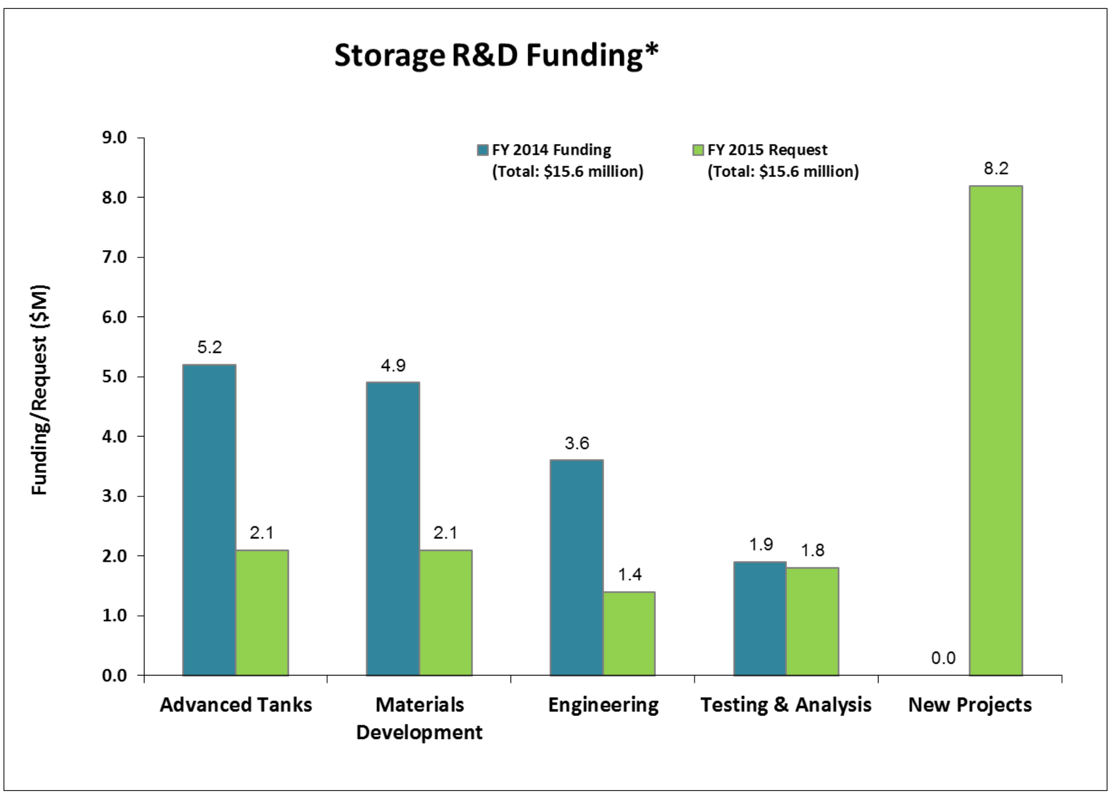
2014 — Hydrogen Storage
Summary of Annual Merit Review of the Hydrogen Storage Sub-Program

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

In fiscal year (FY) 2014, the Hydrogen Storage sub-program portfolio continued its focus on onboard automotive and nonautomotive applications as well as increased its emphasis on new materials and novel concepts to meet performance requirements for portable power and material handling equipment applications. Reviewers commented that the sub-program is well managed and that there is good communication between U.S. Department of Energy (DOE) technology managers and project principal investigators. 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. Reviewers remarked that the sub-program was underfunded, especially with the effort to address both near-term compressed gas storage and longer-term materials-based storage technologies. Overall, reviewers expressed concern that too much emphasis is currently being placed on near-term technologies at the expense of longer-term, potentially higher-payoff technologies. A reviewer recommended trying to structure future funding opportunity announcements to establish “Center of Excellence–like” collaborative efforts.

Hydrogen Storage Funding

The chart below illustrates the appropriated funding planned in FY 2014 and the FY 2015 request for each major activity. The sub-program received $15.6 million in funding in FY 2014, and it has a budget request of $15.6 million for FY 2015. In FY 2014, the HSECoE continued to be a major activity for the sub-program, although it has entered its final phase and has an anticipated end date in FY 2015. Additional efforts aimed at lowering the cost of compressed hydrogen storage were initiated in FY 2014. Work on hydrogen storage materials development is also an important part of the portfolio that will continue to be an area of focus, with three new projects initiated in FY 2014. New efforts on near-term compressed gas storage and advanced storage technologies are anticipated in FY 2015.



∗ 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.

Majority of Reviewer Comments and Recommendations:

The Hydrogen Storage portfolio was represented by 20 oral and 9 poster presentations in FY 2014. A total of 18 projects—via oral presentations—were reviewed. In general, the reviewers' scores for the storage projects were good, with scores of 3.5, 2.5, and 3.2 for the highest, lowest, and average scores, respectively.

Advanced Tanks: Three projects on advanced tanks were reviewed, with a high score of 3.2, a low score of 3.1, and an average score of 3.1. Reviewers considered the work to identify lower-cost precursors for high-strength carbon fiber (CF) manufacturing and efforts to demonstrate pathways to lower-cost advanced tanks to be highly relevant efforts that may have a significant impact. Reviewers commented favorably on the progress being made with both the textile-grade and melt-spinnable CF precursor projects. Reviewers praised the textile-grade precursor project for meeting the tensile strength target. However, one of the concerns raised included a CF manufacturer's purchase of the producer of the textile-grade precursor, which may potentially limit the impact the effort could have on the industry. For the tank cost reduction projects, reviewers commented favorably on recent and future efforts aimed to validate modeled predictions on cost reduction pathways through fabrication and testing of real systems. 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 3.4, a low score of 2.5, and an average score of 3.1. 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 experimental and theoretical efforts as well as place more emphasis on meeting projected material-level property requirements to meet the system-level targets.

Engineering: Nine projects were reviewed on hydrogen storage engineering, with a high score of 3.5, a low score of 3.0, and an average score of 3.3. Reviewers stated that the HSECoE made significant progress in the past year and featured 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. It was recommended that more emphasis be placed on improving system performance for targets furthest from being met. Overall, reviewers thought the HSECoE and its partners were making good progress in evaluating materials-based storage systems and making decisions to meet DOE performance targets.

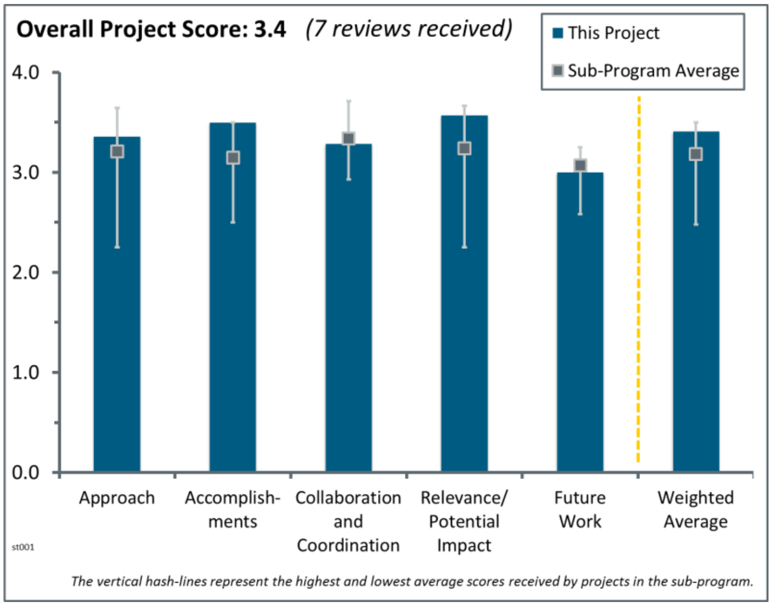
Testing and Analysis: Two projects related to testing and analysis were reviewed, with a high score of 3.4, a low score of 3.1, and an average score of 3.3. Reviewers stated that these projects are critical to the sub-program because they help develop targets and guide research to maximize impact. Reviewers commended the excellent collaboration and cooperation displayed in each project to ensure coordinated assumptions and efforts in the community. The project teams were commended for their use of the Design for Manufacturing and Assembly (DMFA) methodology, which was considered to be a powerful and appropriate analysis tool. Reviewers thought that the validation of models and analysis provides excellent information for DOE and researchers in targeting high-impact areas; however, they also suggested more validation of the results. Overall, reviewers noted that a strong team performed thorough analyses and emphasized the importance of these projects in improving the quality of research in the 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:

This project's objectives are to develop and use models to analyze the onboard and off-board performance of physical and material-based automotive hydrogen storage systems; conduct independent systems analysis for the U.S. Department of Energy (DOE) to gauge the performance of hydrogen storage systems; provide results to material developers for assessment against system performance targets and goals and help them focus on areas requiring improvements; provide inputs for independent analysis of costs of onboard systems; identify interface issues and opportunities, as well as data needs for technology development; and perform reverse engineering to define 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.

- This project is directed analysis work in support of various DOE-supported projects. As such, by definition, it is in direct and indirect support of DOE efforts in surmounting barriers. Analysis work is always needed and valuable to understanding and quantifying barriers. It is difficult to rate the approaches of directed activities, but the techniques used in this effort are very sound.
- This project provides great support to several DOE research, development, and demonstration programs. The principal investigator (PI) deserves an award for his many contributions. The approach is sharply focused on technical barriers; it is difficult to improve on the approach significantly. The team appears to be very accommodating with tight timelines and provides constructive feedback to collaborative partners.
- The PI is collaborating with the Hydrogen Storage Engineering Center of Excellence (HSECoE) to provide models based on empirical data and systems (where available). The intent of the system modelling has shifted recently to provide a sensitivity analysis of what material and system performance is required to achieve targets. This has always been the key objective to come out of the entire engineering effort.
- The Argonne National Laboratory (ANL) approach considers the relevant technical parameters needed to assess the ability of a given storage option to meet both the onboard and off-board refueling performance targets. The ANL team collects and updates inputs from various sources to obtain reasonably complete descriptions of hydrogen storage systems, and the team's analysis methodology seems to be thorough and sound. The team has exchanged information with several partners of the HSECoE, as well as other organizations. The team performs trade studies to determine influence of various parameters to identify those with the most impact on achieving or limiting the performance targets. Unfortunately, this type of analysis does not directly lead to devising specific solutions to the problem areas. For example, it is not enough to continue showing that storage media needs to have greater gravimetric or volumetric capacities or fast reaction kinetics to overcome the barriers.
- Developing and using models is a good first step to gaining information about hydrogen storage systems. The necessary step to validate the simulation results is also addressed. It is not clear how the "Life-cycle-management" barrier was addressed.

- The PI and team's approach is generally sound. There are many different concepts covered, and it takes a sound understanding of the science to model each technology. There is a need to validate the result of the resin additive study because other researchers have had conflicting results, in that they have demonstrated nanofillers to increase mechanical properties. Tank improvements should be ranked or demonstrated in a waterfall to show the improvements and estimated impact on the tank. It is not obvious that the PI allows the experimental researchers to vet their results, and this would seem to be a key requirement since this is a reverse engineering effort. The project needs to do more than just obtaining input for the modeling. Variances should be incorporated in the projections as the values listed are not absolute.
- The approach in the analysis of onboard and off-board hydrogen systems using thermodynamic and kinetic models is effective but could be improved by further explaining the model transfer functions and references to empirical results. Additional assumption justifications and sensitivity analysis would be useful, such as recognizing a tolerance band.

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.

- There has been excellent progress toward objectives to develop models to analyze onboard performance of physical and material properties. The project team was asked at a past DOE Hydrogen and Fuel Cells Program Annual Merit Review to provide a sensitivity analysis of parameters under model review. The back-up slides in the presentation show the message was taken seriously.
- Good progress has been made in resin development and vessel protection (impact resistance). The overview of cold gas systems with regard to volume, capacity, gravimetric capacity, and well-to-engine efficiency was good. On page 5, tasks and accomplishments should be clearly differentiated.
- The PI has provided the storage community with key "material" performance targets that are required to achieve overall system targets. This will undoubtedly cause a major rethink of the materials approach. The sensitivity analysis indicates that the required materials performance is beyond the theoretical maximum of known materials.
- ANL has continued its assessments of several storage systems, reporting results on mechanical properties of carbon fibers; low temperature compressed hydrogen gas storage; and reverse engineering on desirable properties of hydrides, sorbents, and chemical storage materials to meet the DOE performance targets. While the analyses are comprehensive and probably reliable, they do not predict promising new pathways to any significant practical improvements in properties of carbon fibers or compressed gas storage vessels, nor will the low-temperature gas storage option offer much better performance than ambient compressed gas. The requirements predicted for the sorbents to meet the DOE system targets almost certainly cannot be met with real materials.
- The overall accomplishments were very good, especially the reverse engineering of the material parameters for the sorbent system. The physical storage analysis indicated the resin properties did not affect the burst strength but could change the impact damage tolerance. This seems to contradict the results of others, such as 3M, which did achieve a burst strength improvement. The impact analysis seems to imply the addition of foam at 2.5 cm eliminates damage issues without the nanoparticles. The results of the cold gas storage analysis were useful based on the PNNL project, but the project should be careful in making generalizations about the high-density polyethylenes (HDPE) material because there are different grades of HDPE that could operate at lower temperatures.
- The results were generally sound. There is a need to validate nanofiller results, as there are questions.
- During the last year, the analysis team performed a number of tasks on physical, metal hydride, adsorbent and chemical storage components. These included very important well-to-wheel efficiency and reverse engineering to quantify required storage media properties. The modeling of composite impact damage for compressed hydrogen tanks is encouraging and should be especially useful. The reverse engineering calculations for the properties required for a cryo-adsorbent to meet the system target (120g hydrogen/kg adsorbent) will be an extreme challenge for the materials developers. All other work was clearly needed. This project provides clearly outstanding contributions to many DOE-funded projects.

Question 3: Collaboration and coordination with other institutions

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

- This project has excellent collaborations. Especially useful are its roles for, and interactions with, the HSECoE, the Storage System Analysis Working Group and other analysis activities.
- The project continues to have a high level of collaboration with Strategic Analysis (SA) for cost modeling along with many other organizations involved in the HSECoE and hydrogen storage development.
- The PI is working with the HSECoE, to obtain material and system characteristics. The PI is also supporting SA to assist with providing the cost analysis of these systems.
- There has been close, timely, and appropriate collaboration with other institutions; partners are full participants and well-coordinated.
- Contact to all relevant institutes has been established.
- ANL worked with SA in assessing both onboard and off-board costs for several storage systems. There were exchanges of technical information with a number of organizations within the HSECoE, although there appears to be significant duplication of effort with the reverse engineering assessments.
- It was not apparent that the collaboration was multi-way. In a multi-way collaboration, the analysis team would receive input from experimentalists to create the models/projections; the experimentalists would then review the results to vet them. This is a key part of how this relationship should work.

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 has direct relevance and much needed impact on most of the Hydrogen and Fuel Cells Program goals and activities.
- The relevance of this project is high because it provides an independent assessment of various hydrogen storage system concepts.
- The ANL group provides valuable feedback to DOE and the PIs of DOE projects.
- This project is very relevant with regard for the evaluation of hydrogen storage systems.
- This systems analysis arguably provides more value than the fuel cell system analysis that the same PI conducts. While most original equipment manufacturers have their own internal analysis based on their own systems, there are not many complete materials storage-based systems to draw upon. This analysis provides key direction to industry, academia, and the DOE. It provides the system and materials requirements that in turn will guide material developers to take into account many material characteristics other than density. It will allow DOE and the tech teams to make better decisions going forward on funding and targets.
- ANL has provided in-depth systems analyses that supported the Hydrogen Storage sub-program with respect to the assessment of various storage approaches compared to performance targets for light-duty vehicles. While these results previously gave useful insights on the attributes and limitations of current configurations towards meeting technical and cost goals, more recent assessments appear to show levels generally below desired targets.
- This project can give DOE guidance and understanding into the impact of new technologies and is an important tool for the DOE Hydrogen and Fuel Cells Program; however, this should not be used as a standard for what is achievable.

Question 5: Proposed future work

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

- This effort is in its final stages. The PI will finish the promised deliverables.

- The plans build on past progress and generally address overcoming barriers. It is great to hear that there are plans to provide system-level support to new projects.
- There is little need for new assessments (of either high temperature or unstable hydrides as hydrogen storage candidates) because prior work by HSECoE has already documented the impact and imposed requirements rather clearly. Having new evaluations by ANL are unlikely to produce breakthrough discoveries of new materials. As there are no new attractive chemical hydrogen storage properties beyond those previously evaluated by ANL, there is limited potential for more "reverse engineering" of their materials properties or regeneration processes.
- Efforts in metal hydride should be reassessed. Relevant automotive applications should be discussed with DOE.
- The composite work should be continued and is needed to provide guidance. One suggestion would be to take a look at alane regeneration cost and efficiency based on the new project and recent results from Dr. Zidan at Savannah River National Laboratory.
- The future work list makes sense. The origins of the items on the list are not fully clear, but they presumably represent DOE's priorities.
- The future work indicated a continuation of several items that were conducted during the past year. It is recommended that the project does not work on high-temperature metal hydrides in the future work. The addition of compressed natural gas in the future work is a good addition to further assess SA and validate the tank models.

Project strengths:

- The project provides the main analysis service for DOE. It is a versatile, valuable, and much-needed activity.
- The project continues to provide an excellent resource for hydrogen storage system modeling comparisons.
- The project provides guidance to academia, industry, and government as to the limits and possibilities of materials based systems.
- ANL has developed very comprehensive analytical tools for detailed engineering assessments of both the onboard and off-board aspects of hydrogen storage. The results appear reliable and robust from comparisons based upon current knowledge and others' experience with available prototype and demonstration storage systems. Analyses appear to be based upon best available data from various sources.

Project weaknesses:

- The project should continue to pursue opportunities to validate its results based on empirical testing and existing hardware.
- The analyses ultimately need some validations. It is not always clear if and when such validations will be accomplished.
- ANL has been performing these assessments for a number of years and appears to have considered nearly all of the variations in the design and property parameters, but are still unable to specify storage options capable of meeting all targets simultaneously. This situation is especially true for the various materials options based upon available candidates. It seems unlikely that further tweaking of these assessments will be all that productive.

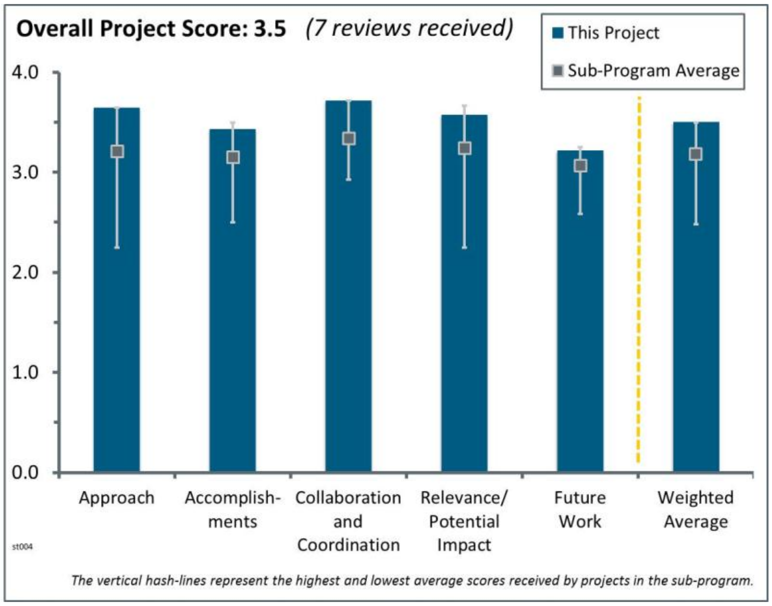
Recommendations for additions/deletions to project scope:

- The project could make a more significant impact on the overall hydrogen storage industry if certain basic models and/or transfer functions were released for the public to utilize. The project has resulted in several publications with excellent explanations of certain assumptions, but additional modeling functions would be useful for the industry.
- As the wrap-up effort, the PI should continue to strengthen the sensitivity analysis. Particular emphasis should be placed on providing guidance on the requirements of future materials to meet the overall systems targets. The PI should be careful to ensure that the message emphasizes all material requirements, such as density, heat conductivity, packing, etc., and provide multiple examples of the trade-offs of each material parameter.

- Keep publishing results in appropriate peer-reviewed journals in a timely manner. Continue to use experimental data whenever available to test and benchmark models.
- It is suggested that ANL either cease (or at least greatly curtail) further "reverse engineering" assessments of the hydrogen storage materials. It is now quite clear what properties are needed to meet the DOE targets from prior analyses by both ANL and the HSECoE, and there have been no new viable candidates identified recently. Further refining requirements via more analyses would be of limited value at this time. Resources should be directed elsewhere for more exploratory research instead of continuing these predictive assessments.
- Proceed as directed by DOE.

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 will design innovative material-based hydrogen storage system architectures with the potential to meet U.S. Department of Energy (DOE) performance and cost targets. The objective for 2013/2014 is to 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 **3.6** for its approach.

- This project gets better each year. The management approach was good at the start and has improved annually. The presentation was a joy to listen to. The approach to overall team organization and interaction is excellent. The emphasis is on defining materials and component performance requirements to meet DOE targets for onboard hydrogen storage. In this regard, the researchers now have this aspect of the project at a point where the final outcome will be successful by most standards. The system/engineering validation models, software, etc. seem to be sufficiently comprehensive, and are now teaching the project participants about how the components should be designed /devised to obtain the best possible outcome. However, the project is also giving a fairly clear signal that some (but not all) of the DOE targets will be met. The decision to go with the metal organic framework-5 (MOF-5)-based adsorbent system, instead of a tank full of highly compressed hydrogen, is a vindication of the work done previously by the three older hydrogen storage Centers of Excellence. At least part of all what those centers worked on is in the final demonstration, even though it will not meet all the targets.
- The project aims at virtually all the important storage system parameters and barriers. It is organizational and coordinative in nature. Each storage medium (adsorbent and chemical hydride) and subtask is compartmentalized in a logical matrix managed by individual organizations and principal investigators (PIs). The structure, objectives, and management structure of the HSECoE seem outstanding.
- The general approach of simultaneous exploration of materials development and engineered systems concepts is excellent. A high level of collaboration is evident on this project, which forces additional scrutiny of the project approach to maintain cohesion. Division into technology areas and system topics (adsorption and chemical hydrides) is logical and seemingly effective.
- The Hydrogen Storage Engineering Center of Excellence (HSECoE) has undergone several down-selects to focus on two systems (different thermal management approach) on sorbents. The center is building scaled down (2L) systems to evaluate the advantages and disadvantages of each approach.
- Similar to one or two of the materials centers of excellence, the HSECoE appears to have hit its stride as the project prepares to end. The researchers have done a nice job of making difficult down-select and go/no-go decisions to arrive at Phase III. The overall management structure and decision-making processes that the HSECoE management arrived at in the end proved to be useful and supported the underlying technical projects. System Architects put into place a consistent basis for comparison of materials and systems. Use of spider charts, while cumbersome initially, appeared to, in the end, provide a readily understandable method of displaying progress toward meeting individual targets, as well as a ready

assessment of the remaining barriers. It was transparent as to how progress was achieved with time in this way. The approach that led to the “reverse engineered” materials properties for future chemical hydrogen storage materials should be the model for other similar activities.
- Although a few minor aspects of the research and development (R&D)/engineering approach can be debated, the overall approach, the strong engagement by multiple partners, and the positive trajectory of this project are first-rate. Over the last two years, the project has become keenly focused on the critical engineering and prototype development issues. The HSECoE has faced the exceedingly difficult problem of designing engineering prototype systems based on storage media that are sub-optimal. The team has adopted an approach that overcomes/mitigates this problem by exploring more general design options that are adaptable to new improved materials that may become available in the future. The results will undoubtedly be useful to the Hydrogen Storage sub-program well after the HSECoE activity has concluded.
- This project was the over-arching activity that had the responsibility of coordinating all other projects. It was effective in this task; hence the score of excellent. One area that is lacking is in a clear listing in how the $35 million in funding was distributed among the various partners.

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

This project was rated **3.4** for its accomplishments and progress.

- Progress on the adsorbent system materials (MOF-5), components (modular adsorbent tank insert [MATI], HexCell, tank, and filter), and system modeling has ranged from good to excellent. The researchers have all the parts, have tested some of the components, and are getting close to some real test data for the system as a whole, but it seems that will have to wait until next year. This reviewer is somewhat skeptical about the MATI until there is real evidence of the device performing as expected. Progress on the chemical system also ranges from good to excellent. The required materials properties are very well established. What is also well established is the fact that neither ammonia borane (AB) nor alane can meet all of the DOE targets. Some of the deficiencies seem insurmountable. The “lessons learned” part of the presentation was most enlightening, specifically the notions about earlier down-selecting and the need to identify and circumvent complexities up front. Also, the findings that would have accrued to a preemptive exploration of balance of plant (BOP) and forecourt issues for the various storage options might have given the team a better idea about how much BOP size, volume, and complexity were going to influence the system targets and costs in the long run.
- The HSECoE is on track to complete the tasks it was asked to do, namely incorporating materials into systems and fully understanding the tradeoffs.
- This is a large, seemingly well-executed project with many achievements. Sometimes it is hard to tell if the achievements are “old,” or were achieved in the past year. However, focusing solely on the past year, most activities have been on preparing designs of fabrication and preparation of test facilities. These are vital activities, but create a Phase III period of lessened output compared to periods of testing or conceptual design formulation. The detailed and extensive listing of SMART milestones is very effective. It provides both a structure to the efforts but also a very convenient way to brief on progress. Inclusion of the “lessons learned” slides shows introspection and insight and is commendable.
- After a few years of finding its way, the HSECoE has begun to really accomplish some very impressive results, and one must assume that in part, the HSECoE approach finally gelled, leading to a greater fidelity of accomplishment across the HSECoE’s quite diverse set of tasks. While progress at times seemed slow, it is now more apparent that aside from the usual project start up issues, a significant amount of effort was required just to get a high-fidelity set of materials properties collected. This must have been a significant challenge, given the great diversity of materials types and the R&D sources from which they were gleaned. Along the way, the HSECoE concept drove the project to be quite innovative in a few areas. Designing sorption systems where rapid fueling has been enabled is a very nice achievement. In the chemical hydrogen storage (CHS) area, which is a technically very challenging one from an engineering perspective, innovative approaches were made in a number of unit operations and were successes. The output of a set of CHS materials properties derived from “reverse engineering” the CHS systems will be a powerful tool for future CHS materials development efforts and will hopefully serve as model output for the metal hydride and adsorbent efforts as the team wraps up the research and compiles the final reports. Where there are still

remaining barriers to be addressed (as evidenced by the spider charts), one hopes that future DOE efforts will be directed at solving these remaining difficult and complex problems.

