpretation of said results is questionable. The researchers are strongly advised to move away from PEGS.
- Rapid progress has been made on the synthesis and screening of new materials. Only the ill-characterized material made upon ball milling "polymerized decaborane" with LiH has been found to undergo reversible

dehydrogenation, and then only approximately 1 wt.% at approximately 300°C, thus little progress has been made toward the DOE goals.

Question 3: Collaboration and coordination with other institutions

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

- The project features good external collaborations with the University of Utah and the National Institute of Standards and Technology (NIST) for BH nanoparticles (former) and characterization (latter).
- There is excellent collaboration within the project team and with researchers beyond this group.
- The project is well organized and coordinated, and the partners appear to be well integrated in the project.
- The collaborations are ongoing and appear to be effective.
- This is a good team effort, with specific expertise provided by all partners.
- The project features reasonably good collaborations.
- The partnership between theory and experiments is well coordinated, with experiments guided by computational results. There is a clear distinction and synergy between the experimental partners. The coordination would be clearer if the future computational work was not presented under its own heading, but instead integrated with the experiments under the materials headings.
- The collaboration was evident during the Q&A session; however, the experimentalists need to work more closely with the theorists to obtain more relevant interaction.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.1** for its relevance/potential impact.

- The project is highly relevant and focuses on new approaches to obtain materials for reversible hydrogen storage.
- Project aspects align with the Hydrogen and Fuel Cells Program (the Program) and DOE research, development, and demonstration objectives, but they are far from practical applications in real hydrogen storage systems.
- The project aligns well with the Program's goals. The materials and approach are somewhat risky and therefore lower the likelihood of making advances.
- The goals of the project are sound, and the results could be very important; however, in their current state, the results themselves are questionable.
- While this project has the potential to identify materials that could meet DOE targets, it is exploring compositional space that seems to at least border territory that has been previously covered by DOE-funded research.
- The researchers are developing a potentially interesting material, but they will need to work on regeneration processes.
- This is an 18-month seed project to investigate two novel, independent approaches to store hydrogen.

Question 5: Proposed future work

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

- The proposed future work is in line with what is needed: testing of the novel chemistry. Doping boranes with more electronegative elements (e.g., C, O, N) makes sense to stabilize potential B-Li species. The team should try to find out what structure is responsible for the 1 wt.% cyclable hydrogen in the polymerization sample. It would not be surprising to find the formation of Li $B_{11}H_{14}$, $B_{12}H_{12}$ and $B_{10}H_{10}$ from pyrolysis of $B_{10}H_{14}$.
- The project is progressing according to plan and will likely fulfill the goals. Overall, this is a very productive and successful research project. A large number of materials can be produced by the project processes, and many could be under consideration.

- The future work is based on the results obtained so far and properly addresses the project goals.
- The researchers will need to optimize the polymerization of $B_{10}H_{14}$ to lose as few hydrogen atoms as possible. The BH nanoparticles are very interesting. The focus of the electronic structure on the solids is good because the computational work on the molecules is of low quality and not carefully thought-out. The researchers need to use composite correlated molecular orbital methods such as G3 and G4. They need to think about the accuracy of the electronic structure calculations. It is not clear how they will predict solubility and critical temperatures.
- The studies of the dehydrogenation of the Mg/Mn borohydrides need to be conducted using in situ IR or Raman spectroscopy so that any elimination of diborane gas can be detected.
- C-substituted boranes (i.e., carboranes) and polyboranes were extensively studied in the past; this part of the future work should be downscaled.
- Given the relatively short term of this project, there are probably too many avenues suggested. Work that is vaguely described (e.g., "optimize polymerized borane," "consider doping") is especially low priority.
- The team needs to utilize other theory approach than PEGS, especially with respect to the lithiated boranes.

Project strengths:

- The project features good integration of theory and experiments to focus the experimental studies, although the theory might need some experimental validation. For example, some dismissed ternary boride systems might have good thermodynamics, and it could be beneficial to test at least one of these.
- The project deserves praise for looking into materials that have a potential for more than 10 wt.% hydrogen content, as well as for studying both mixed-metal borides and borohydrides, plus extended B-B networks.
- The prompt-gamma neutron activation analysis conducted at NIST was a Specific, Measurable, Attainable, Realistic, and Timely (SMART) quantitative approach to measure hydrogen uptake and provides a maximum theoretical hydrogen storage density.
- The synthesis work is quite nice. Other strengths include the development of potentially interesting materials, the good team, and the attempt to integrate theory and experiment.
- This is a very well-organized and productive project. The project aim is highly relevant, and the project has a high degree of novelty.
- The highly efficient synthesis and screening of materials is a project strength.
- The approach used by the experimentalists in this project is a strength.
- The project features good fundamental research.

