Hydrogen Infrastructure Technologies – 2024 Hydrogen Infrastructure Technologies Subprogram Overview

Introduction

The Hydrogen Infrastructure Technologies subprogram focuses on research, development, and demonstration (RD&D) to reduce the cost and improve the reliability of technologies used to deliver, store, and dispense hydrogen for a variety of applications in industry and transportation. Subprogram activities support development of hydrogen infrastructure technologies to enable meeting the goals identified through the U.S. National Clean Hydrogen Strategy and Roadmap, the U.S. Department of Energy's H2@Scale initiative, the Infrastructure Investment and Jobs Act (also known as the Bipartisan Infrastructure Law), and the Inflation Reduction Act. The subprogram addresses technical challenges through a portfolio of projects in two RD&D categories:

- Hydrogen Infrastructure addresses low-cost, high-efficiency technologies to move hydrogen from the point of production to the point of use. RD&D activities investigate the conditioning, transport, and dispensing of hydrogen as a gas, as a cryogenic liquid, and as a materials-based hydrogen carrier. Processes and components of interest include liquefaction and hydrogenation/dehydrogenation processes, compressors, pumps, sensors, dispensers, and bulk transport equipment, including pipelines. Integration of components into complete fueling stations for medium- and heavy-duty vehicles and development of fueling protocols are also being pursued. The Hydrogen Materials Compatibility Consortium (H-Mat) coordinates RD&D on accelerated test methods and novel, low-cost, durable metals and polymers for use in hydrogen service. The HyBlend initiative investigates the potential of blending hydrogen into the natural gas infrastructure.
- Hydrogen Storage addresses cost-effective onboard and off-board hydrogen storage technologies with improved energy density and lower costs. RD&D activities investigate high-pressure compressed storage, cryogenic liquid storage, and materials-based hydrogen carriers. Activities in the latter topic area are coordinated through the Hydrogen Materials Advanced Research Consortium (HyMARC) to accelerate the discovery, development, and demonstration of breakthrough hydrogen storage materials.

Goals

The Hydrogen Infrastructure Technologies subprogram aims to develop technologies so that clean, low-carbon hydrogen can be competitive with incumbent and emerging technologies across diverse applications. These applications include medium- and heavy-duty transportation, power generation, energy storage, and chemical and industrial processes. Specific subprogram objectives include the following:

- Develop hydrogen infrastructure technologies, including hydrogen delivery, storage, and dispensing, with the aim of meeting overall cost targets for delivered and dispensed hydrogen. For vehicle refueling, there is an intermediate cost target, which includes everything from production through dispensing, of \$7/kg H2 and an ultimate cost target of \$4/kg H2.
- Develop low-cost, efficient, compact, and safe hydrogen storage technologies for use with end-use applications, including on board vehicles and at end-use sites. For vehicles, the objective includes meeting an intermediate cost target of \$9/kWh (\$300/kg H2 stored) by 2030 and ultimately \$8/kWh (\$266/kg H2 stored) for Class 8 long-haul tractor-trailers.

Key Milestones

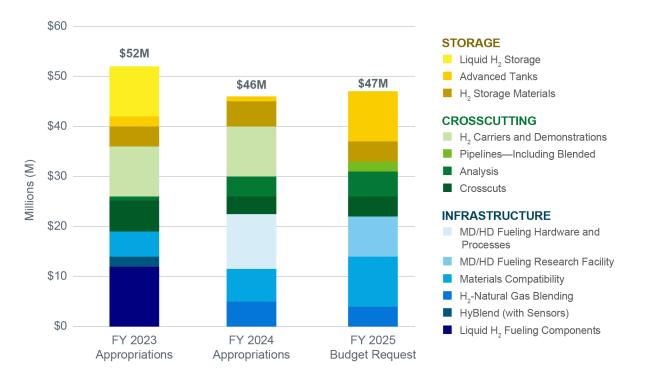
The Hydrogen Infrastructure Technologies subprogram has key milestones for each of the technology areas:

- Develop hydrogen infrastructure technologies for medium- and heavy-duty vehicle refueling to enable meeting an intermediate dispensed cost target of ≤\$7/kg H2 and an ultimate cost target of ≤\$4/kg H2.
- Develop medium- and heavy-duty vehicle hydrogen refueling technologies capable of dispensing to 700 bar onboard tanks at an average rate of 10 kg H2/minute, with a peak rate of ≤18 kg H2/minute, while meeting established safety protocols and regulations.
- Develop onboard hydrogen storage technologies meeting an intermediate cost target of \$9/kWh (\$300/kg H2 stored) by 2030 and ultimately \$8/kWh (\$266/kg H2 stored) for Class 8 long-haul tractor-trailers.
- Develop onboard hydrogen storage systems for Class 8 long-haul tractor-trailers capable of at least a 5,000-cycle life, with pressurized system components capable of at least 11,000 cycles.

Budget

The FY 2024 appropriation for the Hydrogen Infrastructure Technologies subprogram was \$46 million, with \$27 million allocated to hydrogen infrastructure and \$19 million allocated to hydrogen storage. New areas funded in FY 2024 include high-throughput fueling components, hydrogen carrier demonstrations for non-vehicle applications, and bulk sub-surface storage. The subprogram also continues to fund RD&D on materials compatibility for hydrogen service, blending of hydrogen with natural gas, hydrogen carrier materials, low-cost carbon fiber for advanced tanks; and analysis.

The FY 2025 request is \$52 million, with \$30 million allocated to hydrogen infrastructure RD&D and \$22 million allocated to hydrogen storage RD&D.



Annual Merit Review Results

During the 2024 Annual Merit Review, 49 projects funded by the Hydrogen Infrastructure Technologies subprogram were presented, with 12 Hydrogen Infrastructure projects and 12 Hydrogen Storage projects reviewed (a breakdown of number of projects reviewed by budget category is shown in the table on the right). The reviewed Hydrogen Infrastructure projects received scores ranging from 2.8 to 3.6, with an average score of 3.2. The reviewed Hydrogen Storage projects received scores ranging from 2.7 to 3.7, with an average score of 3.3. The complete list of reviewed projects and the average score for each can be found in the Prologue Table.

Following are reports for the 24 reviewed projects. Each report contains a project summary, the project's overall score and average scores for each question, and the project-level reviewer comments.

Number of Projects Reviewed by Budget Category

Materials Compatibility (H-Mat)	2
HyBlend	2
Fueling Components and Stations	6
Hydrogen Sensors	1
Advanced Tanks	2
Hydrogen Storage Materials and Carriers (HyMARC)	8
Analysis	3

Project #H2-041: H2@Scale Cooperative Research and Development Agreement: California Research Consortium (Reference Station, Fueling Performance Test Device, Station Cap Model)

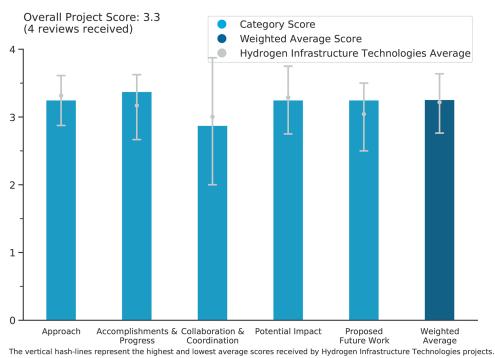
Sam Sprik, National Renewable Energy Laboratory

DOE Contract #	WBS 8.6.2.1
Start and End Dates	10/1/2021–12/31/2024
Partners/Collaborators	Sandia National Laboratories, Argonne National Laboratory, California Governor's Office of Business and Economic Development, California Air Resources Board, California Energy Commission, South Coast Air Quality Management District
Barriers Addressed	 Lack of information on operation and evaluation of high-flow infrastructure for heavy-duty hydrogen vehicles including: Infrastructure examples Tools to evaluate designs Test devices for performance

Project Goal and Brief Summary

This project aims to advance hydrogen fueling infrastructure for heavy-duty (HD) vehicles. Researchers will provide design considerations (by developing reference station designs) and risk analysis for HD hydrogen fueling stations. In addition, a model will be developed to evaluate station dispensing capacity. This project will provide tools and information that lead to more efficient design and commissioning of HD stations with greater capacity and higher flow rates.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The defined approach is well-suited to addressing the barriers/mission of the project in support of HD hydrogen station deployment, namely the derivation of station designs to facilitate cost and design considerations, as well as models and hardware to assess performance. This project is very timely, with HD fuel cell trucks and stations in deployment now. The approach taken for the development of the station testing device (Hydrogen Station Equipment Performance, or HyStEP) is a vast improvement over the previous light-duty (LD) version. It has been clearly recognized that the national labs should focus on this type of approach, i.e., design the system/hardware and perform hazard analysis but allow private industry to build and operate the unit. The approach to hydrogen station capacity model development is sound. A safety plan was not required, but the project team identified safety culture as a tenet of the project and also will consider a hazard assessment in the derivation of the station testing device. Diversity, equity, inclusion, and accessibility and community benefits plans were not required for this project.
- The project's approach is great. Investigating and reporting the codes and standards (C&S) (and regulations) will be a great help to the industry players.
- Overall, the project addresses an important need, is logical and well-laid-out, and can be (has been) positively impactful on HD fueling needs. The HyStEP has been critical to station and vehicle rollout in California, so there are similar expectations for HD.
- It is unclear whether this project is an identified industry need or a government need and how the results will help or limit the implementation of future HD hydrogen refueling stations (HRSs) by developing a set of targets or approaches that have to be met by infrastructure implementers. Hydrogen supply options are too narrow—a general focus on gaseous supply down to 20–50 bar supply that includes all options (pipeline, tube trailer, steam methane reformer, and electrolyzer) would be more valuable for industry purposes on the gaseous supply side and broad industry interests (which will indicate what option in what geographic location is optimal to make a specific business model work). This project appears to be a repeat of a LD/retail HRS exercise, while the industry has no or very limited proven operational experience with targeted HD hydrogen fueling. The experience that does exist is with very few entities, which does not make an industry or preferred path forward for HD hydrogen fueling infrastructure.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and DOE goals.

- The team has made good progress thus far, with the publication of a report detailing the HD fueling station reference design, a C&S review, and risk analysis, the latter already identifying some possible pain points with National Fire Protection Agency (NFPA) 2 and SAE International fueling protocols. Excellent progress has been made on the development of the station testing device (piping and instrumentation diagram [P&ID]), cause-and-effect controls document, process hazard analysis, and operation manual outline). The hydrogen station capacity model is in near-final form, with expectation of the web-based model in 2024. The reviewer has one minor point of feedback for the project presenter who stated that SAE J2601-5 is not an approved fueling protocol: it could be countered that the document was published after consensus derivation by a group of industry experts, and "approval" is technically granted by the authority having jurisdiction, authorizing its use.
- The project was effective and impactful in publishing the reference station guide with significant detail, supporting HD C&S development, and developing the public model. These accomplishments are all significant and impactful.
- The project should provide options and direction for HD fueling station infrastructure providers and toward the DOE Energy Earthshot.
- The project does not address existing truck stop challenges with regard to available space/footprint for hydrogen fueling infrastructure equipment. On slide 9, the top right graph does not appear to have the correct unit for operating expense (OPEX) measurement. It is also unclear if OPEX includes the cost of fuel. For electrolyzer options, the cost of water is not included, and this cost can be significant, as electrolyzers use deionized water. On slide 11, increasing tube diameter to one inch only on hose assembly

rather than throughout the HD station, instead using double piping throughout the HD HRS, might effectively lower the 8× risk increase modeled. On slide 11, it appears (but was not clarified) that the underlying assumption for the presented information is a compressor-based station equipment approach. Cryopump-based stations have fewer components, particularly for HD HRS with high throughput. The team should clarify what the real/practical function of the Hydrogen Fueling Capacity (HyCap) model will be for government-specific use. It is unclear how the HyCap model will be used as a low-carbon fuel standard HD hydrogen credit-related auditing tool and funding-related measurement tool to compare proposed HD HRSs.

Question 3: Collaboration and coordination

This project was rated **2.9** for its engagement with and coordination of project partners and interaction with other entities.

- There is excellent collaboration with other national labs and California state government agencies, but there is a clear lack of industry input. The team should seek input from the National Renewable Energy Laboratory team working with the Heavy-Duty Industry Group on the fueling cooperative research and development agreement. HD station providers and HD fuel cell vehicle manufacturers are included in this industry group.
- The collaboration between labs and California agencies was strong. It was noted that industry was consulted along the way, yet knowing this product needs to be "industry facing," that collaboration could be stronger and more deliberate throughout. The original HyStep device is effective yet also limited, in part by some of the industry feedback on implementation not being considered. While this device has learned from that effort, recognizing how critical these devices will be to market rollout, at least until full in-house certification happens, this undertaking could be expanded (especially in the following steps of implementation).
- Industry involvement would help validate assumptions on the latest market direction and storage requirements. Some of the fuel cell electric vehicle Class 8 truck manufacturers are targeting 80–120 kg of 700 bar H₂. The modeling can be updated to consider such requirements, along with refueling times.
- While the project is using industry feedback (as indicated), it is (very) unclear what the extent of industry influence is on decision-making. If the cost of HyStEP for LD HRS testing is an indication, collaborators should very seriously consider modeled capital expenditures (CAPEX) and OPEX cost and funding as priority parameters for decision-making for the HD HyStEP concept device. If testing targets become requirements for operation, not addressing these cost parameters will become a significant barrier for implementation—particularly considering that HD fuel cell electric trucks are expected to be rolled out throughout the United States (vs. West Coast only).

Question 4: Potential impact

This project was rated **3.3** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The impact will be significant if the resulting HyCap model and HD HyStEP device use become effective and enforce regulatory requirements for HD HRS operations. The test device and capacity tool efforts appear to move beyond the final research and development stage of technology readiness level 8 into commercialization and the auditable HD HRS verification phase.
- The project is doing great work that is essential to HD fueling station infrastructure development and growth.
- The project has a necessary and significant set of outputs—from the device to the C&S inputs. This project is well-done, and the effort is appreciated.
- Overall, the project is highly relevant and impactful, owing to the simple fact that HD fuel cell trucks are launching now and HD stations are in the ground and operating. Much work needs to be done to support the further penetration of these stations for customers in California. An aspect that could be considered for the future includes how existing station sites that already have large installations of stored hydrogen (e.g., at fuel cell bus depots and forklift operations) can be upgraded to allow HD trucks to fuel there at the current 350 bar level and what considerations are necessary to upgrade the stations to fuel at 700 bar.

Question 5: Proposed future work

This project was rated 3.3 for effective and logical planning.

- The proposed future work plan thoughtfully considers the key elements required to conclude the effort covering the station reference design, the station test device, and the capacity model. This work is excellent, and the reviewer is looking forward to the final report.
- The third challenge listed in the presentation is also very important, and the reviewer is looking forward to seeing the work on this challenge: "Identifying other temperatures and pressures that are of interest to vehicle and/or station manufacturers to inform future HD station performance test device concepts."
- The proposed C&S and pipeline work is good. One area that could be expanded is addressing the mediumduty (MD) needs. It is unclear whether the models and effort could support MD vehicle (and station fueling) needs, which is a gap that should be considered. Beyond the scope of this project, however, seeing how the LD HyStEP device was both effectively rolled out in California and insufficient to meet all the station rollout needs, DOE should consider how multiple HD devices can be effectively rolled out based on this work, or the HD fuel cell electric truck rollout may stall.
- The station capacity tool should include pipeline delivery options containing lower-grade hydrogen.

Project strengths:

- The project strengths include a well-defined approach to addressing very important issues facing the deployment of HD hydrogen stations. The team made excellent progress on the deliverables this fiscal year, with good definitions of future work to close out the project. In addition, the team recognizes the importance of safety in the design of the station testing device.
- The project addresses a critical need and sets up development of a needed device. The project has critical inputs to HD C&S development and strong lab and state agency collaboration.
- The project provides five variations of station design for different scenarios. The analysis of capital cost and OPEX is beneficial.
- The project explores future options and considerations for several HD HRS hydrogen delivery and compression, storage, and dispensing options.

Project weaknesses:

- Project weaknesses are minor and include the need to include industry input/feedback. Hydrogen Safety Panel feedback should be sought for a review of the P&ID and hazard analysis of the station testing device.
- The exploration of future options and considerations appears to not include all HD HRS hydrogen delivery options. The inclusion of a capacity modeling tool and HD HyStEP device does not appear to include cost considerations and impact on the speed of the rollout of HD HRSs throughout the country.
- The project should include more industry feedback. There should also be more consideration of how the product is used in the field, mass-produced, or deployed across the United States.
- The project lacks industry involvement, i.e., HD vehicle original equipment manufacturers.

Recommendations for additions/deletions to project scope:

- Recommendations for additions to the project include seeking industry feedback, opening up the reference station design to include the potential use of existing 350 bar stations for 700 bar HD trucks, and engaging the Hydrogen Safety Panel to review elements of the station testing device.
- The involvement of industry representatives would help to make sure the HD fueling station is ready to address the requirements of the vehicles targeted for release in the next decade. It would be good to get input from suppliers of power-hungry equipment (compressors and electrolyzers) on work being done to optimize the energy consumption. This input can be used to update graphs to show projected improvements that would benefit infrastructure providers that intend to set up such HD fueling stations in the future.
- The team should consider potential MD impacts and use. Greater industry input throughout (not just government-to-government interactions) is also recommended.

• The project should add CAPEX and OPEX of the HD HyStEP device; the current approach indicates a sole focus on ability to test and does not include practicality and cost.