- Important results were obtained during this review period on systems utilizing adsorbent media and chemical hydrogen (non-reversible) media. The work on both the HexCell and MATI systems is on track, and preliminary results are promising. Although less promising results were obtained on the slurry-based alane and AB systems, the work established a good baseline for incorporation of either those systems or related media in a practical storage/delivery system. Although the slurry-based reactant delivery system can function adequately with certain materials, it is extremely complex. It seems unlikely that such a complicated system could actually be deployed in a practical transportation application. Cost and maintenance issues should be addressed. A particularly noteworthy aspect of this presentation is the technical and programmatic "lessons learned" discussion. This candid presentation provided a useful look at the critical issues, how they were addressed, and what might have been done to improve the project. For an effort with such broad breadth and scope, this information is invaluable to the reviewer and the DOE Hydrogen and Fuel Cells Program (the Program).
- This is an excellent example of a well-managed and highly productive DOE Center of Excellence. The presentation was excellent and full of valuable detail. There has been much progress on the adsorbent and chemical hydrogen storage materials synthesis, containment, and system integration, more or less on the original project schedules. The adsorbent MATI and HexCell storage systems have been developed to near completion and test stage, with much useful information developed. Many targets have been met, but volumetric system capacity and hydrogen retention properties remain well below goals. The chemical hydrogen storage materials and systems studies have been excellent in their science and engineering. Although alane was found to have some advantages over AB, both media were shown to have serious problems with cost, efficiencies, and gravimetric densities. Work on chemical systems was phased out at the 2013 go/no-go point. Even in the unlikely event that much improved materials lie in the wings, the efforts pursued by this CoE are very unlikely to meet all the targets. Either approach (adsorbent or especially chemical hydrogen storage) is turning out to be excessively costly and complicated from operational points of view, relative to high-pressure hydrogen storage. However, from the beginning it was not really meant to do so; it was intended instead to develop the engineering techniques to optimize a reasonable onboard storage system should better materials come out of the materials projects. The HSECoE should be highly complimented for expertly and objectively developing the base techniques for future use. It seemed some duplications of effort were possible, e.g., demisting and purification efforts for the hydrogen derived from liquid chemical slurries. The presentation was not always clear in precisely differentiating nominally similar efforts.
- In fiscal year (FY) 2013 the project was 70% complete. In FY 2014 the project was 90% complete. This is good progress for this year, but not excellent. Also, it appears that the project was granted a no-cost extension until 2015. Although significant progress has been documented with this presentation, there also has been some slippage in meeting the original milestones on time.

Question 3: Collaboration and coordination with other institutions

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

- Collaboration and cooperation among all partners in the HSECoE are exemplary. This is a multi-disciplinary, broad-based endeavor that is well-managed and fully coordinated. The strong and beneficial interactions among the partners underscore the importance of the "Center of Excellence model" for tackling problems of this magnitude.
- The PI did an outstanding job in coordinating this activity. There were13 different partners, and they all seem very satisfied with the PI's effort in coordinating the work.
- The HSECoE has developed into a very collaborative set of researchers. This is excellent! Collaborations external to the HSECoE were less well-described during the review.
- The Center is working with the appropriate partners from industry, academia and government.
- The communication forums that tie the team together across institutional and geographic boundaries are well established and are working effectively. There are very few overlaps in responsibilities and tasks. All the ongoing work is essential to the remaining goals of the HSECoE.

- The program has many collaborators and entity interactions, almost to the point of unwieldiness. However, the structure maintains focus and is made to work.
- By the nature of the HSECoE, the collaborations are very extensive and clearly productive. It is difficult to see how all this organizational structure can be fully managed and coordinated, but it seems to have been done very well. There were no real indications of serious organizational problems. It would have been useful if there were preliminary statements from the two original equipment manufacturers (OEMs), GM and Ford, as to whether such relatively complex materials/engineering systems have much potential for fueling a fuel cell vehicle relative to high-pressure hydrogen storage systems. Some comments on this matter were briefly covered in the Q&A period.

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.

- Development of engineering solutions to onboard storage issues is critically important. The logical and well-run execution of the HSECoE greatly aids in progress toward the DOE's R&D objectives.
- At this point in time, the HSECoE is as well-aligned with the Program goals and objectives as it could be. In fact, the HSECoE comprehensive final reports will undoubtedly provide much of the definition for the Program goals/objectives in the years to come. Utilization of the models and validation codes on the HSECoE website will undoubtedly contribute to future program planning.
- This project is vital to the success of the Program. In addition to providing important information that will be useful for optimized system development, the project is providing researchers engaged in new materials development efforts with a solid set of system requirements and guidelines that must be satisfied by the materials systems.
- The major products of the HSECoE are a refined look at what materials properties must be to successfully build a system, as well as the various models that describe the engineering properties of the system-level outputs. Currently, the HSECoE is contemplating having only a drive-cycle fuel cell storage system integrated model. To serve the R&D community more broadly, it may be necessary to provide the storage system models as standalone models. There were several comments from audience members that support this vision. Lack of a plan to maintain the models once the HSECoE project ends is a potential weakness and could limit the future impact of this piece of R&D.
- The HSECoE work has had high relevance and potential impact towards the Program goals. The results may not be what was hoped to solve the storage problem right now, but the work has clearly been useful for the future. Even negative technical limitations and barriers must be known and understood. This was an outstanding effort and the work will retain its value.
- The project's overall goal was to design and engineer various onboard hydrogen storage systems. To this end, the project did a good job and made a significant impact toward meeting the Program's multi-year goals for hydrogen storage systems.
- The HSECoE is evaluating storage systems with materials known for being unable to meet the targets. The HSECoE has been careful to proceed in a manner that provides guidance for future materials and to provide results that are universally applicable as much as possible.

Question 5: Proposed future work

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

- The project should continue to develop sorbent systems (complete work), evaluate, and possibly integrate with future work on compressed natural gas solid state storage. Efforts should be reduced on chemical hydrogen storage systems, as they are very difficult materials to deal with, proposed solutions will not be applicable for automotive systems (augurs, separators, etc.), and systems are mostly materials-specific based. Many of these materials have inconsistent handling properties; therefore, they will each need their own unique systems.

- Technical work is defined by the Gantt Chart and the detailed milestones. Extensive use of detailed milestones makes it easy to track progress and explain future work to all team members.
- The plans for the coming no-cost extension year seem to be precisely what is needed to bring the project to a logical and successful conclusion. The HSECoE team is fully focused on the path identified for meaningful testing and validation of the adsorbent system.
- The future work for the last year of the project is directed toward achieving "Technology Readiness Level 4: System Validation in a Laboratory Environment." This is clearly the logical and reasonable progression for this project. However, more detail about the future work would have been helpful. Specifically, several system deficiencies are apparent in the spider charts (especially the loss of usable hydrogen in the adsorbent systems). Specific work to be done (or recommended) to address those issues should be determined. The material requirements derived from the system analyses and prototype development work should be made available to the material science community at the conclusion of the project.
- The close out of the overall project seems to be pointed in a reasonable direction, with the caveat that stand-alone system models be included in the final output.
- The HSECoE is in its last year. The final work planned is fine and is appropriate for completing the effort. The prototype storage unit(s) should be completed, models finalized, and all significant work made public. The time to accomplish all of this seems short.
- The project is 90% complete. Its accomplishments are many. Future work lies in documenting the progress over the past five to six years. To be most helpful to the Program, the final reporting package needs to stress "lessons learned" and identify the "show-stoppers" for the various hydrogen storage systems under study. Future R&D in hydrogen storage systems should start where this project ended by addressing unresolved challenges in meeting DOE's hydrogen storage targets.

Project strengths:

- The project represents an excellent collaboration of diverse experts with excellent management.
- The project provided the storage community with a strong understanding of materials and systems limits. It provided interesting insight on how to handle thermal management of materials (e.g., anisotropic characteristics of compressed materials).
- Excellent management and program execution are the project's largest strengths. Use of detailed milestones is very effective in guiding the program.
- There is strong leadership at the top, along with thoughtful planning and skillful execution of the research. Good go/no-go decisions have been made down the stretch.
- This project is serving as a model for large-scale collaborations that address the daunting challenges faced by the Program. The project is well organized and managed, and the technical effort is keenly focused on the key technical areas that underlie the successful development of a prototype system. The HSECoE team has done an excellent job of taking a rather loosely structured set of material properties that were initially provided and translating and refining them to the point that the team had meaning and relevance to the development of a workable system.
- The project is well-structured, collaborative, and has good communication. It is a well-focused effort at this point. Some areas exhibited some quite innovative engineering thinking. It has a good, capable team. There was a good set of lessons learned, from both technical and project management perspectives. This would be valuable to DOE in the future.

Project weaknesses:

- There are no glaring weaknesses at this point. The project has improved over past years. A potential weakness is determining how the models on the website will be maintained once the funding is gone. In a perfect world, these models would be "living", and someone would be tasked to keep them up to date with improvements as new results from the community emerge in the future.
- Participation of so many collaborations presents challenges (as well as benefits).
- The HSECoE is always subject to criticism from outsiders due to the nature of the materials being used. Everyone involved knows that the materials are inadequate to meet targets. The work on the chemical hydrogen storage material systems may not be universally applicable to future chemical hydrogen storage materials (most chemical hydrogen storage materials have fairly unique handling characteristics).

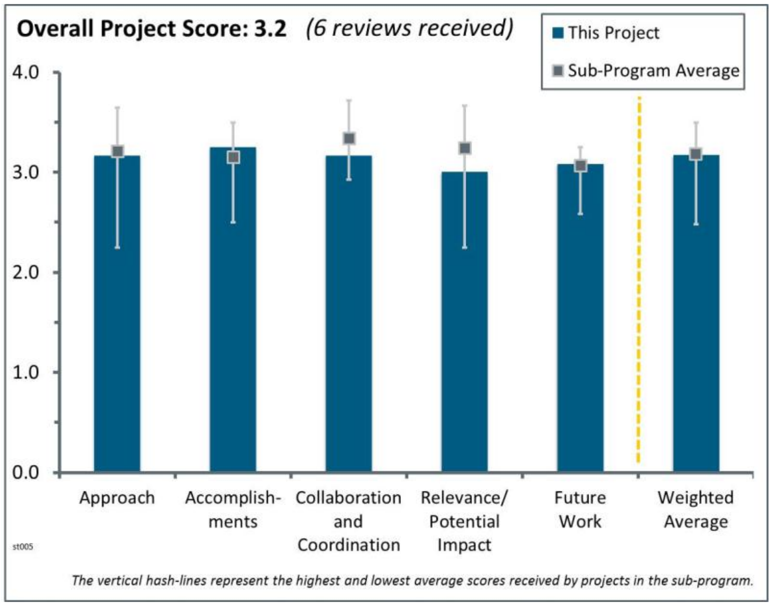
- The greatest weakness of this project is the fact that the three original hydrogen storage centers failed to provide a material that (1) had a chance of meeting the original DOE gravimetric and volumetric hydrogen storage system targets, or (2) gave enough margin in performance to meet even the subsequently down-graded targets.
- It is unfortunate that work on the chemical hydrogen-based systems will not be continuing. Although regeneration remains a serious issue, the chemical hydrogen systems may hold the best promise for meeting (or at least approaching) the challenging DOE hydrogen onboard storage targets. Problem areas and technical obstacles identified by “white spaces” in the spider charts have not been addressed consistently.
- The project has extremely difficult targets, combined with complex storage systems and very limited choices of adequately promising storage materials.

Recommendations for additions/deletions to project scope:

- More explanation as to why the helical thermal management system was down-selected would have helped reviewers.
- The gas-to-liquid separator seems complicated and expensive. Fuller consideration of other approaches is needed. Further attention could be paid to explaining a long-term vision for what the onboard system components might look like. For instance, the HexCell/MATI concepts use a common two-part containment system. [*DOE comment: the referred to containment system is only being used for the prototypes to be able to investigate and modify the systems for evaluation and test purposes; it is not proposed for real systems for use in actual automotive applications.]* It should be determined whether that is considered a long-term feature, as well as exploring whether other perhaps more technically risky (and thus not selected) design concepts emerged that might possibly be a pathway to future development. Further definition of a future aspirational system might serve to focus R&D activities. For example, development of a neat chemical hydrogen storage material (as opposed to a slurry) would perhaps simplify both the storage tank design (settling would not occur) and the gas-to-liquid separator. Quantification of the benefits would then help to gauge whether they should be R&D priorities.
- It should be questioned how much more effort should be spent on the chemical system in the coming year beyond final reporting. Whatever is left of planned but yet to be completed experimental work may not be all that necessary. The best path to a successful final outcome seems to be a focused effort on achieving the best possible demonstration of the absorbent system.
- Greater emphasis should be placed on dealing with the problem areas and technical obstacles identified by “white spaces” in the spider charts. A comprehensive set of material requirements based on system needs should be published in a journal that is widely read by researchers engaged in new material development.
- A key component of the final report should be statements from the OEMs as to the practical potentials they see for the materials and containment designs developed in this project. Whether or not these designs are reasonable for achieving commercial reality needs to be determined.

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:

This project addresses the engineering challenges for materials-based hydrogen storage and provides feedback and recommendations on materials requirements. Project results impact identification, development, and validation of critical components for storage materials in light-duty vehicles, as well as development of models and simulation tools to predict materials performance and development of engineering methodologies, analysis tools, and designs applicable to stationary storage and portable power applications.

Question 1: Approach to performing the work

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

- The project's approach is clearly defined.
- This project team went through a rigorous go/no-go process on chemical hydrogen slurry systems and has quickly adapted its approach, including new tasks in the adsorbent area following the no-go decision on chemical hydrogen storage (CHS). The team performs solid engineering analyses and engineering assessments that are relevant to addressing the barriers the projects present them with.
- The approach is consistent with U.S. Department of Energy (DOE) needs, in particular support of the Hydrogen Storage Engineering Center of Excellence (HSECoE) in the general area of systems engineering. In addition, the project indirectly contributes to high-pressure cryogenic gas storage efforts. In view of the 2013 ending of chemical hydrogen work, the project has expanded efforts on adsorbent tank concepts.
- The approach has been given a score of good in that it was generally effective in addressing the various barriers associated with designing advanced hydrogen storage tanks and estimating balance of plant weight and volume.
- The team combines expertise on hydrogen storage materials, storage tanks, coat modeling, and manufacturing to provide potential hydrogen storage solutions based on various concepts, such as liquid slurry, tank exchange, and compressed hydrogen storage.
- Development of cost and performance models and weight-saving strategies are reasonable approaches for optimizing pressure vessel design and fabrication. Ideally, off-board factors would have been included, but this was out-of-scope.

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.

- The Pacific Northwest National Laboratory effort has made useful progress in the areas of reactor modeling and model validation, system parameters (cost, volume, and mass) and several other contributions. The analysis of alane should be especially valuable to the HSECoE by assessing the relative merits of alane (AlH_3) versus. ammonia borane (AB). Extensive progress was made on containers for AB slurries before the chemical storage effort was terminated, as well as on adsorbent work. The project has accomplished

weight, volume, and cost reductions by balance of plant optimizations. Cost estimates on alane are very useful. The thermos container concept is simple and should help with general DOE efforts on adsorbent storage concepts.
- Progress was good this year, going from 65% complete in fiscal year (FY) 2013 to 80% complete in FY 2014. The only task at risk is the adsorbent cost analysis. The presentation failed to discuss why this cost analysis is at risk.
- The team was able to suggest some potential solutions based on system-level thinking and simulations. The specific accomplishments include (1) combining exothermic and endothermic thermo-bottle system with much reduced foot print and (2) providing proof-of-concept laboratory-scale demonstration. The knowledge gained will be very valuable for future hydrogen storage system design.
- Following the no-go on slurries, the team has picked up on the thermos bottle concept, and has quickly demonstrated proof of principle. The team’s continued work on finishing up on the CHS system model is important. While the current CHS system is highly complex, and still has several significant remaining barriers to be addressed, the model being developed will be very important for future efforts that will hopefully allow the field to take advantage of the high volumetric capacity that CHS enables. The work on identifying opportunities to reduce the gravimetric and volumetric contribution of balance of plant (BOP) components has progressed and impacts many other areas across the Center’s activities. The team’s work and progress on the “tankinator” model was noted by other project presenters.
- Cost analyses results are useful. System mass and energy modeling allow parameter optimization. Reductions and improvements in BOP components resulted in significant weight and volume savings. The thermos bottle is a rather naive approach to heat exchange. More traditional, well-known heat exchanger concepts with internal coolant circulation might have been a better approach.
- The flow schematics with small print and exceptionally thin lines are hard to read. Clarity of system operation is lost as a result of the diagram. Alane cost results are interesting and quite high. Even when not considering the high media cost, the reactor system itself appears cost prohibitive (even at 500,000 systems peryear). No description of cost analysis methods or of pathway to lower cost is discussed. The alane reactor performance model does a decent job of matching experimental data. However, there is no description of type of model, i.e., whether it is empirical or first principals. Reduction of BOP mass and volume is an interesting conceptual exercise and probably worth doing. However, it is important to note that the BOP mass savings achieved is minor compared to the mass of the overall storage system. Thus, resources are being spent on a small part of the weight problem, not the main one. Also, the volume savings probably do not lead to additional usable volume for the system, i.e., the “saved” volume is in unusable locations. It is not clear if the cost of the redesigned BOP unit is considered. The testing of thermos bottle concepts seems well-considered and well-executed. Tests results indicated unexpected zones of high cooling rate. Mixed/alternating use of liquid hydrogen and liquid nitrogen for cooling is an interesting idea. The general amount of cryogens consumed seems to be high. The cost implications of using that much cryogen should be determined.

Question 3: Collaboration and coordination with other institutions

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

- There were excellent collaborations with HSECoE and other entities. Such collaborations are vital as the project continues into the remaining phase.
- There appears to be excellent collaboration among HSECoE members and others.
- As with all projects associated with the HSECoE, the collaboration and coordination between researchers was excellent.
- There are numerous good collaborations within the HSECoE, Storage System Analysis Working Group, and others.
- Adequate collaboration was demonstrated with the CHS partners and across the HSECoE as other areas have received greater emphasis.
- There has been good coordination within the HSECoE, but there is little evidence of collaboration outside of it.

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 **3.0** for its relevance/potential impact.

- This team's approach is highly relevant to achieving overall project goals across several different storage system scenarios, and it has made good progress toward achieving the goals of their specific tasks. The impact of having the best available CHS system model is high, as it will provide future efforts a very solid foundation on which to build. The team's work in cryotank modeling, design, and cost modeling will have an impact in several areas. The thermos bottle' approach may contribute to reducing fill time, which is a high priority target.
- There is a good match to the DOE Hydrogen and Fuel Cells Program goals and objectives for onboard hydrogen storage, mainly via supportive activities for the HSECoE.
- The impact of this work is good. This year, the project experimentally measured cool-down rates for the term's bootleg prototype hydrogen storage tank. The project also addressed methods for reducing the BOP mass and volume by integrating key components.
- This project is very important to understanding/simulating various storage options.
- The relevance of engineering optimization for materials that will never meet targets is questionable.

Question 5: Proposed future work

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

- This project includes an adequate set of tasks to ensure that the close-out phase of the project results in the preservation of the documentation for future efforts.
- Work for this project is almost complete.
- The list of future activities is reasonable to complete the story. DOE has ended the chemical hydrogen storage efforts, but the models should be completed and published.
- The proposed future work is good since it addresses the remaining tasks of this work. These tasks are the design and dormancy testing of a two-liter vacuum thermos bottle, as well as costs modeling for the modular adsorbent tank insert and Hexcell storage tanks.
- The proposed plan is very reasonable. Adsorbent work will take priority in the coming months. It is very important to document the results in open publications and digital models.

Project strengths:

- Comprehensive engineering and cost analysis of systems supported by experimental proof of principle testing are project strengths.
- Project strengths include cost modeling, the tankinator model, and the thermos bottle concept evaluation.
- There is good work on BOP volume and mass reductions.
- The project provides good input to the HSECoE in the area of systems engineering.
- The team has the right expertise and excellent communication/collaborations both internally and externally.

Project weaknesses:

- There is the potential to become distracted with new adsorbent and tank-based tasks and neglect providing the highest fidelity CHS model possible from the existing information.
- The project emphasis was originally on chemical storage without reasonable materials needed to approach DOE targets.
- Feasible hydrogen storage materials are not available for more practical simulations/modeling. The team is asked to perform simulations on materials and concepts that will not be of practical use.

Recommendations for additions/deletions to project scope:

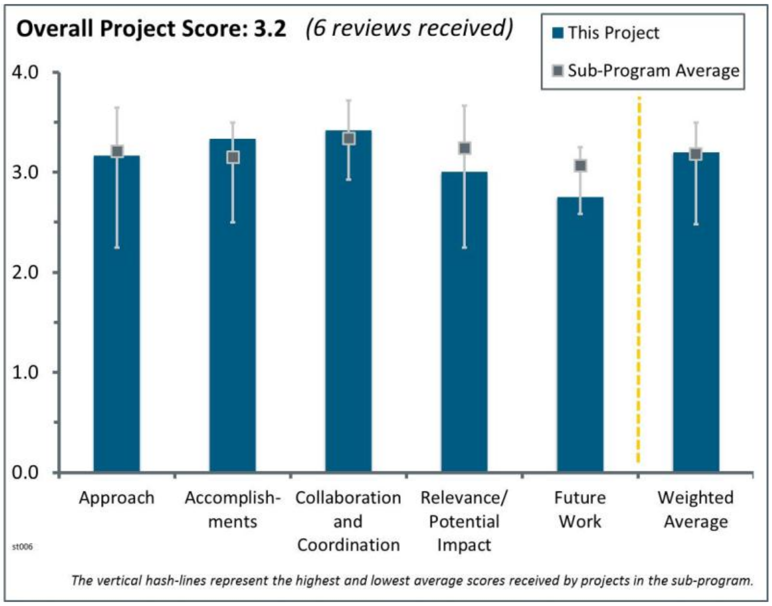
- The project scope is appropriate for the end stages of the HSECoE.
- Include economic results for the costs of coolants needed to cool down a tank.

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 objective of this project is the design of materials-based vehicular hydrogen storage systems that will allow for a driving range of greater than 300 miles. To accomplish this goal, United Technologies Research Center (UTRC) will leverage in-house expertise in various engineering disciplines and prior experience with metal hydride system prototyping to advance materials-based hydrogen storage systems for automotive applications.



Question 1: Approach to performing the work

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

- UTRC plays an important collaborative team role with the National Renewable Energy Laboratory in the development of the graphical user interface (GUI) architecture for the Simulink Model efforts. These frameworks are one of the critical outcomes from the engineering center to facilitate research on new materials.
- The recent and current focus of UTRC has been in two distinctly different areas: (1) developing and demonstrating effective components that deliver purity-free hydrogen gas from the adsorbent and chemical hydrogen systems, and (2) developing and implementing storage system modeling tools that can be utilized not only within the Hydrogen Storage Engineering Center of Excellence (HSECoE), but also by external researchers to clarify materials properties required to meet performance targets. Both of these topics are relevant to the development of viable storage systems for passenger cars, although they do not offer immediate solutions to all problem areas.
- The team has done a nice job of absorbing the no-go decision on chemical hydrogen storage (CHS) systems within the HSECoE and bringing those tasks to an orderly completion. Participating in the team that is developing the GUI for the integrated framework models so that the public release version will be ready by the time the HSECoE ceases work is a very important task for UTRC. The approach to bringing the CHS system components (such as the gas-liquid separator [GLS] and the purification train) to a logical conclusion is important, as this helped to provide proof of principle that even though it is complex, the CHS system can achieve noteworthy volumetric capacity. Thus, the efforts of UTRC will be important for consideration of potential future CHS materials development, and for potential portable power applications. UTRC’s work in particulate clean-up for adsorbent systems was approached in a logical manner.
- The project approach fits in with the HSECoE objectives and thereby addresses several of the problems and barriers. In particular, the specific problems with particulate control in the adsorbent and liquid phase control in CHS beds are covered in this project. In addition, UTRC is also leading the development of the GUI architecture. Importantly, this will allow the models developed by the HSECoE to be made available to the public.
- The HSECoE has taken a reasonable approach to addressing hydrogen quality issues. The project has adopted existing commercially available technologies to address problems.
- The effort is reasonably well defined. The work approach needs to be better correlated with how barriers are being addressed.

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.

- Outstanding progress has been made in all the contractor's areas of responsibility. The principal investigator's presentation was clear, direct, and appropriately detailed. The work on liquid management is apparently finished. With the virtual termination of chemical storage work during the 2013 go/no-go decision, the project has focused more on adsorbent storage problems. Metal-organic framework (MOF) particulate filtration phenomena have been nicely studied. Reductions in balance of plant costs have been achieved. The project has done some outstanding vehicle simulation work, and models were developed. Some of these models have already been placed on the website.
- There has been very impressive work on the GLS, including the design, enabling the reduction in mass and volume, and the testing to validate some of the model predictions. Even if the CHS materials are not going forward in Phase III of the HSECoE the results from the GLS will be valuable, as other liquid materials are considered for vehicular and non-vehicular applications.
- UTRC's work on integrating storage system models into a framework that is readily usable and accessible is an important accomplishment (still in progress) that will be important to DOE goals of providing the storage community and public with usable access to modeling capabilities. The team's work on the CHS major balance of plant (BOP) components, such as gas cleanup and the GLS, was important to demonstrate proof of principle that such complexity could be successfully integrated into an onboard storage system while achieving the target for overall system volumetric capacity. This is a noteworthy accomplishment. The CHS system team, of which UTRC is a member, did a good job of investigating the slurry concept to the point where it was demonstrated to be difficult to implement for CHS. This is a valuable contribution, as knowing where not to go in the future is crucial to future DOE efforts in onboard hydrogen storage. The team's work on particle filtration for adsorbent systems will have an impact on other system types as well, and is an important contribution to achieving DOE goals.
- The modeling effort is clearly valuable in supporting technology development and addressing barriers. It is not clear what the criteria are for an acceptable gas liquid separator.
- Given the no-go status for further chemical storage work in 2013, UTRC satisfactorily completed improvements for a prototype GLS system that included experimental demonstration of its effectiveness, along with major reduction in mass and volume compared to an initial conceptual component that would have been prohibitive. The team also met milestones for ammonia and particulate filter systems that should satisfy targets. The team is making excellent progress on completing web-based system analysis models for the chemical and adsorbent systems that will be available to allow public and independent assessments of alternative candidate materials for comparisons with performance targets.
- Developing a computational fluid dynamic model to allow sizing of GLS was a promising step, but it does not appear to have predicted experimental behavior. Improvements in system capacity are significant steps. The GUI should enhance the model's usability and encourage wider use.