Project weaknesses:

- The researchers need to benchmark the computational methods. DFT is not as reliable as they think. PEGS should not be used for any energetic calculations. The researchers need to use their computational results to help in their spectral interpretation.
- The project is a very long shot to meet the vehicular targets, but it might discover some novel chemistry and should provide some interesting insight into kinetics.
- The project lacks a clear and believable path to meeting DOE targets. The project is too speculative for the Office of Energy Efficiency and Renewable Energy.
- The team may not have enough time to complete the planned experiments, with only about six months left. Li-B materials appear to be irreversible below 100°C.
- Weaknesses include the theoretical approach and the misinterpretation of some x-ray diffraction and IR spectra.
- There is very limited characterization of the novel borides and products upon ball milling "polymerized decaborane" and LiH.
- The project is far away from any practical applications.

Recommendations for additions/deletions to project scope:

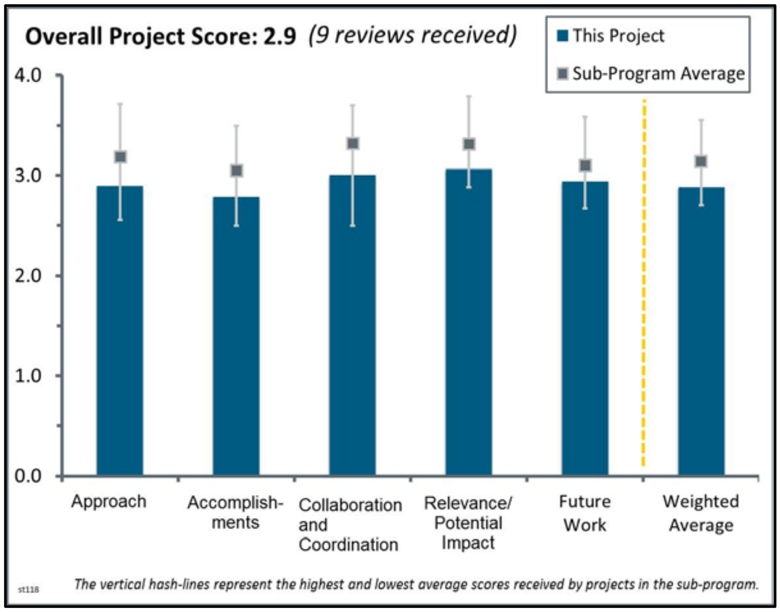
- The team should consider validating the theoretical prediction. The polymeric boranes/LiH composites are produced by high-energy milling and are likely to produce similar compounds, no matter the source. The team should concentrate on one source and pursue compositions that increase reversible hydrogen. Because the maximum observed so far is 1% from a theoretical 7.7 wt.%, this group of compounds could be out-selected if significant improvements are not seen in cycling experiments.

- The researchers need to provide benchmarks of the computational methods. They need to go beyond PEGS for the evaluation of the solid materials. They should consider using nuclear magnetic resonance (NMR) to help evaluate the chemical composition of their materials.
- Another strategy may be to consider Mg-Ni-B, which absorbs hydrogen, but the mechanism remains not fully understood. Understanding the mechanism may lead to new knowledge and other new hydrogen-adsorbing metal borides.
- If the project is unable to obtain more computing power, hence the use of PEGS, the PI should reach out to a national laboratory or an academic institution with the ability to develop more complex modeling systems.
- The team may need to concentrate on the mixed-metal borides and borohydrides because these appear to hold most of the potential.
- The material made upon ball milling “polymerized decaborane” and LiH should be characterized by NMR.

Project # ST-118: Improving the Kinetics and Thermodynamics of $Mg(BH_4)_2$ for Hydrogen Storage

Brandon Wood; Lawrence Livermore National Laboratory

Brief Summary of Project:



The objectives of this project are to (1) combine theory, synthesis, and characterization techniques at multiple length/time scales to understand kinetic limitations and possible improvement strategies in $Mg(BH_4)_2$ with relevance to light-metal hydrides, and (2) deliver a flexible, validated, multiscale theoretical model of (de)hydrogenation kinetics in "real" Mg-B-H materials and use predictions to develop a practical material that satisfies the Department of Energy's (DOE's) 2020 onboard hydrogen storage targets. Current project year objectives are to synthesize and characterize high-purity MgB_2 and $Mg(BH_4)_2$ materials, measure hydrogenation kinetics of bulk MgB_2, and establish and calibrate an initial modeling framework and test its computational feasibility.