Project #IN-001a: Hydrogen Materials Compatibility Consortium (H-Mat) Overview: Metals

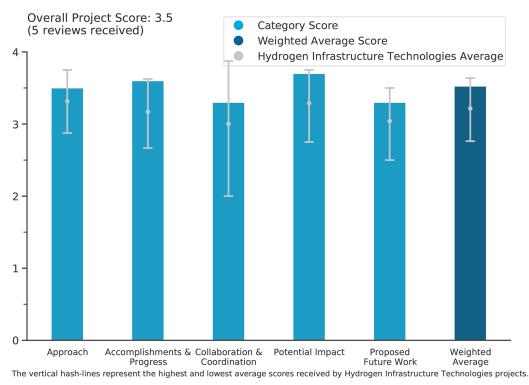
Chris San Marchi, Sandia National Laboratories

DOE Contract #	WBS 8.7.0.1
Start and End Dates	10/1/2018
Partners/Collaborators	Pacific Northwest National Laboratory, Argonne National Laboratory, Oak Ridge National Laboratory, Savannah River National Laboratory, Colorado School of Mines, Rutgers University, University of California, Davis, Swagelok, HyPerformance Materials Testing, LLC, Massachusetts Institute of Technology, University of Alabama, University of Illinois Urbana-Champaign
Barriers Addressed	 Reliability and costs of gaseous hydrogen compression Gaseous hydrogen storage and tube trailer delivery costs Other fueling site/terminal operations

Project Goal and Brief Summary

The primary objective of this project is to evaluate the potential for modern, high-strength steels to inform sciencebased strategies to design the microstructure of metals with improved resistance to hydrogen degradation. Specific goals are (1) to enhance performance and safety through improved understanding of materials compatibility and comprehensive materials data and (2) to reduce the cost of infrastructure and components.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project's goals are all sound: (1) to quantify trends for high-strength steels exposed to hydrogen, (2) to assess the role of oxides on embrittlement, and (3) to assess the testing methods for embrittlement. Proposed work on hydrogen interactions at high temperatures of austenitic stainless steels and superalloys is also very important. Behavior at high temperatures is an emerging field in hydrogen, and Sandia National Laboratories (Sandia) is well-positioned to investigate. Dr. San Marchi mentioned in his presentation that the team plans to investigate the role of impurities in hydrogen gas on dissociation and uptake. Use of impurities in hydrogen gas for embrittlement mitigation is an emerging field, and it is important that the subject be investigated. In the case of high-strength alloys, the role of hydrogen on fracture will be investigated on wrought and additively manufactured (AM) nickel-base alloys. This, too, is an important area to be explored. The project aims to identify best practices for characterizing fatigue crack growth and propagation in ferritic systems, as they depend on frequency, strain rate, and hydrogen purity. The question here is what additional laboratory data are needed over and above those already amassed at Sandia. The proposal to explore issues of similitude between lab and real-world conditions is a sound approach.
- The team has selected five critical topics to focus on and is bringing to bear an impressive combination of topical expertise and unique equipment to address these areas. The identification of key scientific questions and engineering-relevant goals will ground the efforts in each task and ensure the relevance of generated understanding.
- The project is multi-faceted, with several different performers. A discussion of each of the aspects is below.
 - Task 1: Elevated temperatures
 - The experiments were reasonably designed to meet the goals. The condition of the AM materials being investigated is a bit unclear, i.e., whether they are strength-matched, asbuilt, post-processed. These details will be important in evaluating the rigor of the comparison.
 - The data are interesting and compelling for demonstrating an impact. However, the presented data and approach will likely be insufficient to provide mechanistic insight.
 - The elevated temperature improvement is interesting. The presenter mentioned the enhancement for mobility, which makes sense for crack-tip-generated hydrogen, but for internal hydrogen, that seems a little odd. Perhaps the argument is simply that hydrogen will not concentrate at the tip of the crack.
 - Task 2: Surface phenomena
 - The density functional theory (DFT) and x-ray photoelectron spectroscopy (XPS) analyses comprise a rigorous approach.
 - Looking at the long-term behavior is important.
 - As you push to account for long-term behavior, there is clearly an impact on hydrogen accumulation, but there will also be modifications of the oxide during that time. It is not clear whether those modifications are taken into account in the modeling.
 - Task 3: Advanced alloys
 - The approach is reasonable.
 - At room temperature, there is a dramatic impact of pre-charged hydrogen, whereas with the fatigue, there is not. Perhaps the reason is simply that the tensile testing is governed by global processes and interactions, whereas the fatigue is governed by local crack tip behavior that would require a redistribution. Perhaps the project team could explore this by lowering the frequency. This might result in more distinction.
 - Task 4: Similitude
 - The approach is reasonable. However, loading rate plays an important role in intermediate susceptibility material-environment combinations. The observed behavior could be due simply to this effect. Perhaps, if the team were to run a hold in a more aggressive environment (higher hydrogen pressure), a crack would not continue to grow.

- Task 5: Mechanisms
 - Based on what is presented, it is difficult to judge how relevant and appropriate these methods are for such a nuanced and complex mechanistic study.
- The work at the national lab has a good safety track record in hydrogen research and development (R&D), and it would be great if the procedures to perform the experiments safely were also disseminated to the R&D community. It did not seem like a diversity, equity, inclusion, and accessibility plan or a community benefits plan was required. Using pre-charged samples is an attractive approach to testing materials compatibility with hydrogen; correlating it with prior experimental data obtained from tests in pressurized hydrogen is important. It would have been nice if the presentation had provided more details about the equivalence between the two. The rationale for testing at elevated temperatures was not clear. The speaker mentioned interest from one industry partner (Siemens), but it is not clear whether there is a broad need or just one company's interest. Likewise, the justification for expanding the work to nickel-based alloys was not clear.
- Slide 5 shows the goal, objectives, and underlying tasks. Each of these is welcome and will advance the field. However, they do not appear to be organized, inter-related, or combined into an efficient procedure for certifying a material for hydrogen resilience. Such a process-based approach is essential for increasing the efficiency of new material development. For example, Objective 2 and Task 2 begin with hydrogen uptake into a material; if the project starts here, then a decision tree begins to grow out that will encompass each of the other objectives and tasks while clearly identifying knowledge gaps. Objective 2 + Task 2 could then be the role of temperature in these surface phenomena and uptake. Objective 3 + Task 3 now considers how absorbed hydrogen advances microstructural damage within the material. Objective 4 + Task 4 focuses in on how these affect the high-strength alloys. Objective 5 + Task 5 now looks for similitude between the lab and the real world, showing gaps in the decision tree that is now created. It would be wonderful to see this progression carefully done for one material of significance, such as 304L or 316 stainless steel (SS). The lack of order and the jumping around between materials were confusing.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and DOE goals.

- The project appears to be progressing from year to year. The data reported support conclusions and answers to the questions posed.
- Clear progress has been made on all stated objectives, which align with overarching DOE goals.
- Investigation of the tensile ductility of 304L, IN625, and Hastelloy X in hydrogen up to 200°C is complete. Dr. San Marchi argued that, at elevated temperature, interactions of hydrogen with the material microstructure may not be the case, which is a plausible argument. However, there was no reference to any potential trapping mechanism, e.g., vacancy type, that may not be operable. The presentation mentioned that hydroxyl forms rapidly when oxides are exposed to hydrogen and that hydrogen diffusion through oxides is explored through DFT. However, there were no details on how and why hydroxyls are forming or even why hydrogen can diffuse through oxides. Investigation of the fatigue life of IN625 (high strength) and Hastelloy X (low strength) yielded that, whereas the life of IN625 is significantly reduced by hydrogen, the life of Hastelloy X is not. The question is how strength is so important to fatigue life. Answering this question may be important to new alloy development. Regarding the observation that unstable crack growth can occur at a stress intensity factor less than the measured fracture resistance, this reviewer did not manage to capture the underlying hydrogen-related effects during the project's presentation. The progress reported on mechanisms of hydrogen degradation is difficult to evaluate because no details were provided. That level of detail was not possible within the 30 minutes allocated to the project's presentation.
- The slide progression from approach to accomplishments/progress is thoughtful. This can be further improved by some kind of graphical indicator showing how much progress has been made since the start and how much further the project has to go.
- Results on internal hydrogen's effect on ductility at elevated temperatures do not describe details of precharging or the hydrogen pressure to which these tests would correspond. It is not clear how, if hydrogen is mobile at elevated temperature, the team verified that the hydrogen has not diffused out during heating/ holding/testing. The DFT of surface effects is interesting, but relating such highly idealized simulations to realistic conditions (the project goal of lab-real-world similitude) will be a challenge. Key details/

assumptions of the modeling work performed were missing. Results on slip localization in 316SS need to be better explained and put in context with other supporting/conflicting theories/results.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The project benefits tremendously from collaboration with Oak Ridge National Laboratory on advanced microstructures and significantly from collaboration with Swagelok on materials applications and relevant conditions. The collaboration with the Colorado School of Mines is also important, given the corresponding expertise in steel R&D. On the other hand, the importance of collaboration with Rutgers is not clear.
- The work is highly collaborative and is effectively integrating various institutions.
- There are excellent partners from multiple sectors that have a strong chance to build a pipeline of people.
- Overall, the collaborations are reasonable and seem to be well-coordinated. While the Pacific Northwest National Laboratory and Sandia aspects are clear, it would be helpful to have a clearer picture of the role that Oak Ridge National Laboratory is playing in the project and, more particularly, whether there are specific areas in which the lab's characterization and production capabilities were leveraged.
- Coordination across the teams was not clear from the presentation: whether they hold periodic meetings, the manner in which the experimental test matrix is determined, etc. The presentation gave the impression that each of the performers is working relatively independently in that organization's own direction. A cohesive effort was not apparent.

Question 4: Potential impact

This project was rated 3.7 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- Of the projects that this reviewer knows, this project is the best one that serves the DOE Hydrogen Program's goals and objectives for materials compatibility. Sandia's current accomplishments and those attained since more than two decades ago warrant the impact of the project on engineering practice.
- The results of the project will be broadly impactful, as the stated objectives span a number of relevant areas, ranging from high-strength, precipitation-hardened alloy performance to best practices for materials testing.
- Different facets of the work are at different levels of impact, but holistically, this is important work that is addressing relevant materials compatibility issues.
- This project is making excellent progress in an area definitely needed by the hydrogen community.
- The project in general is aligned with Hydrogen Program goals and objectives.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- On slide 20, the deliverables and milestones for "hydrogen interactions at elevated temperatures," "surface phenomena and uptake and transport," "advanced high-strength alloys," and "similitude between lab and real world" are very important pieces of future work to be pursued. On the other hand, in the context of "mechanisms of hydrogen degradation," the focus on analyzing the hydrogen effect on cross-slip for implications of hydrogen-assisted fracture of face-centered-cubic (FCC) metals is not a promising direction. The stacking fault energy of FCC materials is so small that the project will need to demonstrate that a "small" reduction of the stacking fault energy by hydrogen has a very large effect on fracture toughness. This reviewer is not familiar with any such correlation studies. The result reported on slip localization in relation to cross-slip (at the bottom of slide 16) has already been reported in the open literature for decades, and it is not clear whether single-crystal studies can provide any new insights.
- Next steps are logical and driven by existing work outputs. There are two suggestions to consider for future work. First, for the study of precipitation-hardened alloys, the stated focus will be on alloy strength, but it would be interesting to determine whether there are any mechanistic links between fracture behavior and

the changes in precipitate character. Second, while the reviewer acknowledges the experimental benefits of notched fatigue specimens (and the challenges with fully reversed fatigue testing in hydrogen gas environments), the team should consider the application of Dowling's local strain theory to the notched fatigue experiments. Such approaches may facilitate further understanding of the fatigue life data, especially across different alloys.

- Under the proposed work on "advanced high-strength alloys," it is not clear why the work is listed as focusing on "non-pressure containing applications" since the presentation gave the impression that the point of looking at high-strength alloys was for higher-pressure applications. It is not clear what application and strain rates are planned for the work relating to "similitude between lab and real world."
- The proposed future work was a bit vague. This is difficult for such a large project to present in such a short review time.
- It is hard to evaluate the appropriateness of the proposed goals without a systematic structure process framework in which to couch the proposed work.

Project strengths:

- The leadership of the principal investigator (PI), Dr. San Marchi, and the experimental capabilities at Sandia are the two key factors underlying the project's current success and future accomplishments. The project has clearly stated goals and objectives based on the long record of accomplishments at Sandia. These goals and objectives are perfectly aligned with the important engineering materials classes that are needed for hydrogen technology applications.
- The project has targeted research questions with clear relevance. There is a strong team with access to state-of-the-art facilities and capabilities. Results to date are technologically useful and are addressing key areas where further understanding is needed.
- This is a fantastic science project that is beginning to feel comprehensive for understanding hydrogen embrittlement.
- Strengths include excellent collaborations and clear goals. There is generally good mapping between the experiments and the goals.
- The PI is an expert in fatigue and fracture testing and analysis of metallic alloys in hydrogen atmospheres.

Project weaknesses:

- Data generation has been excellent, but the interpretation and takeaways can continue to be improved. Because of the multiple tasks and the limited time, the presentation did not allow for a full engagement and review of the technical details. It is likely that the authors have interpreted these in depth, but it could not be judged in this short review.
- Slide 15, on mechanisms of hydrogen degradation, lists that modeling interpretations for hydrogen-induced damage will be explored in a model alloy system. Sandia should work only with real-world materials and leave the model systems to academia. Unlike with universities, Sandia does have the laboratory resources to focus on real-world systems to impact the engineering of real-world applications. Given the goals and objectives for technology development, it is not clear how the proposed modeling and simulation of, for example, the response of 316 single crystals are impacting the project's goals on real-world materials deployment under real-world hydrogen conditions.
- With the science methods becoming established, a focus should become efficient, targeted tests/simulations that allow engineers with a new material (e.g., 3D-printed) to determine suitability for a given hydrogen application in a pragmatic way.
- It is not clear which aspects of the accomplishments were performed by which of the performers. The desire to connect things "...across length scales...", while noble, is a cliché. Perhaps if there were some specific milestones/go/no-go's that showed connection across length scales, that would have been nice. The project should use more concrete/achievable statements. There's no go/no-go in the project, and the milestones are very weak.
- There are no weaknesses of note.

Recommendations for additions/deletions to project scope:

- The work is properly scoped for the funding.
- It is not clear why the role of impurities on hydrogen dissociation and uptake is going to be investigated for 100–1,000 hours. The importance of this time interval is not clear. The project may explore the effect of yield strength on fatigue life from a mechanistic perspective. This effect has been investigated in the absence of hydrogen for a long time, with the results being inconclusive. Moreover, understanding of the effect in the presence of hydrogen is even more limited. Conservative fracture methodology to measure fracture resistance in gaseous hydrogen is a very important issue, and the project should resolve it thoroughly.
- It is not clear whether there is a limiting temperature below which we just do not need to be concerned with embrittlement. In other words, if we know the ambient pressure, material, and time exposed to hydrogen and are operating cold, it is not clear whether we need to worry about hydrogen embrittlement.

Project #IN-001b: Hydrogen Materials Compatibility Consortium (H-Mat) Overview: Polymers

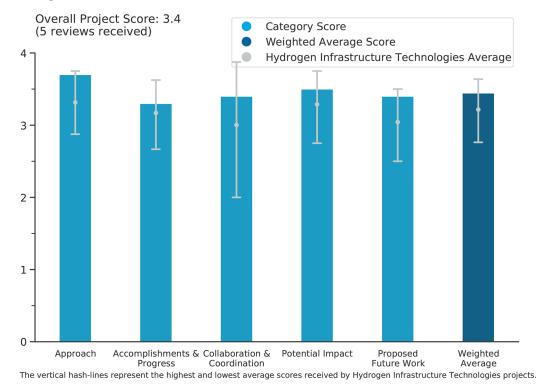
DOE Contract #	WBS 8.7.0.2
Start and End Dates	9/1/2018
Partners/Collaborators	Sandia National Laboratories, Argonne National Laboratory, Oak Ridge National Laboratory, Savannah River National Laboratory, Swagelok, Takaishi Industries, Burke Industries, ARLANXEO, Zeon Corporation, TSE, Chemours Company, Kyushu University (Hydrogenius), INVISTA, Ascend Performance Materials, Solvay, Saint- Gobain, Hummell, Dover Corporation, AMPO, Howden, Solar Turbines, Burckhardt, Green Tweed, Arkema, Kepner Products Company, Nel Hydrogen, Freudenberg Sealing Technologies, Evonik Industries
Barriers Addressed	 Safety, codes, and standards Safety data and information: limited access and availability Insufficient technical data to revise standards Limited participation of business in the code development process No consistent codification plan and process for synchronization of research and development and code development Hydrogen delivery Reliability and costs of gaseous hydrogen compression Gaseous hydrogen storage and tube trailer delivery costs Other fueling site/terminal operations

Kevin Simmons, Pacific Northwest National Laboratory

Project Goal and Brief Summary

The project objective is to fill a critical knowledge gap in polymer performance in hydrogen environments. Investigators are gathering and assessing stakeholder input about the challenges, materials, and conditions of interest for hydrogen compatibility. Findings inform the project's development of standard test protocols for evaluating polymer compatibility with high-pressure hydrogen, characterizing polymers, and developing and implementing an approach for disseminating the information.

Hydrogen Infrastructure



Project Scoring

Question 1: Approach to performing the work

This project was rated **3.7** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project's goal is to understand hydrogen-materials interactions and develop tools for decision-making for material deployment in hydrogen technologies. In particular, the project's focus is on the degradation and computational modeling of performance of polymers in a hydrogen environment. The project's approach through topography of cavities and cryogenic testing, along with simulation for parameter optimization and life prediction, is sound.
- The approach is logical to address each. The knowledge gap in this space is very large. It may be beneficial to establish an overview and clearly articulate/prioritize the material systems, applications, and components that drive this initial work and the extent to which is it is transferable. There should be a larger focus on liners; barrier properties are of importance. The tasks include mechanisms of property changes, computational modeling of long-term aging in a hydrogen environment, and prediction. Some notes and questions from the presentation are below:
 - There was much discussion of the formation and growth of the macroscale defect formation (bubbles, etc.). However, it would be helpful to know whether there are any other fundamental changes earlier associated with the secondary bonds or modification of the polymer back bond, side groups, etc.
 - Silica plays an important role in the formation of micro-voids/micro-cracks.
 - It seems that the volume change is being used a good deal.
- It would be helpful to know whether a framework (almost like an Ashby curve) exists for the expected damage mechanism for a given set of relevant conditions or for some critical material variables.
- It is not clear whether everyone is on the same page for qualification requirements for polymers in hydrogen service; getting everyone in accord seems like a significant challenge.
 - The presenter mentioned the question of whether going to the higher-pressure values is necessary. It would be helpful to clarify what the first indication of the answer is.

- The project has clearly defined goals that are targeted to address pressing questions. It is also wellintegrated into the overarching H-Mat framework. The only comment is that the artificial intelligence/machine learning (AI/ML) implementation could have been more clearly linked with specific goals; for example, the team should make it clearer how these methods are being implemented in the context of the proposed scope and what the true expected outcomes are for these efforts.
- The effort to merge experimental and computational datasets is essential, as it is not fiscally possible just to run an experimental campaign. More emphasis on three-dimensional printed properties at cryogenic temperatures could be beneficial. It is not clear what material classes are being targeted and how data are being generated in a pragmatic schedule for the community. It is not clear whether the researchers just test whatever material they are asked to test. If that is the case, they could be doing this for a while.
- Overall, the project has spent significant time working on rubber materials (e.g., O-rings) that have reliability problems but are not necessarily cost showstoppers. Also, a better understanding of the material needs versus the true hydrogen pathway might provide different relevant problems. Properties such as pressure, temperature, and cycling should be examined. Most of the rubber material work ties back to 700 bar high-pressure refueling and reliability concerns.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and DOE goals.