Question 3: Collaboration and coordination with other institutions

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

- There was close, timely, and appropriate collaboration with other institutions; HSECoE partners are full participants and well-coordinated. The collaboration with the Los Alamos National Laboratory and the Pacific Northwest National Laboratory to come up with material targets based on engineering needs was fantastic.
- The project worked closely and efficiently with various organizations and individuals on implementing and testing the storage systems user-interface software for the web-based models. UTRC also collaborated closely on issues relating to purification of the chemical and adsorption storage materials.
- The project interacts with a number of high-quality collaborators from both industry and national laboratories.
- Collaborations are excellent, but almost entirely within the extended network of the HSECoE.

- The level of collaboration appeared to be adequate, but did not appear to be reported very well. There must have been more effective collaboration within the CHS system team for UTRC to have accomplished what it did. Collaboration will be extremely important in rolling out a usable and effective GUI for the integrated framework models.
- There was adequate coordination within the Center, as well as work with third-party vendors to acquire devices.

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 **3.0** for its relevance/potential impact.

- This project provides great support to several HSECoE research, development, and demonstration projects. This year, contributions include an impressive reduction in the mass and volume of BOP components for the GLS and the ammonia filter for the CHS approach, as well as some initial work on particulate filters for the sorption approach.
- This project is of significant impact, as it has demonstrated that even in systems of high complexity, such as the CHS, there are innovative ways to address gravimetric and volumetric capacity challenges in designing and fabricating critical BOP components. The UTRC results helped to formulate what the materials properties must be for future CHS efforts, particularly in the area of minimizing impurities to reduce the gas cleanup BOP budget, and in particulate cleanup for solid systems as well.
- This project supports the HSECoE in several practical and modeling areas not covered elsewhere, and is thereby directly supportive of the DOE Hydrogen and Fuel Cells Program's goals and objectives.
- UTRC has developed promising concepts and prototypes of purifiers for improving the quality of hydrogen supplied by various chemical storage materials. While these improve the potential for this storage option, they cannot override the significant regeneration issues. The development of robust and flexible analysis models for Internet-based usage could be useful to focus future researchers on candidate materials that address more requirements for the total storage system.
- The effort is contributing to reaching DOE targets. It is not clear what the specific contribution toward reaching targets is attributable to gas liquid separators and filters.
- Work to optimize auxiliary systems for materials that will never see commercialization cannot be justified. Modeling work is probably justified to allow future investigators to build on existing work.

Question 5: Proposed future work

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

- Plans to finalize the Simulink framework models are appropriate, given the remaining time of the project. Hopefully, there are sufficient time and resources to submit a peer-reviewed paper or two on the team's nice work in addition to a final report.
- Final activities are largely centered on the finalization of the Simulink framework development and completion of some of the adsorbent modeling. Plans for the remainder of the project are reasonable for the short project time remaining.
- Future work for simulation portion is reasonably well defined. Future work for GLS and hydrogen quality is not identified.
- For the amount of unspent project funds, (i.e. ~$1 million as of 3/31/14, as shown on slide 2), having only the major technical task to be adding the chemical and adsorption systems to the models for the framework website seems rather costly, along with just performing management activities and preparing the final report. More efforts would have been expected toward either the particle filter assessment or some other support activity to the cryo-testing with at least a portion of these funds.
- It is very important to achieve a practical user interface well in advance of the completion of the HSECoE's work.
- Modeling work should be completed and will add value. The value of continued experimental work is dubious until promising chemical hydrogen storage materials are found.

Project strengths:

- The project has been very responsive to DOE's and the Technical Team's suggestions and directions.
- UTRC has consistently provided diverse, high-quality expertise by developing innovative purification systems, especially for the chemical storage materials, over the past couple of years. It was able to verify experimentally components that greatly improved purification of the hydrogen gas. UTRC has had talented and dedicated staff members contributing to the HSECoE tasks who made substantial contributions over the past five years with both experimental work and system analyses and modeling.
- There has been good integration with the System Architect's vision for the CHS system. While not viable with the slurries, the CHS system team, including UTRC, has provided very valuable information for both potential portable power applications as well as future CHS materials development efforts.
- The simulation development and its migration to a public platform are valuable.
- The project adds important engineering and simulation components to the overall HSECoE.

Project weaknesses:

- The UTRC project did not demonstrate any significant weaknesses in supporting DOE goals.
- There needs to be a clearer quantification of how GLS and hydrogen quality efforts contribute to reaching DOE targets.

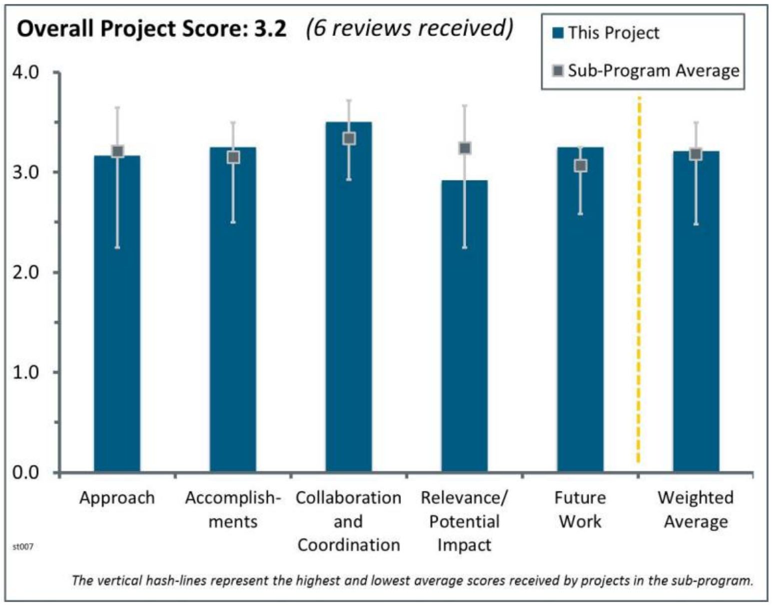
Recommendations for additions/deletions to project scope:

- Particulate filtering of the MOF-5 bed still seems somewhat problematical. Some particles are still passing through the filter and may pose a problem for downstream valves. More mitigation work may be necessary.

Project # ST-007: Chemical Hydrogen Rate Modeling, Validation, and System Demonstration

Troy Semelsberger; Los Alamos National Laboratory

Brief Summary of Project:



The objectives of this project are to develop chemical hydrogen storage system models, develop chemical hydrogen storage (CHS) material property guidelines, and develop and demonstrate advanced engineering concepts and components for hydrogen storage systems. This project will provide a validated modeling framework to the energy research community and provide viable material properties that meet U.S. Department of Energy (DOE) 2017 system targets; identify and advance engineering solutions to address material-based non-idealities and identify, advance, and validate primary system level components; and provide an internally consistent operating envelop for materials comparisons.

Question 1: Approach to performing the work

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

- The project was well-designed and integrated with other efforts on CHS systems.
- The principal investigator (PI) took on many of the key components required for a CHS system, such as liquid carriers, gas-liquid separators, reactors, augers, and bladder tanks. These are very difficult components to provide a universal design for all potential future materials. The PI designed flexible models where possible to make the work more relevant to future materials.
- This project has mainly concentrated on CHS, a clear specialty of Los Alamos National Laboratory. It has recently focused more on alane (AlH_3), in particular slurry-based properties and systems. There is a valuable modeling component, along with system optimization. All the project activities are directed at DOE barriers and needs.
- The approach for system architecture was competently thought out and executed. The fact that a reactor shows different activities for the same space velocity but different auger rates suggests that it is not well-characterized and should not be used for fundamental kinetic measurements. The reactor is not operating in either a continuous flow stirred-tank reactor or plug flow regime. The PI should start with a reactor that it is well-characterized before attempting to measure kinetics that can be interpreted in a meaningful way.
- Adequate approaches have been presented for overcoming barriers raised for chemical hydrogen storage systems.
- The team used its system-level expertise in simulation to help address the various materials property trade-offs and balance of plant requirements. The approach is sound; unfortunately, the unavailability of really workable hydrogen storage solutions forces the team to employ various hard-to-implement strategies.

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.

- Progress on systems, components, materials properties, and modeling is very impressive and clearly contributes to the understanding needed for practical systems. It is not always clear when the cited progress was made, i.e. whether it was within the last year or earlier. The materials properties required to meet DOE system targets have been better defined. The work has clearly shown difficult problems for both ammonia borane (AB) and alane in the areas of fuel cost, system cost, efficiency, and gravimetric density. These properties are far from the DOE targets, and it is difficult to see how materials improvements can be made to counter these problems in the near to mid-term. Such negative impressions are indeed important to know. This activity, along with others, has led to the discontinuation of chemical hydrogen work. However, system designs developed during this project for liquid slurry and solution approaches should be applicable to DOE storage projects in general and to chemical hydrogen-storage activities that may be revived later.
- System design, construction, and validation have been well done.
- The project provided a good summary of the system design examined and lots of new information on the endothermic CHS system with the alane results.
- There have been numerous component and system design concepts delivered for CHS components.
- The establishment of critical parameters required for hydrogen storage materials provides a benchmark that will allow researchers to quickly assess the potential of their materials for meeting the DOE targets.
- The PI tried several approaches (particularly slurry formulation) to achieve desired formulations; however, the materials are difficult to work with.
- Considering the unavailability of really feasible solutions, the team did the best it could in (1) developing chemical hydrogen storage system models for alane and AB slurries; (2) providing guidance through system-level analysis in terms of materials properties for slurry stability, impurity quantification, and kinetics; and (3) demonstrating laboratory-scale systems and components. The models and experience significantly enhanced the knowledge on how to deal with chemical hydrogen storage options.

Question 3: Collaboration and coordination with other institutions

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

- This was a part of the Hydrogen Storage Engineering Center of Excellence (HSECoE) and is an excellent model that other teams should follow. The PI worked with the appropriate industry, government, and academic partners.
- There was successful collaboration with United Technologies Research Center (UTRC) and Pacific Northwest National Laboratory (PNNL) to develop guidance for future materials development.
- There is a wide range of outstanding collaborations, both within and beyond the HSECoE. There is good communication between the team and various stakeholders who provided inputs to the models.
- There was good collaboration within the HSECoE, but little work with non-HSECoE members.

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 relevance and impact of this project on the DOE Hydrogen and Fuel Cells Program is clear and substantial. It has contributed to the termination of chemical hydrogen storage work. This is a valuable output of the project, even if it is disappointing.
- This project is directly relevant to the hydrogen storage requirements of DOE.
- This project worked with UTRC, PNNL, and other members of the HSECoE to develop a system model recommending material properties for chemical hydrogen storage approach. This was one of the most

important expected outcomes from the HSECoE, and they teamed up to accomplish this in a timely manner.

- It is unlikely that these systems (CHS) will make it into automotive use. The complexities of moving liquid slurries are very difficult to manage, particularly on automotive systems. Many of the components worked on will likely not be suitable for future materials because of the specific material handling requirements of most materials.
- Work on materials that have no chance of commercialization is not a responsible use of funds.

Question 5: Proposed future work

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

- Considering the short amount of time left for the project, the proposed future work is reasonable and achievable.
- The project is largely complete.
- Because of the down selection, the PI is winding down work and providing the final reports. Future work should concentrate on developing neat liquid systems and robust bladder systems.
- Peer-reviewed manuscripts will be a great complement to the models available through the Internet.
- The project is near its end. The remaining activities are naturally limited, but appropriate.

Project strengths:

- Mapping of materials properties needed to meet DOE targets was a project strength.
- The project provided very useful expertise on chemical hydrogen carriers and component and system engineering.
- Models are well-developed and seem to be working for each system.
- Project strengths include good team expertise and system-level simulation experience.
- Developing the scalable model for the liquid-gas separator is a useful tool that can be used for future materials and systems. The PI should have spent more time on describing the bladder system that was developed; this was not a trivial exercise, and it could have applicability for future systems.

Project weaknesses:

- Progress was always hampered by the breadth of components that needed to be worked on and their lack of universal suitability for all materials.
- Kinetics measurements were questionable.
- It is questionable whether the models will work for materials/systems that are really useful.
- Not many good solutions were available to the team.

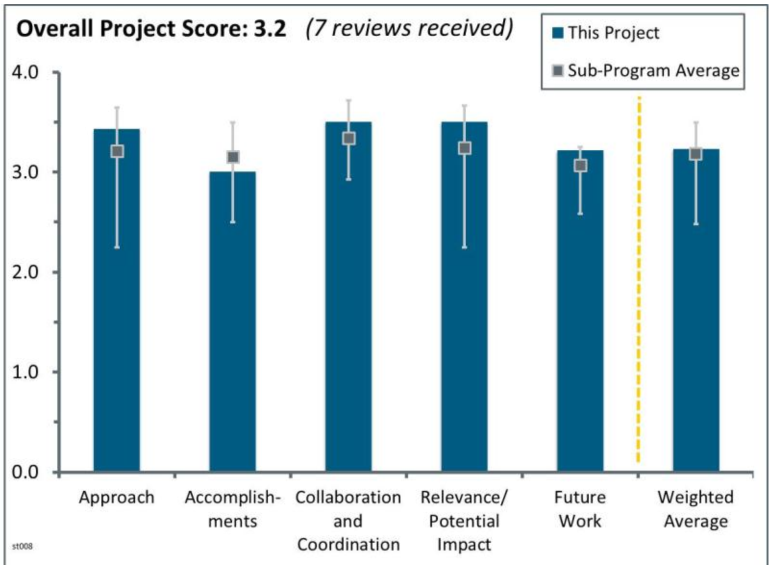
Recommendations for additions/deletions to project scope:

- In order to achieve a neat liquid that does not hurt system density, novel and innovative ideas are required to develop solutions that are stable, light, liquid at all conditions, and support the regeneration efficiency of the materials. Future materials studies on chemical hydrogen storage materials need to place equal emphasis on the carrier materials and the storage material itself.

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

Matthew Thornton; National Renewable Energy Laboratory

Brief Summary of Project:



The vertical hash-lines represent the highest and lowest average scores received by projects in the sub-program.

Objectives for this National Renewable Energy Laboratory (NREL) project are in support of the Hydrogen Storage Engineering Center of Excellence (HSECoE) with system design, analysis, modeling, and media engineering properties for materials-based hydrogen storage systems. Vehicle performance research will develop and apply a model for evaluating hydrogen storage requirements, operation, and performance trade-offs at the vehicle system level. Energy analysis focuses on coordinating hydrogen storage systems well-to-wheels to evaluate off-board energy impacts. Media engineering properties research assists in the identification and characterization of adsorbent materials that have the potential for meeting U.S. Department of Energy (DOE) technical targets for onboard systems. The project leads the effort to make select HSECoE wide models available for use by other researchers via a web-based portal.

Question 1: Approach to performing the work

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

- Providing vehicle-level modeling is necessary to provide the correct operating framework for the storage systems. Even a simplified system can provide good guidance to the HSECoE to develop suitable and relevant systems.
- The team has made good use of past experience and expertise to facilitate Internet access of the HSECoE models.
- Analysis of correlation between vehicle performance and storage performance is very helpful. Availability of models on an Internet portal will help researchers worldwide to define their projects. There was a good response from 2013 comments with regard to fixed volumes.
- The project has a logical approach that generates insight into the usable hydrogen based on standard vehicles drive cycles.
- Development and application of hydrogen storage system models and storage system trade-offs can have significant impact on improving future engineering system design and development. System models that encompass metal hydride, chemical hydrogen, and adsorbent systems are being (or have been) developed on the project. These models could ultimately provide important predictive capabilities. The use of a web-based portal will ensure that the models are available to the entire hydrogen storage and system engineering communities. The emphasis has been placed almost entirely on model development; insufficient attention has been paid to model validation.
- Providing a graphical user-interface for HSECoE models will increase usability tremendously and allow generalists to access the models. Internet access will allow users without MatLab/Simulink access or experience to use models. The approach is appropriate and well-defined, and it integrated well with a number of other efforts.

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.

- The project is on a good track. A metal hydride model, physical model, and cost model are complete. The 2014 presentation does not show whether the open milestones in the 2013 presentation are complete or still open. The status of the open 2013 milestones should be clearly documented in the 2014 presentation.
- Good progress has been made on incorporating Phase II performance data into the system models and on developing plans for making the models available to the public. Solid work has been performed on developing generic user-interfaces that should make the models more accessible to the user community. Useful information has been provided about user analytics; this should help to guide and fine-tune future embodiments of the models. Very little emphasis seems to have been placed on model validation. That work should be a critical element of the project going forward. Without experimental confirmation, it is exceedingly difficult to ascertain whether the models accurately (or adequately) address hydrogen storage issues in real-world situations.
- There is good progress on releasing models. The download page should include requirements for running model (such as Excel, MatLab, etc.).
- Current efforts to expand the user base are generally beneficial and should help to refine the models and the environment/interface.
- Work on the graphical user interface and populating the models with data seemed behind schedule, especially considering that the HSECoE is nearing completion. Much of this work could be done in parallel with other HSECoE functions.
- Given the reduced resources, NREL is more in a support role than in a lead role for technical accomplishments.

Question 3: Collaboration and coordination with other institutions

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

- Extensive and beneficial collaborations with HSECoE partners are evident. Especially noteworthy are the collaborations between NREL and Pacific Northwest National Laboratory/Savannah River National Laboratory on coding and conversion to Simulink framework, as well as collaborations with United Technologies Research Center (UTRC) on development of generic user interfaces and collaborations with multiple partners on model documentation.
- There has been close, timely, and appropriate collaboration with other institutions; partners are full participants and well-coordinated with the HSECoE and UTRC, in particular.
- It seems that all relevant partners/institutes are involved.
- It is clear that appropriate collaboration within the framework of this project exists.
- The principal investigator (PI) is working with all the appropriate HSECoE partners. Input from the vehicle original equipment manufacturers is critical to the success of this project.
- The project encompasses participants from industry, national laboratories, and academia, with important contributions being made by the collaborators.
- There is significant collaboration within the HSECoE, but limited interaction with non-HSECoE entities.

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.

- Publishing models on an Internet platform is very good. Models for all storage systems will be available to be used by everybody.
- The project helps guide the development of materials with potential of meeting the DOE targets.

- Development and implementation of robust models capable of analyzing HSECoE vehicle performance, cost, and energy balance, as well as hydrogen storage system performance and trade-offs, are important to understanding and improving current future storage systems. The development of models with accurate predictive capabilities addresses most of the technical barriers identified in the DOE Hydrogen and Fuel Cell Program (the Program), and it is clearly relevant to the Program needs.
- The methods and models developed here will be useful to future investigators.
- Vehicle performance modeling provides storage system developers with valuable information to help direct development efforts.
- Providing vehicle-level modeling is necessary to provide the correct operating framework for the storage systems. Even a simplified system can provide good guidance to the HSECoE to develop suitable and relevant systems.
- The NREL project is small in size, but it is obviously providing a valuable service to enable the outcome from the HSECoE to be made available to the scientific public. The project provides great support to develop and apply models for evaluating hydrogen storage requirements at the vehicle systems level.

Question 5: Proposed future work

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

- The future work is well-defined and incorporates updates from collaborators. Trade studies are of particular value.
- The proposed future work is a direct extension of the solid modeling work already conducted on the project. Additions of the chemical hydrogen and adsorbent systems to the modeling framework are important. The presentation (slide 26) states that the focus of future work will be on “Model Validation and Model Web Access.” The former is vital; however, no details are provided concerning the approach for experimental validation of the models. A clear and compelling statement about plans for model validation is needed. Likewise, a statement about how (or if) the models will be maintained after the project is completed would be helpful.
- The list of future work is reasonable.
- It will be necessary to adjust the model based on the Phase III results that will be generated from planned HSECoE efforts. However, it is unclear whether this will be possible within the duration of this project.
- It would be useful if models could be made internet-accessible.
- The PI needs to catch up on previous slow progress and finish the models as proposed. This will be an excellent tool for future systems and materials developers to use to understand the operating environment of their materials and systems.

Project strengths:

- This is a useful and highly relevant project that is being conducted by a capable team that is well-coordinated and closely connected with other partners in the HSECoE.
- The project generates very useful information that related basic material properties all the way to standard vehicle drive cycles. This is expected to guide the researchers and engineers as they propose new/improved hydrogen storage materials/systems.
- The relationship between storage system characteristics and vehicle performance/operability is a valuable tool for storage system developers.
- The graphical user interface will provide a useful tool to visualize a complex system operation.
- The project has been very responsive to DOE and U.S. DRIVE Hydrogen Storage Technical Team suggestions and directions.
- Good model development is a project strength.

Project weaknesses:

- The project relies on the results generated from Phase II within the HSECoE program. Although there exists a plan to adjust the model per the results produced in Phase III, it is unclear how this could be possible within the remaining duration of this project.

- Progress seems slow. It is unclear how much can be done in parallel with other HSECoE activities.
- There is a lack of clear and compelling plans for model validation. More attention seems to have been paid to web-based access and evaluation of user analytics than to the crucial task of model validation.

Recommendations for additions/deletions to project scope:

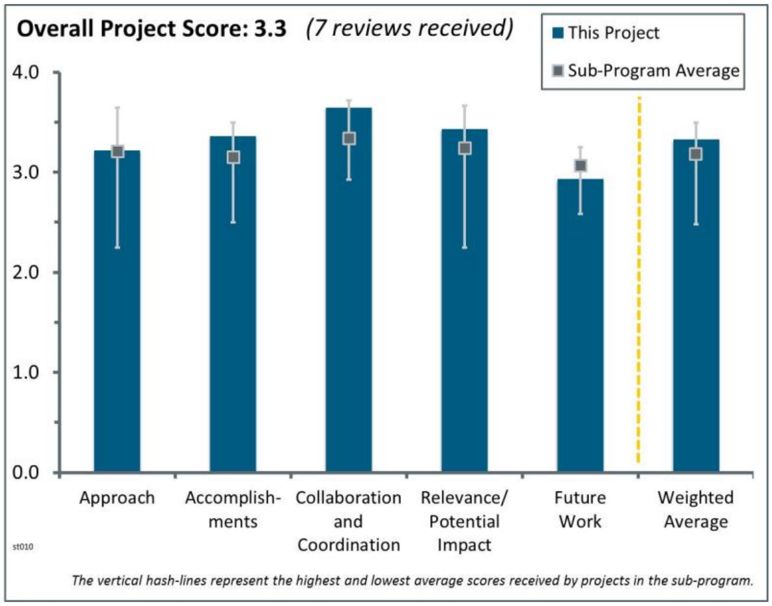
- Anything that can be done to make the modeling more widely accessible and user friendly will be invaluable.
- After the project ends and the models are completed and uploaded, all assumptions, material properties, and specifications should be updated on a regular basis to make sure that these models can be used in the future as well.
- It will be necessary for the sorbent model to be adjusted per the results produced in Phase III.
- A description of plans for maintaining the models after completion of the project would be helpful. A more robust validation plan is needed.
- As the public rollout continues, mechanisms to gather user feedback regarding utility and usability should be established.

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:

Material-based hydrogen storage systems have higher potential to meet U.S. Department of Energy (DOE) targets but have increased complexity over physical-based storage options. This project, led by Ford, is focused on three technical tasks that contribute to the overall Hydrogen Storage Engineering Center of Excellence (HSECoE) mission. Task 1 is to develop a dynamic vehicle parameter model that interfaces with diverse storage system concepts. Task 2 is the development of robust cost projections for storage system concepts, and Task 3 is 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 **3.2** for its approach.

- This project is a key contributor to the HSECoE. It is well-integrated and provides valuable research and development and an automobile perspective to the onboard storage challenge. In particular, the project provides key input on adsorbents, e.g., metal organic frameworks (MOFs) and vehicle integration of hydrogen-storage systems. It aims to provide very valuable original equipment manufacturer (OEM) input.
- The project has clear goals and provides extensible inputs for modeling to account for variations in potential MOFs, should they become available. Unfortunately, MOF-5 will ultimately fall short of the DOE targets, but the efforts to maximize MOF-5 give perspective on perhaps a better MOF (some have been identified).
- The accomplishments are very good. The analysis and characterization techniques have been well-developed. However, it would be nice to see the HSECoE apply these developed methodologies to some of the new materials sets that have been developed since the HSECoE was initiated. There are limited materials that can be synthesized in the quantity needed, but the processes should still be validated for another framework material.
- The Ford/BASF/University of Michigan (UM) team plays many important roles in the overall HSECoE program. This includes the system architecture for the adsorbent system, most of the manufacturing and testing associated with MOF-5, coordination of failure mode and effects analysis (FMEA), and performance/cost-model development. The automotive industry perspective provided by Ford is invaluable. At the present time, this particular project seems to be a nerve center for the entire HSECoE because it performs (or interacts closely with those performing) pivotal aspects of the HSECoE's overall effort. The focus of work throughout the HSECoE (including this project) has reached the point where lack of relevance to critical barriers is a non-issue. The entire HSECoE effort is locked in on a successful demonstration of an adsorbent-based onboard hydrogen storage system.
- The approach is well-formulated and includes optimization of MOF performance in an adsorbent-based hydrogen storage system, scale-up of the MOF-5 manufacturing process, and failure mode analysis of MOF-5 under real-world operating conditions. The approach addressed important remaining issues in the successful development and deployment of a prototype system from an OEM perspective. An important addition to the overall effort was the assessment of the properties of alternative (known) MOFs that may

have volumetric and gravimetric capacities superior to MOF-5. This effort directed toward "enhancement of MOF performance potential" represented a mid-course correction to the original approach, and it has produced valuable findings that could significantly impact the Hydrogen Storage sub-program.

- The approach is generally effective but could be improved. It contributes to overcoming some barriers. The main barrier is the storage capacity of the absorbent. The choice of MOF-5 is driven by material availability. At the same time, (see slide 9 of the presentation) MOF-5 volumetric versus gravimetric capacity is close to optimal, which leaves relatively little room for further improvements.

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

This project was rated **3.4** for its accomplishments and progress.