Question 1: Approach to performing the work

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

- The team uses a combination of experiments, models, characterization, and synthesis to demonstrate a new approach to fuel design in solids. This approach is similar to the approach of the Chemical Hydrogen Storage Center of Excellence. The multiscale computational framework is good. The phase-field approach for a mesoscale model combining experiments and density functional theory (DFT) electronic structure calculations are good. Synthesizing very pure materials is a very good idea. The project is using x-ray spectroscopies at the Advanced Light Source at Lawrence Berkeley National Laboratory. DFT electronic structure data collection and subsequent analysis is not new in chemistry or in solid materials. The team has good ideas about connecting the properties of phases to kinetics and has done good work connecting interfaces to bulk thermodynamics and kinetics. The only weakness is that the material is not very exciting.
- This project combines advanced theoretical models with selected experimental measurements on high-quality samples to investigate phase formation and atomic transport in light-metal hydrides. The emphasis is on identifying the atomic processes that control hydrogen absorption and desorption in order to understand and enhance the rate-controlling reactions that impact the hydrogen storage properties of these materials. Attention is focused on the hydrogen interactions at surfaces and interfaces for non-equilibrium conditions. Two explicit example systems are Li-N-H and Mg-B-H.
- The team is using a good approach. It is nice to see well-integrated theory, synthesis, and characterization. Multiscale characterization and modeling are essential for understanding these complex reactions and identifying ways to improve their properties.
- The project has a good team and a good balance of theory, modeling, synthesis, and characterization.
- The theory approach to investigate multiple length and time scales is very ambitious. The principal investigator (PI) has the background and tools to initiate this task. It is not completely clear how much the team will use published work in the literature or perform kinetic measurements in its laboratory. There are advantages to both approaches.
- The multifaceted approach adopted in this project provides a solid strategy for gaining a more complete understanding of kinetic limitations and rate-limiting steps in complex hydrogen sorption reactions in light-

metal hydrides. Although there are reasons to have serious reservations about $Mg(BH4)_2$ actually emerging as a practical material that meets DOE goals, the understanding that will be gained from the studies of that material will undoubtedly extend to other light-metal systems as well. A combined theory (DFT and phase-field modeling), synthesis, and characterization approach conducted at multiple length and time scales should provide important insights into the daunting challenge of inhibited kinetics in those materials.
- The combination of DFT and phase-field modeling is a very powerful tool for probing the $Mg(BH_4)_2$ dehydrogenation process. However, these studies are not focused on the pathways established through solution studies in the 1960s or recent solid-state studies for the reversible dehydrogenation of $Mg(BH_4)_2$ to polyborane anions. Instead, the approach has been to validate the modeling on a $LiNH_2$ system, which is irrelevant to the $Mg(BH_4)_2$ system. Likewise, the approach of characterizing the "B-H" products through x-ray absorption spectroscopy (XAS)/x-ray emission spectroscopy (XES) rather than nuclear magnetic resonance (NMR) techniques is off target.
- The budget appears to be low for this formidable task of improving the kinetics and thermodynamics of such a well-studied material as $Mg(BH_4)_2$. The researchers appear to rely heavily on collecting their own experimental results versus analyzing results that have been already reported by others. There is already a lot of information available about the effect of nano-confinement on $Mg(BH_4)_2$, the reduction of the dehydrogenation temperature, and the high temperature that is required to form some $Mg(BH4)_2$ upon hydrogenation. The project will benefit from incorporating existing information in its analysis. The laboratories involved in this project have extensive analytical and computational capabilities, but it is not clear whether the right analytic capabilities have been made available to quantify the different phases that form upon $Mg(BH_4)_2$ dehydrogenation and during hydrogenation of its reaction products. It is not clear how the project plans to collect all the properties of the intermediate phases and the interaction between the intermediate phases in order to complete a phase-field analysis.
- The approach for the project is not clear; several theoretical methods and multiple experimental methods are mentioned without a clear plan for their utilization.

Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

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

- The researchers have been successful in using a combination of experiments, models, characterization, and synthesis to demonstrate a new approach to fuel design in solids. They have developed a multiscale computational framework. They have connected a phase-field approach for mesoscale model combining experiments and DFT electronic structure calculations, which is good. They have synthesized and characterized very pure materials. Their work on connecting the properties of phases to kinetics is of high quality. They have done good work on connecting interfaces to bulk thermodynamics and kinetics. One issue is how they will make the software and data sets/materials available to the community, which is the basis of success for the project, not the hydrogen storage material they are initially focusing on, which is not very exciting. Automation of the DFT calculations based on the missing data in a spreadsheet is a good idea, but it has been previously addressed in computational chemistry applications.
- Considerable progress was shown regarding the development of the theoretical framework of integrating a range of modeling techniques to predict the different phase pathways for the reactions of bulk and nanoparticles in Li-N-H. The experimental effort seems to have been somewhat slower. For example, while presumably high-purity samples of MgB_2 and $Mg(BH_4)_2$ were synthesized, and a number of experimental methods are shown on slide 7, only powder x-ray diffraction (XRD) and XES/XAS results were presented.
- The successful development of a theoretical and computational framework for predicting phase fractions as a function of pressure, temperature, and particle size is a critical advancement. It will be challenging to adapt these tools to address multiple reaction intermediates. As pointed out in the presentation, this will carry a very high computational cost. Noteworthy progress was also achieved on developing a construct for exploring phase nucleation and non-equilibrium effects in the mesoscale kinetics code. These effects may be critical to understanding kinetic pathways in hydrogen sorption reactions in light-metal systems. It was unclear why the team "switched gears" from its preliminary studies of the Mg-based system to studies of the Li-N-H system. It is not clear whether this was because of major obstacles (e.g., prohibitively slow kinetics) in the Mg-system or whether there were other reasons for taking that detour. Some clarification

would be helpful. The identification of challenges, obstacles, and proposed mitigation strategies was important and led to useful additions to the presentation.

- This is a new project but good progress has been made on synthesizing and characterizing MgB_2 and $Mg(BH_4)_2$ and on establishing the theory and models.
- The preliminary synthesis and hydrogenation results look interesting. Spectroscopy shows some B-H formation, but it is not clear what progress is being made with XRD. This could be tracked (in situ) at a number of synchrotron facilities. The team should be able to see hydrogen insertion or the formation of new phases. Preliminary results with nano-Li_3N look interesting. A more detailed understanding of reaction pathways is critical to further improving the properties of these reactions. It is unclear how the internal structure of the particles is determined (especially at intermediates states of reaction). This will likely play an important role in the reaction pathway, but measuring this will not be easy—transmission electron microscopy has many challenges, the biggest of which may be beam damage.
- It will be helpful to use theory in combination with other spectroscopic techniques such as IR and NMR to better understand the evolution of structures involved in the hydrogenation of MgB_2. The addition of catalysts may be required to increase rates, but this will add some additional variables to the computational modeling.
- A small hydrogen uptake in MgB_2 was detected, but the reaction product remains unclear. This contrasts with the system MgB_2-LiH (and other similar composites), which readily absorbs hydrogen. $Mg(BH_4)_2$ was successfully prepared, but it is not clear what the next step is in the experimental characterization process. A high number of polymorphs of $Mg(BH_4)_2$ are described in the published literature, along with decompositions using different additives. This experimental information needs to be taken into consideration.
- The studies of the lithium amide system, which appear to have dominated the efforts today, have contributed little toward improving the kinetics of the reversible dehydrogenation of $Mg(BH_4)_2$. The most meaningful accomplishment to date has been the benchmarking of the hydrogenation of bulk MgB_2. Unfortunately, the extremely slow and low-level hydrogenation that is observed at >350°C brings the feasibility of hydrogenating MgB_2 in a practical system into serious question.
- The synthesis of bulk MgB_2 and $Mg(BH_4)_2$ is well known, and the study of the hydrogenation and dehydrogenation of the material in its bulk form is unlikely to result in new information that will improve the kinetics and thermodynamics, because the bulk properties have already been studied for such a long time. There is information in the literature about the dehydrogenation of nano-confined $Mg(BH_4)_2$, but such information, even if incomplete, does not appear to have been introduced to the modelers to test their models. Instead, the modelers tuned their models to the lithium amide system, which does not appear to be relevant to $Mg(BH_4)_2$. It will be important for the modelers to review the nano-confined $Mg(BH_4)_2$ literature first because it will take considerable time before the project will have collected and analyzed data about the hydrogenation of nano-confined MgB_2 and the dehydrogenation of $Mg(BH_4)_2$.