- The team has made clear progress on stated objectives, has developed interesting new experimental capabilities (the in situ O-ring test system), and is actively pursuing ways to expand and amplify project impact (via AI/ML method implementation).
- Solid progress was reported based on the report from last year.
- Using molecular dynamics (MD) simulations, the project researchers investigated the strength of the interface between crystalline and non-crystalline regions as a potential source of cavitation damage. Phase field modeling and hydrogen diffusion were used to investigate gas bubble evolution. Finite element modeling was also used to investigate bubble growth in conjunction with hydrogen diffusion. The concern here is that phase field models are not mechanistic; they require laws/rules for damage initiation that were not mentioned in the presentation. For instance, it was not clear how interfacial strength obtained from MD simulations was implemented with the phase field models. In addition, it is not clear how the simulations treated bubbles created through "empty space" due to straining and bubbles created through "open volume" expansion at interfaces. Lastly, there was no elaboration on insights from the finite element simulations of bubble growth, e.g., onset of instabilities, etc. X-ray computed tomography (CT) studies were used to observe defect formation in model EPDM (ethylene propylene diene monomer) filled with carbon black and silica. The studies are interesting, but there was no report of lessons learned. The new EPDM and NBR (nitrile butadiene rubber) elastomer systems were experimentally found not to experience dramatic swelling in comparison to other model compounds (slide 14), but again, there was no mention of the impact of this experimental observation on technology. The studies on O-ring behavior (slides 15 and 16) look very promising, but it is not clear what the objectives are. More specifically, the studies were presented as if swelling is a new phenomenon that the researchers are now beginning to explore.
- While the results are valuable and highly relevant, they stop one step short of what is needed—a quantifiable rule that shows us what pressure swing to stay below to avoid blistering for specific polymer classes. Slide 11 states that "Helium is Inappropriate as a Surrogate Gas for Hydrogen"; the project team must be careful with broad statements like this, as they are often applied out of context. This is likely a thermochemical temperature effect and not generally true (slide 11 shows only pressure; no temperature is provided). It would be surprising if hydrogen acted differently from helium when absorbed in materials at cryogenic temperatures.
- There is much effort on understanding bubble formation and technical understanding, but there is not a correlation to how this work can be used to develop real-world component-/system-level understanding.
- Question 3: Collaboration and coordination
- This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- Only one university partner—in Kyushu, via Hydrogenius—does not build the sustaining research pipeline necessary to keep this work going after 2027. The prior Hydrogen and Fuel Cell Technologies Office infrastructure workshop emphasized the need for more independent testing labs for cold hydrogen, and this project could be a mechanism to make that happen.
- Collaborative efforts and engagement are excellent.
- Coordination and collaboration are strengths of this effort.
- The collaborations and associated coordination are clearly defined and scoped.
- Testing and characterization at Sandia National Laboratories (Sandia) are very important and beneficial to the project. Benefits from atomistic simulations at Sandia are not evident. Collaboration with Oak Ridge National Laboratory (ORNL) (slide 17) is not clear. Equipment was shown, and neutron/x-ray scattering testing was mentioned—but not in relationship to the fundamentals and technology questions that the project aims to tackle.

Question 4: Potential impact

This project was rated 3.5 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- Polymer material data at cryogenic temperatures is desperately needed by the community for pump seals. This cannot be underemphasized.
- The project clearly will make a positive impact on understanding polymer-hydrogen interactions and is actively seeking to transition developed understanding to industry partners for broader implementation.
- This work is of high need and is addressing important knowledge gaps.
- It is not clear how the project's Phase II continues on the basis of the accomplishments and progress of Phase I. In fact, it seems that the project has started as if previous studies for elastomer swelling, polymer composites, and O-ring behavior do not exist. The project's "relevance and objectives," as mentioned on slide 5, are very important, but it is not clear how the presented accomplishments address these objectives in progression from Phase I through previous years.
- The project always has relevance but needs to take a deeper dive into the industry needs.

Question 5: Proposed future work

This project was rated 3.4 for effective and logical planning.

- Proposed future work is driven by current results and appears reasonable. The only suggested area for consideration is actively seeking to leverage the impressive datasets being developed to create "consensus relationships" akin to those now being implemented for fatigue crack growth and subcritical cracking thresholds in pipeline steels. It seems like significant data are available to at least begin drawing some conclusions on possible relationships that could be readily implemented into governing test standards.
- The polymer tribology work at cryogenic temperatures will be enabling for many in the industry. However, there is a need for new test capabilities such as a cryogenic nanoindenter or coefficient of thermal expansion (CTE) measurements.
- Identification of challenges was good, but discussion of specific action items and project actions to address the challenges was vague.
- The remaining challenges as outlined on slide 22 are on target regarding the project's future impact. These challenges can be used to focus the project. The proposed future work on slide 23 also needs to be focused. The bullets "Continue pressure cycling with varied decompression conditions and temperatures" and "Thermoplastic focus for testing" are rather vague. It is not clear how these two themes are related to the material that was presented.
- As Phase II starts, it is unclear how the work scope will align with deployment needs.

Project strengths:

• The project's strengths are the principal investigator, Dr. Kevin Simmons, and the collaboration with Sandia. Dr. Simmons has an extensive research record in the area of polymers and hydrogen behavior. He

knows what is needed for the project to have impact on technology development and how the relevant experimental and simulation tools can be used to serve the goals of the project.

- The project has an excellent team, is well-organized, is clearly linked to industry, and is pursuing questions of merit.
- Strengths include addressing important data and knowledge gaps and the unique data being generated.
- The project is a great transition to thermoplastics after the much-needed work in seal blistering.

Project weaknesses:

- There are no weaknesses of note.
- Polymer swelling and elastomer blistering are well-investigated fields, and the researchers need to outline the technology-related issues for O-ring design that they are concerned with and how their results are applied in the direction of technology impact. The project, as presented, seems to be at a beginning stage. In other words, there were no conclusions drawn from progressive accomplishments and developments over the years on polymer behavior in the presence of hydrogen. In fact, there were no definitive research results that would enable technology improvement or new technology concepts, promising new materials compositions, etc. It is not clear that phase field studies or AI/ML have produced any impactful results so far.
- It is hard to use AI/ML with cryogenics because no data exist to train an AI/ML system. The project team should make sure to generate the necessary experiment data and process first; then AI/ML will exponentially expedite new material validation.
- Interpretation was somewhat vague, and it was difficult to understand what information is extracted. The project could benefit from a clearer definition of how this work fits in for the wide range of applications and material systems that are being considered.

Recommendations for additions/deletions to project scope:

- The role of hydrogen on the silica-polymer interface needs to be systematically investigated if phase field models are to be used to ascertain life and degradation of the polymer composites in hydrogen. The presenter mentioned that there is a concentration-dependent diffusivity of hydrogen. This needs to be discerned from the deceleration of hydrogen transport by interfacial trapping. In fact, the presenter did not mention how the hydrogen diffusivity was measured. The project needs to clearly outline why AI/ML is to be used on measuring transport properties. The diffusion predictions listed on slide 18 were not explained during the presentation. The project needs to define what specific technology roadblocks the numerical simulations aim to address. As the project was presented, it was not clear how the simulations support the experiments or are informed by the experiments. In particular, how phase field modeling is used to elucidate real-world composite polymer behavior needs to be clarified.
- The project should consider adding funds to develop additional cryogenic test capabilities—or partner with a university that can.
- This portion of H-Mat is well over \$2.5 million per year (the presentation did not include Sandia's and ORNL's budget contributions), and there needs to be focus on the right activities.

Project #IN-015: Optimizing the Heisenberg Vortex Tube for Hydrogen Cooling

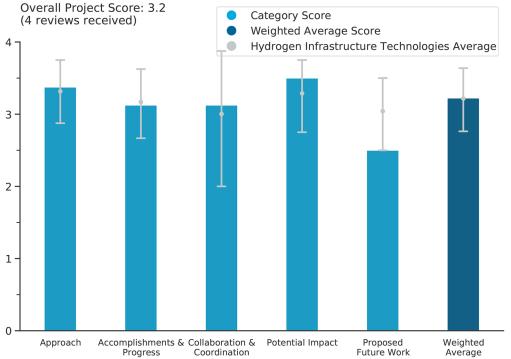
Jacob Leachman, Washington State University

DOE Contract #	DE-EE0008429
Start and End Dates	1/23/2019–5/30/2024
Partners/Collaborators	Plug Power Inc.
Barriers Addressed	 Reliability and cost of liquid hydrogen pumping High cost and low efficiency of liquefaction Other fueling site/terminal operations

Project Goal and Brief Summary

This project aims to establish that Washington State University's Heisenberg Vortex Tube cooling system can achieve the following improvements to cryogenic hydrogen storage systems: (1) a 20% increase in liquid hydrogen (LH2) pump volumetric efficiency through vapor separation and subcooling, (2) a 20% decrease in LH2 storage tank boil-off losses through thermal vapor shielding, and (3) an increase of supercritical hydrogen expansion from 31% to more than 40% through greater isentropic efficiency.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project has a very clever idea that utilizes the unique properties of hydrogen to decrease boil-off. The project has made great use of different modeling techniques, such as computational fluid dynamics (CFD) and atomistic simulations, to aid in understanding this complicated process and design the system.
- The project uses boiled-off H₂ to serve as energy to drive a para–ortho converter to make the remaining LH2 more resilient to future boil-off. The idea is novel and clever. The researchers had other uses that they thought about but focused on storage, so the project had plans B and C. This is an idea worth pursuing and one that addresses relevant barriers. The project is testing multiple designs to improve the odds for success, and a reasonable project plan is being executed.
- The project was successful, but it had to overcome several project challenges with cost and supply from vendors. The vendor changed the price on the project after the quote when the industrial partner was willing to purchase the material. The project was able to overcome and adapt to the impacted cost change while reducing the size of the project approach.
- The overall approach and information gathered in the study is very sound and sufficient for a system designer to consider this technology option. One area that has not been directly addressed is the potential maintenance and reliability of such a system. Presumably, the simplicity of the vortex tube makes this a particular advantage, but it would be helpful if these factors could be quantified. Similarly, it would be useful to know whether there is potential for any degradation in performance over time or any potential lifetime-limiting aspects to the system.

Question 2: Accomplishments and progress

This project was rated 3.1 for its accomplishments and progress toward overall project and DOE goals.

- The CFD model was first validated versus NASA data, and a Heisenberg vortex tube was tested in the lab. Learnings from this initial work were incorporated into a system to reduce boil-off gas from an LH2 storage vessel.
- The project was successful in demonstrating the cooling effect in tanks using the gas interacting with the project's surface-coated catalyst. The team worked with an industrial partner and demonstrated the project's success. The project is at its end, and the industrial partner is continuing to work and demonstrate the technology on a full-scale system. The presentation did not provide any new direction or opportunities for how this technology could be used in other ways or for future research.
- The goals are clear, and the progress toward them is well-demonstrated. It is not clear how important the effects of stratification are to the overall system performance. The team should expand on this topic to understand how the system could perform in other tank layouts.
- The project modeled the system in CFD, set up a test stand, built and tested field articles to check performance, and started the trial on the customer site. The initial improvement is two-thirds of CFD results but still a reduction in loss of about 2.7% in near-full tank. The project could not provide the more important part—full tank results—because of multiple delays.

Question 3: Collaboration and coordination

This project was rated **3.1** for its engagement with and coordination of project partners and interaction with other entities.

- The project has good collaborations with Plug Power and among different groups at Washington State University. It is great that this concept has been demonstrated with a commercial partner.
- The project team is strong, and having a direct end user (Plug Power) as a developer and test partner provides a level of validation that some other projects would be well-suited to copy.
- The project lead worked with an industrial partner and demonstrated success in the project. The industrial partner had challenges in Task 3, but they were overcome, and the partner successfully demonstrated the effectiveness of the cooling system.

• Plug Power is a suitable partner, but a station owner or dispenser maker to show impact in transport would be preferable. It is good that Plug Power allowed onsite testing, but more upfront input would be preferable.

Question 4: Potential impact

This project was rated 3.5 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The initial results seem very promising, and the system has no moving parts, so essentially, there are zero operating costs. Given that hydrogen boil-off is a large problem, it seems like this system could enter the marketplace quite quickly.
- The continued improvement in liquid-handling equipment is critical to the hydrogen industry. Boil-off and system off-gassing will become ever more important aspects of design and technology development. After a few decades of limited LH2 equipment development, projects such as this one begin to move the industry toward the next stages of improved efficiency and performance.
- The team should aim to increase LH2 pump efficiency and lower boil-off, which will support filling of HD vehicles, a major DOE goal. However, this could also serve in any application where LH2 is moved regularly. The ability to improve the ortho-para ratio using existing boil-off could help with extending the time until boil-off starts, which could be of value in any mobile operation, as well as stationary ones.
- The project is aligned and addresses an issue with boil-off gases. More work needs to be done in this space, and continued improvements to the existing work to further the performance could be valuable and benefit the Hydrogen Program.

Question 5: Proposed future work

This project was rated **2.5** for effective and logical planning.

- This is where the end of the project could have provided new insight and direction on what needs to be accomplished: how good this system can be and how else this system can be used. The presentation did not provide a new direction on where the project would go next.
- Basically, the team intends to complete the plan.
- The project is essentially finished at this point.

Project strengths:

- The project was successful, with the partner developing and demonstrating a solution to cooling gases back through the storage tanks. The static process would save energy and money, as gas would flow across the catalyst, thereby benefiting the system.
- The project includes a great use of different modeling techniques, such as CFD and atomistic simulations, to aid in understanding this complicated process and design the system.
- A weakness in the previous year's presentation was the lack of performance data; this weakness has now been addressed, and a more complete picture of system performance is now available.
- The project has a novel idea that uses lost hydrogen to cool remaining LH2.

Project weaknesses:

- This is where the end of the project could have provided new insight and direction on what needs to be accomplished: how good this system can be and how else this system can be used. The presentation did not provide a new direction on where the project would go next.
- It would be good to see the performance of a fully catalytically coated Heisenberg Vortex Tube and over a wider range of fill levels, but it is great that some preliminary data arrived prior to the Annual Merit Review cutoff date.
- The study is limited to impact on horizontal tanks; this could be expanded to consider other tank sizes and shapes to provide a more comprehensive design analysis.
- The project has had significant issues getting the device the team wanted and operating it in the field.

Recommendations for additions/deletions to project scope:

- The team needs to try this out at a scale and for a long enough time to prove it works at scale and has durability in order to get non-government funding, which is where the project is, and the team needs those data.
- It would be interesting to measure the ortho-para percentage of the hydrogen going into the tank and coming out through the Heisenberg Vortex Tube to verify the performance of the system.
- A follow-up field implementation/demonstration would be very interesting.
- There are no recommendations for future work.

Project #IN-019: Ultra-Cryopump for High-Demand Transportation Fueling

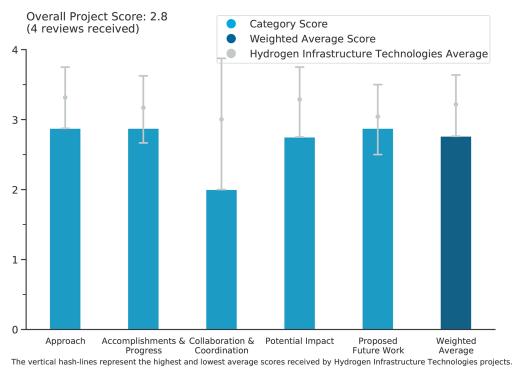
Kyle Gross, RotoFlow

DOE Contract #	DE-EE0008819
Start and End Dates	2/1/2020–9/30/2024
Partners/Collaborators	N/A
Barriers Addressed	Reliability and costs of liquid hydrogen pumping

Project Goal and Brief Summary

This project aims to help advance hydrogen refueling infrastructure for heavy-duty transportation by designing, building, and testing a liquid hydrogen (LH2) pump with the flow and pressure necessary for bus and truck refueling. The work addresses challenges caused by refueling operating conditions (e.g., extreme pressure), in part by upscaling existing RotoFlow technologies and making improvements to pump design, seal design, and motor–drive configuration. The intended final product is a cost-effective, reliable, high-flow, high-pressure reciprocating LH2 compressor system.

Project Scoring



Question 1: Approach to performing the work

This project was rated **2.9** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

• The project team will develop an LH2 pump that meets the 10 kg/min flow target. The team will also develop a vaporizer to warm to ambient temperature, as well as a bypass loop to inexpensively deliver subcooled compressed gas at the desired temperature and pressure. This approach is direct and effective. Testing is only to vent. While acceptable, testing would have been more useful if it were interfaced to a dispenser and a

vehicle to increase the odds of noticing any integration issues. All the above are aimed at barriers that apply to the project. The team employed good safety measures and responded to feedback well.

- The continued work is progressing well, and there are good data being generated on improved seal performance compared to previously used materials. It does appear that there is still a need for continued work on materials and the design to minimize wear without impacting efficiency. The team is aware and continues to work on that challenge.
- Seals for high-pressure cryo-pumps are a large problem; it is good that this project has spent a good deal of time trying to de-risk this issue and improve reliability. It is not clear what tests on seal materials have been performed or what metrics will be used to determine a winner.
- "Other developments will continue long after project completion" is not a statement upon which this proposal can be objectively assessed, unless it leads to new potential for collaborations, but none were specified. LH2 testing should have been included in the original proposal, as liquid nitrogen (LN2) testing limits the value of the work.

Question 2: Accomplishments and progress

This project was rated 2.9 for its accomplishments and progress toward overall project and DOE goals.

- The project progressed, completing the design, which is ready to be sent back to the Hydrogen Safety Panel for review. The project also completed wear testing in LH2, demonstrating a greater than 50% reduction in material wear from the current material. This is good progress. With the design work completed on the warm and cold ends, once the procurement is completed for the cold end, the project will progress toward testing for the remainder of the fiscal year.
- The pump motor has been built, with the whole device nearing completion, and the facility is also nearly ready. The project is progressing on time and presumably on budget, which is pretty good progress.
- The statements of work received for budget period 2 (which is stated as completed) are not SMART (Specific, Measurable, Attainable, Relevant, and Time-bounded). The proposers need to quantify improvements in a non-arbitrary way, even if it is relative to their own prior systems. Without this quantification, the return on the taxpayer investment cannot be assessed. The slide 8 graph, which includes quantifiable data, is helpful. While >200% improvement is great, if the initial test lasted only a minute, it is not going to be good enough, so more is needed. Some kind of order of magnitude should be sufficient while not giving away anything too proprietary. On slide 10, the N₂ purge is directly opposite the main vent stack line and will not accomplish a proper sweep purge of the area near the high-pressure seals, at least not as interpreted by the reviewer.
- Some progress has been made, but it seems slow, considering that this project has been ongoing for many years. More details about the testing process used to evaluate the wear rate would be good, as well as how the longevity of the piston ring design was determined to aid in evaluating progress.

Question 3: Collaboration and coordination

This project was rated **2.0** for its engagement with and coordination of project partners and interaction with other entities.

- The project team received integration help from Hydrogen for Mobility (H2fM), but this is a design and build effort and thus not highly collaborative.
- There is no partner listed on the proposal. Credit is given to the working collaboration with the Hydrogen Safety Panel for review of the design and the testing to be performed.
- The slides specifically state there is no collaboration or coordination, in response to prior reviewer comments.
- The sponsor organization has no external partners. There seems to be little transfer of knowledge outside of the sponsor organization. It is unclear who makes the seal materials and whether there is collaboration with an outside company to improve them.