- The extent of accomplishments reported for the past year and the degree to which milestones were met is most impressive. Many technical issues concerning MOF-5 have been resolved. Fully formed MOF-5 pucks with enhanced thermal properties have been delivered to Oregon State University (OSU) for modular adsorbent tank insert (MATI) fabrication. FMEA and safety assessments have been completed. Ford has continued to serve the HSECoE in regards to research planning and execution, modeling and analysis, and being an effective liaison to the external community.
- Most milestones and extra work have been performed successfully working towards developing an understanding and methodologies that could potentially take advantage of a better MOF material. Methodologies and experimental tests have been developed to quantify properties. The system architecture has been developed significantly, and new efforts to identify potential MOFs to replace MOF-5 are promising. There are several items in the milestones that are underway and maybe on target for completion. For instance, only initial cycling has commenced on evaluation of degradation, and the FMEA plan has just been initiated. The scale-up and characterization of MOF-5 are the most developed aspects of the project, and additional MATI puck issues have been addressed.
- The approach is effective and contributes to overcoming most barriers. The main remaining barrier is the availability of an absorbent material with good hydrogen storage capacity, which is outside of the project's scope.
- Significant progress has been achieved. However, on slide 16, relating to the MOF-5 scale up, while there may be "performance" metrics within experimental error, the size distribution has been significantly altered. There may be deleterious or beneficial effects from long-term cycling that should be addressed in future work.
- Solid progress has been made on all tasks during the present reporting period. Especially noteworthy is the new work on enhancing MOF performance potential. Four new MOF candidates having gravimetric and volumetric capacities superior to MOF-5 were identified. This is an important result that could have positive impact on the adoption of MOF materials as viable media in a practical hydrogen storage system. The manufacturing scale-up to produce 9 kg of MOF-5 with properties similar to laboratory-scale material is an important accomplishment. Likewise, the identification and analysis of possible failure modes for the adsorbent system in Phase II has been an important accomplishment that is leading to the development of robust strategies for mitigating risks.
- A lot of good engineering and associated work has been done. Numerous potential new adsorbents have been surveyed theoretically, showing some potential for improvement. Manufacturing scale-up, cycling, and integration of MOF-5 have been mostly worked out. The failure mode work is very useful. Although MOF-5 is better understood, it is still not evident if this material (or any adsorbent) has significant medium-term chances of leading to a practical onboard vehicular hydrogen storage system that will compete with high-pressure gas. There is a lack of preliminary OEM (Ford or General Motors) perspective on this important question.
- One key accomplishment was the production of 9 kg of MOF-5, thereby allowing manufacture scale-up and material improvements in thermal conductivity. The project also presented data on puck formation, but did not discuss how the pucks were made and if there were any difficulties in making MOF-5 into pucks.

Question 3: Collaboration and coordination with other institutions

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

- There has been close, appropriate collaboration with other institutions; HSECoE partners are well-coordinated.
- Collaboration and coordination seemed to be well-handled throughout the HSECoE as a whole.
- As with every Center of Excellence, collaboration is at the heart of its success.
- The importance of the active involvement of a major OEM in the HSECoE cannot be overstated. The Ford/BASF-SE/UM team is well-coordinated with other partners in the HSECoE, and that close collaboration and attention to “real-world” issues have become extremely valuable elements in the success of the HSECoE.
- There is excellent collaboration with the HSECoE members and a few others.
- This team (led by Ford) is as well-connected to the greater HSECoE as any among the pack of aligned contributors. The principal investigator (PI) projects a level of leadership that clearly benefits the entire HSECoE and fosters a much-needed inspirational connection to the automotive industry. The interest of that industry in the work of the HSECoE should be important to and much appreciated by the DOE.
- Collaboration exists between partners, but it was not clear who will make the MOF-5 pucks for later testing at OSU and Savannah River National 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 **3.4** for its relevance/potential impact.

- The project is well-designed and implemented. It is moving forward in parameterizing the laboratory-to-OEM production and implementation of a physisorption-based solution. It is clear that many of the obstacles and solutions generated here will impact any MATI-puck storage solution.
- The HSECoE system models and knowledge gained from MOF-5 will be extremely valuable to materials scientists as the researchers look to design and develop new materials for transportation applications.
- The relevance and potential impact of this project are fully aligned with the Phase III goals and objectives of the HSECoE. This is essentially true of all the remaining ongoing projects that collectively form the HSECoE. Their targets for Phase III are clearly defined, and all teams are properly focused. It is clear that all these efforts form one well-oiled machine, which is good news. The problem is that the Phase III targets are not nearly ambitious enough to justify a compelling argument for a higher level technology demonstration sponsored by, e.g., the DOE.
- This project is addressing important problems in the development of an engineering system based on adsorbent media. The OEM perspective incorporated into the HSECoE by the investigators from Ford contributes greatly to the success of the technical effort. The project has significant positive impact on advancing progress toward meeting DOE research, development, and demonstration (RD&D) goals, and it is a vital component of the overall HSECoE project.
- This project has direct relevance to the DOE Hydrogen and Fuel Cells Program goals via expert participation in the HSECoE. These partners have participated well.
- The project is aligned with DOE RD&D objectives by developing material-based adsorbent hydrogen storage systems. The project should have pointed out that the MOF material volumetric capacity needs to be doubled from 20 g/L to 40 g/L to meet DOE target. *[DOE note: the 40 g/L target is a system-level target and not at the material level.]*
- The impact of this project may be seen in multiple areas that may not be directly related to hydrogen storage for automotive applications.

Question 5: Proposed future work

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

- The project is entering its last year. The remaining planned work seems reasonable.
- The project appears to have a one-year extension. The future work plan for fiscal year 2014 completes this project.
- There are reasonable plans for wrapping up the project.
- The project is quite linear and does not seem to rely on contingency plans and risk management in most of its fact finding/understanding role. Several options may prove themselves as the Phase III tasks progress, but they are not discussed.
- The role of Ford/BASF/UM in Phase III mostly involves (1) completing ongoing MOF-5 optimization/testing, FMEA activities, and related tasks based in part on results from Phase III experiments, and (2) supporting the Phase III modeling and validation efforts. It is likely that most of this work during Phase III will be done by Ford.
- The proposed future work is clear and succinctly stated, and it is a logical extension of the excellent work that has been conducted thus far on the project. It is unclear if support exists for additional work on enhanced MOF performance (new material candidates). That will be an important issue for the DOE Fuel Cell Technologies Office to consider.
- It would be beneficial to see another material evaluated beyond MOF-5, as well as more long-term cycling of larger batch materials.

Project strengths:

- This was an overall strong project performed by a good team of researchers. The potential impact of the project's results, outside of hydrogen storage, is one of its major strengths.
- The project consists of clear goals, actionable items, and a good balance between university/laboratory and industry partners.
- The project features a strong team.
- There has been strong leadership from the PI. The team is productive and skilled in the disciplines required to perform the proposed research.
- A well-coordinated project team is conducting work that is vital to the overall success of the HSECoE effort. The technical effort on this project has produced important new results that are directly relevant to the development and implementation of a practical hydrogen storage prototype system. The investigators should be commended for seriously considering the recommendations from the 2013 DOE Hydrogen and Fuel Cells Program Annual Merit Review and expanding the technical effort to include the valuable new work on identification of MOFs with potentially enhanced gravimetric and volumetric capacities.
- The project demonstrates excellent expertise on MOFs and other adsorbents.

Project weaknesses:

- This team has no obvious weaknesses.
- This is a strong project with no notable deficiencies. The only criticism is that the HSECoE in general (and this project specifically) has failed to adequately address the important system problem related to loss of usable hydrogen in the prototype design.
- Using MOF-5 as the tested hydrogen storage material is a weakness.
- The project is unlikely to develop a real physisorption solution that meets DOE goals.
- The limitation of the project to MOF-5 is a weakness. There are limitations instilled by project milestones-deliverables etc., but another materials set would be beneficial, even though it is not possible at this late date in the project.

Recommendations for additions/deletions to project scope:

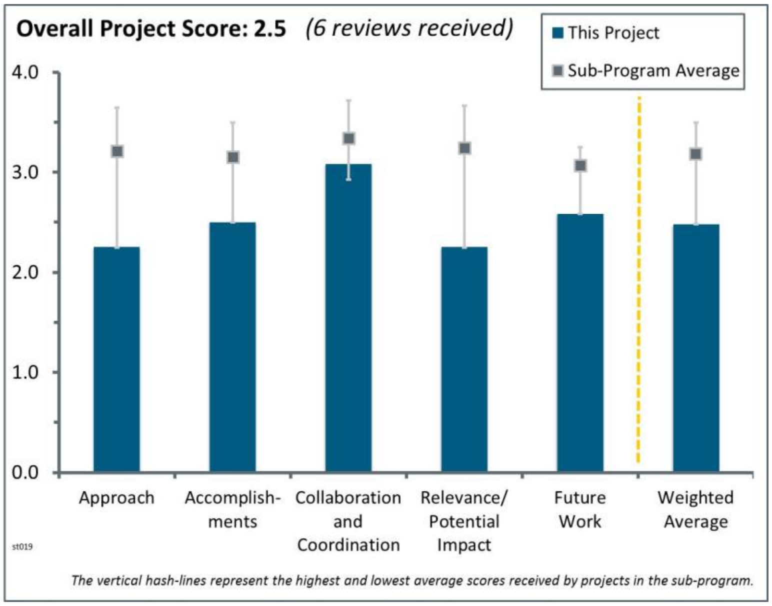
- Make sure the PI stays deeply involved. When the work of the HSECoE comes to end next year, someone will have to go before the Technical Team, the DOE, and perhaps others to convince them that follow-up to the HSECoE is warranted.
- It will be important for the project team to work closely with the Hydrogen Storage sub-program to consider how the work concerning synthesis and testing of new candidate MOFs can be expanded/extended.
- There should be frank judgments from OEMs on the real-world practicality of adsorption systems for automobiles.

Project # ST-019: Multiply Surface-Functionalized Nanoporous Carbon for Vehicular Hydrogen Storage

Peter Pfeifer; University of Missouri

Brief Summary of Project:

The objectives of the project are to (1) fabricate boron-doped nanoporous carbon (particulate and monoliths) for high-capacity reversible hydrogen storage, and (2) characterize materials and demonstrate storage performance.



Question 1: Approach to performing the work

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

- The University of Missouri (UM) project continues to explore the feasibility of enhancing hydrogen adsorption in high-surface carbons by partial substitution with boron (B) into the graphitic lattice via decomposition reactions using either liquid or gas phase decaborane ($B_{10}H_{14}$) followed by decomposition at elevated temperatures. While first principles computations are used to rationalize possible mechanisms for stronger chemical bonds for hydrogen molecules on boron-carbon (B-C) surfaces, most of the project's efforts have been empirical variations of the processing steps to search for improved storage capacities and higher heats of adsorption. The goal is to surpass behavior of more traditional adsorbents to allow greater capacities near room temperature. However, it does not appear that this approach produces a high fraction of the desirable B-C bonds or especially large surface areas for greater storage capacities. It is also unclear whether truly high volumetric capacities are realistic in spite of the extrapolations shown on slide 16.
- The approach seems good, but whether the boron atoms are in the right positions and are uniformly distributed is still questionable. Nevertheless, the team's initial idea/approach is good.
- The presented results and approach are primarily geared towards improving the physisorption amount at relevant temperature and pressure for onboard vehicular storage. Due to the nature of the materials being researched, the researchers will also potentially address thermal management, charging/discharging rates system cost, and system weight and volume. The efforts to incorporate boron into carbon frameworks is primarily pushed by the theoretical predictions that this can meet and exceed material goals at room temperature of which their previous work shows potential to achieve these goals. The researchers have changed their methodology to incorporating boron through gas-phase delivery of $B_{10}H_{14}$. Experimental characterization and uptake properties are relevant to benchmark the materials and compare to DOE goals.
- The principal investigator's (PI's) understanding of B-C chemistry is limited. This leads to an interpretation of results that is artificially optimistic. It also limits the advancement of the project. The interpretation of the x-ray photoelectron spectroscopy (XPS) data and the resultant assumptions about how much BCx (boron-carbon material) and other boron containing materials are significantly skewed from the reality of the materials set investigated. Considerable efforts need to be made to improve the focus of the researcher's efforts to more promising avenues. With this rudimentary understanding and its effect on their effort, it will be almost impossible for them to succeed or disseminate useful information to the scientific community at large.
- After nearly six years and numerous changes to the project's focus, it seems like focusing on boron substitution in carbon a few years ago should have resulted in much more progress. However, the lack of progress can be directly attributed to the very poor synthetic approaches chosen and the inability of the project to develop and perform accurate measurements for hydrogen storage and materials characterization, including the exact amount of sp^2 hybridized boron bonded in the carbon lattice.

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.

- The team performed computer simulation, experimental synthesis trials, and characterization. The results are impressive in comparison with the accomplishment of last year.
- The team is working toward increasing the enthalpy for hydrogen adsorption, while maintaining a high surface area. The results of the team's best materials are marginally better than MSC-30 activated carbon due to the reported small amounts of the correct boron-character being incorporated. It is unclear how definitive the XPS results for the B-B and B-C components are, but there seems to be boron distributed throughout the samples and lower oxygen content in the current materials. The higher temperatures needed to incorporate nominally increased boron content results in just a smaller population of similar pore volumes, but essentially no increase in surface-area normalized uptakes. Despite the apparent low sp^2 B content, there are some effects (perhaps also due to morphology changes) on the isosteric heats of adsorption. Slide 13 details the results for a pristine carbon- and boron-doped system where there is a significant increase of enthalpy for the latter. This is a surprising effect if only 2% of boron is incorporated in to the carbon. There are some concerns about the enthalpy data presented, in part because of the aforementioned discrepancy, but also due to the scatter in these data points that are much larger than the 0.2 kJ/mol indicated by the PI in person. Slide 26 details the methodology for obtaining these results from the isotherms of various temperatures, and this seems quite reasonable. Surprisingly, the data on slide 26 does not appear to present such a large variation with adsorption. Slide 16 indicates a very high film density (over 50% larger than the liquid hydrogen), which seems unrealistic. A scenario of such dense packing is not presented. A detailed description of these plots would be welcome as the captions are somewhat cryptic.
- After several years of effort, the UM team still finds rather low levels of B-substitution for its higher surface area materials. While its XPS results do indicate some improvement in the amount of B-C bonds during 2014 processing, there is still a substantial amount of B-B and B-O bonds, which are not useful for improving the hydrogen adsorption properties. Furthermore, while stronger binding with hydrogen is indicated at very low contents, these energies fall rather quickly and seem to be similar to conventional graphitic surfaces at 1 wt.% or higher. It also appears that the UM researchers have had difficulties with obtaining accurate and reliable hydrogen capacities from their Hiden Analytical, Ltd equipment that negated several of their prior claims for enhance performance.
- The PI has to be given credit for his efforts on validating and correcting his capacity numbers. He did spend significant time working with researchers at the National Renewable Energy Laboratory (NREL). It was refreshing to see that his numbers on standard materials were validated and that his approach was significantly altered after working with NREL. It would be of value to see this same level of effort on establishing reproducible materials sets. The limitation seems to be in the B-C chemistry. The overall concept of the proposal is sound; the interpretation of the characterization of the materials and how to apply those results to a future approach is the limitation.
- There does not appear to be any demonstrated advantage of the B-doped carbons over commercial carbons such as MSC-30.
- After nearly six years, and the project ending in November 2014, the team has failed to meet nearly all of its objectives and has come nowhere close to meeting the DOE hydrogen storage targets for light-duty vehicles. This is evident in several areas and for several reasons including the following:
    - The graph on slide 3 showing the predicted hydrogen storage capacities reaching over 12 wt.% at 77 K with 10% boron is clearly wrong and based on using only a "Langmuir"-type approach for modeling the isotherms. At low temperatures (77 K), the gravimetric excess capacities might go up a little, but because of the cold temperatures, the surface will become saturated whether boron is there or not. The only thing boron will do is perhaps increase the density of hydrogen on the surface a little. This minor increase should have virtually no effect on the total capacity difference with different concentrations of boron at 77 K. The main increase in capacity should only be observed at higher temperatures, i.e., 298 K. This means that the project's projections for volumetric capacity are also wrong throughout the presentation. For example, see the figure on slide 4.

- While better than in the past, the authors continue to report excess adsorption numbers that are too high, e.g., slides 6 and 11. This probably also impacts their isosteric heats of adsorption results as well (i.e., slide 13). Clearly, the error in this data and the fact that the low amount of adsorption for the higher heats can be completely attributed to structure rather than boron is indicative of the poor data being taken. The authors also continue to report "total" adsorption numbers that are way too high due to wrong calculations. They need to work with others to get their calculations correct (e.g.., see the NREL presentation at this DOE Hydrogen and Fuel Cells program Annual Merit Review).
- There are numerous papers in the literature that specifically identified real ways to increase the amount of sp^2 hybridized boron coordinated in carbon lattices. There is no recently demonstrated way to do this through chemical substitution from a vapor that results in high boron concentrations (i.e., 10 wt.%). The impetus for this project to spend several years working on this approach seems very unreasonable, considering the general understanding that the higher the processing temperature, the lower the boron saturation level becomes. It is amazing that the project even got 1% to 2% loading. But based on their interpretation of their XPS results, it is a good bet that they did not achieve even this level of loading. Having virtually no sp^2 coordinated boron would explain their anomalous results that showed no difference in hydrogen storage based on boron loading. Clearly other literature results demonstrated such dependence, but the literature results also indicated that achieving more than 1% to 2% sp^2 coordinated boron loading was very difficult.
- On page 7, the authors provide conclusive proof that their approach used temperatures that are way too high to get boron into carbon. Instead of accepting the data, the authors claim to actually demonstrate new chemistry. However, they base this on conclusions from data like that on slide 12, where there is no obvious peak due to sp^2 coordinated boron. Published XPS results of sp^2 coordinated boron have clear peaks and thus, at best, the author's interpretation of 20% boron in the data and 1% to 2% boron in their samples is a gross overestimate.

Question 3: Collaboration and coordination with other institutions

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

- The UM team has interacted very well with a number of outside organizations, especially for structural and spectroscopic characterization of their B-dope carbons. The XPS, transmission electron microscopy (TEM) and electron energy loss spectroscopy (EELS) results are most welcome additions to show chemical compositions of the samples. It was also useful and informative that hydrogen capacities were determined at NREL, revealing some issues with prior measurements done at UM.
- The team has a great mix of expertise.
- Working with NREL was a good step forward. Taking a new approach to data evaluation was a direct result of this collaboration.
- Collaboration with NREL should be helpful.
- There are several partners in the project that are mostly contributing to the goals. The monolith and industrial scale collaborations did not seem to contribute to the presentation, nor was any prompt-gamma neutron activation analysis (PGAA) data presented.
- The project should have worked more closely with a number of institutions that had previously performed a large amount of this work to minimize duplication.

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 **2.3** for its relevance/potential impact.

- Such exploration is the kind of idea deserving support from DOE. Hydrogen storage remains a daunting challenge except for tanks.
- The development of B-substituted carbons has the possibility of improving the potential adsorption storage properties if greater gravimetric and volumetric capacities were achievable above cryogenic temperatures. However, the associated larger heats of reaction would complicate the engineering issues associated with thermal management during both adsorption and desorption of hydrogen, and it is not fully evident whether this is really that much of an advantage.
- The limited advances in boron incorporation have restricted the impact of the project, but the materials development goals are well aligned with the DOE goals.
- The materials have potential, but it will not be realized with the current approach at UM
- After nearly six years of trying, it seems unlikely that this project will make a significant impact.
- The project did not improve any materials or successfully meet any targets.

Question 5: Proposed future work

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

- The tasks described on slide 19 are all relevant to addressing some outstanding issues with the nature and distribution of B-substitution in the UM carbons and their subsequent impact on observed hydrogen storage properties. With only a few months remaining for this project, it is not clear how much will actually get accomplished. The PI is strongly encouraged to complete as much of the planned experimental efforts as possible and to report the findings.
- There is limited time left for this project. There are several items listed that the researchers will pursue, but prioritization, proportioning of efforts, and risk mitigation are not discussed.
- There are only a few months left and thus it is uncertain if the proposed list of future work is realistic. The best course of action is to do a good job in summarizing the results in publications.
- With the short time left, there is virtually nothing the project can do to achieve its goals. The project has not developed any materials with significantly improved capacities.

Project strengths:

- The idea is good and the team is strong.
- The UM team has involved personnel with great expertise in boron chemistry, as well as equipment and experience for working on the adsorption properties of porous carbons and other materials. These capabilities have contributed toward using $B_{10}H_{14}$ for adding boron to carbon hosts.
- The project has a combined theoretical and experimental approach. There was broad team experience with materials development and characterization efforts.
- The current understanding of how to determine the gravimetric capacities of the materials is a project strength, as was the PI's willingness to work with DOE to better evaluate the materials. The PI has shown that the B-doped materials have promise; unfortunately, the current approach has not led to a more in-depth understanding of the possibilities.

Project weaknesses:

- Throughout the life of this project, there has been considerable disorder in the approaches used to select and investigate the C-B candidates. Synthesis methods and characterization techniques seem to have been selected because they were either convenient or available at the university or research group. There was little discrimination on whether they are the most appropriate to address the stated objectives and needs. It appears that there have been improvements over the past year or so. In particular, there finally seems to be more appreciation on the challenges of accurately measuring the hydrogen storage parameters.

- There have been limited efforts to mitigate risks or try alternative methodologies for boron incorporation. Several mistakes in previous isotherms are discussed at the end of the presentation (even though these discrepancies have been identified), indicating poor data management practices in the team at some points in the past.
- The interpretation of the spectroscopic and thermal characterization of the materials is a project weakness. The volumetric capacity calculations need to be updated.
- The PIs have shown (slide 11) that the addition of boron does not result in an increase in hydrogen-binding energy and lowers the surface area. Further work on these materials is not recommended.
- The project did not meet any of its goals.

Recommendations for additions/deletions to project scope:

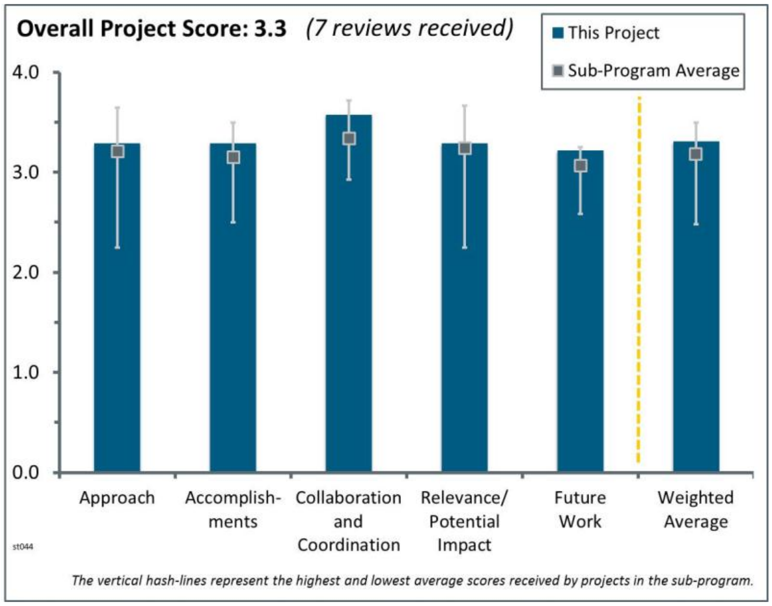
- The UM researchers should concentrate on completing the proposed experimental assessments that address the composition and structure of their B-C adsorbents, as well as perform careful measurements on the hydrogen storage properties on the most promising candidates.
- With only a few months left, the authors should use techniques in the literature to make sp^2-coordinated boron samples, and at the very least show that all their materials they have made in the past did not contain any sp^2-coordinated boron. The lack of progress of this project should not be viewed by DOE as evidence one way or the other for sorbent materials or boron-doped sorbent materials. The project's lack of results cannot be used to gauge the success of future projects that use more appropriate approaches to investigate these types of materials.

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:

The Phase III objectives of the project are to (1) design, fabricate, test, and decommission the subscale prototype hydrogen storage systems for adsorbent storage materials; and (2) validate the detailed and system model predictions against the subscale prototype system to improve model accuracy and predictive capabilities.



Question 1: Approach to performing the work

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

- This year's approach of testing sub-scale adsorbent prototype systems is what is needed to successfully complete the Hydrogen Storage Engineering Center of Excellence (HSECoE) program. This testing will improve model accuracy and predictive capabilities, which has been the goal of this Center of Excellence.
- The design and fabrication of prototype systems with validation of modeling to contribute toward their predictive capabilities is well executed. The medium-scale testing before large-scale testing has proven valuable. Step-wise approaches to measure system properties have been advantageous in determining contributions to physical properties. Modeling and system properties are strongly integrated and well aligned across the center.
- There is a logical, step-by-step approach, involving designing and testing first with a 0.5 L vessel, then with a 2 L vessel, as well as testing with and without various media in HexCells.
- The project has a reasonable and straightforward approach, comprising development and application of gas transport models, testing and validation of a cryo-adsorbent system model, and final design and testing of the HexCell adsorbent heat exchanger. Understanding gas and heat transport is crucial to optimizing the HexCell and modular adsorbent tank insert (MATI) adsorption systems. The experimental effort is complemented by a well-focused modeling effort that should provide a powerful predictive capability.
- Some fundamental data can be accumulated to overcome the engineering barriers.
- A small-scale approach is the logical first-step test to test a new storage system.
- The principal investigator (PI) investigated two different thermal modelling approaches. More explanation could have been provided as to why the helical system was rejected (while the explanation has been given before, it should be communicated consistently for new reviewers).

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.

- There is good progress in changing from the 0.5 L vessel to the 2 L vessel. There is good progress in performing test results and comparison to simulations.
- Important and useful results were obtained on evaluating power distribution non-uniformities in resistively heated HexCell assemblies and understanding the effects of the adsorbent media and heat exchanger

assembly in homogenizing the thermal distribution. Initial results using metal organic framework (MOF)-5 in the HexCell assembly are promising. The construction of a MATI prototype test facility at Savannah River National Laboratory (SRNL) is a valuable addition to the project. It will allow the MATI assembly to be tested under conditions commensurate with actual fuel cell operation. The complementary modeling and experimental efforts are contributing to a solid understanding of gas flow phenomena and thermal transport in the two adsorbent media assemblies that have been adopted in the project.
- The charging and discharging experiments were well done, and the model works for replicating the experimental conditions.
- The project milestones are significant to achieving project goals, with many potential stumbling blocks along the way. This was highlighted quite well by monitoring the heater cartridge temperature response and determining the non-uniformity, but testing proved that it behaved quite well because of the thermal distribution of the MOF in the HexCell, matching model predictions quite well. This has led to significant progress toward the 2 L storage tank and test facility. The MATI test system is on track.
- Accomplishments in this reporting period appear largely focused on the 0.5 L vessel, with a plan arranged for the 2 L system. While substantial work was accomplished, the budget for this project is quite high, (approximately $1 million per year). A cost breakdown between experimental and modeling efforts would be interesting.
- The PI delivered two systems. This was a very complicated task with very sensitive materials and systems.
- The project is listed as 90% complete, but has not completed the most important tasks of actually testing these adsorbent storage systems, which have been under study since 2009.

Question 3: Collaboration and coordination with other institutions

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

- Strong and fruitful collaborations between SRNL and the other partners working on the adsorbent systems are readily apparent. They are contributing significantly to the success of the technical effort.
- As with all projects under the HSECoE, the collaboration and coordination between partners have been excellent.
- As part of the HSECoE, the PI is working with all of the appropriate industrial and academic partners.
- Close collaboration is needed and well-executed with partners in this project. Significant progress is made through the combinations of design, testing, and modeling in the different institutions, with added perspective coming from external collaborations.
- Contacts to all relevant partners and institutes are established.
- It continues to be difficult to estimate how much collaboration actually occurs between HSECoE participants. However, since there do not appear to have been problems that interrupted the test schedule, the collaboration must have been at least adequate.
- Roles are unclear.