Question 3: Collaboration and coordination with other institutions

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

- A well-qualified team with expertise in all areas of ab initio theory, phase field modeling, nanostructure synthesis, and characterization is conducting the work on this project. Extensive collaborations with external partners are also evident, and they should generate important, new information that complements the core work on the project.
- The project has a strong team. The challenge is to perform the modeling in parallel with the nanoparticle synthesis, testing, and characterization. The modelers first will need to depend on literature data before experimental results will become available from the materials that have been synthesized as part of their own project.
- The interactions with the theoretical team appear very strong and clearly integrated to the Sandia National Laboratories (SNL) experimental group. It is much less clear whether outside researchers (e.g., the National Institute of Standards and Technology for neutron scattering) are actively involved.
- The project has a good technical team with excellent capabilities, and it is very commendable to develop a Google tools platform to share DFT data, but it might also be good to have some additional outside collaborators identified.

- The project has a strong team with a number of active collaborations. In general, the new materials projects seem to be working somewhat independently. More coordination among all materials projects (forming a mini-materials Center of Excellence) would be worthwhile to minimize overlap and ensure the expertise and capabilities of all partners are fully utilized.
- There are good collaborations with SNL on nanophases and nano-confinement.
- The project has good connections and collaboration between experiments and theory.
- The collaboration among team members seems adequate. However, this effort seems completely insulated from the many other ongoing worldwide efforts to develop $Mg(BH_4)_2$ as a practical hydrogen storage material.

Question 4: Relevance/potential impact on supporting and advancing progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Multi-Year Research, Development, and Demonstration Plan

This project was rated **3.1** for its relevance/potential impact.

- Understanding kinetic limitations in hydrogenation and dehydrogenation reactions in light-metal hydrides is critical to overcoming existing barriers to successful use of those materials in practical hydrogen storage systems. Gaining a deeper fundamental understanding of kinetics and reaction mechanisms will be key to developing improved low atomic number, lightweight metal hydrides that operate at temperatures and pressures commensurate with fuel cell operation. This work is highly relevant, and it directly supports the goals articulated in the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan.
- The project addresses interesting concepts that are of real interest and value to the hydrogen storage community. Success will be measured by the release of codes, data sets, and materials to the storage community and their use by the community. The linking of theory and experiments is good. The mesoscale work is good and relevant, as is the development of theories to cross scales.
- The project goals and approach to "combine theory, synthesis and characterization…to understand kinetic limitations," are critical to providing insight into the development of a rational approach for enhancing kinetics.
- Efforts from this work should lead to a better understanding of the mechanisms that control the absorption and desorption of hydrogen in lightweight hydrogen storage materials.
- This project has the possibility of providing very insightful descriptions of the processes that limit the light element hydrides from meeting storage capacity and reaction rate targets. It may provide guidance to changes in chemical compositions, phase dimensions, and structures that lead to overcoming some of the barriers. However, it probably will not provide major modifications of the equilibrium thermodynamics parameters or address the role of volatile decomposition products, such as NH_3 or B_2H_6, or the irreversibility and degradation of these storage candidates.
- Overcoming the high kinetic barrier to the reversible dehydrogenation of $Mg(BH_4)_2$ is key to the development of this highly promising hydrogen storage material. Thus, the modeling studies could be of high relevance and impact. It would be good to get at least some preliminary results on the dehydrogenation of $Mg(BH_4)_2$ (not $LiNH_2$) to see whether it is useful and in agreement with previous studies on $Mg(BH_4)_2$. MgB_2 nanoparticles will, of course, not remain nanoparticles on reversible hydrogenation to $Mg(BH_4)_2$. However, the nanoparticle studies can at least determine whether the "nano-MgB_2" approach is worth pursuing.
- The impact of the project likely lies with the models and their online and open-source tools. $Mg(BH_4)_2$ has been exhaustively studied, so it is somewhat difficult to imagine that the performance will be improved substantially. However, the importance of this project will come from better understanding the reaction pathways and kinetics, and how these properties are affected by particle size and catalysts.
- Magnesium borohydride is a highly relevant compound to study in detail.
- $Mg(BH_4)_2$ is a well-known hydrogen storage material, and many groups have tried nano-confinement as a means to establish reversible hydrogen storage at moderate conditions, but so far these efforts have been unsuccessful. The project has not reported what it will be doing differently from the previous attempts to turn $Mg(BH_4)_2$ into a practical hydrogen storage material, other than working with a purer starting material.