Question 4: Potential impact

This project was rated 2.8 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The project is well-aligned and is aimed at important infrastructure to enable high-pressure refueling using pumps, rather than compressors. Since LH2 could be the delivery preference, reducing power to achieve 350 or 700 bar pressure and the desired low temperature enables hydrogen transportation.
- The targeted flow rates are significant for DOE to be able to achieve to reach Hydrogen Program goals. The project is well-aligned and appears on track to test out the approach to achieving project goals. The testing will be performed with LN2, but future work will need to be validated with LH2 and at the 950 bar pressure. This is not a trivial task, but good plans are laid out for future testing at Air Products post-project.
- Improvement of cyro-pump reliability is very important, but the slow progress of this project may indicate that it is not a priority for the sponsor organization. Additionally, it is unlikely that the learnings from this project will be transferred to other organizations.
- There seems to be nothing here that is shareable to help the broader community. It seems like the work will advance this company's proprietary pump line. However, improved longevity is the primary problem, and no estimates of this were provided.

Question 5: Proposed future work

This project was rated 2.9 for effective and logical planning.

- A good plan is laid out for completing the project. RotoFlow also has plans beyond the project to test with LH2. This is a demonstrated commitment to product development.
- The proposed future work is exactly what is needed. The project will basically finish on time.
- The LN2 pump curves will be helpful. Specificity is suggested regarding what form the pump curves will take and how the parametric studies will be conducted.
- It would be great to see testing of this system this fall, as planned.

Project strengths:

- The project has completed the objectives set out for completion at this point in the project and has an excellent plan moving forward and post-project. The project is on track to meet the targeted flow rates at pressure.
- Seals of high-pressure cryo-pumps are a large problem; it is good that this project is tackling that and spending time trying to de-risk seal wear and improve reliability.
- Improvements to LH2 pumps are desperately needed, and this work addresses that need.
- The project is valuable to transportation where LH2 is the form used for transport.

Project weaknesses:

- Future materials testing for wear should be addressed at higher pressure. This can be addressed in the future when the team begins testing under higher pressure.
- No real durability data seem likely to be gathered in testing. The project is simply venting the hydrogen pumped, which is sub-optimal.
- It would be good to see some of the knowledge from this project transferred to others, considering taxpayers are contributing the bulk of the funding. Progress has been slow.
- The lack of collaboration that does not advance the general community is a major weakness.

Recommendations for additions/deletions to project scope:

- If possible, the team should find a partner who would value the chance to accept hydrogen testing to verify use in the partner's own hydrogen equipment.
- Actual LH2 testing should be conducted. (It is unclear who will do it if this team cannot.) Specification of the pump curves that will be characterized for project completion would also be helpful.
- It would be good to see test results using LH2, rather than LN2, to verify the improvement in performance.

Project #IN-025: Hydrogen Delivery Technologies Analysis

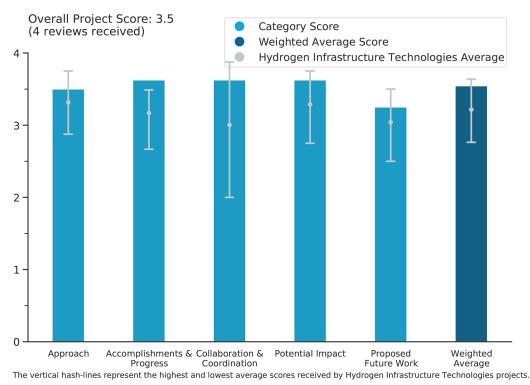
DOE Contract #	WBS 3.4.0.1
Start and End Dates	10/1/2005
Partners/Collaborators	Energy Technology Analysis
Barriers Addressed	Inconsistent data, assumptions, and guidelines

Amgad Elgowainy, Argonne National Laboratory

Project Goal and Brief Summary

This project aims to evaluate the economic and environmental costs and benefits of hydrogen and ammonia delivery technologies. Researchers will analyze various hydrogen and ammonia technologies throughout their life cycles and identify the technologies with the highest cost-effectiveness and lowest environmental impacts. Argonne National Laboratory (ANL) is collaborating with Energy Technology Analysis on this project.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- This project provides a good approach to alternative hydrogen delivery options via ammonia as a carrier while leveraging established modeling tools from ANL that have been upgraded from established models, e.g., the Hydrogen Delivery Scenario Analysis Model (HDSAM). The pathways chosen (trucking, pipeline, rail, and ocean vessel) are appropriate.
- Hydrogen delivery options—NH₃, liquid hydrogen (LH2), gaseous hydrogen (GH2), and pipeline—are well-covered. Ammonia has both an established infrastructure and clear pathways that include incentives.

The model includes all necessary elements, and the finding that the NH_3 cost is lower than that of H_2 is interesting.

- This analysis clearly fits into and is needed in the lifecycle assessment suite developed at ANL. A direct comparison of the NH₃ and LH2 pathways becomes a critical element for project investments. As this is a direct comparison between NH₃ and LH2, it would be helpful to include this comparison in every possible case. For example, slide 8 would be well-suited to include the NH₃ data (shown) overlaid with the LH2 equivalent. With ammonia, the last leg of delivery needs to be properly accounted for in the analysis. In many cases, the end market will require high-pressure GH2 or LH2, which must be factored in after the dehydrogenation step.
- A wide range of production and transportation strategies were considered, providing a complete picture of the different options for using ammonia as an energy carrier.

Question 2: Accomplishments and progress

This project was rated 3.6 for its accomplishments and progress toward overall project and DOE goals.

- The HDSAM modeling tool was successfully updated specifically for ammonia applications, providing a comprehensive techno-economic model evaluating production, transport, and decomposition. The new Hydrogen Carrier Scenario Analysis Model (HCSAM) tool provided insightful cost results for transporting ammonia using various delivery options (trucking, pipeline, rail, and ocean vessel). The analysis also includes decomposition costs of NH₃ by case study region, which provides a more thorough look at the larger picture of NH3 transport and conversion to useful hydrogen.
- NH₃ transport is better than hydrogen—this is a very important finding. Pipeline vs. rail vs. truck is an interesting comparison and very useful for Regional Clean Hydrogen Hubs (H2Hubs). Ocean tankers are the lowest-cost option at <50 cents per kilogram. NH₃ cracking—Ni vs. Ru and 800°C vs. 550°C—yields 35 cents per kilogram, which is very promising. A very good tool is emerging to compare H2Hubs options for hydrogen infrastructure.
- The goals for this comparison are clear and have been well-articulated by the study. Expanding the scope to evaluate the carbon footprint of the NH₃ and LH2 pathways would add an interesting and necessary part of the analysis.
- The project carried out a very detailed analysis of the various factors affecting the use of ammonia as an energy carrier.

Question 3: Collaboration and coordination

This project was rated **3.6** for its engagement with and coordination of project partners and interaction with other entities.

- ANL has been the leader in this type of assessment and is considered the standard for developing tools and comparisons for these pathways. Having industry input to validate the methodology is critical, and it is good to see that this input has been included.
- Overall, collaborations on this project are strong and appropriate for the highlighted scope. The project references external sources of information from consultants, DOE's Hydrogen and Fuel Cell Technologies Office (HFTO), and industry experts. Other NH₃ cracking technologies are currently being modeled in Aspen Plus for incorporation in HCSAM, in coordination with Dennis Papadias from ANL.
- This work relies heavily on collaboration with industry to determine all the costs that factor into the analysis.
- NH₃ industry experts may help fine-tune the model. Compression station sizes will be different for each mode of transport.

Question 4: Potential impact

This project was rated **3.6** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The project is providing a comprehensive techno-economic assessment of NH₃ production, transport, and decomposition through a new modeling tool (HCSAM) that will eventually be released to the public. The results are valuable for assessing the viability of NH₃ use in hydrogen applications.
- This work is critical to understanding what the current state of the art costs and what areas of research the community should focus on to drive down costs. The work also provides a solid and necessary basis for comparing various technologies.
- The continued development of the tools and analysis of pathway economics is important as we make the long-term investments necessary to make hydrogen a national and international commodity. In addition to evaluating the greenhouse gas (GHG) impacts of these pathways, there is a similar need to conduct economic evaluations on an equivalence basis for comparison.
- Hydrogen infrastructure is a critical element for delivering hydrogen cost-effectively. The modes being evaluated are very competitive and practical. This analysis tool is valuable.

Question 5: Proposed future work

This project was rated 3.3 for effective and logical planning.

- It is great that HCSAM will be publicly available so interested parties can run their own scenarios and leverage all of this work. There is increasing discussion about methanol as an energy carrier, particularly for shipping via ocean tankers, so this addition would be worthwhile.
- The future work actions listed in the presentation are appropriate for the scope of work. The project should work to release HCSAM to the public by the end of the fiscal year, model NH₃ cracking technologies in Aspen Plus/HCSAM, and consider incorporating additional hydrogen carriers for incorporation in HCSAM.
- It would be beneficial to consider comparing the small hydrogen user (shown on slide 19) with a large user where onsite NH₃ cracking could make more sense. This comparison would be particularly relevant for power generators, steel, refineries, etc. Moreover, making similar comparisons with a methanol pathway and accounting for the capital expense uncertainty with respect to LH2 and NH₃ might be useful.
- The work is nearly complete. The proposed remaining effort is consistent with open items.

Project strengths:

- The HDSAM modeling tool was successfully updated to HCSAM, specifically for ammonia applications. The new model provides a comprehensive techno-economic tool for evaluating production, transport, and decomposition of NH₃. The HCSAM tool provided insightful cost results regarding the transport of ammonia using various delivery options (trucking, pipeline, rail, and ocean vessel). The analysis includes decomposition costs of NH₃, which provides a more thorough look at the larger picture of NH₃ transport and conversion to useful H₂. Overall collaboration on this project appears appropriate for the scope. The project is referencing outside sources of information from consultants, HFTO, and experts from industry.
- The comparative evaluation of NH₃ versus LH2 and GH2 is very valuable. The modeling tools are based on good assumptions; flexibility for new applications is very good. All modes of transport are included—a very important aspect.
- A very detailed analysis was carried out accounting for the various factors affecting the use of ammonia as an energy carrier, providing stakeholders with information on how it compares to transporting GH2 and LH2 via various means.
- The team consists of recognized leaders in the field, and this work adds to the portfolio of studies previously developed.

Project weaknesses:

- GH2 cost at \$1/kg is the future goal and an important one. However, it would be beneficial to include transition cost numbers. Currently, in California, the cost of GH2 delivered to a fuel cell vehicle is well above \$30/kg. It is not clear how the project includes LH2 benefits in dispensing; no pre-cooling is required. It may be worth considering NH₃ vs. hydrogen safety costs during loading and unloading, insurance costs, etc.
- More information about the uncertainty in assumptions would be useful to the community. It would be helpful to incorporate uncertainty and propagate it through the models so we have a better idea of how sensitive the output is to a specific assumption and how settled or certain the assumption is.
- The project should work to incorporate updated cost data from industry, partners, and DOE, as appropriate. This omission remains a challenge for all projects related to total cost of ownership in the hydrogen space.

Recommendations for additions/deletions to project scope:

- While not related to the scope of the project, the following safety comments might be considered for future reporting on NH₃ transport methods. In this reviewer's experience, there is a significant concern from the rail and trucking industries regarding the transport of ammonia because of safety concerns. Rail organizations have specifically communicated that transport of ammonia is a non-starter because of many observed fatal safety incidents. The analysis completed on this project is appropriate and informative regarding the chosen metrics.
- This tool is very valuable. A webinar for potential users would be beneficial and would provide valuable guidance to individual H2Hubs, as well as new technology start-ups, in evaluating economic benefits. In the future, perhaps compression stations for pipelines may be included.
- GHG emissions should also be tracked and reported for each of the processes, as the main goal of transitioning to hydrogen as an energy carrier is to reduce GHG emissions.

Project #IN-034: HyBlend: Pipeline Cooperative Research and Development Agreement (CRADA) Cost and Emissions Analysis

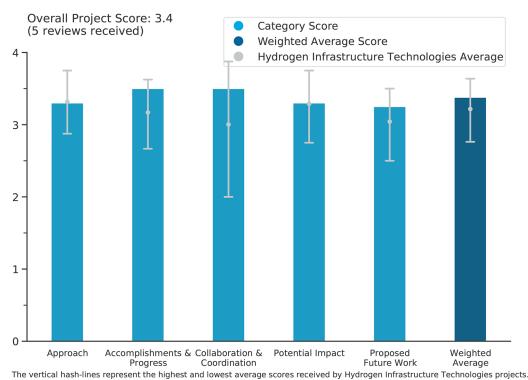
Mark Chung, National Renewable Energy Laboratory

DOE Contract #	WBS 8.6.2.1
Start and End Dates	10/1/2021–9/30/2024
Partners/Collaborators	Argonne National Laboratory, Sandia National Laboratories, Pacific Northwest National Laboratory, Air Liquide, Chevron Corporation, DNV, Enbridge Inc., Electric Power Research Institute, ExxonMobil, GTI Energy, Hawaii Gas, Hydril Company, National Grid, New Jersey Natural Gas, ONE Gas, Inc., Pipeline Research Council International, Sacramento Municipal Utility District, Southern Company, Stony Brook University, Southwest Research Institute
Barriers Addressed	Inconsistent data, assumptions, and guidelinesInsufficient suite of models and tools

Project Goal and Brief Summary

This project will develop tools to quantify the economic and environmental impacts of blending hydrogen into U.S. natural gas (NG) pipelines. Existing national laboratory tools (e.g., the Hydrogen Analysis [H2A] model) will be leveraged to estimate and quantify the value proposition with the goal of accelerating early-market hydrogen technology adoption and short-term emissions reduction. Scenarios will be designed to evaluate the application of hydrogen blending across different sections of the U.S. NG pipeline system, helping to provide pipeline operators with a pathway to converting existing assets into clean infrastructure.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- This project represents a good adaptation of the existing DOE/lab tools to address the key issues of cost and emissions from blended delivery systems. The modeling basis is well-founded and based on previously proven models that provide a strong basis for continuing this work.
- The project team has an excellent approach to evaluating the costs, life cycle emissions, and benefits of blending hydrogen into NG pipelines. The approach includes three processes: modeling, designing, and quantifying.
- This project is well-thought-out, well-organized, and appropriately focused on meeting the targets. The included cost analysis and attention to detail in the three ASME design approaches are very good. This work clearly shows the techno-economic analysis (TEA) values, given the concentration mix and design approaches. It is somewhat intuitive that cost goes up with increased hydrogen concentration and up with increased hydrogen addition. The detail, however, showing TEA for different designs (no fracture, option A, and option B) is instructive. Options A and B will require lab work; no fracture produces a base case. This project is very well-executed, but there are issues. There is no mention of diversity, equity, inclusion, and accessibility (DEIA) in the description of the work. Even if the work itself lacks DEIA considerations, the application of the work to make hydrogen blending both safe and cost-effective is relevant to DEIA principles.
- The project's approach, based on open-source modeling, incorporates the two key components of TEA and greenhouse gas life cycle analysis. The model can then be applied on various scenarios of hydrogen blend rates, end uses, locations, and pipeline design options.
- The issue of rotational machinery used to generate power as an end-use technology is often overlooked in discussions of blended fuels. Turbines used for this purpose are prone to developing acoustic interactions between the combustion process and the power turbine blades. This interaction is a function of the chemical ignition delay time and the rotation of the turbine. Turbine manufacturers are well aware of this issue and can design their machines to function with a given set of characteristic times. For example, a turbine can be designed to operate well in San Francisco, but the same turbine may not operate as well in Texas because the chemical makeup of the fuel is different and thus the chemical kinetics are different. The addition of hydrogen to the NG fuel dramatically changes the kinetics, but it can be designed for with a stagnate mixture space so that it is not a problem. However, if the concentration is dynamically changed, there could be a major problem in that one can easily drive the acoustic resonance to the limit cycle. This issue, at minimum, needs to be discussed by the project team.

Question 2: Accomplishments and progress

This project was rated 3.5 for its accomplishments and progress toward overall project and DOE goals.

- The project team's progress toward the goals and milestones is outstanding. The ASME design space is well-covered, and the base case with additional designs (i.e., no fracture base case, parallel piping, and additional compressors) considered is well-done. The study includes the effects on criterion emissions (NOx). The project team points out the overwhelming contribution to the NOx emissions is done at the production and at the consumption side of this transport issue, which should put to rest the criticism that the pipe distribution system is a significant contributor. This is well-done.
- This project represents one of the biggest accomplishments to meet DOE goals with respect to life cycle emissions blending hydrogen with NG.
- The release of the tools for others to use is an important step, as more users will provide feedback and validation of the HyBlend toolset.
- The cost and greenhouse gas analysis results from the Blending Pipeline Analysis Tool for Hydrogen (BlendPATH) are clearly demonstrated for a range of hydrogen blend rates. The application to the two specific case studies is especially useful. However, the assumptions for the synthetic NG are unclear.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- It was good to see that the authors used existing project data and industrial partner input on projects for validation, as this information was lacking in past presentations and thus a perceived weakness.
- The project includes excellent collaboration and coordination with other entities such as the DOE national labs and industry stakeholders, as well as knowledge-sharing through meetings and seminars.
- The project team describes great collaboration and coordination.
- The laboratory consortium for this work is excellent; it is the correct balance of modelers and material scientists needed to execute this work. The industrial partners mix is very good for pipeline consideration. However, the list of industrial entities did not include any end users (turbine manufactures specifically), and this project needs to include that sort of talent.
- The collaboration with several industry partners from various sectors (e.g., industrial gas, energy producers, utility companies, non-profits, universities, and research institutions) led by principal investigators from four national labs is very impressive. However, the relative contribution from the industry partners is not clear from the presentation.

Question 4: Potential impact

This project was rated 3.3 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- This project has significant potential impact toward the future with respect to achieving the Hydrogen Program goals and objectives. The market impact can be determined by modeling the economic impact and life cycle emissions associated with blending hydrogen, designing and evaluating various scenarios to evaluate the hydrogen blending, and quantifying the value of the hydrogen blended.
- Hydrogen blending is becoming an increasingly important part of the hydrogen ecosystem and, in the case of power generation, is likely to be accelerated in the coming years with the new U.S. Environmental Protection Agency power plant rulings.
- The potential impact of the model is significant, especially for early adoption cases in which there are limited upgrades to existing pipeline infrastructure and end-use equipment.
- The project is well-focused and has made excellent progress in achieving the stated project goals.

Question 5: Proposed future work

This project was rated 3.3 for effective and logical planning.