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 potential impact this project will have on the U.S. Department of Energy’s (DOE’s) research, development, and demonstration is rated excellent, because the plan testing of adsorbent storage systems under design for several years is needed to validate the modeling of these systems to access balance of plant (BOP) mass and volumes.
- The adsorbent system has emerged as the primary candidate for prototype development in the HSECoE. The SRNL effort forms the centerpiece of the modeling, testing, and prototype development effort. It is critical to the success of the project and is highly relevant to the overall goals of the DOE Hydrogen and Fuel Cells Program.
- Focus is currently on mostly adsorbent based systems. The results of this work are universally applicable to compressed natural gas systems and future sorbents.

- The system focus of the project is geared toward DOE goals and will have significant impact even in the advent of another storage material being used, as the design and modeling are all extensible. Several challenges and design improvements have been made, and the testing capabilities will provide the backbone for further development. The downside is that these will not be stand-alone tanks that will be useful as-is on a vehicle at the moment. Further integration with insulation, etc. will need to be considered in the end.
- Even in the case that it is obvious that this kind of storage system cannot fulfill some DOE goals, it makes sense to complete this project. Results of this project will help to set the focus on future projects.

Question 5: Proposed future work

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

- The proposed testing of these adsorbent storage systems will provide the data validating BOP models. The goal of the HSECoE is to determine BOP mass and volumes, so without these experiments, the HSECoE will have fallen short of its goal.
- Significant barriers to achieving the project's future goals are not apparent, though perhaps present. The work is logical, building on successful tank manufacture and test facilities to parameterize the tank performances.
- The PI should focus on evaluating effects of vibration on the system performance.
- Future work will capture MOF testing in both the HexCell and MATI designs. This will be the true measure of project success, as it will validate both the modeling and the system designs.
- Test and validation of the 2 L vessel make sense and is the logical next step. There should be an outlook or recommendation for the usage of other materials (not MOF-5) with better performances to be tested in that vessel. A follow-up project should be established to build up a full-sized system (MATI and HexCell). Upscaling to a full-sized system will reveal more issues with the realization of material-based storage systems.
- A clearly stated and detailed plan for future work is presented. The plan addresses important work in both the HexCell and MATI systems. A better understanding of the thermal contact resistance between the heat exchanger and the adsorption media may be needed to optimize system efficiency. It is unclear how "the loss of usable hydrogen" problem is being addressed.

Project strengths:

- This project is vital to the success of the HSECoE. It is dealing with important engineering issues in a straightforward and compelling way. The project is being conducted by a well-qualified, highly capable team, and it is well-coordinated with other technical efforts in the HSECoE.
- The project used available storage materials, and the PI was able to deliver working systems.
- Project strengths included integration across the HSECoE, smart choices in deciding the path forward, and step-wise monitoring of tank properties, etc.

Project weaknesses:

- An actual onboard tank design with integrated insulation, etc. would be desirable.
- The project does not satisfactorily address the key technical deficiencies illustrated in the "spider charts," most notably the loss of usable hydrogen. Approaches and plans to mitigate problems that are system-dependent (e.g., loss of usable hydrogen) should be considered.
- MOF-5 does not seem to be an ideal hydrogen-adsorbent. It is questionable if the data accumulated for MOF-5 will be of use for any useful hydrogen adsorbents.

Recommendations for additions/deletions to project scope:

- An evaluation of packing density versus cooling channels for the HexCell system should be included in future work. The HexCell system selected was an off-the-shelf material for aeronautical applications. More work can be done to optimize the channel design for improved material packing and heat transfer.

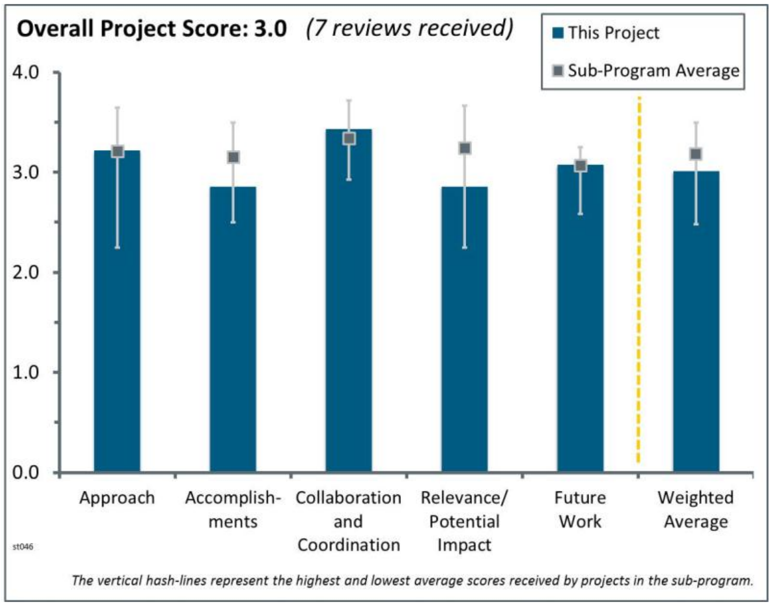
- There needs to be consideration given as to how the HexCell system is loaded with MOF. There also needs to be attention given to keeping the MOF tightly packed against the heat exchange surfaces.
- There should be an increased focus on formulating approaches for dealing with the “white spaces” in spider charts; for example, loss of usable hydrogen.

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

Kevin Drost; Oregon State University

Brief Summary of Project:

The objectives of this project are to use the enhanced heat and mass transfer available from arrayed microchannel processing technology to: (1) reduce the size and weight of the hydrogen storage system, (2) improve the charging and discharging rate of the storage system, and (3) reduce the size and weight and increase the performance of thermal balance of plant (BOP) components. The project will use enhanced heat and mass transfer available from arrayed microchannel processing technology to design, fabricate, and test a modular adsorption task insert (MATI) prototype.



Question 1: Approach to performing the work

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

- The arrayed microchannel processing approach adopted in this project has emerged as one of the two principal approaches for adsorbent system prototype development in the Hydrogen Storage Engineering Center of Excellence (HSECoE). The approach is keenly focused on design, simulation, and experimental validation of MATI subsystems capable of facilitating efficient mass and thermal transport in a metal-organic framework (MOF)-based adsorbent prototype system. The combination of modeling, simulation, and acceptance testing of MATI subsystems optimized for densified adsorbent media is a crucial component in the overall HSECoE technical effort.
- The design and fabrication of prototype systems with validation of modeling to contribute toward their predictive capabilities is well executed. Step-wise approaches to measure system properties have been advantageous in determining contributions to physical properties. Modeling and system properties are strongly integrated and well aligned with HSECoE goals. Improvements have been significant from last year's presentation in design and performance.
- Generally, the approach for the project is rated good, because it addresses system reduction in size and weight, charging and discharging rates, and determining BOP. Having Oregon State University (OSU) performing acceptance testing and Savannah River National Laboratory (SRNL) performing performance testing is also a good approach and an effective use of capabilities.
- The OSU effort is focused on a pivotal piece of the final feasibility testing and validation in the HSECoE's signature proof-of-concept demonstration of an onboard hydrogen storage system. If successful, it will represent one of the first such demonstrations for a non-compressed hydrogen approach and will include cyclic charging and discharging of hydrogen into a tractable storage system for a fuel cell-powered vehicle. The MATI is a highly innovative (but also complex) structure requiring careful attention to all aspects of the fabrication/assembly. This approach is intriguing in principle, but also risky. Whether or not it will be "insensitive to mechanical failure of the medium" remains to be seen.
- Overall, the approach is well constructed and suitable for the work as defined. There needs to be a better explanation of how experimental system requirements and acceptance testing criteria relate to eventual onboard system requirements and criteria.
- As a partner in the HSECoE, OSU has been employing microchannel technology (MT) that enhances heat and mass transfer within components to reduce weight, volume, and cost of the storage systems. This

project does not directly influence the selection of composition of the storage materials themselves. The primary focus of OSU during Phase III of the HSECoE is upon adsorption hydrogen storage by compacted materials.

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.

- Progress appears to nearly be on target, with fabrication of the subscale system nearly complete. Should testing of the 2 L scale prototype be completed this June, work will be on schedule.
- The goal is to demonstrate the feasibility and validate simulations of a 2 L MATI storage unit. To this end, there has been smart consideration of the cooling and charge/discharge functions within the prototype, a new cooling plate, and parallel modeling. The overcoming of difficulties in manufacturing/testing has been worthwhile, but full tests are still needed.
- The progress over the past year has been generally good, but this reviewer expected the project to be further along in terms of the MATI testing. While most of the key components of the MATI have been fabricated and tested to some extent, getting a MATI assembled, started up, and tested remains to be done in the coming year.
- Solid progress was made on meeting 2013 SMART goals for this project. Computational fluid dynamics modeling, fully instrumented MATI enclosures, and MOF pucks provided useful information to assess the design functionality and to guide and optimize on-going subsystem development. OSU investigators have worked closely with other HSECoE partners on optimizing the pressure vessel, cooling plates and headers, and media puck characteristics to ensure adequate subsystem performance. A more tightly focused effort on timely development and delivery of a MATI subsystem for acceptance testing at SRNL was an important research and development direction during this reporting period.
- During Phase III of the HSECoE effort, the OSU researchers have been working on the design and fabrication of a prototype MATI for experimental verification of its performance potential. The MATI could potentially facilitate heat transfers within the tank using compacted adsorbents, but its validation is still lacking. OSU has recently completed a detailed design review along with fabricating most of the MATI components for a prototype, as well as constructing a setup for acceptance testing of the prototype. However, assembly of the prototype seems to be at least a few weeks behind schedule, so meeting the Phase III goal of prototype delivery to SRNL for performance testing starting in August 2014 looks to be at risk.
- This year, the project was 82% complete from last year’s 72% completion. A 10% progress is rated satisfactory. The accomplishment this year was a complete pressure vessel design for the 2 L MATI storage system. The presentation showed a Computer-Aided Design (CAD) illustration of the MATI, but it only showed about eight MOF-5 puck layers. It depends somewhat on assumptions on the material properties, but a 2 L tank (10 cm diameter with 1.5 cm thick walls) should have more than 12 puck layers. If the storage system is to be tested in June 2014, then a drawing of the actual tank should have been in the presentation.
- It is not quantitatively clear how technical accomplishments such as improved heat transfer and temperature distribution contribute to improved system performance or durability, or how they ultimately improve metrics relative to DOE targets.

Question 3: Collaboration and coordination with other institutions

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

- Coordination and collaboration within the HSECoE has become a true strength of the Center. The OSU connection seems to be solidly in place. This is probably because OSU is tasked with supplying a critical piece of the final demonstration.
- The OSU effort was tightly coordinated with relevant work by other partners in the HSECoE. The collaborations with Ford and the University of Michigan (UM) (adsorbent puck development), Hexagon Lincoln (HL) (pressure vessel/header development), and SRNL (acceptance testing and code validation) are

particularly noteworthy. Those interactions have strongly enabled and supported the technical effort at OSU. They reinforce the relevance and merits of a "HSECoE model" for this kind of activity.

- Most identified collaborators appear to be actively involved in project planning and execution.
- There appears to be excellent collaboration between Ford and OSU on delivery of the MOF-5 samples. However, it was not clear who was responsible for making the MOF-5 pucks with enhanced conductivity.
- OSU interacted mostly with SRNL, HL, Ford, and UM regarding the development, fabrication, and testing of the MATI prototype. There do not appear to be any active relationships with the other HSECoE partners during Phase III.
- 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. It is not possible to tell if there is also input from these partners regarding the system designs being developed, besides HL.
- The MATI subsystem is to be integrated with a vessel being fabricated by HL. Based on progress reported by HL, no issues are reported and integration of the MATI insert is the next scheduled step.

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 high level of relevance of the OSU work to the goals of the HSECoE is unequivocal. In fact, the perceived success of the project a year from now will be based in large part on how well the MATI performs. The HSECoE has already done many good things in the form of (1) significant insight and knowledge relative to onboard hydrogen storage, and (2) analysis tools designed to probe and validate system performance. Failure to demonstrate a functional hydrogen storage system at some level would not bode well for a successful closure of the project.
- The system focus of the project is geared toward DOE goals and will have significant impact even in the advent of another storage material being used, as the design and modeling are all extensible. Several challenges and design improvements have been made, and the testing capabilities will provide the backbone for further development. The downside is that these will not be stand-alone tanks that will be useful as-is on a vehicle at the moment, and further integration with insulation, etc. will need to be considered in the end.
- The use of arrayed microchannel processing technology for adsorbent-based hydrogen storage prototype development is a key component of the technical effort in the HSECoE. By facilitating a reduction in storage system size and weight, improving sorption rates and thermal transport, and addressing key BOP barriers, the OSU project is closely aligned with DOE Hydrogen and Fuel Cells Program goals and DOE research, development, and demonstration objectives.
- Potentially, the MATI may reduce mass and volume of adsorption storage systems while enhancing thermal performance, providing the hydrogen permeation is sufficient within the compacts, the liquid nitrogen flow within the microchannels and discs provide efficient heat transfer into/out of the compacts, and the configuration of components within the storage vessels do not require extraneous volumes. Initial analyses indicate that higher costs due to fabrication and integration of these MATI components will make the overall storage system more expensive than using powder absorbents. OSU has yet to experimentally demonstrate the performance levels and robustness of MATI components during pressure/temperature cycling as well as their durability during extended operation. Fabrication of the internal structures using aluminum materials (necessary for reducing bed weight) and assembly of the MATI within light-weighted storage vessels have been incompletely addressed so far.
- The engineering challenge is to provide in situ cooling or heating within a vessel to make pressurized hydrogen storage through densified adsorbent media economically practical. The evaluation provided by the team indicates the MATI approach can provide more media per volume than other packing arrangements such as finned tubes, as well as meet functional goals necessary of the overall system to work. Alternatively, this allows more room for the hydrogen, given the presence of the thermal control apparatus. For this densified hydrogen storage concept to be successful, the MATI approach must not compromise overall system capabilities on the amount of hydrogen stored.

- It is not clear how the incorporation of improved heat transfer mechanisms "moves the ball" closer to DOE targets.
- The project was rated satisfactory in advancing progress in hydrogen adsorbent storage because of its good design of the 2 L MATI prototype reactor.

Question 5: Proposed future work

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

- The future plans for work at OSU are as sharply focused as they could be. Its target in terms of a successful outcome seems to be well understood. A statement in the listing of Phase III MATI Functional Criteria caused some disappointment: "Provide data for model validation instead of meeting specific DOE goals." It seems to imply that either the DOE goals have become unimportant or that achievements will be so far from the goals that they are no longer embraced.
- During Phase III, resolution of fabrication issues and laboratory testing of the MATI prototypes are critical tasks that are mandatory to verify simulations of enhanced thermal performance. They also need to address issues and problems during component building and operating conditions (i.e., pressure/temperature cycling and fluid flow rates). Based upon the level of testing previously performed at OSU, it is unclear whether sufficient assessments of thermal performance and component robustness will be completed on new prototype MATI devices during the remaining duration of the project.
- The work has logical extensions to finish the assembly testing and validation. No significant risks are identified at this point in the project.
- The planned future work is appropriate for completing the approach as identified.
- The proposed future work is scored as good. The project addresses the remaining tasks of model validation and performing acceptance testing on the MATI hydrogen storage system.
- Future work entails assembly of a larger scale prototype, acceptance testing, and delivery to SRNL for performance tests. This work is followed by model validation and trial of "conduction enhanced pucks." This appears straight forward.
- The project is nearly complete. The future work is tightly focused on remaining project issues, especially completion of the MATI prototype and delivery to SRNL for acceptance testing. Although the plan for future work is reasonably complete and compelling, it is not entirely clear if there are any technical obstacles that could impede that effort. A succinct statement about remaining barriers (if any) to achieving final project goals would be helpful. The OSU investigators acknowledge that some thermal enhancement in the adsorbent puck may be needed to meet SMART goals. Although a potential solution (embedded aluminum pins) has been proposed, it is not clear whether that solution can be fully implemented and tested prior to the conclusion of the project.

Project strengths:

- The team at OSU has exceptional skill in the area of modular mass and heat transfer technology. Up to the present time, planning has been excellent and execution has been successful.
- This is an innovative project that comprises a solid technical approach implemented by experts in the field of microchannel array technology. It has significant relevance and importance to the overall technical effort in the HSECoE. The project benefits greatly from extensive collaborations and technical support from HSECoE partners.
- The goals and execution of the project are straightforward.
- OSU has unique experience with developing and fabricating MT devices for various purposes that suggest these assemblies may be suitable for those hydrogen storage components requiring improved heat and mass transport without sacrificing system weight and volume.
- Collaborations within the HSECoE are strong. The considerations in MATI design are detailed and provide an extensible test bed.

Project weaknesses:

- It has not yet demonstrated by laboratory testing at OSU whether the as-conceived MATI configuration will operate reliably under the variable pressure and temperature conditions that will be necessary for long life components in hydrogen storage systems. In particular, leaks between the different fluids could lead to very serious problems. While the project's models do predict high performance behavior from MATI under idealized configurations and operating conditions, robustness after fabrication and assembly of the components has not been sufficiently verified.
- There is some concern about the pace of work at OSU. It is unclear whether it has enough funding left to support the manpower needed to complete their remaining work in a timely manner.
- A comparison of cost, efficiency, and mass/thermal transport characteristics of the MATI subsystem with other competitive technologies is needed. A specific and candid description of technical risks and potential limitations/problems with the MATI approach to mass and thermal transport in an adsorbent-based hydrogen storage system would be helpful.
- There needs to be clear connections made between technical goals and accomplishments and progress toward achieving (or approaching) DOE targets.

Recommendations for additions/deletions to project scope:

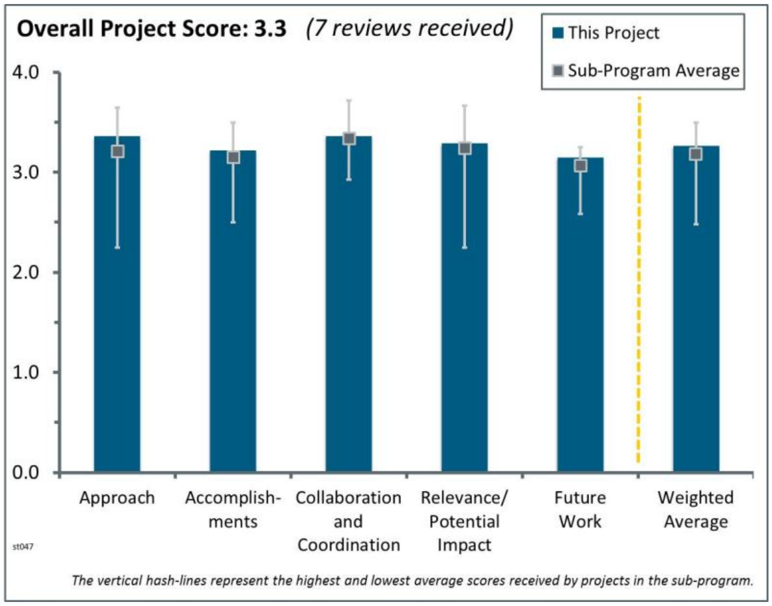
- The project is nearly complete, so significant additions to the project scope would be difficult to implement. However, a useful addition would be the development and testing of a method for enhancing the thermal conduction within the adsorbent media puck.
- OSU should confirm conceptual designs for the MATI devices via experiments. In particular, these demonstrations should show complete and reliable separations (i.e., no internal or external leaks of heat exchange fluids or pressurized hydrogen gas) during operation.
- The MATI is the most complex piece of the adsorbent bed test. It is recommended that the team stick with the plan of having several MATIs constructed in parallel for the validation tests. If one has a problem, it will be very beneficial to the progress of the project to have several backups. It is doubtful that one can put a MATI together overnight.

Project # ST-047: Development of Improved Composite Pressure Vessels for Hydrogen Storage

Norman Newhouse; Hexagon Lincoln

Brief Summary of Project:

The objectives of the project are to: (1) meet the U.S. Department of Energy (DOE) 2017 hydrogen storage goals for the storage system by identifying appropriate materials and design approaches for the composite container; (2) maintain durability, operability, and safety characteristics that already meet DOE guidelines for 2017; and (3) work with Hydrogen Storage Engineering Center of Excellence (HSECoE) partners to identify pressure vessel characteristics and opportunities for performance improvement, in support of system options selected by HSECoE partners.



Question 1: Approach to performing the work

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

- Milestones are very specific and relate directly to the project. The approach keeps HexCell and modular adsorption task insert (MATI) tank designs as similar as possible.
- Hexagon Lincoln (HL) has performed good work in design and fabrication of the prototype pressure vessels. The finite element analysis performed to verify integrity represents best practices.
- The effort takes a systematic approach to storage development. More details regarding go/no-go requirements should have been provided.
- The approach undertaken is a bit different than other efforts. There is an attempt to build in flexibility in order to modify goals to accommodate changes or incomplete development in other coordinated research. This is realistic.
- The project built reusable tanks for testing the systems. The systems are probably over-built for automotive uses, but that is not the focus of this project.
- Cost and weight reduction are some of the most important criteria regarding the vessel development. Involvement of a vessel manufacturer is the best approach to gain results with a high confidence level. To start with a small-scale approach makes sense. It is good that not only performance, but also durability, safety, and operability are addressed. However, the strategy is not 100% clear. Design work of Type 1, 2, and 4 vessel designs are involved at different phases. It is unclear whether the goal is to develop a material-based or physical-based storage system.
- HL has a clearly defined role in the HSECoE program: to design, fabricate, and test tanks. Tanks are an essential part of the hydrogen storage approaches that remain under study, whether they are compressed gas- or adsorbent-based. HL's contribution is pivotal to the success of the planned adsorbent system demonstration.

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 principal investigator (PI) built and delivered functioning systems to the HSECoE for incorporation into the systems.
- The project is on track and seemingly conducted in a very professional manner.
- Accomplishments of small-scale vessels include improvements in weight, volume, and cost. However, because there is no prediction to full-scale system, there is no correlation to DOE goals.
- HL has completed all the tasks assigned to it for Phase II. All the results reported in the presentation related to Type 1 tank performance were encouraging, which is critical to the success of Phase III of the project. The liner problem for Type 3 and Type 4 tanks remains to be solved (or so it seems). It is unclear how important this is in the context of planned system demonstrations for Phase III, or whether Phase III will include any tests of Type 3 or Type 4 tanks containing metal-organic framework (MOF)-5.
- HL has done a good job of meeting project timelines and milestones. The project is on target to meet all milestones. Down-selection to 2 L design and subsequent construction are on schedule. Weight reduction with 1-piece design is significant.
- There has been continued progress on separable Type 1 tank weight reduction. Work towards a number of Phase III milestones is still in progress.
- Progress continues in many areas, despite waiting on results from other coordinated projects.

Question 3: Collaboration and coordination with other institutions

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

- All relevant partners/institutes are involved.
- The PI is working with the HSECoE, which has the suitable academic, industrial, and government partners.
- The HSECoE structure of monthly/quarterly meetings appears to ensure close collaboration with performers.
- It is clear that HL is solidly connected to the HSECoE in terms of communications, coordination of design, fabrication, and testing details, as well as meeting delivery deadlines, e.g., for the Type 1 tanks.
- There has been good collaboration with other center members to establish design parameters and requirements.
- Work is well coordinated with HSECoE and other collaborators.
- This is a strong team that exhibits detailed coordination (e.g., communicating subcomponent dimensions for mating equipment).

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.

- There are several desirable impacts of this work:
    - Demonstration of improved capability with improved cost-effectiveness.
    - Demonstration of improved vessel subsystem capabilities (strength of carbon fibers at cryo temperatures, suitability of metallic liners, etc.).
    - Development of vessels designed as flexible “test beds” to help demonstrate the use of other technologies (e.g., MATI) that in conjunction will produce overall system gains.
- Low-pressure tanks for sorbent materials are required.
- Cost, weight, and volume reduction of a pressure vessel are very important, especially when a tank manufacturer is the project lead.
- HL’s contributions are critical to a successful outcome in Phase III of the overall HSECoE program. On the other hand, it was noted in slide 6 that the Type 1 tank is “designed to meet team needs for engineering

demonstration, but less responsive to overall DOE targets." Similar statements have appeared in several other HSECoE project presentations. It makes one wonder how far short of the original DOE targets the Phase III demonstrations will fall.
- The project is providing necessary tanks to HSECoE partners to facilitate other development efforts. It is not clear what the specific targets for the tank portion of a storage system are.
- The strategy of designing tanks for materials that are unlikely to ever be commercialized is highly questionable.

Question 5: Proposed future work

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

- A very good summary of future work activities was presented.
- The completion of tests with a 2 L vessel is good, as is the outlook for moving forward from upscale to a full-size system vessel.
- Future efforts should focus on methods to reduce cost and determine whether cheaper materials can be used.
- Future work is well-defined and will address several important development areas, including cryogenic Type 3 and Type 4 liners, external vacuum shells, and storage media installation into monolithic tanks.
- There is no issue with the proposed future work, as it directly pursues the goals of current work.
- Many of the Phase III tasks listed on slide 21 of the HL presentation seem ancillary to the remaining key outcomes that will ultimately define the overall success of the HSECoE program. For example, it does not appear that the results of these Phase III tasks will be incorporated in any storage system feasibility demonstration. At best, the results of HL's Phase III effort will provide some guidance for future technology development/demonstration beyond the HSECoE.
- Given the unlikelihood of current sorbent materials to ever see commercial use, the design and construction of additional tanks can hardly be justified. This is not a comment on the capabilities of the PI, but a programmatic issue.

Project strengths:

- The strength of project is the professional manner in which the activities are conducted on schedule, as well as achieving targeted results. Demonstration of a resin liner would be a novel and potentially significant achievement.
- HL's contributions to the HSECoE have been strong and steady. It is not the tanks that have limited the success in meeting DOE targets. Clearly, HL is a qualified, engaging tank manufacturer and a very good choice for the role it has played in the project as a whole. The PI has demonstrated great competence as the leader of the tank development effort. The work on the Type 1 tank for the adsorbent system tests looks to be exceptional.
- There has been solid design work and testing. There are strong analysis capabilities supporting design and construction.
- This project is providing needed and responsive support in the development of tanks for historically uncharacteristic operating conditions.
- The project directly pursues incremental improvements in vessel construction to improve performance. It does so with several different vessel constructions so that several potential paths of improvement are being simultaneously examined.

Project weaknesses:

- The only weakness (and it is simply a perceived weakness) is that HL's Phase III contribution may not bring much luster to the final list of HSECoE accomplishments.
- Other than the complexity of pursuing several different elements of vessel construction at once, no weakness is noted.