Question 5: Proposed future work

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

- The proposed work on transport is good. The team must focus on developing the toolset and making it available to the community. The team needs to discuss its plans for how to release its tools and data sets for use by others. The Office of Energy Efficiency and Renewable Energy should sponsor a materials library for benchmarking experiment and models.
- There is a good mix of experimental and modeling activities planned for the rest of fiscal year (FY) 2015 and FY 2016.
- The future work planned is appropriate for this project. The team may want to investigate nano-confined $Mg(BH_4)_2$ (if it is not already part of the plan).
- The proposed DFT studies on $Mg(BH_4)_2$ and hydrogenation of MgB_2 nanoparticles for the coming year are much more on target than the work that has been accomplished in the previous year.
- The future work is clearly stated and represents a straightforward and reasonable extension of the work conducted thus far. However, the critical issue of how multiple-phase formation during sorption reactions will be addressed was not adequately described. Likewise, the diversion of the initial effort on the Mg-based systems to studies of the Li-N-H system should be described more thoroughly. Both “nanosizing” and catalytic doping are entirely reasonable pathways to enhancing sorption kinetics. However, the project team must clearly recognize that hydrogenation/dehydrogenation cycling in media containing “free” nanoparticles can frequently lead to unwanted agglomeration and clustering of the nanoparticles, thereby defeating the purpose of creating the nanoparticles in the first place. This is far less problematic in nano-confined media (e.g., nanoparticles confined within a framework or template structure). Adapting theory and modeling tools to nano-confined media should be an important research thrust.
- The team provided a list of “remaining challenges,” but having more details of how the challenges will be addressed would be beneficial.
- The work on the lithium amide system appears to be distracting the team from making progress on the $Mg(BH_4)_2$ system. The characterization method that is being proposed in the future work may not be able to identify quantitatively the fraction of all the intermediate phases that occur during $Mg(BH_4)_2$ dehydrogenation and the intermediate phases that form during an attempt to hydrogenate the reaction products. The researchers have not indicated whether they would consider limiting the dehydrogenation of $Mg(BH_4)_2$ to a point at which hydrogenation of the nano-confined material would still be feasible. The researchers appear to have selected MgB_2 as the starting point for hydrogenation, which may be very difficult.
- Additional experimental work (i.e., macroscopic kinetic and XAS/XES measurements) is planned for the Mg-B-H samples, but no indication of any supplemental studies using neutron scattering or insightful spectroscopies (i.e., Raman, NMR, or mass spectrometry) was given. It is not clear that the proposed kinetics and x-ray techniques will be sufficient to validate the theoretical predictions reliably.
- It is not clear how experimental science will proceed and be correlated to the theoretical work in the project.

Project strengths:

- Gaining a deeper understanding of the kinetic limitations to hydrogen sorption reactions in light-metal hydrides is a critical need. This project offers an important and valuable opportunity to gain keen insight into reaction kinetics and mechanisms in these systems. Although the challenges are numerous and difficult, the extensive expertise and experience of the project team in all areas relevant to the proposed studies provides confidence that solid progress will be achieved.
- This project has assembled a diverse collection of theoretical tools to model and predict phase transitions and possible reaction pathways in great detail. With appropriate experimental results, a substantial increase in key reaction processes may result. The ability to produce high-quality sample materials should help with obtaining more reliable test data to compare with calculated properties.
- Project strengths include the development of new computational toolsets and databases for the hydrogen storage community, the development of new theoretical methods, the development of data sets, and the new very pure materials for testing.

- The models and the “platform for collaboration, data management, and data sharing using online and open-source tools” will be an important contribution to the community. In addition, a better understanding of the kinetics and reaction pathways will help guide future work in this area.
- The research team has successfully prepared pure $Mg(BH_4)_2$, following a published procedure, which is a good starting point for further experimental research. Some theoretical results are also presented using different approaches.
- The project has a strong team of experts and a good balance between theory and experimental activities.
- The project has a strong team. It has great analytical and computational capabilities.
- The project demonstrates good connections and collaboration between experiments and theory.
- The combination of DFT and phase-field modeling has the potential to provide valuable insights.