- The proposed future work is excellent and has much potential. For example, the TEAs will include development of a model to assess the feasibility of blending hydrogen and reflect changes to any standards. In addition, the life cycle assessment will investigate the impact of global warming potential on hydrogen life cycle emissions of blended hydrogen and any pipeline upgrades and modifications.
- The project will end in September and, short of final documentation and release, is essentially complete.
- The proposed work is an appropriate extension of the current effort. It is exciting to see HyBlend fully in the public domain, but the project team must give attention to the end-use combustion systems, particularly rotational machinery.
- The proposed work is reasonable for achieving incremental improvements. However, it is not clear what the basis is for extending model capability to assess higher blends up to pure hydrogen.

Project strengths:

• The modeling effort is well-balanced and is simply excellent—typical of the Argonne National Laboratory work. The project work is strengthened by the inclusion of the materials science (Sandia National Laboratories and Pacific Northwest National Laboratory). This is excellent.

- The project's strengths include the use of real pipeline and industry validated test cases. This is a good extension of existing, proven DOE toolsets.
- The project has considerable strengths, including the team's modeling, designing, and quantifying.
- The project's strengths are strong collaboration with industry and the well-framed basis and objectives for building the tool.

Project weaknesses:

- The project team's inclusion of TEA and life cycle analysis on the synthetic NG production options should not be given that much space, given that there are no synthetic NG markets to speak of. It is unusual to see that the model's TEA output in gas cost uncertainty bars for the established fossil NGs and future fuel synthetic NG (at least as shown for ethanol and ammonia) look the same.
- The project has challenges with respect to obtaining the test emission data on NG and hydrogen production, usage, and transportation with various blending ratios. It is also difficult to obtain gas transmission pipeline data since such data are considered critical infrastructure information.
- This project must include analysis of the end use of this blended fuel. The behavior of stationary burners, boilers, etc. is of interest, particularly the behavior of rotational machinery as a varying function of hydrogen concentration.

Recommendations for additions/deletions to project scope:

- The project team should consider the following additional scenarios for future modeling:
 - A scenario with multiple hydrogen injection points along the NG pipeline scenarios in which the blend rate may vary by pipeline segment. In practice, this scenario is more likely to occur than a single upstream hydrogen production facility that can satisfy the high blend rates to a typical NG pipeline volume. An additional challenge is to model these small hydrogen production sources with potentially varying carbon footprints along the pipeline route (with or without hydrogen storage).
 - A scenario in which there may be more than one end use with potentially different "optimal" blend rates, because the current scenarios seem to assume a single end use with a fixed blend rate at the initial hydrogen injection point.
- Expansion beyond 30% blending has some potential and should be included in the next steps. These higher concentrations bring in many more challenges beyond the modeling work (i.e., metallurgy, pipeline assessments, burner impacts, compression).
- The project team should include a discussion of the combustion characteristics as a function of dynamically varying the hydrogen concentration. The rotational machinery is of particular concern.
- The reviewer looks forward to Phase II of the project.

Project #IN-035: HyBlend: Pipeline Cooperative Research and Development Agreement (CRADA) Materials Research and Development

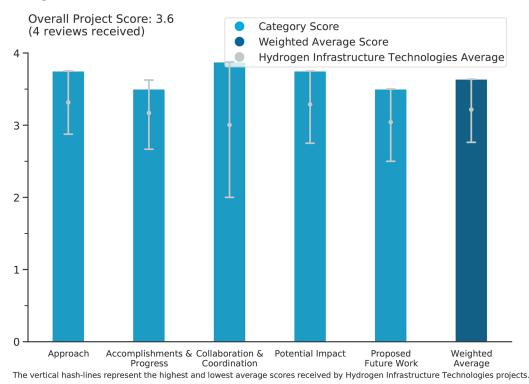
Chris San Marchi, Sandia National Laboratories

DOE Contract #	WBS 8.6.4.2
Start and End Dates	10/1/2021–9/30/2023
Partners/Collaborators	Argonne National Laboratory, National Renewable Energy Laboratory, Pacific Northwest National Laboratory, Air Liquide, Chevron Corporation, DNV, Enbridge Inc., Electric Power Research Institute, ExxonMobil, GTI Energy, Hawaii Gas, Hydril Company, National Grid, New Jersey Natural Gas, ONE Gas, Inc., Pipeline Research Council International, Sacramento Municipal Utility District, Southern Company, Stony Brook University, Southwest Research Institute
Barriers Addressed	Inconsistent data, assumptions, and guidelines

Project Goal and Brief Summary

This project aims to provide a scientific basis for the assertion of pipeline safety for hydrogen service. More specifically, the project aims to develop a scientific understanding of variables and mechanisms that contribute to hydrogen-induced degradation of piping and pipeline materials. National lab capabilities will be leveraged to examine materials performance in hydrogen environments, and the project will design probabilistic analysis tools to quantify the structural integrity of pipeline networks for hydrogen service. Converting networks for hydrogen blending within the natural gas pipeline system may offer a low-cost pathway to distributing clean hydrogen, and the data gathered for this project will help ensure the safety of decarbonized energy infrastructure for both transitional and long-term strategies of hydrogen conveyance.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.8** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project has a vision for (1) the development of science-based probabilistic analysis tools to quantify structural integrity of piping and pipelines for hydrogen and (2) providing community guidelines for structural integrity of pipelines carrying pure hydrogen or hydrogen blends with natural gas. This vision serves the DOE goals for safe and reliable hydrogen infrastructure and decarbonization. In the area of polymer research and development, the project aims to study slow crack growth behavior for lifetime prediction by understanding how hydrogen affects the molecular structure of polyethylene materials. These studies also serve the DOE goals. The development of a probabilistic life prediction model, as outlined on slide 12, is promising for assessing structural integrity and reliability. However, the use of results from accelerated testing with polymers vis-à-vis reliability should be validated. On the other hand, the development of the probabilistic lifetime prediction tool, along with subscale component testing and hydrogen-assisted fatigue and fracture, is a well-thought-out approach. The description and status of this approach (shown on slide 14) is very satisfactory.
- The project's proposed approaches are directly addressing key needs for pipeline infrastructure, especially with respect to (1) developing tools that can help users predict pipeline infrastructure lifetimes and (2) implementing work into industry standards and code cases.
- The metals activities for the HyBlend initiative, similar to those of the Hydrogen Materials Consortium (H-Mat), are shifting to support real-world deployments. The Hydrogen Extremely Low Probability of Rupture (HELPR) platform could be a great tool for industry.
- The project approach is reasonable and effective for the stated goals. There are several points that could use clarification:
 - Regarding HELPR, whether there is availability to handle the variable amplitude loading, with transients going from different environments.
 - Whether, going forward, there is flexibility to incorporate the data for different frequencies and R ratios that were generated.
 - Whether HELPR is configured to take into account the load and environment spectrum shown on slide 15.
 - Regarding the internal versus external flaws, whether the project team assumed a homogenous distribution and the same growth kinetics—although perhaps this information is not relevant.
 - Regarding the smaller-scale test, whether the project team focused on initiation or growth or whether the team seeded a flow. The issue with smaller-scale tests will be much more prevalent for initiation where the distribution of defects is constrained as compared to growth, which should work well.
 - Whether the project team has started to think how this would transition into structural management.
- Whether the difference between the internal and the external flaw cases is the contribution of hydrogen at the crack tip in addition to the charged hydrogen (if present).
 - Whether the project team has any plans to use the sub-scale test to look at the oxygen impacts.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals.

- The project team has made great progress on all fronts. The full release of HELPR, successful implementation of sub-scale testing for metallic pipes, vintage pipeline work, and measurement/modeling of crack growth in polymer pipes are all exciting developments.
- The project team has made excellent progress since last year.
- The project team has presented good accomplishments and good progress toward project goals. It is unclear why a Phase II was necessary for the project since it was initiated under a cooperative research and development agreement.

• In the area of polymer research and development, the project found that slow crack growth behavior depends on the polyethylene resin system and how hydrogen affects crystallinity by affecting chain mobility. However, it is not clear why hydrogen may improve or hinder performance, as slide 10 presented results without further explanation. The development of accelerated testing (outlined on slide 11) needs to be justified because polymers are rate-sensitive. The experimental studies and results at Sandia National Laboratories on hydrogen's effect on pipe failure in the presence of internal or external defects are state of the art. However, it is not clear why the threshold stress intensity factor range for crack growth is the same in hydrogen and air, as previous literature (e.g., Suresh and Ritchie) indicates otherwise and indicates a strong dependence on R ratio.

Question 3: Collaboration and coordination

This project was rated **3.9** for its engagement with and coordination of project partners and interaction with other entities.

- The project's collaborations and coordination with ASME, the Electric Power Research Institute, Oak Ridge National Laboratory, Southwest Research Institute, Det Norske Veritas (DNV), and industry (e.g., the Southern California Gas Company) ensure its relevance and real-world impact.
- The project team is broadly involved with key industry stakeholders (e.g., joint industry projects and the Pipeline and Hazardous Materials Safety Administration) and provides support in a number of capacities.
- The project has strong collaborations and coordination with relevant industry players.
- The project is highly collaborative, and its collaborations are integrated well.

Question 4: Potential impact

This project was rated **3.8** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The project's life prediction interface and the data it generates will be critical to the design and management of pipelines.
- The open-source probabilistic tool for failure assessment of both polymeric and metallic materials holds promise for the future of reliable hydrogen transport and use.
- The impact of the project is clear. There are strong impacts in a number of areas.

Question 5: Proposed future work

This project was rated 3.5 for effective and logical planning.

- The proposed future work is well-aligned with current work outputs. The metals team has made significant progress in developing and implementing consensus relationships for fatigue cracking, which should be an area of focus for the polymers side wherever possible.
- Future work on hydrogen-induced morphological changes in polymeric materials, and the attendant effects on polymer viscoplasticity, is required for the development of crack growth models. For the case of metallic materials, the study of welded microstructures is highly important, Conversely, it is unclear where and how the investigation of hardness can provide any additional input to understand and quantify hydrogen-induced fracture.
- The future work is a reasonable extension of the current progress.

Project strengths:

- This project has clear goals and impressive data generation. It addresses important knowledge gaps to enable safe implementation of its science. The project team's use of low-energy electron microscopy builds off of well-developed science for this application.
- The development of the probabilistic lifetime prediction tool, along with subscale component testing and hydrogen-assisted fatigue and fracture, is a well-thought-out approach and an important and impactful accomplishment.

• The project team is top-notch, and the questions being addressed are of technical relevance. The development of HELPR is a significant achievement and should continue to be refined with additional capabilities moving forward. For example, it would be useful to implement multiple fatigue crack growth relationships for environmental spectrum conditions.

Project weaknesses:

- The project team needs to continue to refine the modeling capability to capture all of the subtleties of the application. The modeling approach also needs additional verification and proof-testing.
- The project team did not include a plan to assess the hydrogen effects on polymer viscoplasticity toward understanding and modeling slow crack growth.

Recommendations for additions/deletions to project scope:

• The project team needs to justify and assess the reliability of developing accelerated testing (outlined on slide 11) regarding polymer research and development. This assessment is needed because polymers are rate-sensitive. It is unclear whether the project team has assessed the reliability of using accelerated test results for probabilistic life prediction, which needs to be thoroughly investigated.

Project #IN-036: Cost-Effective Pre-Cooling for High-Flow Hydrogen Fueling

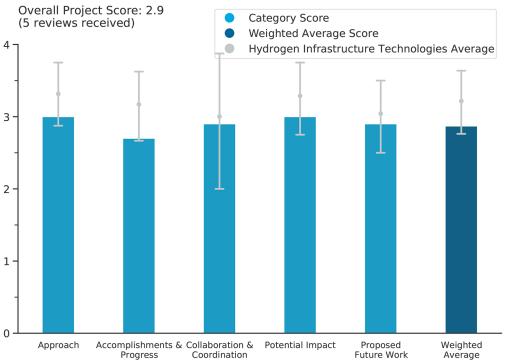
Devin Halliday, GTI Energy

DOE Contract #	DE-EE0009625
Start and End Dates	8/1/2022–7/31/2025
Partners/Collaborators	Creative Thermal Solutions, Argonne National Laboratory
Barriers Addressed	Lack of commercial pre-cooling technology

Project Goal and Brief Summary

This project aims to deliver a validated high-flow chiller design for heavy-duty (HD) hydrogen fueling stations. The product will be designed to withstand evolving regulations. Researchers will begin by developing a detailed understanding of requirements and use the findings to identify the optimal configuration. A pilot-scale chiller will be constructed for testing, and results will be used to update the design. The final stage is technology transfer activities to ensure market adoption.

Project Scoring



The vertical hash-lines represent the highest and lowest average scores received by Hydrogen Infrastructure Technologies projects.

Question 1: Approach to performing the work

This project was rated **3.0** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

• The approach to the work is well-designed to address some of the barriers facing the HD fueling space, including the need for high-throughput hydrogen, at a reasonable cost of capital and energy intensity and the use of environmentally friendly refrigerants. The team has done an effective job of planning the work through the three-year term to include defining the duty cycle, down-selecting refrigerants, designing the

system, and testing it at the sub-scale level. There is good mention of the process safety management system employed, along with an expectation that the safety plan will be reviewed by the Hydrogen Safety Panel. There was no mention of a diversity, equity, inclusion, and accessibility plan and community benefits plan (CBP), so presumably they were not required for this effort.

- The team has taken a thoughtful approach, with steps to ensure that the chiller will meet market demands.
- The approach appears to be sound and well-constructed.
- This project provides an overall good approach to the design, build, and demonstration of a high-flow chiller design ready for manufacture and installation in an HD fueling station. The methodology to scale the design by one-fifth allows the project to save on costs. The original scope provided estimates on key performance metrics (precooling temperature, average pressure ramp rate, system volumes, etc.) that were based on DOE Hydrogen and Fuel Cell Technologies Office (HFTO) truck targets and the Argonne National Laboratory (ANL) Hydrogen Station Cost Optimization and Performance Evaluation Model (H2SCOPE). New medium-duty (MD)/HD fueling protocols are now available in either published form or draft form. The key design metrics should be updated to meet MD/HD fueling protocol and industry requirements as appropriate. While in most scenarios, -40°C fueling is not required for 700 bar systems, targeting -30°C for a design metric does not fully account for the range of fuel delivery temperatures that might be required in fast-flow fill scenarios. The decision to use -30°C relies on ANL's analysis and appears not to align with DOE HFTO truck target precooling requirements (the only other metric available at the time the project was funded). The project should reach out to organizations performing fast-flow fueling research and development (R&D) (i.e., the National Renewable Energy Laboratory [NREL], SAE International [SAE], European Union [EU] Protocol for Heavy-Duty Hydrogen Refuelling [PRHYDE], and the FirstElement Fuel (FEF) Oakland project) to assess design requirements, performance metrics, and computational fluid dynamics (CFD) results based on current DOE HFTOfunded work.
- It is unclear why the cycle that matches duty the best is not selected before determining the optimal refrigerant. The team should consider trying the liquid overfed refrigerator paradigm instead of cascade/ liquid suction on the lower stage. The cold liquid refrigerant storage tank with a variable speed pump is particularly advantageous for transient cooldown problems like this one. The reserve tank capacity can be increased depending on demand, allowing for more flexibility in selecting the compressor, which can be continuously operated at lower power draw and would not require a second hydrogen heat exchanger. This approach could even be done on both loops to handle peaking. It is not clear why cascade was selected over other approaches. The liquid overfed paradigm is also particularly advantageous for ammonia-based refrigerants, as was selected.

Question 2: Accomplishments and progress

This project was rated 2.7 for its accomplishments and progress toward overall project and DOE goals.

- The project makes good progress toward addressing DOE goals, such as building clean infrastructure, lowering greenhouse gas (GHG) emissions, achieving lower-priced hydrogen at the pump, and providing pathways to private-sector uptake. The project is highly relevant to supporting HD fuel cell truck rollouts in the near term, which are needed for rapid deployment of modular HD fueling stations and the modification of existing large inventory hydrogen sites, such as at bus depots and forklift facilities, where hydrogen may be fueled only at ambient temperatures.
- The overall accomplishments and progress appear appropriate for the original project plan. Significant advancements have been made in the MD/HD fueling infrastructure realm, and the project should realign with recently released fueling protocols (i.e., SAE J2601 and MCF-HF-G [(MC Formula High Flow General]) and available R&D data.
- The team used modeling to estimate the performance of the system using different configurations and working fluids. It would be nice to see numbers associated with the different options. Rather than state that option X is slightly better than option Y, it would be good if the exact metrics and their values from the modeling were shared.
- No design calculations were presented showing the suitability of the heat exchanger effectiveness or number of transferred units. It would be helpful to know the minimum heat exchanger performance

required for the design to be successful. The SAE J2601 refueling standard requirements do not prefer - 30°C; it is not just an "industry-leaning" sort of thing.

• While some progress has been made, the project appears not to be moving rapidly forward, and it is unclear why more progress has not been made.

Question 3: Collaboration and coordination

This project was rated **2.9** for its engagement with and coordination of project partners and interaction with other entities.

- The project appears to be well-coordinated and well-communicated.
- The project has good collaborations with Creative Thermal Solutions and ANL, but it would be good to see a commercialization partner early on so that the team does not go down a path that is not viable and the commercial partner learns from the design process.
- The project team has been coordinating efforts with ANL and a prototype manufacturer specializing in refrigeration/cooling system design, but no commercialization partner has been identified yet.
- The project has a fine team involving national laboratories, companies, and GTI Energy. The fact that there is still no industry partner for technology transfer and commercialization is troublesome; this should be emphasized to continue project progression. Involving universities could help with CBP outcomes while training future researchers.
- The project should consider collaborations or consult with outside organizations working on HD fast-flow fueling work. Other DOE HFTO-funded work in this area could provide key information to the project regarding design requirements and specifications. Real-world data now exist for HD fast-flow events with published fueling protocols. Also, it is unclear whether the partner organizations are capable of supplying hydrogen gas at the required mass flow rates and/or pressure ramp rates required under new HD fueling protocols.

Question 4: Potential impact

This project was rated 3.0 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The potential impacts of the successful development of the cost-effective pre-cooler include meeting DOE goals for supporting GHG reduction and reduced capital and operating costs (which translate to lower hydrogen costs to the customer). The technology is highly relevant to achieving these goals, and the project itself is making good progress in meeting its objectives.
- The overall project potential and impact/relevance are good and will hopefully lead to a scalable high-flow chiller design ready for manufacture and installation in an HD fueling station. Reliable, higher-efficiency, and lower-cost chillers are critically needed by industry.
- Development could lead to more reliable and low-cost infrastructure, if this project works out.
- The ability of the proposed cycle to match or address surge requirements is not clear. If the cycle cannot address these requirements, it is unlikely to have a significant impact or be enabling for industrial partners.
- It is still unclear what the best hydrogen storage system will be for HD trucks and, therefore, how relevant this work is to the future of HD filling with hydrogen.

Question 5: Proposed future work

This project was rated **2.9** for effective and logical planning.