Recommendations for additions/deletions to project scope:

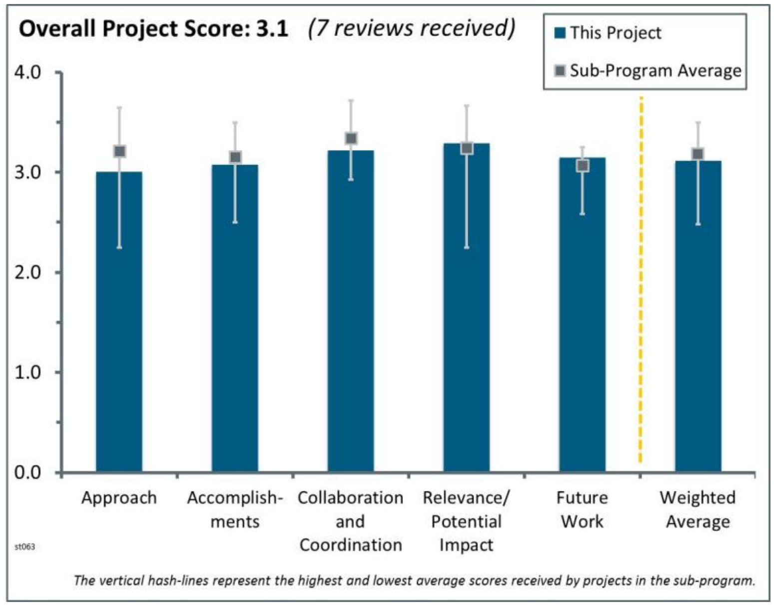
- The PI should provide more details or future study on designing liner robustness for cryogenic conditions. The PI should provide a list of suitable materials and operating parameters.
- “Resin liner” gas permeability needs to be explored.
- To counter the concern regarding the ultimate value of HL’s Phase III results, DOE should consider going a bit further with the adsorbent system feasibility testing. If the Type 1 tank/MATI combination is a rousing success, there is no reason not to go one step further and do the full system demonstration using a Type 3 or Type 4 tank/MATI combination.
- It would appear that pre-formed storage media and monolithic tanks could be incompatible. Trade studies should be undertaken (not necessarily by this project) to evaluate the usefulness of monolithic designs with anticipated storage media configurations if completion of tank construction with media installed is not feasible.

Project # ST-063: Reversible Formation of Alane

Ragaiy Zidan; Savannah River National Laboratory

Brief Summary of Project:

The overall objective of the project is to develop a low-cost generation/regeneration process for alane (aluminum hydride, AlH_3), a promising hydrogen storage material. Key activities include characterizing the material's stability, thermodynamics, and kinetics, and evaluating its potential for fulfilling the U.S. Department of Energy (DOE) onboard hydrogen transportation and portable power performance targets.



Question 1: Approach to performing the work

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

- The Savannah River National Laboratory (SRNL) alane (AlH_3) project continues to make steady progress toward an electrochemically driven alane regeneration scheme. Its approach is logically driven by cost, and currently it is mainly directed toward niche applications, such as potential military applications. Here it appears that the cost of regeneration is either completely unimportant or of secondary concern, as the project appears to be concerned mainly with one-time use, disposing of the spent fuel canisters. The approach has added a small company involved in developing soldier-based fuel cell systems, where the cost of 'first fill' is still crucial, and so the project's continued interest in reducing cost of regeneration of alane makes sense for first fill for niche applications. As the path forward to reduce alane regeneration costs so that it could eventually be viable for onboard application, the SRNL approach is a good one. Although, in the end, it seems unlikely that the project will be able to meet DOE fuel cost targets for onboard/off-board regenerable systems.
- Electrochemical approaches for reversible formation of alane are interesting.
- The approach, an electrochemical generation of aluminum hydride, has been known for some time. It was attempted in the past (German patent DE 1141623 and Osipov, O. R.; Kessler, Yu. M. Elektrokhimiya (1971), 7(7), 923-7.) but never really implemented in larger-scale manufacturing. The main value of the current work is an attempt to design a "real life," scalable set of processes, which can be used to generate a high-capacity hydrogen storage material and regenerate the spent fuel.
- Off-board regeneration has many limitations. It appeared that the thermodynamic "costs" were going to limit the applicability of this approach for application to transportation beyond early market systems.
- Alane with 10 wt.% hydrogen is barely likely to make the 2017 DOE system target (when the entire storage system weight and volume is taken into account) and is highly unlikely to achieve any higher system targets, e.g., 7.5 wt.% hydrogen. It is no longer a candidate for demonstration in Phase III of the Hydrogen Storage Engineering Center of Excellence (HSECoE) program. Its contribution to overcoming barriers to the targets is not great. Therefore, in the context of achieving compelling Phase III accomplishments, further work on regeneration of alane seems unnecessary at this time.
- The electrochemical approach has great potential for efficiently regenerating alane. However, in the past, only very limited and general information was provided about process efficiency and process-limiting mechanisms. A more detailed examination of these issues and potential obstacles was a very positive addition to the approach employed during this review period. In this reporting period, there was a much sharper focus on identifying and implementing electrochemical methods to reduce alane regeneration costs. This is the critical issue for successful deployment of an alane-based system in either stationary or transportation applications.

- It looks like the electrochemical process touted by the principal investigator (PI) as the saver of the alane world is not working well after all. The team is back to using the traditional solid reaction method.

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.

- Most targeted objectives have been accomplished. The progress is excellent.
- The science involved in this work on alane is actually quite good. The thermodynamic and electrochemical aspects are thoughtfully applied with modest success. Some barriers associated with regeneration have been overcome, but other barriers raised by the use of alane for vehicle applications seem insurmountable.
- Solid progress has been made in several areas, including more efficient $NaAlH_4$ regeneration using a new and less expensive catalyst, solid state alane production from $NaAlH_4$ via "dry" processing, understanding and quantifying costs and inefficiencies in electrochemical regeneration of alane, and use of alane-diethyl ether adducts for improved process yield. This work is providing increased confidence that a truly scalable electrochemical process for alane regeneration can be developed. A more detailed and understandable analysis of process-limiting steps and costs of individual process steps was an important (and welcome) addition.
- SRNL continues to exhibit good progress at every meeting, dealing with the multitude of problems it uncovers. One accomplishment has been to show that the kinetics of electrolyte recycle are quite slow, which may limit the overall efficiency and cost of the process. Nonetheless, this is an important observation, and the team is now focused on removing this barrier.
- Although positive results have been presented on a laboratory scale, the scalability of the electrochemical processes remains to be seen. The advantages of the electrochemical process over conventional chemical approaches may not materialize because of technical challenges associated with the need to run the electrolysis in a highly flammable and volatile organic solvent and the limited overall yield of alane.
- The PI has made steady, significant progress over the past few years. However, there appeared to be an overpotential limitation that the PI was unable to explain. The kinetic and thermodynamic barriers are significant, and a direct pathway to overcome these limitations was not clearly defined.
- The team accomplished relatively little in the past year. The electrochemical process did not look promising. The solid state reactions are not really different from what has been done before. The team demonstrated recycling of $NaAlH_4$ electrolyte with > 70% yield. The surface treatment is not any different from what was done by the Russian scientists.

Question 3: Collaboration and coordination with other institutions

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

- There has been close, appropriate collaboration with other institutions; partners are full participants and well-coordinated.
- It would be good to see collaboration with possibly the hydrogen storage group at the University of Hawaii or an International Energy Agency – Hydrogen Implementing Agreement member. A new external collaboration would give new insights and directions to approach the overpotential limitations mentioned above.
- A close collaboration with Ardica Technologies and SRI International (SRI) has been established. This is a positive and critical step to developing a scalable and cost-effective electrochemical process. A new DOE project, led by Ardica Technologies, will build directly on the work conducted in the SRNL effort.
- This project appears to be as plugged into the HSECoE as it needs to be at this time. It is not clear what the contributions of Ardica Technologies and SRI have been over the past year.
- This is a small project, and thus by its nature, collaboration may not be as extensive as in larger projects. It has recently added a small company partner, and that collaboration will likely assist the project in a higher fidelity cost model for its process.
- The extent of the collaboration is not very clear.

- The team is not really collaborating with other teams on the technical side. This is mostly a solo play at SRNL. The so-called collaboration is a Cooperative Research and Development Agreement to explore potential use of alane.

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 project aligns well with the DOE Hydrogen and Fuel Cells Program (the Program) and DOE research, development, and demonstration (RD&D) objectives and has the potential to advance progress toward DOE RD&D goals and objectives.
- Development of an efficient and cost-effective method for regenerating alane would have significant positive impact on the overall direction and success of the Program. The electrochemical process being developed at SRNL and partner organizations is the leading candidate for regenerating alane at costs and quantities that are useful for the Program needs. The project is highly relevant and directly supports the overall DOE RD&D objectives.
- The project is relevant for early market applications.
- Of all the tractable hydrogen storage materials that have been studied as part of the work of the HSECoE, alane is certainly one of the best in terms of coming within reasonable range of the system targets. However, the spider chart for alane (notably missing from this particular presentation) still shows many substantial deficiencies, system gravimetric density being one of them.
- This small project may have an outsized impact on short-term DOE goals in the area of portable power and niche applications of hydrogen storage materials if the team can continue to make progress in improving efficiency and reducing cost.
- The advantage of alane to alanate is not clear. There is higher hydrogen capacity for alane, but since alanate is needed as a precursor, there is lower energy efficiency and one more step for regeneration.
- Alane looks attractive in terms of the high hydrogen content, but the cost of synthesis will be hard to overcome to make it practical. The electrochemical process was thought to be able to make a difference, but the results so far are nothing but disappointing.

Question 5: Proposed future work

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

- Future work plans are well defined within the scope of the current project.
- The proposed future work is a logical and reasonable extension of the current effort. It would be helpful if critical remaining technical issues could be stated and addressed more explicitly, i.e., the main obstacles that (may) limit scalability and efficiency and how they will be addressed. Maintaining clean electrode surfaces during the complex electrochemical process is critical for limiting over-potential in the reactor. Methods for mitigating electrode surface contamination should be addressed.
- The question here is about what the overall impact will be in regard to the feasibility of alane-based onboard hydrogen storage if this project is highly successful with their proposed Phase III research. In truth, more work on alane is hard to justify at the present stage of the HSECoE.
- The PI identified during the question and answer session that the kinetics of electrolyte recycle are slow (something around 50% conversion overnight, or some lengthy time). This may impact overall cost in a significantly negative way. It should become a focus of the project's future work to identify whether the kinetics impact capital costs significantly, and if so, determine ideas to accelerate the kinetics of electrolyte recycle. The fluid bed electrochemical reactor concept is intriguing and could help lower downstream separations costs as well as lend more of a continuous aspect to the overall process.
- The team is doing what is planned for the project, but it seems the final results will be far from anything practical.

Project strengths:

- The project has a strong team of materials scientists. Research results are independently confirmed (see German patent DE1141623 and Osipov, O. R.; Kessler, Yu. M. Elektrokhimiya (1971), 7(7), 923-7). There have been good collaborations.
- The progress the team has made has been good. The industrial partners' insight in batch processing of the samples is evident.
- The project involves smart people with good ideas doing high-quality science.
- Alane is a leading candidate for a storage medium that meets DOE targets. However, the problems associated with regeneration of the material have limited its use in practical applications. The SRNL project employs a novel electrochemical approach that may overcome the limitations and problems encountered in more conventional regeneration methods. Solid progress has been achieved in demonstrating the viability and scalability of the electrochemical regeneration approach. The results from this project have provided the basis for a new project led by Ardica Technologies to extend the electrochemical approach to produce large quantities of alane at greatly reduced costs.
- The project has a small team with potentially outsized impact, if the research and development continues to proceed successfully. SRNL has brought on a small company with a vested interest in its success, and this should help bring additional focus to efficiency and cost.
- The passionate PI is a project strength.

Project weaknesses:

- With the addition of a small company partner, there will be no weaknesses.
- There are thermodynamic and kinetic barriers that will be very difficult to overcome.
- A more detailed description of efficiency-limiting steps (especially kinetics-limiting processes) is needed. Although conceptually straightforward, the electrochemical process comprises multiple steps, each of which has its own potential limitations. These should be addressed explicitly. Without that information, it is exceedingly difficult to assess the potential for achieving an efficient, scalable process.
- The advantage of alane to alanate needs to be clarified.
- The cost analysis does not seem to include the extensive processing cost (labor cost and capital expenditure). The loss of $NaAlH_4$ or $LiAlH_4$ also seems not to be included (only about 73% recovery).
- The high level of risk associated with scaling up the electrochemical process is the major drawback for the project. From the practical standpoint, if alane is really desirable in substantial quantities in the near future, it is recommended to back the current approach up by developing an alternative way of making alane in a safe and efficient manner.
- Working on a material that has little to no potential of meeting future onboard hydrogen storage targets that are at a level the automotive industry will consider attractive is the project's weakness.

Recommendations for additions/deletions to project scope:

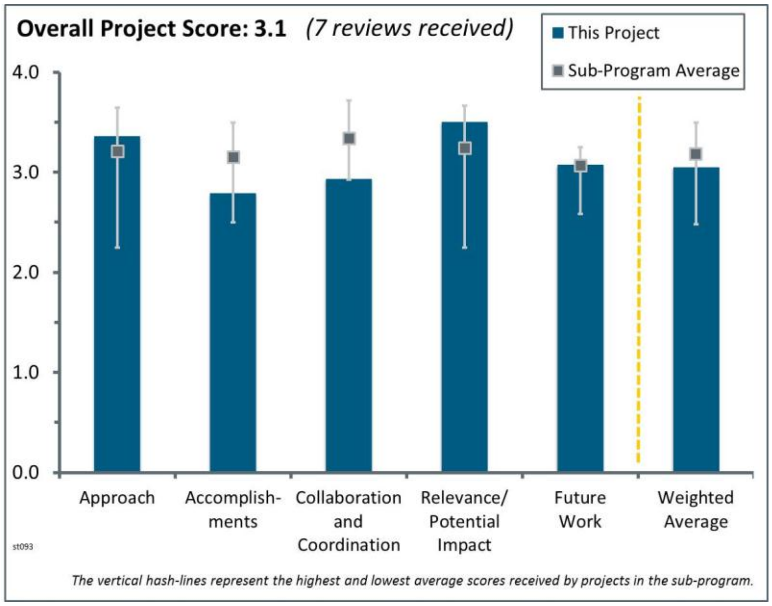
- It would be interesting to know what Ardica Technologies and SRI are bringing to the table where this project is concerned.
- The inclusion of the Ardica Technologies/SRI collaboration into the project is an excellent addition that will provide expertise and experience needed to develop a scalable process.
- There should be more attention to the impact on kinetics on overall process costs.

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 the project is to significantly reduce the manufacturing cost (>25%) of high-strength carbon fiber (CF) via: (1) development of alternative formulations for advanced precursors capable of being melt spun in high volumes; (2) enhancement of high-quality polyacrylonitrile (PAN) precursor melt spinning techniques for practical application; (3) development and demonstration of appropriate conventional and/or advanced CF conversion technologies; and (4) advancement of properties, scaling, and overall economics to meet high-pressure storage targets.



Question 1: Approach to performing the work

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

- This effort fits in very well with the other projects in CF. The learnings of this project can be extended to other programs. The goals of this specific project are well defined, and the project plan seems sound.
- Continuing the work from BASF to produce a precursor with a different method (melt-spinning) is a good way to reduce CF costs significantly.
- Focusing on the precursor chemistry before the filament processing appeared to be an effective approach. It is good to see that the project is moving toward the use of PAN-methyl acrylate (MA), which will allow for a better chance to achieving the targets. The approach should accelerate the cost model effort to understand the critical drivers in the processing that could affect the cost savings of the melt spun fiber.
- The approach of addressing costs of aerospace-grade CF by reducing the energy and cost for spinning a precursor is valid and should have an impact on the industry, specifically on storage technologies.
- Simplifying the preparation process of the CF has a direct impact on cost reduction.
- This project has effectively addressed the barriers encountered by previous work that was similar in nature and set a plan to overcome these obstacles. The approach is also aimed at creating a commercially viable solution to move this work forward. Switching PAN chemistry to use MA is an example of addressing barriers that have been discovered during this project.
- The comparison between the "melt" processing being investigated against the conventional "solution" processing makes it clear why melt processing is desirable to pursue. However, at the start of the presentation, it was made clear that while the use of PAN-vinyl acetate (VA) chemistry is feasible, the evaluation had to change to the use of PAN-MA because of material availability issues, a realization reported at the previous DOE Hydrogen and Fuel Cells Program Annual Merit Review. At this point, the impression given is that details of the approach involve a lot of trial and error work and the methodology cannot be presented because of Intellectual Property (IP) issues. Note that a subsequent presentation in this area was able to make clear the logic of testing through discussion of the test matrix and did not invoke IP issues. This did not seem like an adequate explanation by the principal investigator (PI).

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.

- This project is meeting its goals. The main thing holding this effort back is resources (both equipment and human).
- The project appeared to take a significant step towards the feasibility of the melt-spun processing. It was useful to observe progress and results using PAN-MA.
- There have been good accomplishments up to now, but the delay of extruder delivery could cause a no-go decision at the next milestone. The target of >300 ksi is not shown in the presentation. Potential risks and future challenges should be documented.
- It looks like the project is starting to come together and produce solid results with new plasticizers developed, but still lacks consistent production of long segments that can be carbonized for mechanical testing. It will be interesting to see if the team can meet the third milestone with the extruder delays. The project is expected to really increase progress once the new extruder is in place.
- Much knowledge was gained last year on the barriers in using PAN-VA. The project responded well to this technical challenge, but in the process it needs to readdress the ability to achieve the project objectives. However, the team has remained focused on the project objectives while addressing the technical hurdles encountered.
- The status of progress was not clear because the PI stressed how complex and interdependent development is, and how coordination is critical in each area. Progress was reported as hampered by delayed receipt of equipment and a June milestone in jeopardy. No impact was indicated for fiscal year-end milestones. Accomplishments involving chemistry, spinning, and conversion were claimed.
- The feasibility that the melt-spun process could meet the costs target of the project has not been established.

Question 3: Collaboration and coordination with other institutions

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

- The project has well-chosen partners.
- All relevant partner and institutes are involved.
- Collaborations between Oak Ridge National Laboratory (ORNL) and Virginia Tech (VT) seem to be increasing, which is positive. Reaching out to BASF is also a positive; however, it is not a U.S.-owned company. It would be nice to see a U.S.-owned company, such as Dow Chemicals or DuPont, become a partner.
- The project has good collaboration with VT but has discontinued effort with BASF, and there have been some delays due to the extruder. It is acknowledged that the project is searching for other partners. As the project develops the cost model, it would be helpful to have an industrial partner to confirm the manufacturing and feasibility assumptions. The project presentation indicated additional partners may compromise longer-term options, although a strong industrial partner may increase the probability of commercialization.
- Comments from previous reviews indicate additional collaboration may be desirable, but the presentation states that this may compromise longer-term options.
- The collaboration between VT and ORNL appears to function very well. However, the change in PI at VT may impact that collaboration and change this dynamic. The broadening of the collaborative team appears necessary at this point to optimize the PAN-based dope formulation from both a cost and performance standpoint. The project should consider adding a full industrial partner that can assist in and provide a steady supply of PAN-based dope.
- Collaboration with CF manufacturers (original equipment manufacturers [OEMs]) does not seem to be present.

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.

- It is clear that despite the risk of being unable to accomplish goals, success would be a quantum leap for the manufacture of CF in reduction of complexity, reduction of cost, and reduction of environmental impact.
- This project can provide a significant reduction in high-quality CF costs and seems to be in very good alignment with the Hydrogen Storage sub-program goals.
- CF is the number one cost driver for pressure vessels. Reduction of more than 25% in manufacturing cost (as predicted) would be a huge step.
- If successful, this project could have significant impact on the cost of composite-wrapped pressure vessels by lowering the cost of CF. This will be very dependent on the CF industry adopting a new process.
- This project has high relevance because of the potential of advancing towards the DOE research, development, and demonstration cost objectives for pressure vessels. It would still be helpful to have a detailed cost model that confirms the cost savings to further highlight the opportunity of this project.
- If the feasibility could be demonstrated, high impact on cost reduction is expected.
- This project represents an opportunity to change the landscape of CF production. This is not only important to the DOE Hydrogen and Fuel Cells Program (Program, but may be more critical to Lightweight Materials and other CF-based programs. The higher strength CF needed by the Program may be too advanced for this technology, as this "game changing" approach may fall short of those strength targets; however, the results of this portion of the Program would still be considered extremely successful if properties adequate for lightweight applications are achieved.

Question 5: Proposed future work

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

- The proposed future work is clearly outlined and has the appropriate steps toward developing the melt-spun fibers.
- Future efforts that target overcoming the technical challenges and in scaling up the process appear well planned. The feasibility of the project requires more urgent attention as to verify the economics of this approach and of changing to PAN-MA. The development of patentable IP requires a more definitive plan that includes how to add a PAN dope partner and protect the work accomplished to-date.
- Aside from current difficulties, planned future work appears to make sense.
- To produce a specific amount of CF tow is the logical next step. The PI should increase efforts to get a new extruder as soon as possible.
- The future work looks straightforward, but the precursor formulation work might be in jeopardy because of the passing of the PI at VT.

Project strengths:

- The excellent approach and use of previous work are project strengths. The approach as outlined is technically sound, and it represents an opportunity to change how CF is made and to impact its cost and use. This is a very important project and should be continued through scale-up.
- If successful, the process in development could change the industry.
- The project has an excellent team, and the team has learned a lot.
- The project strength is the potential impact on reducing CF cost for pressure vessels.

Project weaknesses:

- The project seems to be utilizing a trial and error effort towards optimizing the fiber. It would be helpful to have a better understanding of the systematic approached used to optimize the precursor and filament processing parameters.

- The project has not yet demonstrated cost reduction feasibility. The project also lacks collaboration with OEMs.
- Feasibility studies need to be continually readdressed as technical challenges are experienced and overcome. The data behind these feasibility studies, such as dope cost, processing throughputs, and quality impacts, should be made known to the program managers and project reviewers so that verification of project objectives can be addressed.
- It is not clear if there is some disorganization and if IP issues are compounding progress.

Recommendations for additions/deletions to project scope:

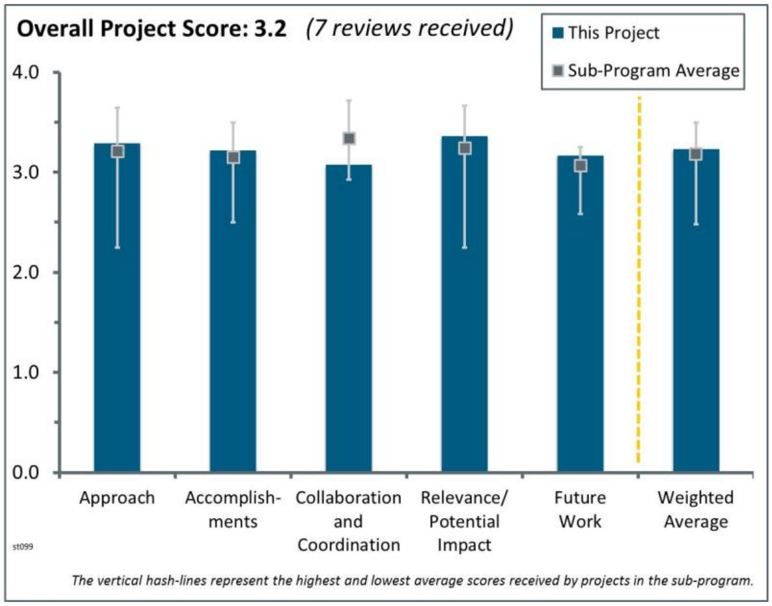
- Collaboration/regular communications with OEMs is recommended.
- The project should accelerate the cost model analysis and consideration of industrial partners. Also, the optimization of fiber parameters should be further developed and communicated as a key outcome of the project.
- This project's fit within the Program should be reevaluated at Milestone 8. Achieving Milestone 8 but not Milestone 12 does not deem this project a failure, as this project represents a key CF development that will have an impact on the entire industry (even if the strength goals of Milestone 12 are not met).

Project # ST-099: Development of Low-Cost, High-Strength Commercial Textile Precursor (PAN-MA)

Dave Warren; Oak Ridge National Laboratory

Brief Summary of Project:

The objective of the project is to develop a low-cost precursor fiber that can be converted to low-cost carbon fiber (CF) with at least 650 ksi tensile strength. Fiber production cost modeling is also performed. For the precursor cost model (7,500 t/year line capacity), the precursor manufacturing will be evaluated at the level of two major process steps: (1) polymerization and (2) spinning. For the CF cost model (1,500 t/year line capacity), the CF manufacturing will be evaluated at the level of nine major steps.



Question 1: Approach to performing the work

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

- This is a good approach that addresses fundamental issues in CF. What is learned here can have implications in other related programs.
- This is a good overall approach to decrease the cost of the main cost driver, that is, the cost of CF. Starting with precursor selection, followed by process optimization, simulation, and final validation, is a comprehensive approach.
- The general approach of the project has been effective to optimize the fiber and exceed the objectives. The update on cost using the information from the Textile Research Journal was useful, but the independent cost model results are needed to confirm the opportunity of the textile fiber. Delivering fiber to a tank manufacture is an excellent addition to the approach.
- The approach of optimizing the processing of a textile grade precursor for yarn manufacturing has shown great promise in exceeding cost targets. An issue is that the SGL Group (SGL) now owns the precursor producer, but it might be converted in the United States. This will still create jobs, but ultimately will not contribute significantly to the Gross Domestic Product.
- The approach is well organized, and early coordination with FISIPE is well planned. The statistical analysis of the CF process optimization should be more evident in the work. The development of influencing factors and the rate of influence should be more evident and related to the down selection of the precursor formula. The effect of such key cost influences, such as CF conversion yield and A-quality spool yield, needs to be addressed.
- Exploring alternate synthesis of CF is necessary for reducing the tank cost.
- Despite the complexities of the CF fabrication process and elements of the fabrication process that are more art (trial and error)-based, the approach to cost reduction appears practically organized to achieve results.

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 has made excellent progress from last year by exceeding the targets and improving the tensile strength from 400 ksi to almost 600 ksi.

- Performance targets are being met or exceeded.
- The project is on a good track. Results from the past are showing a continuous improvement of tensile strength (ksi). In addition, it was mentioned during the presentation that the target of 650 ksi was reached and that the "roundness" issue was resolved. However, the presentation still shows "kidney"-like fiber shapes. The correlation between fiber shape and performance (strength) is not clear, that is, it is not clear whether the strength of a round fiber is higher than a "kidney"-shaped fiber.
- The project has shown steady improvement over time and steady efforts to overcome processing obstacles. The speed of property improvement could have increased once the precursor formula was identified.
- The effort appears on track and is exceeding planned technical goals.
- The modulus was exceeded (which was not that difficult), but the tensile strength target was exceeded by over 30%, which is a major accomplishment with textile fiber. Further optimization should demonstrate a textile fiber with tensile strength of over 650 ksi.
- It would be useful to investigate the potential of the preparation process on the properties of the CF.