Project weaknesses:

- The PI is relatively new to the research topic and will make a greater impact after having more time to catch up on published work in the field. A few reviewers seemed to think the team missed an opportunity to test some of the modeling using literature data on nanophase $Mg(BH_4)_2$ instead of Li_3N.
- Selecting an Mg-B-H system may have been a problem because of the system’s very slow kinetics. While $Mg(BH_4)_2$ has high potential as a storage material, it might have been better to select $NaAlH_4$ as a baseline material, especially to better understand the effects of catalytic doping.
- It is unclear whether adequate attention has been given to characterize enough properties of the Mg-B-H and Li-N-H materials experimentally to confirm that the modeling correctly includes actual species or intermediate phases that are responsible for the kinetic and capacity behavior during the hydrogen absorption and desorption reactions.
- The project team is tackling a very difficult problem. The team must avoid the temptation to solve the “entire problem” and instead concentrate on tractable pieces of the puzzle. However, it is not entirely clear whether information gained from one simple system is readily transferrable to others. This is especially true in cases where multiple phases are at play. Also, the team must recognize that nanoscale “free particles” most likely will not remain small upon cycling. It seems that a more thorough investigation of nano-confined media should be included in the research plan.
- The storage material is not very interesting. The team has no plans for releasing software and data sets.
- It is not really clear what is expected from the XAS measurements. These studies take considerable time and planning, but it was not exactly clear what the team hopes to learn from them. If it is just a test for hydrogen absorption, as indicated on slide 12, there are probably easier spectroscopic methods (e.g., Fourier Transfer Infrared Spectroscopy or Raman Spectroscopy to look for B-H modes). $Mg(BH_4)_2$ has been well studied, so it seems unlikely that tailoring particle size or catalysts will significantly improve performance (kinetics) beyond what has already been reported. The project should focus on understanding the materials and reactions.
- The project has been sidetracked on studies of $LiNH_2$. The project is apparently being carried out with no connection and very little awareness of other research efforts on the dehydrogenation of $Mg(BH_4)_2$.
- A high number of experimental methods are mentioned without a clear plan of utilization. The work does not take published literature into account to a sufficient degree. Therefore, it is not clear what the outcome of the research may be and how experimental and theoretical research will be combined. The theoretical work appears to “stand alone” with little correlation to published knowledge and the experimental part of the project.
- $Mg(BH_4)_2$ has so many intermediates, which can also be different upon dehydrogenation and hydrogenation, that it appears to be an overwhelming task to quantify all the model parameters that will be required for phase-field modeling. It will be important to verify whether DFT calculations can be accurate when applied to borohydride materials. It is not clear how thorough the literature search has been for data that could help the modelers with setting up their models for $Mg(BH_4)_2$. It is not clear how the researchers plan to further improve the $Mg(BH_4)_2$ kinetics and thermodynamics beyond the doping and nano-confinement that has already been reported in literature.

Recommendations for additions/deletions to project scope:

- The team should extend the "nanosizing" studies to include nano-confined media (e.g., nanoparticles confined within structure-directing frameworks or templates).
- It is useful to understand some of the unique properties of the nanophase; however, in cyclable material, there has been little precedence to describe how the nanophase will be reformed after the initial hydrogen uptake or release step, so it will be imperative to study "real systems." SNL has the capability of kinetic measurements in bulk materials, as outlined in the presentation. The experimental measurements are a critical component to benchmarking the computational work, but the focus with limited resources should be on bulk, not nanophase, materials.
- In order to adhere to the project schedule, the team should perform an extensive literature search for data about nano-confined $Mg(BH_4)_2$ that can be used to start developing and evaluating the computational models while data collection efforts start for experimental data (which is time consuming).
- The authors need to study the published experimental literature in detail (rather old literature is mentioned on slide 5).
- Opening the project to look at other materials, especially if the kinetics of $Mg(BH_4)_2$ becomes a problem, is recommended. It might be better to validate the models against better-known materials, similar to what was done with the Li-N-H system.
- Additional techniques should be included in the experimental portfolio to establish whether the models are for the actual processes that are responsible for these hydrogen storage materials.
- It is not clear what is new in the Google spreadsheet. The team should connect to the computational chemistry community that has developed some of these types of tools. Also, the team should develop a plan and approach to release software and data sets.
- The team should stop all work on lithium amide immediately.