- The barriers to this effort are well-understood and include understanding the duty profile, giving due consideration for upcoming standards for refrigerants, and understanding the impacts of new fueling protocols on the design. Each of these potential barriers has been addressed in the future work plan.
- The future work plan seems logical.
- The overall proposed future work proposed is adequate for the original scope of the project. The presenter mentioned that the project will work to realign with recently published fueling protocols and reassess the overall design requirements and specifications. The project should consider collaborations or consult with

outside organizations working on HD fast-flow fueling work to integrate lessons learned and leverage R&D data. It is unclear whether the partner organizations can complete HD fast-flow fueling experiments with the demonstration system (a non-trivial task with current technology limitations).

- "Future" work cannot be projected when existing work is still in process.
- The project did not show modeling results indicating that it is on track to meet the milestones or what minimum performance metrics are required for the low-stage unit to be considered successful.

Project strengths:

- This project provides an overall good approach to the design, build, and demonstration of a high-flow chiller design ready for manufacture and installation in an HD fueling station. The methodology to scale the design by one-fifth allows the project to save on costs. The project partners appear well-aligned and well-coordinated to execute the original scope of work.
- Project strengths include a well-defined project plan with a sound overall approach to the project deliverables, including a definition of the requirements, design iteration loops, testing using a subscale specimen, etc. The project team is strong, and the future work is reasonable, given the potential barriers at play.
- The project includes a simple, low-cost approach that should be able to be commercialized. The ability to adapt to liquid overfed or include thermal mass of heat exchanger in analysis is a bonus.
- The project uses modeling to guide the project direction and subdivides the different component testing to de-risk the final design.
- This project addresses a need and is laid out logically. The leading partners are appropriate.

Project weaknesses:

- A minor project weakness is the need to identify a commercialization partner, but the barrier should be surmountable.
- Basic specifications of the heat exchanger, such as minimum effectiveness or number of transfer units, are essential. The presenter said the supplier did not provide these numbers; as the system integrator, the presenter calls the shots on the specification. The project team should know the minimum heat exchanger performance metrics and how easily the heat exchanger hits the requirements.
- The project should provide more details about the modeling work since these details are driving the design. The approach and software used are unclear. The results from the modeling should be shared. It is unclear what metrics were used to go one direction or the other. The values for each of the options should be compared.
- The key design metrics should be updated to meet new MD/HD fueling protocol and industry requirements as appropriate. While in most scenarios, -40°C fueling does not appear to be a hard requirement for 700 bar systems (and is more than adequate for 350 bar systems), targeting -30°C for a design metric does not fully account for the range of fuel delivery temperatures that might be required in fast-flow fill scenarios. The project team should reach out to organizations performing fast-flow fueling R&D (i.e., NREL, SAE, EU PRHYDE, and the FEF Oakland project) to assess design requirements, performance metrics, and CFD results based on current DOE HFTO associated work. This information would provide further justification for this design choice. It is unclear what size fueling infrastructure and demand profile was used in the modeling to align the precooling design requirements and specifications. It is unclear whether the partner organizations can complete HD fast-flow fueling experiments with the demonstration system (a non-trivial task with current technology limitations). This work should be addressed in future project updates.
- Progress seems limited. Until additional progress is made, no projections can be made.

Recommendations for additions/deletions to project scope:

• There are no suggestions. The team has a good grasp of the performance metrics expected for HD fuel cell vehicle fueling: 70 kg dispensed, 10 kg/min, T30 (-33°C to -26°C) cooling, and ambient temperatures of 20°C and 40°C. Excellent effort is shown, and the project should keep going.

- The project team should consider consulting other organizations performing fast-flow fueling R&D (i.e., NREL, SAE, EU PRHYDE, and the FEF Oakland project) to assess design requirements, performance metrics, and CFD work. Outside partner organizations could help answer the questions listed on slide 17 for "Remaining Challenges and Barriers" and provide real-world data. This information could also be used for model validation at ANL.
- The liquid overfed refrigerator paradigm should be considered. It should make everything simpler, even at this late date in the game.
- The project team should consider whether this system could be tested at NREL or a station following the final build.
- The project work should be completed.

Project #IN-039: Analytic Framework for Optimal Sizing of Hydrogen Fueling Stations for Heavy-Duty Vehicles at Ports

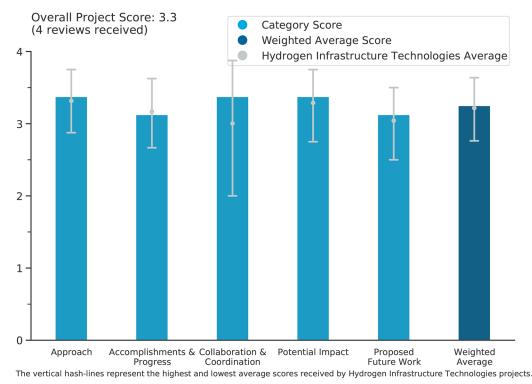
Todd Wall, Pacific Northwest National Laboratory

DOE Contract #	WBS 8.6.5.1
Start and End Dates	3/31/2021
Partners/Collaborators	Sandia National Laboratories, Seattle City Light, Port of Seattle
Barriers Addressed	Initiate transition to clean hydrogen for portsIdentify potential scale-up opportunities

Project Goal and Brief Summary

The project aims to develop a framework and guide for sizing and siting industrial hydrogen nodes at U.S. ports. The work involves designing modular and commercial-scale hydrogen nodes using proton exchange membrane electrolysis, compressed gaseous storage, refueling for fuel cell vehicles, and fuel cell power generation. The project seeks to provide guidance to stakeholders and potential market participants on designing commercial hydrogen nodes, estimating the potential for cost savings and emission reduction, and advancing private-sector participation in clean hydrogen infrastructure.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

• The project has an excellent concept of hydrogen for grid support, refueling, and more. The project also has a great team, good stakeholder engagement, and a good modeling plan. The approach has a modular design

for 300 kg/day using a 770 kW electrolyzer. The assumptions of 10-day resiliency and 10,000 kg storage for the Port of Seattle are good. The peak shaving benefit for both a grid and hydrogen station is a great high-value strategy to use excess power for hydrogen.

- The reworked scope is appreciated; it still has value and is significant, considering extreme power demands at ports. The consideration of power as backup and for fueling/charging equipment (and the balance/ shifting between them) is well-received.
- The project team identified a new approach to accomplishing the project goal related to commercial scaleup and size. The revised approach seems more logical; the capability of the distribution feeder is directly related to the node size, and the team correctly utilizes the electrolyzer sizing to support the analysis. There was no mention of a safety plan or diversity, equity, inclusion, and accessibility and community benefits plan, so presumably they were not required for this effort.
- It appears that the project was hijacked by an electrolysis onsite approach. While the focus is on port grid system robustness, this focus does not have to result in inflexibility regarding production and storage location within the port premises. If this technology concept is to be considered in context, a short pipeline from a nearby location may economically be more optimal and contribute to the robustness of a port system. The revised 2024 approach shows improvement over the original approach, which had too many uncertainties, especially in project context that partners did not receive specifics on port fleet make-up, as well as other future regulations related to power demands (for example, shore power to reduce maritime vessel emissions while docked).

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and DOE goals.

- The team has made good progress despite the early pivot, including the creation of a hydrogen node design for resilience scenario, development of constraints mapping to power availability, and calculations for the levelized cost of hydrogen for a maximum energy purchase price.
- Hourly load data and anticipated growth are useful for hydrogen production economics. Feeder thermal limit versus carrying capacity are useful tools to guide hydrogen. The levelized cost requires that the cost of energy (COE) be \$1-\$2/MWh for \$3/kg, which is a good input to the DOE goal of \$1 per 1 kilogram in 1 decade ("1-1-1") for hydrogen by 2030.
- The project has good outputs on power availability, variability, and options. It has a strong node design on variable uses of said power. Recognition of value beyond price (e.g., production) is significant.
- It is unclear how the mix of different fleet equipment/vehicles came together. The presenter indicated that input was not received; the presenter also did not mention how it is reflective of the Port of Seattle fleet. The fleet emphasis appears to be on "all battery electric" and efficiency at any cost. The coloring of bars and lines in graphs on slide 8 is confusing because the use of the same color for different purposes creates the impression of a relationship (in addition to notation of graph 1 + graph 2 = graph 3). It is only infrequently possible to achieve a minimum hydrogen production cost of \$3.45/kg if \$1.61/MWh is the average electricity price. The project needs more realistic assumptions on the topic of maximum price for electricity or better rationale on why regional actors (Port of Seattle) would be willing to pay this rate, as it appears not to be an economically competitive alternative to using diesel (or renewable diesel) or natural gas (or renewable natural gas) for power production and running the fleet (particularly considering the Pacific Northwest is not California, where rates are already in this range for grid-connected properties).

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- The project includes excellent collaboration among national laboratories, utility and port authorities, and industry. For example, Fortescue is a very strong partner and industry advisor, which will truly benefit the project outcome.
- The project has very nice collaboration. The Port of Seattle and Seattle City Light are key stakeholders; the project has done a great job getting their guidance and real data for modeling efforts. Pacific Northwest

National Laboratory as the project lead is quite effective. The Port of Seattle can use the data for decarbonization and to eliminate pollutants from onshore operations, as well as the ships idling.

- The project has strong laboratory, power, port, and industry partners and reflects the diversity of port and power operations.
- The project would benefit from direct involvement or feedback from the gas utility Puget Sound Energy and terminal and equipment operators. The Port of Seattle should provide an indication of how its actual fleet makeup reflects the project fleet selection.

Question 4: Potential impact

This project was rated 3.4 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The project is highly relevant since port authorities are responsible for significant greenhouse gas (GHG) emissions. There is considerable opportunity to site hydrogen generation and fueling infrastructure there to support the adoption of heavy-duty fuel cell trucks. An analysis of the robustness and availability of distribution feeders to support generation, fueling, and other end uses is critical for ports to achieve GHG reduction goals. The project is very timely and important.
- This concept potentially has a game-changing impact. Multipurpose uses of hydrogen and matching peak versus excess in the grid with hydrogen and fuel cells are very important for hydrogen infrastructure. This project could result in lower-cost hydrogen for grid support and other uses. The project is very well-aligned with DOE goals and is a valuable tool for hydrogen hubs.
- The project has significant impact potential for ports regarding hydrogen and electrical use. The pivot of the project approach is recognized and appreciated. Although the original focus would have been beneficial, the reworked approach still has value and is worth pursuing.
- This worthwhile project will undoubtedly show many interesting outcomes. Based on the apparent choices and focus on "all battery electric fleet/equipment," however, it is unclear to what extent Seattle City Light and the Port of Seattle are considering the inclusion of hydrogen as an option.

Question 5: Proposed future work

This project was rated 3.1 for effective and logical planning.

- The project can be expected to provide a baseline understanding of hydrogen nodes in a port setting from modeling, local preferences, and education perspectives.
- The proposed work is linked well with the project goals and progress made. The project team should review 5–10 years of real operation data to determine load-following capability and its limitations.
- The proposed future work is well-defined and should achieve the objectives of the project, but there are self-identified challenges associated with timing constraints.
- The project team could look into more power details and the publication of results.

Project strengths:

- Project strengths include the high relevance of the topic for GHG reductions at ports, the derivation of tools to assist with designing and sizing commercial nodes for hydrogen generation and fueling, and the strong project team, including excellent collaboration among national laboratories, utility, port authority, and industry advisors.
- The use of an electrolyzer and fuel cell in grid balancing, as well as hydrogen for multiple uses, is very beneficial for hydrogen infrastructure. There is good grid data showing peak at noon and excess at night. Thus, an electrolyzer can use lower electricity cost. Hydrogen can provide grid peak shaving, which creates a better value for hydrogen infrastructure.
- A project strength is the development of an initial framework model for a hydrogen node in a port setting. The project provides insights into how regional policy preferences impact technology solutions choices.

• The project has strong and appropriate partners. It addresses the significant need around ports (power) and diverse energy approaches that can be considered. A project strength is the ability to pivot from the original scope and still have a valuable project.

Project weaknesses:

- The assumption that an electrolyzer can load-follow must be supported by operational data. In general, load-following is likely to impact useful life negatively and may require more maintenance. It is unclear how the project supports the COE of 0.1 cent per kWh, which is too low. The project could have a graph that shows the parametric impact of 1, 5, and 10 cents per kWh. The role of the City in guiding the design basis or module development is unclear.
- It appears that the fleet makeup combination received limited input from port stakeholders. The title of the project is not reflective of the reality of this project, which has emphasis on an "all battery electric equipment fleet" approach with a small addition of a hydrogen refueling station for heavy-duty vehicles.
- A project weakness includes the risk that the total effort may not be finished on time.
- It is not clear why the scope shifted; an explanation should be provided.

Recommendations for additions/deletions to project scope:

- This project is very high-value. Data for port electrification groups should be shared with hydrogen hubs. The project should have a workshop for ports to help them better understand the multiple benefits to them.
- It is recommended that the project results be published. It is also recommended that the project get additional feedback from other related stakeholders on what could be built off this project.
- The project should be completed as soon as possible.

Project #IN-040: The HyRIGHT Project: 700 bar Hydrogen Refueling Interface for Gaseous Heavy-Duty Trucks

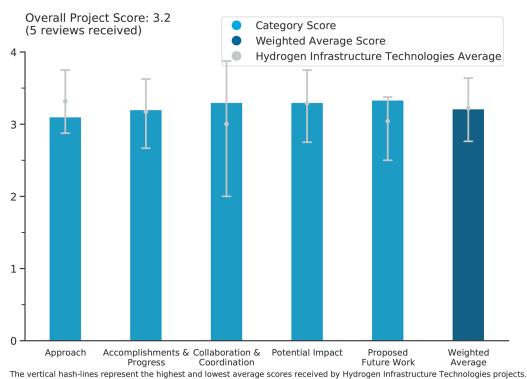
Will James, Savannah River National Laboratory

DOE Contract #	WBS 8.6.3.304
Start and End Dates	10/1/2021–9/30/2024
Partners/Collaborators	Argonne National Laboratory, Sandia National Laboratories, Nikola Motors
Barriers Addressed	 Lack of understanding between precooling performance and cost for high-flow fueling (both station and vehicle impacts) Potential communications cyber vulnerabilities Risks associated with high-flow fueling

Project Goal and Brief Summary

The project aims to support the development of 700 bar hydrogen refueling processes for gaseous heavy-duty (HD) trucks, with a focus on optimizing precooling strategies, creating a cyber vulnerability assessment, and disseminating the results to relevant standards development organizations. By utilizing a dynamic model, the project seeks to develop an optimized precooling strategy based on real-time communications and initial precooling status. The outcome of this project will contribute to the development of fueling protocols for HD trucks, enhancing efficiency and safety in hydrogen refueling processes.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project team has made excellent progress using the presented approach. The reviewer looks forward to the final presentation on this project (per timeline and conclusion of project in September 2024 and its presentation at the 2025 Annual Merit Review).
- Overall, the project approach seems aligned with the original scope of the project. The project covers a diverse set of topic areas within medium-duty (MD)/HD fueling. The direct connection between the various topic areas is somewhat difficult to follow in terms of an overall project end goal. However, research and development within the MD/HD fueling space is critically needed, and the partners/organizations on the project are well-equipped to perform the required analysis and work.
- It is important for the analysis to state the obvious for those trained in the field. For example, it is intuitive that the pressure drop down a pipe is a very strong function of pipe diameter, and indeed it goes approximately 1/d⁵. The hybrid approach to the hydrogen exchange is also intuitive. While it is important to demonstrate this information to those in the audience who are less knowledgeable, it would also be nice to allude to that during the discussion—for example, "Our results clearly show the known dependence on pressure drop due to the pipe diameter (see Figure X)." It is nice to have the well-known demonstrated with specific, detailed calculations. In sum, the team should let the reader know that the authors know that and that the value added here is the application to this specific task. The project did not mention any diversity, equity, inclusion, and accessibility (DEIA) efforts.
- The three aspects of the project (i.e., precooling assessment vs. risk assessment vs. tank testing) seem somewhat disconnected, and it is not clear why these topics are included in a single project, as each has the potential to be a project in itself.
- It is not clear why the project team included computational fluid dynamics (CFD) analysis of the thermal pressure relief device (TPRD) release in the scope, as this seems to deviate from the primary project goal.

Question 2: Accomplishments and progress

This project was rated **3.2** for its accomplishments and progress toward overall project and DOE goals.

- The current accomplishments and results for the dynamic modeling of precooling systems and technoeconomic analysis (TEA) subtasks were addressed, but new information on the cyber vulnerability assessment and standards development was missing for 2024 (2023 information was in the backup slides). The analysis and resulting chart on pipe diameter influence on pressure drop, mass flow rate, fill time, etc. was very interesting and confirms some aspects of fundamental HD station design. The results of average pressure ramp rate, initial tank temperature, and ambient temperature were good to confirm and will be helpful metrics for future HD station and precooling system design. It was unclear whether the SAE J2601-5 fueling protocol was fully implemented for fueling tests or if aspects of the fueling protocol were omitted because of known hardware implementation challenges. It would be great to elaborate more on the level of fueling protocol implementation and highlight any technical challenges or lessons learned (since the protocol was just released to the public). It was unclear how the 300 g/s tests were completed without high-flow hardware, but it appears the FM90 fueling protocol was used, resulting in significant pressure drop. These tests should be redone with an FM300 protocol with high-flow (HF) coupling hardware to confirm variation in flow rate and pressure drop results. The integration of a 90 g/s capable on-tank valve (if understood correctly) is a great addition to the project and a technological step forward for enabling HD fast-flow hydrogen fueling. The thermophysical results will be very interesting to review, especially internal tank temperatures at peak mass flow rate. The partners should consider performing a CFD analysis on the scenario with an SAE/5 fueling profile to confirm safety aspects.
- The reviewer appreciated that the project team used open-source software in Python and HyRAM+ (Hydrogen Plus Other Alternative Fuels Risk Assessment Models).
- At the conclusion of the study, it is still not clear that there is sufficient information to assess the performance or the economics of precooling system designs based on this study alone.
- The accomplished results and progress are not stellar but are on track.