Question 3: Collaboration and coordination with other institutions

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

- There are well-chosen partners that have the resources to expand and commercialize this work.
- The addition of a tank manufacture to evaluate the finished fiber for a tank application is an excellent improvement in the collaboration to gain confidence for potential commercialization. It would still be helpful to identify other partners or collaborations that could ensure the technical results further improve the industry besides just SGL.
- All relevant partners are involved. However, the principal investigator (PI) should clarify the CF requirement with Hexagon Lincoln (HL). Because HL was selected to validate the CF performance, the PI has to make sure that the provided CF will meet HL specifications to ensure that the validation tests provide appropriate results.
- The collaborations appear to have worked well within the framework developed by the partners. The ability of Oak Ridge National Laboratory (ORNL) to provide information back to the precursor producer, even when ORNL could not directly influence the corrective actions of the precursor, appears to have worked well.
- The project is limited in the collaborations because of the proprietary nature of the work. SGL-FISIPE will define the sharing.
- Collaboration with tank manufacturers would be helpful for this project to ensure that requirements for tank materials are met.
- Given the nature of the industry, the collaboration is international in scope. There is an issue of U.S. tax dollars helping an industry that is global in scope, as well as partners who have headquarters in other countries. However, it seems there is little alternative at present. It could be argued that the target of this research is the automotive industry and, since it is international in scope, aiding any party will benefit everyone.

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 **3.4** for its relevance/potential impact.

- CF is the main cost driver of a compressed hydrogen storage system. Significant cost reduction was shown based on the simulation results.
- Direct reduction of the cost of major factors in the production of composite overwrapped pressure vessels (COPVs) is relevant. The presenter did a good job of explaining how the various factors were being addressed despite the confidentiality of some aspects of the work.
- The project has high relevance because it relates to the key cost driver (precursor) for CF that is the main cost element in hydrogen tanks. The cost pie chart in the presentation should be updated based on the current cost analysis by Strategic Analysis.

- This project could have a direct near-term impact on the cost of COPVs, as these precursors could be adopted right away by CF processors.
- The project could have a strong impact on reducing the cost of the high-pressure tank.
- This project has shown the capability to reduce precursor cost significantly (25%). Successful accomplishment of the cost savings level will clearly have an impact on the CF industry and ultimately the overall DOE Hydrogen and Fuel Cells Program (the Program). However, the ability to commercialize appears to be overstated, as the strategy of the precursor supplier and whether this precursor will becomes available to the industry remain unknown. A definitive path to commercialization is required by the precursor producer.

Question 5: Proposed future work

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

- The approach presented for proposed future work is straightforward and includes the following:
    - Completing fine-tuning the conversion protocol
    - Addressing scale-up
    - Completing the cost model
    - Delivering sample fibers for fabrication into a vessel
    - Testing and comparing to existing fibers
- The future work appears to be appropriate for overcoming the barriers and completing this project. The key items would be the cost modeling, achieving the >650 ksi tensile strength, and the fiber demonstration with the tank manufacture.
- Refinement of conversion protocol should be completed. Transferring the process from pilot precursor line to industrial fiber line and delivering fiber to a tank manufacturer are reasonable and important next steps to finalizing this project.
- The extent of refinement, partnering, and delivering 20 kg of CF to a tank manufacturer will directly demonstrate the impact of the project. However, it is possible that the surface treatment and sizing will need to be optimized prior to filament winding a tank.
- The optimization of the preparation process and its impact on the cost is missing and needs to be addressed.
- The future work aligns itself with refining the cost model and with continuing to approach the CF properties. Both of these tasks are necessary and appropriate; however, more effort may be required within these tasks. The cost model needs to include any yield loss and impact on A-quality spool yield. The impact of yield and product quality needs to be addressed in the CF optimization work, as only mechanical properties are targeted. Product quality and yield will be affected by each change in the CF process, and the future work needs to address this in more detail. The unknown factor is whether the quality of the precursor can achieve the variability targets, and if the precursor process could be modified to enhance its ability to maximize oxidation stretch. Consequently, the future work represents the right approach, but needs to include more in-depth effort and analysis to be considered fully successful.

Project strengths:

- The project strengths include good cooperation between FISIPE and ORNL and relevance to the overall goals of the Program. The steady improvement is also representative of a solid approach and an effective team.
- The project strength is the focus to reducing CF cost with a known “textile” grade polyacrylonitrile (PAN) precursor. The project has made significant steps towards meeting the ultimate goal for the CF strength.
- The strength is that the approach is practical in scope and addresses readily made improvements.

Project weaknesses:

- Unfortunately, SGL acquired FISIPE, so the precursor is now linked with SGL. This may have the effect of reducing flexibility in the supply chain—this remains to be seen.
- The delay in the cost model and evaluation of CF is a weakness that should be corrected prior to the completion of the project. Additional explanations for the optimization parameters would also be useful.

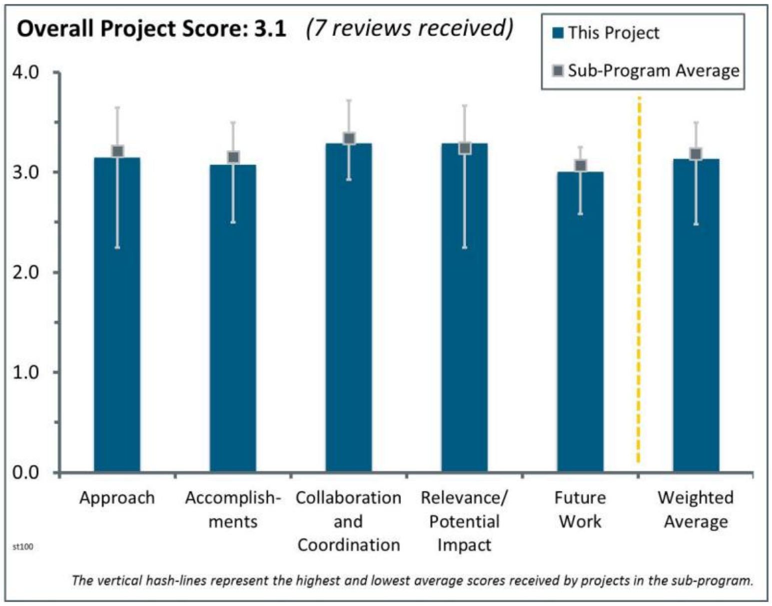
- The future work requires more detailed focus on the use of the textile precursor in a full-scale operation. For instance, questions concerning overall yield and optimized ability to stretch during oxidation need to be fully addressed. In addition, the commercialization plan needs to be identified. Efforts should be taken to ensure that this technology, once proven to meet all targets, is available to the industry.
- Perhaps more could be achieved if understanding extended to the “trial and error” portions of the research.

Recommendations for additions/deletions to project scope:

- The outcome of the project should include a transfer of knowledge and/or methods that can be used to optimized textile grade PAN precursors in order to benefit other CF manufacturers and avoid only helping a single supplier (SGL). The optimization parameters and effects in the CF processing should also be documented in detail.
- Product quality standards and cost impacts due to product quality need to be added to the cost models. The influencing factors of the precursor, such as filament shape, filament diameter variability, tenacity, etc., need to be identified so that a specification can be produced. Composite data in flat panels should be included, as pressure vessels are very complex structures and may not reflect such key aspects as fiber bonding and shear, flex, and compressive properties.

Project # ST-100: Ongoing Analysis of Hydrogen Storage System Costs

Brian James; Strategic Analysis, Inc.



Brief Summary of Project:

The overall objectives of the project are to: (1) perform a process-based cost analysis of current and future hydrogen storage technologies, (2) gauge and guide U.S. Department of Energy (DOE) research and development (R&D) efforts, and (3) validate cost analysis methodology so there is confidence when methods are applied to novel systems.

Question 1: Approach to performing the work

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

- It is a good strategy to focus on highest-cost balance of plant (BOP) items first (piping/fittings 26%, pressure regulator 12%, fuel tank controller 9%, and integrated in-tank valve 13%). The "Design for Manufacture and Assembly" (DFMA) method appears to be a very powerful approach to costing components. The limits are unclear, as is when the DFMA approach is and is not feasible. The team appears to be accommodating and providing timely analyses.
- To use compressed natural gas (CNG) BOP to make cost estimates for hydrogen BOP and the vessel is a good approach. It is a good idea to use DFMA for cost analysis.
- The principal investigator (PI) used systems from the DOE Hydrogen Storage Engineering Center of Excellence (HSECoE). While these systems are still in the prototype phase, they are the only publicly available models.
- For the current review period, Strategic Analysis (SA) has been primarily assessing costs for compressed gas hydrogen storage systems, with the major focus on the impact of the configurations and production volumes on the BOP components. Most attention has been on the numerous fittings in the baseline storage system configuration, as well as on the large ticket price components, such as the integrated valve and pressure regulator. The team's analysis methods are based upon scaling of the manufacturing processes and making comparisons to current production levels for both hydrogen and natural gas storage tanks. While this approach is reasonable and does permit some validation of the team's methodology, projected cost reductions at production rates exceeding 100,000 units/year probably do not fully account for safety inspections and verification of such high pressure (e.g., circa 700-bar), and it is likely that regulations will be imposed by various government agencies. Furthermore, significant reductions in BOP costs are probably only achievable with much more highly integrated and multifunctional components with demonstrable reliabilities.
- It seems like the team is drilling down and further understanding the impacts of BOP on the tank costs. The approach to cost analysis is standard DFMA methodology, with validation through quotation and modeling.
- The approach is okay; however, it would be useful for the BOP diagram to be carefully re-examined.
- The approach of this project is a process-based cost analysis to guide DOE R&D efforts. Previously, the project evaluated 350-bar and 700-bar tanks using DFMA. This year focused on the DFMA for the BOP components, especially the top cost components. In addition, the approach included a helpful comparison of CNG tanks and balance of components.

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 PI did a good job costing out all the components and providing a scaling factor for sales volumes and system size.
- There has been significant effort on and significant results from BOP cost analysis. The project goal of guiding DOE R&D efforts was not as transparent. It is suggested that future cost optimization may be realized by component integration. It should be determined whether the project will provide recommendations as to which components should and should not be integrated.
- Validation of the DMFA analysis tool using CNG tanks was an important result.
- SA has completed significant revisions and updates to its past detailed assessments of costs for compressed gas tank BOP components that provide refined predictions during large-scale production. It has considered some variations and made good efforts to vet its results with several sources, including component manufacturers, commercial suppliers of hydrogen, and natural gas vendors, as well as some automobile original equipment manufacturers (OEMs). While its assessments may be adequate for parts manufacturing and assembly, this reviewer is concerned that SA has underestimated the degree of quality and safety inspections that will be necessary for delivery of large quantities of components to the downstream users. Furthermore, the high-pressure tanks will require very close tolerances and interface surfaces for the fittings, valves, etc. to minimize leakages upon integration into the vessel plumbing for long-term robust operation. SA does not seem to have addressed directly how this is done during high-volume production rates. SA has done only initial assessments on costs for lower-temperature gas storage and for updating the carbon fiber-resins compositions and configurations.
- "Life-cycle-assessment" is listed as a barrier in this project. However, it is not clear how this barrier was addressed. Some components have a high variant with regard to cost, e.g., fittings. This was well-understood and documented. The 2014 presentation is dealing with these high variants by additional investigations and increasing the level of technical details.
- The BOP understanding and refinement is needed to drive the efforts of the project. The DFMA analysis of the integrated valve does suggest routes for cost improvements. Validation through the use of CNG tank costs is a good approach since they are currently manufactured in significant volumes.
- The project was very focused on the dominant cost items in the BOP, which were the fittings/piping, integrated valve, and regulator. Additional details were added to the schematic to evaluate the fittings. The fittings assessment was based on price quotes and the DFMA analysis of Parker fitting, which had results similar to electric vehicle metal fitting. The analysis included error bars with sensitivity of assumptions. The integrated valves were estimated at $130 for CNG to $2,000 for hydrogen. DFMA aligned well with CNG but was lower for hydrogen than price quotes and slightly higher at high volume. The regulator was not analyzed with DFMA but had updated quotes. The result of the BOP analysis was similar but had higher confidence in results. The CNG comparison was a helpful and appropriate approach to gain confidence in the cost model. It was difficult to confirm the validation based on slide 18 due to different feedback from suppliers in comparison to the DFMA.

Question 3: Collaboration and coordination with other institutions

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

- The PI worked closely with the HSECoE and Argonne National Laboratory (ANL) to pull together the necessary costs.
- There has been close, timely, and appropriate collaboration with other institutions; partners are full participants and well-coordinated. The project team includes ANL and the National Renewable Energy Laboratory (NREL) to provide complementary analysis.
- SA appears to work closely with its project partners ANL and NREL as well as with various outside sources, such as component and storage tank manufacturers.
- The project has a high collaboration with ANL in regards to system analysis and has made efforts to verify results using both other DOE projects (e.g., Pacific Northwest National Laboratory [PNNL]) and supplier

quotes. The role of NREL is not evident. The project has done an excellent job in collaborating with industry companies beyond its formal partners.
- Collaboration with ANL is good. The team seems to have a good relationship with tank vendors, which is a requirement for this project.
- While collaboration with ANL is visible, it would useful to show how the collaboration is conducted with OEMs, i.e., automotive and component suppliers, to ensure that the estimates provided represent a real-world scenario.
- At this level of design details, there should be more cooperation with component manufacturers.

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 project has high relevance to guide the DOE portfolio and establish cost baselines for hydrogen storage technologies. It is important to have an independent cost assessment from this project to serve as a public reference showing options for storing hydrogen on a vehicle.
- The project provides great support to several DOE research, development, and demonstration programs.
- This project is currently assessing key issues associated with the overall costs of compressed gas storage tanks, especially related to BOP components. Methods for reducing these costs are certainly necessary for greater acceptance and usage of these vessels in vehicles. However, knowing and understanding these cost drivers does not necessarily lead to innovative engineering solutions. Much more highly integrated BOP subsystems, along with significantly reduced costs for the wall materials of the tanks, will also be necessary.
- An understanding of the cost of these systems is required to compare the materials-based approach to conventional 700-bar technology. The analysis provided a surprising cost savings as compared to 700 bar (due mainly to the pressure reduction of the system). The PI is encouraged to continue to integrate new discoveries and progress into the analysis as they become available (as the project has always done).
- Decreasing costs for BOP are necessary, but not as important as decreasing the costs for the vessel, which is the main cost driver (BOP ~30% and vessel ~63%).
- This project gives the Hydrogen Storage sub-program (the sub-program) a gauge to guide the development of technologies.

Question 5: Proposed future work

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

- The future tasks proposed by SA are reasonable extensions of its current efforts and are worth continuing. It should place greater emphasis on reducing the number of components and fittings via higher integration, as well as incorporating the least expensive structural materials (e.g., fibers and resins) and most efficient designs. SA should also continue to explore options for reducing costs of the higher-priced BOP components. There is little value at this time in looking into refining cost models for either onboard or off-board properties of the various solid storage media, because no candidates capable of meeting the DOE performance targets have been identified. On the other hand, extending the cost analyses and scale-up methodology to compressed hydrogen gas storage vessels now being used rather extensively in forklifts and similar vehicles would seem to be a useful means to validate its predictive capabilities.
- The future work seems to be effectively scoped to progress the cost analysis, which included the BOP integration and alternative materials along with the analysis of the PNNL cold gas system.
- Future work should include an analysis on the following:
    - The kind of break in period required
    - Manufacturing facility clean room requirements
    - System validation testing
    - Ability to withstand noise, vibration, and harshness (NVH)

- The new areas for analysis make sense, e.g., cold storage; however, it is not as clear how examining lower cost components in the BOP will make a great difference in cost analysis. For cost reduction strategies, it is not clear whether the project will provide recommendations for which BOP components should and should not be integrated. This could be the most valuable contribution. It is also unclear whether the project could do this with a life cycle analysis of individual components. It may not be advantageous to integrate components with a shorter life cycle with components of a greater life cycle, assuming replacing an integrated component would be more expensive than individual components. Cost analysis for other projects at greater maturity, e.g., Small Business Innovation Research projects, could be useful for benchmarking vehicular cost targets.
- Further integration of components and examination of lesser BOP should be reviewed with OEMs. At this level of detail, the design could be very dependent on the final vehicle application. It is not clear whether there are alternatives for stainless steel as the main material for the integrated valve housing. If yes, it would be good to know the potential risk of a material combination (galvanic corrosion).
- Proposed future efforts applying true DFMA to BOP components for reduction in BOP could be beneficial. Validation of PNNL pressure/volume improvements should be accomplished.
- Moving forward, it would be useful to have a representative BOP diagram. Caution is needed when considering other material of construction because of hydrogen's embrittlement properties.

Project strengths:

- The project strength is the independent assessment of system cost and associated cost drivers. Another strength is the disciplined DMFA approach and full disclosure of assumptions and results (which is often not provided by others that perform cost analyses).
- The project was well coordinated with the HSECoE and modelling from ANL.
- The project team was very responsive to DOE and U.S. Drive Hydrogen Storage Technical Team suggestions and directions.
- SA has applied a systematic analysis methodology to evaluate manufacturing processes and cost analysis. It has recently revised its assessments with further refinements of the models and selection of input variables. SA revealed the sensitivity of predicting costs for large-volume manufacturing of compressed gas storage vessels.
- Project strengths included DFMA modelling and validation.

Project weaknesses:

- The project does not have significant weaknesses, but it could develop further recommendations to reduce costs based on the cost drivers.
- The systems available for modelling are based on the current prototype systems. These systems' primary goal is to demonstrate operation and good system density. These systems are likely not amenable to high-volume manufacturing. More input from industry will be required in the future in order to scale up these processes.
- Any current cost assessments being performed by SA are hampered by two situations: (1) lack of accurate and comprehensive manufacturing and pricing levels being supplied by BOP and tank suppliers, since they usually consider this information proprietary; and (2) current low production levels (i.e., at most hundreds or low thousands) of either CNG or hydrogen high-pressure storage tanks, which greatly increase the risk of unreliable extrapolations to the desired 100,000s production levels. Consequently, the SA-projected cost levels will have larger uncertainty than indicated in its presentation.
- Collaboration with OEMs is not visible. The estimate may not represent a real-life scenario.

Recommendations for additions/deletions to project scope:

- The PI showed nice agreement between the DMFA-estimated cost for integrated valves and fittings, as well as CNG vessel prices, demonstrating and benchmarking the utility of the DMFA approach. The PI also mentioned using DMFA to find new places to reduce cost. This can be a great advantage to the sub-program goals and should be pursued.

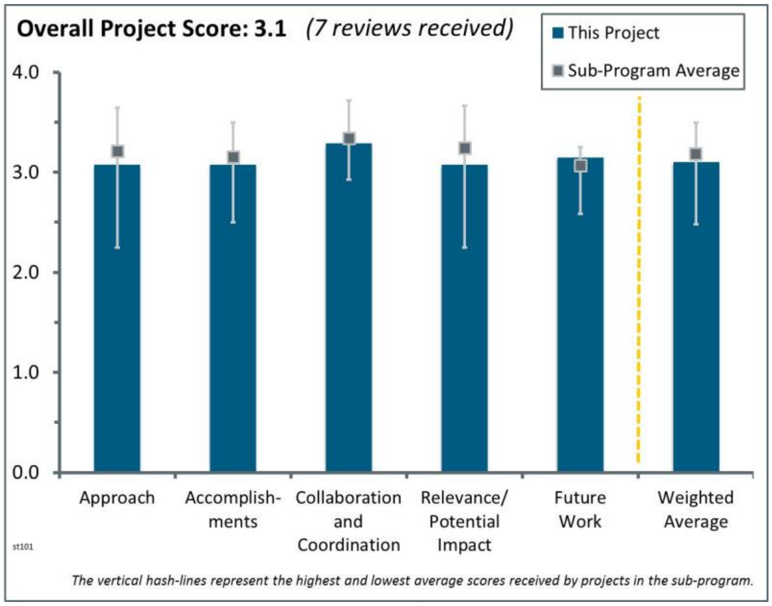
- It would be useful to have a sensitivity analysis based on potential cost reduction opportunities (e.g., integration of components or utilizing alternative materials) or hypothetical requirement changes such as burst or permeation modifications.
- Next time, more time should be spent on describing the loading procedures of the materials into the systems, i.e., determining how robust the process is, what room conditions are required, etc., if a large clean room is accounted for in the costs, or if glove box operations can be upgraded for high-volume manufacturing.
- SA should look much more closely into the impacts of higher inspection demands and verification of the safety aspects and robustness of the BOP components at maximum operating/acceptance pressures. It does not seem reasonable that costs for pressure and leak testing can be greatly reduced during large volume production rates compared to smaller manufacturing lots. A similar issue exists with pressure/leak testing of the final assembled storage vessels. Extending SA assessments to the status of costs for hydrogen storage tanks in forklifts and similar applications could be a good test for its assessment schemes.
- Sensitivity analyses would be useful, especially if it is not possible to access information from BOP charts.

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

Kevin Simmons; Pacific Northwest National Laboratory

Brief Summary of Project:

The objective of this project is to develop a feasible pathway, through cold gas enhanced operating conditions, to achieve at least an additional 20% cost reduction for compressed hydrogen storage tanks above the 15% (13.5 kg composite, 9.6 carbon fiber [CF]) accomplished in fiscal year 2013 through resin modification and fiber placement. This will be accomplished through at least an 18.7 kg reduction in the required amount of composite (13.3 kg reduction in required CF) and demonstrated through detailed cost modeling of specific low-cost thermal insulating approaches.



Question 1: Approach to performing the work

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

- The project team has done a good job of addressing obstacles and creating a path forward to achieve the target savings. The development of cold gas storage represents the step change needed to achieve the targeted savings. The impacts of the resin modification on the actual winding process including pot life, gel time, viscosity, etc. are being properly addressed. With the focus on cold gas storage, the other efforts remain in focus, providing a solid, full-system approach.
- The approach is addressing project goals.
- Minimizing the amount of CF used in order to reduce cost is an interesting approach.
- This Pacific Northwest National Laboratory (PNNL)-led project seeks to lower the costs during high-volume manufacturing of Type IV tanks for hydrogen storage at 700-bar through: (1) changing the composition of the CF-resin composites and wrapping the fibers more efficiently, and (2) reducing quantities of fiber/resin material via decreasing operating pressure and temperature to ~500-bar and ~200 K, respectively. The project's modeling assessments suggested the first approach could decrease costs by probably no more than ~10%. The second option might reach a net 30% cost reduction, but there would be penalties, such as needing insulation for retaining dormancy during storage, as well as uncertainties in mechanical and structural properties of the tank polymeric liner, resins, and fibers at lower temperatures. This project apparently does not consider the off-board impacts to the infrastructure that arise with cryogenic filling of the tanks or probable modifications to the balance of plant components.
- It seems much of the composite property work has been done with epoxy resin (the additive put into vinyl ester [VE] resin). The VE/CF interface is known to be poor. It seems some assumptions are made that the property translations will be the same even when the resin is changed from epoxy to VE.
- CF is the main cost driver for a 700-bar hydrogen storage system. Therefore, it is very important to improve the design of the pressure vessel and to compare it with a baseline. Because a 700-bar system cannot reach the U.S. Department of Energy (DOE) goals, it is a good approach to include a cold gas tank in the cost analysis. A cost breakdown of the manufacturing costs (TIAX estimated $290) should be shown to review the assumptions.
- The approach of the project is to model projections, prove the concepts empirically, and then build tanks and demonstrate as a system. So far most of the savings have only been demonstrated through computations, but some of the empirical studies in composite properties have validated the modeling.

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.

- This project has advanced significantly over the year, with the presentation much improved from last year's. Efforts to address gas dormancy versus cryogenic storage are a notable example of the advances within this project and show the understanding of the team in pursuing the cold gas approach. The path toward the DOE goals is on pace, with all relevant and key topics showing continued progress.
- Further cost reductions are shown. The project is on a very good track.
- Technology advances sought are shown to meet cost objectives. Progress is on track with goals.
- The project has apparently completed its initial phase of developing and modeling a pathway for lowering costs of Type IV tanks through improving fiber/resin composition and adapting a lower pressure and a 200 K storage concept. The team has performed some testing of material properties and behavior of resins with nano-phase additives, but apparently is just starting to build and evaluate prototype vessels for validation of their models and predictions. It was not apparent from the team's presentation whether there are actually any attractive candidates with the appropriate properties that have been found to-date. The properties of these resins at cryogenic temperature were also unclear, and there did not seem to be any plans to evaluate them. There are issues with the number of test tanks that have yet to be built and evaluated, as indicated in the table on slide 20.
- There are many parts to this project. It seems most of the individual components are progressing and meeting goals, but there are many assumptions being made on how they will all come together.
- Most of the impactful accomplishments have been computationally based, but the team has done a great job in demonstrating properties of matrix modifications, nanofillers, and catalysts for curing. The team did demonstrate a burst of a baseline tank, but the real meat of the project will come in the third year, when all improvements will be combined and demonstrated empirically.
- It would have been beneficial to calculate the cost reduction based on the real processing function of the material and processes used.

Question 3: Collaboration and coordination with other institutions

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

- All relevant partners/institutes are involved.
- All team members—PNNL, AOC, LLC (AOC)., Toray Carbon Fibers America (Toray), and Hexagon Lincoln (HL)—seem to be communicating often and appropriately. The team also communicated well with Strategic Analysis, Inc. and Argonne National Laboratory (ANL) to baseline the composite modeling efforts.
- Collaboration with original equipment manufacturers (OEMs) is visible.
- The collaboration between partners is following a systematic approach where the level of involvement adjusts depending on the priorities. AOC's efforts with the resin have been a key element of the project during the year, whereas HL's efforts will greatly increase over the next phase. Toray's efforts are not evident, as the surface treatment and sizing efforts expected from Toray were not made visible during the presentation. Toray's supply of fiber and data is obvious, but its surface-related topics require more discussion.
- No apparent issues on collaboration were noted.
- While most of the effort seems to be at PNNL and HL, it does appear that the other partners in the project are also reasonably well involved. It is less clear whether interactions with outside organizations have been occurring. In particular, it is unclear whether the project is directly communicating with ANL and Lawrence Livermore National Laboratory concerning issues with cryogenic temperatures on materials and dormancy, which are likely to be problem areas.