• This note is for DOE. Project H-2041 uses a baseline pipe diameter of 9/16" to assess risks compared to the use of 1" piping throughout an HD hydrogen refueling station (HRS), and the researchers draw conclusions related to safety factors/risks, while this project appears to use 3/4" as the baseline pipe diameter. While this difference is not major, it may be worth considering assessing the use of a consistent piping diameter between projects so the results can align in various areas of research that involve piping.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The project's laboratory partners are good, and the industrial partner is also good. This team is appropriate for the task this project is meant to accomplish.
- The project's group of partners is sufficient, as long as the partners continue sharing results.
- The overall collaboration with other organizations on this project is good. The partners/organizations on the project are well-equipped to perform the required analysis and work. The project should consider leveraging fast-flow fueling data generated by the National Renewable Energy Laboratory (NREL) high-flow facility to assist with modeling and analysis efforts and to compare to Nikola's data.
- It is valuable to have an original equipment manufacturer on the project team, but it would have been stronger if there were a station developer involved as well.
- The project has a great team of several national labs and industry. The team should consider adding academia to the cohort to train future contributors to this field.
- Question 4: Potential impact
- This project was rated **3.3** for supporting and advancing progress toward Hydrogen Program goals and objectives.
- The project works to meet the current administrations goals of the electrification of MD/HD vehicles to reduce harmful emissions and minimize climate change. The project addresses key aspects of hydrogen precooling, cyber vulnerability assessments of vehicle-to-dispenser communications, and assistance to safety, codes, and standards organizations.
- The correct stable application of the fill physics is critically important to the safe and durable fast fill needed for an HD vehicle fill, as well as for the deployment of hydrogen-fueled HD vehicles in our economy.
- The project creates a robust body of knowledge for industry to continue to move forward on the topic of moving toward higher-flow HRS systems for HD applications and to reduce the fueling time for H70¹ fueling.
- The project has great results showing filling while meeting SAE J2601, backed up with experimental verification.
- Hydrogen precooling remains a critical issue for refueling and is even more challenging when applied to the HD markets. This project is relevant to better understanding these issues.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The project team's correct stable application of the fill physics is critically important to the safe and durable fast fill needed for a HD vehicle fill and critically important to deploying hydrogen-fueled HD vehicles in our economy.
- The project intends to finalize testing for the FM90 and FM300 fueling rates with SAE/5. The presentation was missing updates on the future status of the other associated project subtasks. Any future work completed on cyber vulnerability assessment of vehicle-to-dispenser communications could be very

¹ The H70 designation indicates a dispensing pressure of 70 Megapascals (MPa).

valuable to the newly created International Organization for Standardization (ISO) 19885-3 sub-working group.

- In context of the use of H70 hardware and the FM90 fueling protocol to achieve the accomplishments presented, it is unclear whether the project team will repeat some of the tests with the FM300 protocol when the H70HF interface hardware is available.
- The project is essentially in its final stages, with completion planned for the end of this summer.

Project strengths:

- Research and development within the MD/HD fueling space is critically needed, and the partners/ organizations on the project are well-equipped to perform the required analysis and work. The project leverages upgraded legacy modeling tools from Argonne National Laboratory and brings in other sources of information from industry, the DOE Hydrogen and Fuel Cell Technologies Office, and other organizations. The current accomplishments and results for the dynamic modeling of precooling systems and TEA subtasks were addressed. The results provided were informative and will be a helpful metric for future HD station and precooling system designs. The project integrated the newly released SAE/5 fueling protocol into the test results.
- This project covers a long overdue area of research, and the results have been shared publicly.
- The topic is critical to HD station developers.
- This project includes a great partnership between a national lab and a leader from industry.
- It is important for the project team to validate its work with calculations and experiments. It goes to validating what might be considered intuitive.

Project weaknesses:

- There are no obvious project weaknesses.
- It is unclear how the project results will steer toward cost reduction of hardware required for HD applications. The project covers a diverse set of topic areas within MD/HD fueling. The direct connection between the various topic areas is somewhat difficult to follow in terms of an overall project end goal. It is unclear whether the project will provide a final report or disseminate information to safety, codes, and standards groups. It was unclear whether the SAE J2601-5 fueling protocol was fully implemented for fueling tests or if aspects of the fueling protocol were omitted because of known hardware implementation challenges. It would be great for the project team to elaborate on the level of fueling protocol was just released to the public). New information on the cyber vulnerability assessment and standards development—and how this information would apply to future work—was missing for 2024 (2023 information was in the backup slides). The work completed on cyber vulnerability assessment of vehicle-to-dispenser communications could be very valuable to the newly created ISO 19885-3 sub-working group.
- Regarding FM90 and FM300 fueling, it appears that cooling for HD fueling, owing to receiving HD vehicle compressed hydrogen storage system characteristics, does not need the same cooling requirements as light-duty fueling and therefore may require significantly less energy per kilograms of hydrogen dispensed.
- It is unclear whether the project results are sufficient to have a station design basis.
- It was not clear how TPRD actuation was a part of this project scope and not something the industry leader should have analyzed for its own product.

Recommendations for additions/deletions to project scope:

- The project should stay the course.
- The project partners should consider performing a CFD analysis on the new 90 g/s on-tank valve design with an SAE/5 fueling profile. The thermophysical results—especially internal tank temperatures at peak mass flow rate—will be very interesting to review. These results could provide critical safety information

to the MD/HD hydrogen community. Tests should be redone with FM300 protocol and HF hardware to confirm variation in flow rate and pressure drop results. The project should consider leveraging fast-flow fueling data generated by the NREL high-flow facility to assist with modeling and analysis efforts and to compare to Nikola data.

• The project team should carefully articulate that these are calculations of a specific application of pipe flow and of heat exchanger behavior. This information is intended to provide evidence of the fill behavior during a fast-flow event.

Project #IN-043: Detection System Comprising Inexpensive Printed Sensor Arrays for Hydrogen Gas Emission Monitoring and Reporting

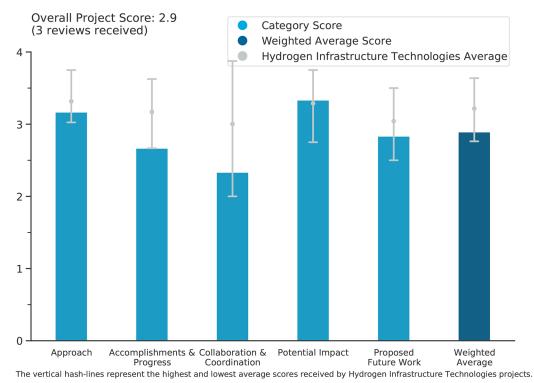
Rahul Pandey, Palo Alto Research Center

DOE Contract #	DE-EE0010745
Start and End Dates	9/1/2023–8/1/2026
Partners/Collaborators	Pacific Gas and Electric Company
Barriers Addressed	 Low hydrogen sensitivity and selectivity Inaccurate concentration quantification Lack of low-cost technologies

Project Goal and Brief Summary

The project addresses the challenge of continuously monitoring hydrogen gas emissions by developing a distributed network of low-cost sensors. These sensors utilize carbon nanotube (CNT)-based transducers chemically modified to selectively detect low concentrations of hydrogen gas, targeting sensitives below 10 parts per billion (ppb). This technology aims to enhance safety by providing real-time monitoring of hydrogen levels, minimizing the risk of undetected leaks. The project seeks to improve the efficiency and reliability of hydrogen production and storage systems through leveraging advanced sensor technology and network integration.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project approach is very solid, with clear milestones and go/no-go decision tree steps in place. The specific targets for meeting the project's overarching goal are clear. A definite plus is incorporating field testing. There are also clear diversity, equity, inclusion, and accessibility (DEIA) and community benefits plan considerations rolled into the project.
- The IN-043 project intends to develop a distributed network of hydrogen sensors comprising low-cost sensor arrays printed with CNT-based transducers chemically modified to selectively detect low concentrations of hydrogen gas with <10 ppb sensitivity in ambient conditions. The system will use a signal processing and data analysis platform powered by machine learning (ML) to identify, quantify, and report hydrogen concentrations with high accuracy and enable environmental monitoring. The approach to performing the work is well-presented but lacks some detail. The objectives are identified, and the barriers are addressed; however, none of the milestones has been achieved so far-all of them are in progress. This could indicate a slight delay in project progress. A safety plan is required for this project. The recommended changes have been implemented, and the safety plan was updated. A conference call has been scheduled with the Hydrogen Safety Panel to address all comments. The safety plan will be updated again and resubmitted for review in Quarter 6. To implement the safety plan, all team members have completed a general lab safety training, new oxygen and volatile organic compound sensors have been installed in the laboratory to detect leaks, and new pressure transducers and gauges have been installed on pressurized lines. A DEIA plan is also required for this project. Three specific, measurable, achievable, relevant, and time-bound (SMART) milestones have been created for the project to create a diverse project team and increase awareness about DEIA within the team and in the local community: (1) completion of at least one DEIA training per year by the project team, (2) encouragement of and reporting on efforts for hiring from minority-serving institutions (MSIs), and (3) the principal investigator's participation in at least one volunteer activity for science, technology, engineering, and math (STEM) outreach in MSIs.
- The project is based on chemically modified CNTs that have the potential to achieve high sensitivity.

Question 2: Accomplishments and progress

This project was rated 2.7 for its accomplishments and progress toward overall project and DOE goals.

- The project has shown steady progress toward its goals. The project team synthesized 15 CNT-based transducers used for detecting hydrogen and interferent gases. The project team printed sensor arrays with 15 CNT-based transducers and tested against hydrogen, methane, and carbon monoxide. Hydrogen concentrations down to 1 part per million (ppm) were detected using CNT-based transducers. The sensor testing system upgrade is in progress to enable large dataset generation for developing robust database models. The sensor device design is also in progress to fabricate a safe low-power device. The project, however, is already getting close to the end of its first year, and many of the early key milestones and go/no-go decisions are still in progress: (1) >80% accuracy in predicting sensor response to temperature and relative humidity (RH) changes, (2) hydrogen limit of detection <50 ppb in air, and (3) >80% accuracy of hydrogen selectivity in air. This could lead to a slight delay in the project. Detection of hydrogen concentrations is still far from the target. Additionally, to achieve the milestone on sensitivity, advances are needed on the influence of morphology, size, and density of nanoparticles in the functional groups on the CNTs. Monitoring a change of 25 ppb has been currently achieved by the sensors, but a change of less than 15 ppb is the target that needs to be achieved by the end of the first year.
- The project has achieved 1 ppm hydrogen sensitivity, which is good progress. The fabrication process is mature and cost-effective. The project still needs to work towards ppb-level sensitivity.
- Although the project is still in its early stages, there is concern that the recent system upgrade pushes back the timeline to collect necessary data and iterate/improve upon the technology to reach critical targets and milestones.

Question 3: Collaboration and coordination

This project was rated **2.3** for its engagement with and coordination of project partners and interaction with other entities.

- Coordination within the team was presented, including a safety plan and review by PG&E. More external collaboration is encouraged.
- Collaboration with a large natural gas utility is a plus but also limiting, as this utility does not currently have active hydrogen operations and the proposed field test location is contingent on state regulatory approval.
- There is one single partner in the project, PG&E. Its role and activities are not very well-defined—just participation in field testing the sensors in its facilities, which will take place in the last year of the project.

Question 4: Potential impact

This project was rated **3.3** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The project aspects align with the Hydrogen Program's goals and objectives in terms of advancing hydrogen sensor technology for high hydrogen sensitivity and selectivity. The project has the potential to advance progress using a configurable and robust low-cost distributed sensor network with concentration quantification abilities. The performance targets are to selectively detect low concentrations of hydrogen gas with <10 ppb sensitivity in ambient conditions.
- This project very much supports the DOE objective to advance hydrogen detection technologies capable of sensing and quantifying at the ppb level and is a critical pathway toward understanding hydrogen's indirect global warming impact.
- A low-cost distributed hydrogen sensor network is appealing to large-area hydrogen monitoring, if this project can fully deliver the performance parameters as a sensor system beyond the sensor devices.

Question 5: Proposed future work

This project was rated 2.8 for effective and logical planning.

- The proposed future work is reasonable and aligned with the project objective.
- The proposed future work is logical and supports the overall project goals, but some line items are not clearly laid out, such as steps to improve sensor lifetime and increase accuracy to greater than 80%.
- The project is still at an early stage. Future work has been mapped out but lacks detail. Further definition of the subtasks to achieve the goals is necessary. The goals are stated, but the tasks to achieve them are not thoroughly described, as listed below:
 - CNT-based transducer development for (1) achieving <10 ppb hydrogen sensitivity with high selectivity in the presence of interferents, (2) minimizing degradation for long sensor lifetime, and (3) estimating and improving sensor lifetime. The methodology to achieve this was not specified.
 - Sensor device development for (1) low-power and low-voltage requirements and (2) ability to read
 resistance change for hydrogen concentration change ≤10 ppb. This would be achieved by tuning
 morphology, size, and density of nanoparticles in the functional groups on the CNTs, but the
 approach is not thoroughly defined.
 - Creation of large sensor data sets for development of database models using ML for enabling >80% accuracy in identification and quantification. There is a lack of detail in the methodology to achieve this goal.
 - Field tests to evaluate deployment of a distributed sensor network at PG&E's facility for demonstrating and improving system capabilities. This will be achieved through the collaboration with PG&E, but detailed tasks are missing.

Project strengths:

- The novel sensor development is based on CNTs bound with chemical functional groups, tuning the sensor's response to the presence of gas. The project has ambitious targets on detection limits, selectivity, and accuracy.
- CNT functionalized resistance-based chemical and gas sensors are relatively established to achieve high sensitivity. The team has prior experience in low-cost sensor fabrication and design.
- The project has strong alignment with DOE objectives and has clearly laid out steps for achieving key milestones. Success is clearly defined by the project goals and objectives.

Project weaknesses:

- It is unclear what progress has been achieved according to the DEIA plan. The achievement of early milestones and go/no-go decisions seems to be slightly delayed. The project lacks definition of the sub-tasks to achieve the milestones/targets. The project has only one partner. PG&E seems to be an industry partner on its own. It is unclear in the slides how well this collaboration is coordinated and tied into this effort.
- A project weakness is collaboration. Partnering with only a single field test partner that currently has no hydrogen operations is an inherent risk to the project.
- The team still needs to show progress toward sub-ppm level and 10 ppb level hydrogen sensing; the current progress shows only 1 ppm sensitivity.

Recommendations for additions/deletions to project scope:

- The project should identify additional partners, including those that have extensive hydrogen operations and experience, for field testing/demonstration steps.
- The project should provide an assessment of sensor lifetime. It is a short project to assess durability, but this is an important requirement that should be added to the project scope. The project should provide clearer reporting of the progress achieved according to the DEIA plan milestones. The project should expand collaborations with industry partners. Clearer definition of the methodology and definition of the sub-tasks to achieve the milestones/targets is necessary.
- There are no recommendations for changes in project scope.

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

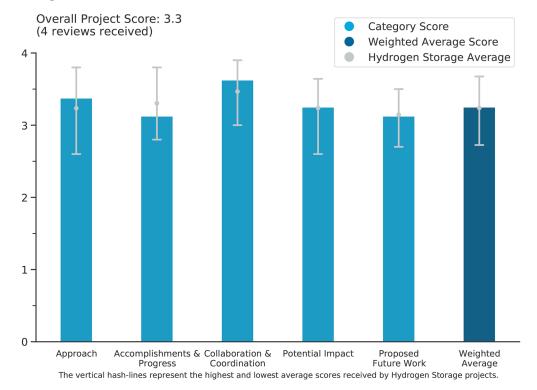
DOE Contract #	4.4.0.2
Start and End Dates	10/1/2009
Partners/Collaborators	Hydrogen Materials Advanced Research Consortium (HyMARC), Pacific Northwest National Laboratory, Lawrence Berkeley National Laboratory, Hydrogen Interface Taskforce, Argonne National Laboratory – Hydrogen Analysis (H2A) model, Argonne National Laboratory – Hydrogen Delivery Scenario Analysis Model, Hydrogen Materials Consortium, U.S. Army Tank Automotive Research, Development and Engineering Center, Lawrence Livermore National Laboratory, Ford Motor Company, Strategic Analysis, Inc.
Barriers Addressed	 System weight and volume System cost Efficiency Charging/discharging rates Thermal management Life cycle assessments

Rajesh Ahluwalia, Argonne National Laboratory

Project Goal and Brief Summary

The project aims to develop and use comprehensive models to analyze renewable hydrogen production, transmission, and storage systems (both onboard and stationary), including compressed hydrogen, liquid hydrogen (LH2), and hydrogen carriers. This evaluation study supports DOE in determining the performance of these systems against established targets, aiding material developers in focusing on critical areas for improvement and providing cost assessment for onboard systems. Given the importance of LH2 storage in heavy-duty applications and in national renewable production and transmission scenarios, this project addresses critical barriers in hydrogen storage, including system weight, cost, efficiency, and thermal management, and is integral to advancing hydrogen technologies for a sustainable energy future.

Hydrogen Storage



Project Scoring

Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project has good modeling work that contributes to determining the importance and relevance of the different components of the project.
- This project has a comprehensive approach, with a strong cast of partners to conduct the system-level analysis for hydrogen delivery and storage.
- The work on comparing onboard hydrogen storage systems is critically important to helping understand how all the different storage systems compare to one another. The study helps highlight the pluses and minuses of each system.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and DOE goals.

• The team's analysis is well-done, but it may be too optimistic at times. A differentiation between "current status" and "future technology if everything goes well" could be relevant. This may be similar to what is done with the onboard LH2 pump (i.e., two cases are analyzed, one that includes an onboard pump and one that does not, as it is uncertain how rapidly these may develop). The presentation showed very little information on the LH2 system, but it included results for cost, weight, volume, etc. It would have been interesting to see what the team assumed since relatively little is known outside the group of institutions doing the development. The two methylcyclohexane (MCH) scenarios have lower costs than dibenzyltoluene (DBT), with the MCH-A scenario¹ having the lowest cost outside of salt caverns.

¹ In the MCH-A scenario, natural gas is used to provide the heat to dehydrogenate MCH.

Presumably, other options remain to be modeled. Otherwise, an explanation is needed as to why MCH is so highly regarded.

- The team conducted a thorough study comparing different onboard hydrogen storage systems. The team looked at many different configurations, and the study contained many key details needed to allow comparison. The second half of the study was more difficult to follow, and the explanation of the motivation for it could be improved.
- The presentation demonstrated strong progress and summarized the level of completion for each task.

Question 3: Collaboration and coordination

This project was rated **3.6** for its engagement with and coordination of project partners and interaction with other entities.

- The team collaborated with a wide range of companies and institutions to ensure that their models reflected state-of-the-art systems, which is critical for this type of study.
- A very strong list of collaborators was utilized to collect data and analyze a broad set of options.
- The project has extensive collaborations with many relevant organizations.

Question 4: Potential impact

This project was rated 3.3 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- This project's type of modeling is critical so stakeholders can understand how all the different technologies compare to one another. There is quite a bit of uncertainty as to which onboard storage solution is best for heavy-duty trucks, and this project takes good first steps in understanding how all the current frontrunners compare. This work also helps to identify the weaknesses of some systems and where additional research and development is needed.
- The data provided by this study will be very useful in making future decisions regarding hydrogen transport and storage.
- This project is very relevant, as the team can evaluate the value of the different technologies.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- A wide breadth of topics is proposed for future work. Most of these topics seem quite important to understanding how hydrogen can impact our energy system and what the biggest research needs are to make it more efficient and cost-effective.
- Future efforts will focus on completion of hydrogen production and transmission scenarios, as well as onboard storage for heavy-duty applications.
- It seems that the project is shifting from vehicle and fueling station modeling to production and distribution. The reviewer was under the impression that this work was being done by another research group at Argonne National Laboratory (Amgad Elgowainy). This should be carefully considered to maintain a relevant effort and avoid scattering and duplication.