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 models show significant cost reduction that will meet the goals.
- Costs are one of the main barriers for a hydrogen tank system. This project is very important because it shows a pathway to reducing the costs by 37%, compared to a baseline model.
- This project is very relevant to the near-term deployment of fuel cell electric vehicles. These advancements could be adopted and implemented quickly by a tank manufacturer such as HL.
- The project is relevant to reducing the costs of the tanks related to CF.
- This project is now showing very good relevance with the accomplishments associated with cold gas storage and use. This was not necessarily evident last year. This project is now well focused on achieving the goals and making a significant impact on the DOE goals for hydrogen storage.
- The project estimated cost reduction opportunities of 48% before insulating costs. When the projected insulating cost margin is included, the projected cost saving for a composite tank is estimated to be 37%, which is significant.
- According to presentation slide 10, there would be only modest improvements toward the mass and volume targets (along ~10% cost reduction) of 700-bar Type IV tanks from this project. Only the much more risky low-temperature storage option would lead to the significant enhancements alluded to in this project. More radical materials or designs are probably necessary to reach the DOE goals.

Question 5: Proposed future work

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

- It is very good and important to validate the estimated cost savings; therefore, the proposed future activities support the overall goals in a very good way.
- The future work of combining the individual empirical and modeled improvements and validating them with an actual tank system will be critical to the success of this project.
- The future work is well planned and properly addresses the necessary steps. The pressure vessel characterization requires additional insight other than burst testing. The final composite is very complex and requires additional thought as to proper characterization, including critical use analysis such as cycle and drop testing where shear, impact, and compressive properties are influential, as well as thermal effects.
- There are no issues with proposed future work.
- It would be useful to optimize the materials and processing function of the properties and costs saving.
- It would be great if the project can complete all of the tasks outlined in slide 28. However, it does not seem probable that prototype and full-scale tanks will be fabricated and tested, given the current status shown in slide 19. There appear to be both unresolved materials and test facilities issues to be dealt with.

Project strengths:

- The strengths of this project lie in the leadership and direction provided by PNNL. The potential impact this project could have on the DOE goals can be viewed as a strength as well.
- Probably the best aspect of this project is PNNL forming a team with a vehicle OEM, a tank manufacturer, and materials (i.e., fiber and resin) producers to address issues with improving the design and construction of Type IV storage vessels in order to decrease costs. This has allowed specialized resources and expertise to be directed toward a common purpose. The fabricating and testing of prototype tanks is also an excellent aspect.
- The project has a skilled team and appropriate collaboration with stakeholders.

Project weaknesses:

- The 2013 presentation shows some open milestones. The completion of these milestones should be documented in the 2014 presentation.
- It seems that there is somewhat too much dependence on cost estimates, which are not based on the optimized materials and processes created within the scope of this project. It would be beneficial if costs reductions were measured based on the optimum processes found.
- The pressure vessel characterization could use some further review to better understand the influence of hybrid fiber designs, resin matrix usage, and temperature on properties beyond burst testing.
- The only viable pathway for this project to reach its 30+% cost savings goal is to implement a reduced pressure and cold gas operation, as only minor improvements in mass, volume, and costs targets will occur at ambient temperature. However, the robustness of the resin, liner, and fibers being considered are either unknown or highly uncertain at cryogenic temperatures and probably will not be sufficiently evaluated by the team. There also seem to be issues with the fabrication and testing of prototype vessels (see slide 19), with just a little over a year remaining in the project. It does not appear that any full-size tanks will be made and evaluated. The project seems to underestimate the impacts on both performance and cost targets of providing sufficient thermal insulation to the tank for acceptable storage dormancy and robustness.

Recommendations for additions/deletions to project scope:

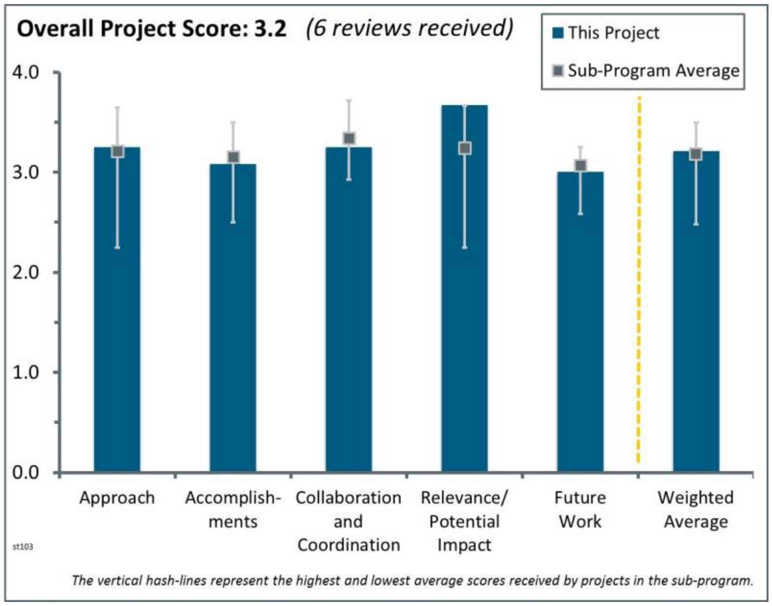
- It is suggested to include costs estimates based on the optimized resin material and related processes.
- The scope is well planned and continues to address key aspects of the project. Added focus on fiber surface chemistry influences using the proposed resin system should be added and demonstrated during the next year.
- There are no suggestions for deletions to the project; however, more screening of the cryogenic properties of fiber/resin materials would be valuable in order to see whether any of the proposed candidates do actually have appropriate behavior to be used for cold gas storage. The project team should also look more carefully into the requirements and impacts of improving thermal isolation and insulation materials for the cold gas storage option.

Project # ST-103: Hydrogen Storage in Metal-Organic Frameworks

Jeffrey Long; Lawrence Berkeley National Laboratory

Brief Summary of Project:

The objectives of the project are to: (1) research and develop onboard systems that allow for a driving range greater than 300 miles, (2) seek materials that offer the potential for meeting the U.S. Department of Energy's (DOE's) targets of reversible uptake, and (3) synthesize new metal-organic frameworks (MOFs) capable of achieving the -15 to -20 kJ/mol adsorption enthalpy required to be used as hydrogen storage materials operating under 100 bar at ambient temperatures.



Question 1: Approach to performing the work

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

- The team's approach is excellent in terms of exploring higher enthalpy binding sites of MOFs. The expertise in synthesis of MOFs, the first-principles calculations of the structure and binding energy, and the neutron characterization is an excellent mix. MOFs are an attractive class of compounds to be explored for hydrogen storage.
- Unsaturated metal centers with multiple bound hydrogen molecules is one of the few ways that any materials are going to be able to meet DOE hydrogen storage targets for light-duty vehicles.
- The approach for the project appears to be effective in progressing the exploration and characterization of MOF materials. The high-pressure measurements have significant error bars, which should be reduced prior to utilizing them as a conclusive result of the project, and/or the error bar should be shown as a function of pressure. The approach seems to be focused on improving gravimetric density without improvement in volumetric density, which is an issue in achieving the ultimate goal of a driving range greater than 300 miles.
- The approach is generally interesting. However, it is based on some high-risk assumptions, namely, that Mg-based MOFs can contain unsaturated/open metal sites capable of binding substantial amounts of hydrogen, which may not work out.
- It would be beneficial to see more detail on the specifics of materials synthesis and characterization. The principal investigator (PI) mentioned several times the stability of the "new" MOF materials; specific experiments on how those were evaluated would be helpful.
- Achieving multiple hydrogen-metal bonds is a laudable goal, but likely very difficult. The computational component could be improved if it were to operate in a more predictive fashion on a wider range of compositions. Fewer than 10 compositions were examined for their hydrogen binding energies. It is not clear that computation is truly guiding synthesis efforts. Thus far, the neutron diffraction experiments are providing information (e.g., one hydrogen molecule per metal site) that can be discerned from the uptake curve and crystal structure alone. It is unclear what new insight is being derived from this activity.

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 is making steady progress toward the project goals and deliverables.

- Authors have demonstrated, through structured studies, a preferential absorption near the cobalt site in the MOF. However, the hydrogen storage capacity of such systems is rather limited.
- The PI has made significant efforts and progress. It appears that this work may be more of a DOE Basic Energy Sciences (BES)/National Science Foundation future effort than an applied DOE Office of Energy Efficiency and Renewable Energy effort. It appears there is some confusion as to whether the gravimetric milestones of the project are hydrogen total or excess, which should be clarified. Also, specifics of how volumetric capacity is calculated should be outlined in the additional slides.
- The project made progress in evaluating various MOFs for the potential increased binding enthalpy. The synthesis of the M_2(m-dobdc) was a useful accomplishment as a potential cost reduction to the MOF-74 linker (although the cost benefit was not quantified). The Ni_2(m-dobdc) resulted in a significant increase in the isosteric heat of adsorption, which is a step in the right direction. The neutron powder diffraction provided good insight regarding the polarization of the hydrogen molecule. The project, through the computational analysis, provided the influence of the initial adsorbed hydrogen on the other binding hydrogen energies based on the open metal site concept.
- In general, the project has shown good progress, and it is great to see the project team reporting room temperature results as its metrics. While total adsorption on slide 14 is interesting to see, the more important metrics are excess adsorption and/or the amount of adsorbed hydrogen at the system level. The total absorption has too many misleading components to be very usable for evaluating the progress of materials development. A simple calculation indicates that the present approach to put one metal atom on an organic linker in the MOF structure will at best produce materials with less than 1 wt.% of additional hydrogen storage capacity because of the metal centers. This can only be changed by substantially increasing the number of metal centers, perhaps even by more than an order of magnitude. A simple calculation shows that if there are only four carbon atoms used to support one Mg atom, then the hydrogen storage capacity at best, with four hydrogen molecules adsorbed per Mg, is around 10 wt.%. If there is one Mg atom per 40 or more atoms, then even if with four hydrogen molecules per Mg atom, the additional hydrogen storage capacity will be less than 1 wt.%. The use of a single temperature isotherm to calculate the isosteric heats of adsorption should be minimized, and the use of two or more temperatures should be instituted as routine.
- Thus far, there is no indication that achieving adsorption of multiple hydrogen molecules per metal site is possible. Given the large budget allocated to this project, disappointingly few new compounds were synthesized/tested during the past year.

Question 3: Collaboration and coordination with other institutions

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

- There has been close, appropriate collaboration with other institutions; partners are full participants and well-coordinated.
- There has been strong collaboration across the team members: Lawrence Berkeley National Laboratory, National Institute of Standards Technology, and General Motors.
- The project has a good team with appropriate interactions and collaborations.
- It is not apparent based on the oral presentation and the presentation slides whether collaboration has been very effective.
- Capacity levels should be verified through an independent 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 **3.7** for its relevance/potential impact.

- The project, should it produced the material desired, would be very well aligned with the DOE Hydrogen and Fuel Cells Program research, development, and demonstration (RD&D) objectives. It would have the potential to substantially advance progress toward DOE RD&D goals and objectives.

- The project is very relevant to the DOE hydrogen storage targets. The potential impact is high if the project is successful. A systematic exploration of new MOFs for hydrogen storage is one area that DOE should be supporting, and this team seems to be the best in this area.
- If the project continues to develop materials with increasingly higher hydrogen capacities, then these materials would have a significant impact on future materials design and implementation for both transportation and stationary applications.
- The objectives of the project are well aligned with the DOE RD&D goals.
- The project approach is one of the only ways to meet DOE targets. The main issue is whether the appropriate metal sites can be made and the solution contaminants adequately removed.

Question 5: Proposed future work

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

- The future work is well aligned with the project deliverables, including finding the right ligands for metal insertion (especially Mg), characterization of the MOFs and their interactions with hydrogen, and high-pressure adsorption measurements, as well as first-principles predictions of optimal metalation conditions and the best metal cations for optimal metal-hydrogen interactions.
- The future work proposed is well designed. However, it does not guarantee that final goals will be met. It is still not obvious that a high-capacity Mg-based MOF, containing stable unsaturated coordination sites on Mg, can be successfully synthesized.
- The future work is clearly defined in order to progress each task. It is uncertain if the defined future work will make significant steps towards the multiple binding site concept in order to achieve the projected adsorption isotherm on slide 5.
- Task 4 (high-pressure isotherms) seems unnecessary given the stated goal of <100-bar operating pressure. Redirecting funds devoted to this task elsewhere is suggested.
- In addition to improving processing and finding appropriate ways to form metal sites, the project needs to focus on increasing the density of unsaturated metal sites by an order of magnitude or more.

Project strengths:

- The team has excellent expertise on synthesis, modeling, and characterization. The focus on charge-balancing ligands as well as high-valence metal cations is a promising direction. The team is paying close attention to the stability of the MOFs while considering potentially higher binding energy and thus higher desorption temperatures. The Co_2(dodc) has already reached 2.5 total wt.% hydrogen at 298 K and 140 bar. New MOFs are expected to achieve even higher hydrogen storage capacities.
- The project has a strong research team, well-thought-out collaborations, and good fundamental science.
- The PI's insight and advanced knowledge of framework materials is evident. The approach and extensive characterization of the materials set leaves little doubt as to the team's performance.
- The project is well-aligned with DOE goals and has a knowledgeable team.
- The project has all the right capabilities to perform the work, as well as an appropriate approach and focus. The synthetic components of the project are very appropriate, and the understanding of the very difficult challenges appears to be good.
- The strength of the project is the focus on achieving the ultimate goal of sorbents, which is to increase the adsorption enthalpy at room temperature.

Project weaknesses:

- There has been limited progress during the past year.
- The project clearly requires a material that can bind hydrogen to multiple binding sites per metal. The project includes theoretical projections of the multiple binding site concept, but the path to demonstrate the concept and protect the binding site needs to be further developed.
- There is limited applicability of the project's results for real hydrogen storage systems. This is a high risk project more appropriate for BES. Practical implementation aspects of the expected results are left out. For

instance, even if they were possible to make on a laboratory scale, Mg-based MOFs with free coordination sites may be not scalable or may be impossible to handle on a commercial scale.

- There are two main issues:
    - It will be challenging to develop appropriate metal centers where the chemical contaminants can be adequately removed. This may require a fundamental change in the way the materials are made and the way the contaminants are removed.
    - To meet DOE targets, even if every metal atom reversibly adsorbed four hydrogen molecules, only a few (i.e., four or five) carbon atoms per metal site would be allowed. In the relatively large MOF structures being discussed, it appeared that there will be dozens of atoms associated with the support for every single metal atom. Therefore, the materials presently being discussed will only have, at absolute best, a 1 wt.% or 2 wt.% hydrogen storage system capacity at room temperature.
- It seems that first-principles calculations are not providing enough up-front guidance to experimental exploration. The success of the project depends on the right metallation and activation of the charge-balancing ligands during synthesis. The ability to synthesize the predicted MOF structures/compounds may be a more significant challenge than the team has envisioned, and may be physically impossible.

Recommendations for additions/deletions to project scope:

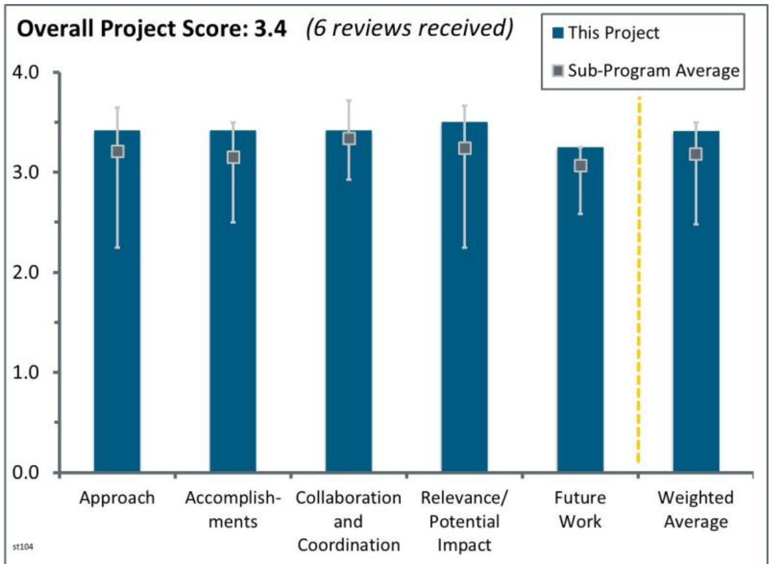
- No additions or deletions are suggested at the current stage of the project.
- Clarify the capacity numbers; please report in excess, not total. Clarify how volumetric capacities are calculated.
- Delete Task 4.
- There is a need to focus on increasing metal site density and access. The use of a single temperature isotherm to calculate the isosteric heats of adsorption should be minimized, and the use of two or more temperatures should be instituted as routine.
- The project should either reduce the measurement errors or eliminate the high-pressure adsorption tasks. Additional priority should be placed on developing materials with improved volumetric density. The project should include some preliminary material cost analysis because a complex material may improve the binding energy, but it will not be feasible if the material cost is too high.

Project # ST-104: Novel C-B-N-Containing Hydrogen Storage Materials

Shih-Yuan Liu; Boston College

Brief Summary of Project:

The objective of the project is to develop novel chemical hydrogen storage materials that have the potential to enable non-automotive applications and meet the 2017 U.S. Department of Energy (DOE) targets for vehicular applications with focus on three classes of materials: (1) liquid phase, (2) potential reversible, and (3) high capacity.



The vertical hash-lines represent the highest and lowest average scores received by projects in the sub-program.

Question 1: Approach to performing the work

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

- In a primarily materials discovery activity, this team continues to follow an excellent approach to seek out new materials. Along the way, the team quickly assessed key properties and continuously down-selected to the most promising materials. As the team has learned more about the chemistry of carbon, boron, and nitrogen (CBN) heterocycles, it has continued to be able to adjust its synthetic approach to explore new concepts in the reactivity or physical properties of these CBN heterocyclic compounds. As in previous years, this approach incorporating computation, experiment, and some practical assessments of performance continues to answer crucial questions that enable better understanding of novel chemical hydrogen storage materials. The project represents a well-coordinated effort directed at potentially reversible systems in the novel class of CBN heterocyclic compounds. The team demonstrates an active down-select mentality to rapidly assess materials, cease work on less promising compounds, and focus on the most promising candidates. This approach provides valuable insight to DOE and the current and future materials discovery efforts. It is very valuable to make a complete and accurate assessment of such new materials concepts. DOE should stay the course while this very competent team continues to make sure the research and development (R&D) is well performed, and the R&D team completes a reasonably comprehensive survey of the possibilities that these novel compounds may provide.
- Effective approaches from both experimental and theoretical sides have been presented for overcoming barriers toward reversible hydrogen storage materials with high hydrogen capacity. “Liquid phase” with “heterocyclic CBN compound” is a correct direction, and the methodology adopted in this project is adequate.
- The team has an excellent combination of expertise on synthesis, computer simulation, and characterization. It is doubtful that other teams could do better than this team. The team explored several types of compounds, but Mother Nature has not been too kind in revealing any one that would be a home-run success for hydrogen storage. It is suggested that the team focus on exploring new compounds instead of spending too much effort on existing compounds that are unlikely to meet the targets. It is critical to find compounds or mixtures that will stay liquid before and after desorption. The team is encouraged to venture outside the composition space that was specified in the original proposal.
- The project combines the expertise of participating partners to develop novel hydrogen storage materials that have potential to meet the 2017 DOE target. The approach is adequate to achieve the project objectives.
- It is an interesting idea to modify ammonia borane (AB) by including it into an organic ring system, which would be more stable and low-melting. However, every carbon atom added reduces the overall capacity.

Also, the formation of an aromatic system during dehydrogenation makes the reverse hydrogenation reaction more difficult.

- There are only two compounds addressed in this project (compounds H and J) that have any chance at all of meeting the 2017 DOE system gravimetric target. To do so, compound H requires reversibly removing all 10 hydrogens in the structure without destroying the rest of the structure along the way. The possibility of doing this is expressed in a way that leaves little hope of success. Considering where the Hydrogen Storage Engineering Center of Excellence (HSECoE) is today and where it is headed in the coming year, it seems hard to justify continued effort on work of this type.

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

This project was rated **3.4** for its accomplishments and progress.

- The team made steady progress toward the overall project goal. It developed fuel blends of compound B + AB, which has a hydrogen storage capacity of 6 wt.%.
- The synthetic capability to gain entry into these difficult to prepare CBN heterocycles continues to impress, as does the ability to characterize the molecular products/outcomes of dehydrogenation reactions. These products themselves are new and novel. A rather large library of CBN heterocycles has now been prepared and assessed, with a focus on the most promising compounds. With this larger number of compounds available and the assessments that have been carried out to date, a valuable number of lessons have been learned, and it is a nice accomplishment to summarize them for the community as the team did in its presentation. Exploring blends of compounds to achieve a liquid "fuel" and "spent fuel" is another valuable accomplishment, and it highlights a potentially useful pathway to providing liquid fuels. Some additional attention to regeneration of these mixtures may be in order. Identifying a heterogeneous catalyst that acts on both the boron-nitrogen (BN) fragment and the carbon-carbon (CC) backbone of a CBN heterocycle is a nice and necessary accomplishment, in that it provides proof of concept that hydrogen may be released from the entire molecular backbone, not just the BN unit.
- A rich group of liquid-phase heterocyclic CBN compounds has been carefully investigated, along with combinations with some other BN hydrides. The properties of several of them have been made clear. The results have shown high potential toward the goal of reversible hydrogen materials with high hydrogen capacities.
- The project has very interesting fundamental results. Researchers may also want to look into phase diagrams of different mixtures, which could help to create liquid or low-melting materials.
- The chemistry is interesting and the go/no-go decision making is reasonable. It seems a waste of effort to study materials that have low hydrogen content. Any material with less than 10 wt.% hydrogen is probably going to be useless in terms of meeting DOE onboard hydrogen storage targets. The argument that something important might be learned is hard to appreciate at a time when the HSECoE is in the final stages of feasibility demonstrations.
- The team did an excellent job in performing, testing, and narrowing down the compounds for further study. Unfortunately, what is left behind is not as attractive to a real hydrogen storage system.

Question 3: Collaboration and coordination with other institutions

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

- There has been good collaboration; partners participate and are well-coordinated.
- The team maintains quarterly conference calls, complemented by more frequent and necessary two-way exchange of information. The team also collaborates with researchers/institutions outside the team.
- The roles for each member of the project team and the outside collaborators are clearly spelled out. The connection/interface with the HSECoE is mentioned.
- As in the past, there is a record of excellent collaboration among the team members. This is perhaps best exemplified by the fact that the (excellent) presentation was given by the Pacific Northwest National Laboratory partner, as the PI was unavailable. The communication within the small project is clearly top notch.

- The project has a well-balanced team with experts from both experimental/theoretical fields and university/laboratory/industry. The team has shown efficient performances to overcome difficult barriers with effective cooperation. It has become clear that reversibility might be achieved by the design of such heterocyclic CBN molecules and efforts made in this project have shown hopeful enhancement of hydrogen capacity.
- Team collaboration seems very effective.

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 critical to the Hydrogen Storage sub-program and has potential to significantly advance progress toward DOE research, development, and demonstration goals and objectives.
- The project tested liquid fuel blends and potential reversible materials while also exploring high-capacity liquid materials. It is highly relevant to achieving the DOE hydrogen storage targets.
- This project continues to provide valuable information regarding the viability of molecular systems as hydrogen carriers for hydrogen storage applications. The range of thermodynamics, kinetics, and other physicochemical properties that are spanned by these types of compounds is thought provoking. This approach, while it may appear to be "too complex" to some, provides DOE with valuable insight into what might be possible with continued research into these molecular systems that have such a wide range of hydrogen release properties and regenerability.
- A completely new and correct direction with very high potential for future breakthrough. More efforts by more groups on a longer time scale will definitely increase the possibility of reaching the DOE targets.
- The work is directly related to DOE hydrogen storage targets.
- Without convincing evidence that there is a CBN compound out there with real potential to deliver >10 wt.% hydrogen reversibly, it is hard to get excited about the work going on in this project. If it were purely a science program, the science would be considered interesting by most. But if the goal is to identify a material the HSECoE can really use to meet its desired targets, there does not seem to be hope for success in a timely manner.

Question 5: Proposed future work

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

- There are good future work plans. Phase diagram studies may help to answer the question on slide 25, "Can compound J be a liquid at room temperature?" and similar ones.
- The project lists CBN cyclohexanes, room temperature solid materials, in the future work. These compounds can be synthesized and will be characterized. These efforts are in line with the project scope.
- Future work should focus on compounds H and J. Working in the molten state with compound J seems like the only real chance for success. Diluting compound H with a liquid carrier will of course lower the effective reversible hydrogen content. Work on compound G is not valuable for vehicular applications.
- While the regeneration of some of these compounds with lithium aluminum hydride ($LiAlH_4$) is chemically facile, it is not likely to be practical, as the recycle of $LiAlH_4$ is energetically problematic. As was pointed out during the question and answer session, were one to use $LiAlH_4$, one might as well just put it onboard and hydrolyze it rather than go to the effort of preparing CBNs, etc. Thus, the future work should acknowledge that for non-reversible systems regeneration must proceed through plausible reaction pathways that can achieve the DOE off-board efficiency metrics.
- The proposed future work is adequate.
- The proposed future work is very reasonable, considering the short remaining duration of the project.

Project strengths:

- This is an excellent team that integrates superb synthesis expertise as well as computational expertise and characterization. Several new compounds were synthesized and characterized. These compounds are not easy to synthesize or characterize. The team did a superb job in delivering the promised results. The understanding obtained from the synthesis and characterization will be very useful for future explorations.
- The project is novel and innovative with a high potential to lead to breakthrough.
- The project has a strong research team and yielded interesting fundamental results.
- The project uses the expertise of the participants to address the project objectives and DOE targets. The project combines the strengths of each participating institutions.
- The project has scientists who are knowledgeable about the relevant chemistry. The project's down-selected materials are well considered based on the results to date.
- The project has an excellent, productive, and experienced team working on a high-risk, potentially high-reward project. The project continues to impress with its synthetic prowess, computational integration, and good knowledge on what the key barriers are to a chemical hydrogen storage (CHS) material, and how those interact with potential CHS engineered systems (which is not the focus of the project).

Project weaknesses:

- Although this is a DOE Office of Energy Efficiency and Renewable Energy (EERE) project and physical understanding of the materials behavior is not at the top of the agenda, understanding the mechanism is critical in improving overall efficiency. For example, the mechanistic understanding would be truly useful to understand the kinetic measurement and improved system performance.
- There is a lack of chemical industry partner(s). The goal to "develop novel chemical hydrogen storage materials that… meet the 2017 DOE targets for vehicular applications with focus on three classes of materials" may be very difficult to achieve with the studied materials.
- The project team is working on a class of materials that others have investigated with little success.
- There is limited time left. A successive project is needed.
- Though it is unclear whether the team has looked into the composition space broadly enough, continued work in this space will likely be unfruitful; instead, new compounds/composition space should be explored (even though such an approach may not fit into the existing deliverables).

Recommendations for additions/deletions to project scope:

- Focus on compounds H and J in the coming year.
- With the little time remaining, the team may wish to focus on those materials that are directly able to be regenerated onboard with hydrogen. Even a low capacity of a few weight percent that is reversible may provide an entry into low pressure, portable power applications.