Project strengths:

- This project is a detailed modeling study that helps the community understand and compare various hydrogen onboard storage technologies and renewable hydrogen production technologies. The team has good collaborations with external partners to ensure the project's models are relevant.
- The project covers a broad spectrum of analysis for hydrogen production, transmission, and storage scenarios. This work is accomplished by teaming with an extensive list of collaborators.
- The project displays good modeling skill and relevance to the Hydrogen Program.

Project weaknesses:

- It would be good to see how the model results compare to experimental onboard storage tanks and thus where some of the model assumptions break down. It would also be good to understand what the largest sources of uncertainty for the models are and how sensitive the results are to these uncertainties.
- Perhaps the scope is becoming too broad. The project team should make sure that the project does not become too scattered.
- The reviewer cannot point to a project weakness; there is so much information that it is difficult to analyze all of it.

Recommendations for additions/deletions to project scope:

- It would be good to understand how the different onboard storage systems behave over different drive cycles and how the end state of the remaining charge affects the fill performance of the system. There was an interesting paper by Faurecia and Air Liquide that looked at some aspects of this. It would also be interesting to look at how sensitive the different cryogenic storage systems are to insulation performance.
- Closer interaction with industry and researchers may be useful in determining whether all assumptions used for the analysis are realistically applied to the systems being analyzed.
- The project has so much information; hopefully, the final report can summarize the key points and findings to simplify decision-making.

Project #ST-127: Hydrogen Materials Advanced Research Consortium (HyMARC) Overview

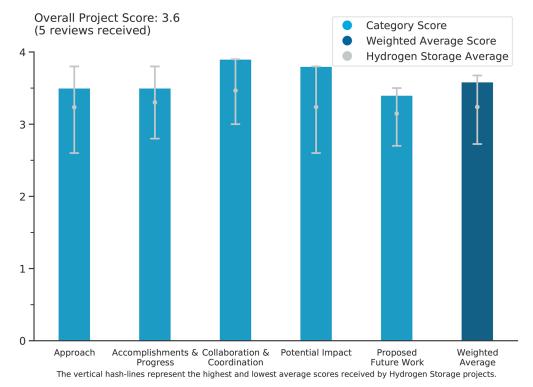
Mark Allendorf, Sandia National Laboratories

DOE Contract #	WBS 4.1.0.805 (SNL); 4.1.0.501 (NREL)
Start and End Dates	10/1/2015
Partners/Collaborators	National Renewable Energy Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Pacific Northwest National Laboratory, National Institute of Standards and Technology, SLAC National Accelerator Laboratory, Immaterial Inc., GKN, Southern California Gas Company, OCOchem, Honeywell, Stoke Space Technologies, Airbus, Microsoft, Colorado School of Mines, University of California, Berkeley, SyZyGy Plasmonics, NuScale Power
Barriers Addressed	 Cost Weight and volume Efficiency Refueling time Hydrogen capacity and reversibility Understanding of hydrogen physi- and chemisorption Test protocols and evaluation facilities

Project Goal and Brief Summary

Critical scientific roadblocks must be overcome to accelerate materials discovery for hydrogen storage. The project objective is to accelerate discovery of breakthrough storage materials by providing capabilities and foundational understanding. Capabilities include computational models and databases, new characterization tools and methods, and customizable synthetic platforms. Foundational understanding is needed for phenomena governing the thermodynamics and kinetics-limiting development of solid-state hydrogen storage materials.

Hydrogen Storage



Project Scoring

Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project uses the best approach for materials development and theory-guided experiment with feedback. The project also uses techno-economic analysis (TEA) guidance for material and system selection but with initial preference for abundant materials wherever possible. Industry advises the project team to focus on more valued areas of effort. This approach will also yield the advantage of involving industry directly earlier, when a result is seen that industry wants to fund to product. There is good safety effort and practice, even though no plan was required. The project has a wide breadth of material types, looking at so many ways to succeed. It continues the seedling project program, which gives smaller amounts of funds to very early work, either to prove it out as worthy of full funding or to fail fast and move on. There are far too many subprojects to comment on their individual approaches, but, in general, there are good approaches at that level, too. The diversity, equity, inclusion, and accessibility (DEIA) plan has provided authentic value to disadvantaged students (one ended up hired, and the other went to graduate school), and the bridge program may diffuse value to students outside the program, which is great. However, more efforts should be expected from a project this large—everything is in Denver, and the program is national.
- HyMARC has done an excellent job keeping focused while investigating a wide range of technologies. The consortium is very well-integrated and includes a wide range of expertise to overcome any challenges. The addition of the levelized cost of storage (LCOS) model for each technology is a great idea that helps integrate the work being done under HyMARC into the analysis work being done at DOE as a whole. The DEIA plan is high-quality and provides an excellent opportunity for students. It is a bit limited in scope, covering four students total, but it is still early in the program. Expanding the summer internships would be a great way to expose more students to scientific work.
- Overall, the approach of HyMARC has improved significantly over the years with the introduction of the LCOS model and tankinator models. With the introduction of more materials such as liquid organic hydrogen carriers (LOHCs) that will impact pathways more significantly than onboard storage, some metric to compare their potential is required. Developing targets is admittedly difficult due to the sheer

number of permutations of possible routes and different materials/methods, etc. A possible suggestion is to pick a reference pathway (such as liquid hydrogen or ammonia) to evaluate costs relative to a more wellunderstood pathway or aligning a new LOHC with a "best fit" pathway from Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) modeling. It would help to insert a short summary of pathways from Dr. Elgowainy's presentations to give the audience context of where an LOHC can fit into the production/delivery big picture and what incumbent it must improve upon to be of true value.

- The evolution of incorporating TEA/use-case analysis to focus the center's approach over the past few years has begun to pay off to large effect. The previous lack of a sound energy/cost/life cycle basis for go/no-go determinations for materials approaches across the center's efforts had been a barrier to progress that has now been largely mitigated with the integration of Dr. Breunig's expertise across many of the project's areas of interest.
- The approach to the work appears quite effective. Specifically, it is arguable that the development and continued improvement of the TEA for predicting LCOS is providing a clear framework for HyMARC to evaluate materials/fuels/processes for the future hydrogen economy. This TEA development is clearly dependent on useful data, and as such, the direction HyMARC is going to maintain and expand this useful data feedback loop appears to be the approach/direction of the team. However, some aspects of the research conducted appear quite fundamental, and the leaders/participants in the project understandably need to find the appropriate balance as HyMARC enters its third stage of funding/direction that leans toward application of learned knowledge.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals.

- With the improved systems analysis approach being integrated into the experimental projects, the center has made significant progress in defining specific materials property attributes against specific use-case scenarios, enabling some prioritization in effort going forward. This approach has also highlighted which materials systems attributes require attention in order to move forward (e.g., rates of release/ rehydrogenation, in the case of the LOHCs that were described). With the consortium's nascent industrial advisory board shaping up, perhaps then additional validation of the center project area will be explored and further focused. The consortium has also improved capabilities in making and testing materials and processes at more than typical laboratory scales, as highlighted by the continuous flow capability for LOHC development, the kg H2-scale metal hydride bed system, and the sorbent/fuel cell demo work that is in its early stages. These activities point to the future opportunity to validate the systems analysis and provide additional data to refine the systems modeling efforts in what can be a nice feedback loop to optimize and improve materials and processes.
- HyMARC has achieved several notable successes toward DOE goals, including developing a model to pair sorbents with end uses, developing a capital cost model for metal hydrides, refurbishing an old test reactor for future research and validation, developing an LOHC reactor for small batch testing, and developing polymer-coated sorbents. HyMARC has done an admirable job transitioning from vehicle-focused research and applications to the wider range of applications discussed in the presentation. These applications can and will support future developments at DOE.
- The work conducted is progressing toward project objectives effectively, on multiple fronts. This includes obtaining fundamental understanding of the most promising materials for multiple avenues of hydrogen storage and coupling this understanding to TEA. Developing large-scale applicable data—such as scaling of materials and LOHCs—and constructing and demonstrating metal–organic framework (MOF)-based tanks are notable examples of accomplishments for the current/future goals of HyMARC.
- There are abundant results; it is not possible to list them all here, but there is progress across all areas. All are making progress that is focused on a cost-effective alternative to gas and liquid storage. It is commendable that the researchers are looking at value that materials can offer other than solving storage directly, e.g., aluminum formate, which charges slower and needs cool temperatures but could serve as a boil-off capture material to avoid losing the energy value of that hydrogen. Analysis suggests a metal hydride that rivals 350 bar compressed gas on capital cost. Another example of service to the whole hydrogen research effort is the improvement in enthalpy measurement.

- Overall, several new concepts/directions were presented this year.
 - Pros: Of particular note were projects such as ST-212, ST-213, and ST-218, which all provide new ways to tune hydrogen storage and release mechanisms. These projects are nearing their completion, but this reviewer encourages the HyMARC team to encourage next steps and continuation of such projects.
 - Cons: With the exception of Craig Jensen's "accidental" discovery of a potentially new LOHC material, there has not been much in disruptive storage material discovery work. Much of the focus is on previously studied materials that may have been rejected in previous years, such as mobility-focused goals, and reintroduced as possible candidates for the center's expanded roll to include production/delivery and grid applications. While these materials may find real applications in these new areas, there is still change needed in improvement of mobility storage materials to significantly improve range and reduce cost of onboard hydrogen storage systems.

Question 3: Collaboration and coordination

This project was rated **3.9** for its engagement with and coordination of project partners and interaction with other entities.

- HyMARC is highly integrated, and there is great evidence of collaboration leading to successful research projects. The team is also working very closely with a minority-serving institution to develop its DEIA efforts, which have been successful. Beyond the collaboration between the labs, there is also great collaboration with industry and academia.
- Heavy collaboration is inherent in the format of the consortium, but there is extensive partnering outside as well. Also, the consortium serves the seedlings very well and assists in their success.
- With the long-term tenure of this consortium, the team members have developed into a very cohesive, collaborative organization and appear also to work nicely with the seedling projects where appropriate, most of the time. (Dr. McGuirk at Colorado School of Mines seems to be having problems getting critical high-pressure sorption data measured at the National Renewable Energy Laboratory center partner's facility.)
- HyMARC connects with all relevant stakeholders, from labs to universities. There was not much international collaboration seen, though—perhaps that is a limitation with funding mechanisms requiring funds to be mostly spent in the United States.
- There is clear evidence of collaboration and coordination with other institutions, including industrial partners. The industrial partners, however, appear conflicted on how best to participate with others in the team (especially other companies, understandably). The project will need to work on how best to find utility with corporate involvement, intellectually and even financially.

Question 4: Potential impact

This project was rated **3.8** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The potential impact/relevance is undeniable. The team comprises the leaders in this field and is tasked with finding material/fuel solutions to an entirely new source/supply chain of energy. The work discussed in this overview provides evidence for relevance, especially the growing feedback loop between fundamental data and establishing levelized cost of use of materials/fuels.
- The impact and relevance of the consortium's work has encountered a watershed moment with the integration of Dr. Breunig's systems-based analysis of consortium materials and processes. The consortium can now make much better headway against the project goals and targets, armed with direction from the focused use case scenario analysis.
- Work done in HyMARC could lead to step-change breakthroughs in current hydrogen production/delivery and storage pathways. The appeal of a stable, non-toxic LOHC to provide an energy delivery system similar to today's petroleum-based supply chain is appealing on many levels and critical if hydrogen is to become more widely used in more applications.
- Despite the breadth of HyMARC's portfolio, the team appears to be laser-focused on working past technical barriers to develop technology that meets or exceeds the project's goals. The structure of the

consortium allows for high-impact materials to be studied from multiple angles quickly, increasing the likelihood of high-impact results that work toward the project's goals.

• The project is developing the materials that will be needed for storage in many different paths, so there are several ways to succeed. All paths are appropriate. This is well-aligned with the DOE mission on hydrogen, the strategy and roadmap, and the needs of the country and its industries.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The proposed future work is highly relevant to DOE goals and is a logical progression of the work already under way. The tools being developed can be applied to multiple applications, and the experimental capabilities will be key to test whether materials discovered or optimized through the screening tools actually perform as expected.
- The future work proposes to continue to increase the overlap of materials and processes with systems analysis/TEA. The future work discussion could have been even more impactful had the project team proposed to use the spectrum of the analysis outputs to prioritize projects going forward and de-emphasize project areas that are not showing as much potential so that the center's resources can be best optimized on the most promising materials systems and processes and postpone work on less impactful projects. With new seedlings coming on, a discussion of how HyMARC will anticipate their needs could have been addressed, particularly in the case of the new plasmonic seedling that might or might not be complementary to the ongoing HyMARC effort in that area.
- Future work is logically and effectively planned. Finding the balance between fundamental materials data on burgeoning and known materials will need to be carefully established.
- Future work should move the needle in areas where progress would have meaning for DOE goals.
- Most of the projects this person reviewed were nearing the end—and most do not have a clear Phase II on what could come next after project completion, such as down-select or evolve the project to the next stage. The project should build upon projects such as ST-212, ST-213, and ST-218, which provide valuable system tuning levers on both existing/potential future materials and de-emphasize projects based on thermodynamically taxing materials, such as anything borohydride-based.

Project strengths:

- The team has done a great job of keeping things focused while exploring a wide range of technologies and applications. The close-knit relationships between the labs, industry, and academia have fostered significant advances and developments. The DEIA plan is well-designed, has been executed effectively, and shows promise for providing a more inclusive path to technical careers. The development of the LCOS model is extremely helpful in comparing work across the analyses performed by other organizations.
- This project is highly collaborative among multiple institutions. Well-integrated TEA/systems analysis function to guide development in a feedback loop. Furthermore, the project focuses on developing the best match of materials/processes to use cases. There is new focus on developing capabilities for scale-up and/or continuous processes; some instances include coupling to fuel cell testing of the produced hydrogen.
- Stronger leadership is emerging, especially with the introduction of system modeling tools to help filter feasibility of projects from a cost perspective. The particular credit goes to Dr. Breunig, who shows strong leadership and presentation skills.
- Clear cost metrics are being established to guide materials use and design. Expansion of this concept, which is dependent on "real-world" data, will be key to better understanding and impact. The team knows this and is finding better ways to integrate this concept throughout HyMARC.
- The project strengths are the principal investigators and their institutions, facilities, breadth of scope, and collaboration.

Project weaknesses:

• In transitioning from vehicle-application-based research, the scope of HyMARC has expanded significantly. Perhaps the development of application-specific targets could help guide the research, similar

to the sorbent end-use pairing that was developed. There does not seem to be a clear path for technology developed in the labs to transition to industry. Perhaps HyMARC could include some form of incubator or mentoring to spin-outs to encourage technology developers to scale up and out into commercial applications.

- There is difficulty in evaluating and providing targets for the many new emerging pathways for LOHC materials in particular. There is continued reliance on traditional materials such as borohydrides, which makes it difficult to identify breakthrough opportunities and new techniques.
- Certain materials studied appear more interesting than useful. This is sometimes how research can go (as the answer is not known until the work ends), but the team must be careful to avoid the sunk-cost fallacy if certain materials arguably lack cost-effective utility.
- The progress has not flowed up into projects of higher technology readiness levels to the extent the project team likely desires.

Recommendations for additions/deletions to project scope:

- The project should increase the budget for novel breakthrough storage materials that have nearthermoneutral performance (could be hybrid systems of exothermic/endothermic systems) or an entirely new class of materials. It is okay to take a high-risk approach for a portion of the budget, now that hydrogen funding has increased significantly over the years. It is also recommended that the project reduce work on borohydrides or any thermodynamically difficult materials that have extremely high desorption temperatures. They will have very limited use-case scenarios, even in stationary cogeneration-type projects where waste heat may be available. Making use of systems that need low-grade waste heat will open up many more industrial opportunities. The project should include a holistic view of grid-balancing services (frequency regulation, peak shaving, load shift, line packing, etc.) to help optimize storage projects to be targeted services.
- It would be worth investigating the addition of some form of program to help encourage technology transfer from the labs to industry. That could potentially be an incubator of some sort, offering mentoring to spin-outs or startups, or some other development program to encourage technology transfer.
- For this size, one would expect more effort on a community benefits plan, even moving the current Denver project into other areas of the country with a strong HyMARC presence (such as Livermore [California] and the Tri-Cities [Washington]).
- With the ability to assess materials and processes with the tools of TEA, a more aggressive go/no-go determination could be performed to focus the consortium's attention and resources on the most promising approaches.

Project #ST-209: Hydrogen Materials Advanced Research Consortium (HyMARC) Seedling: Theory-Guided Design and Discovery of Materials for Reversible Methane and Hydrogen Storage

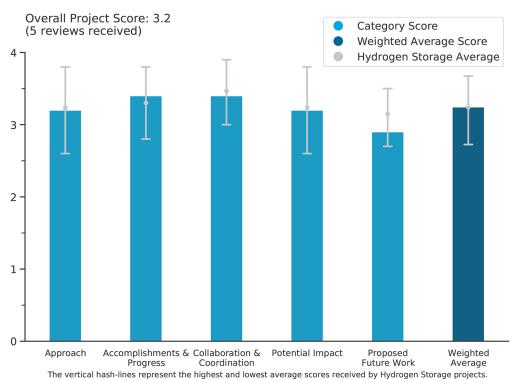
Omar Farha, Northwestern University

DOE Contract #	DE-EE0008816
Start and End Dates	1/1/2020–12/1/2024
Partners/Collaborators	National Institute of Standards and Technology, National Renewable Energy Laboratory
Barriers Addressed	 System weight and volume System cost Efficiency Durability/operability

Project Goal and Brief Summary

This project aims to exploit high-performance metal-organic framework (MOF) sorbents by combining synthesis with machine learning to find stable and scalable materials for hydrogen storage while maintaining a reasonable cost of production. The project researchers use a machine learning algorithm to screen a database of materials for hydrogen uptake. Having identified the top candidate MOFs, researchers synthesize and characterize them and study their behavior under pressure- and temperature-swing (PT swing) operation. The project team is also looking at removing solvent molecules from MOFs to yield open metal sites for storing molecular hydrogen at near-room temperature. If successful, this project will advance economical hydrogen storage technology.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project is focused on achieving useful storage of hydrogen at close to room temperature using highsurface-area MOFs, some with open metal sites. This approach is well-thought-out and addresses the principal barriers and objectives of the Hydrogen Program (the Program). A novel portion of the approach is to incorporate "defects" into the MOF structure by partially replacing a framework linker with a modified, near-isostructural linker that results in open metal site "defects" within the MOF structure that may enhance hydrogen sorption at ambient temperatures. The open metal site strategy is ongoing in several other projects; the approach to developing open metal sites in this project is different and complementary to the others.
- The approach to the work is sound. Necessary collaborations, such as with the National Institute of Standards and Technology (NIST), add verification of performance that is needed for material characterization. The combination with computation materials discovery and modifying a leading candidate lends credence to the proposed work and its prospects.
- The approach has clearly identified several key metrics and has developed a well-thought-out approach to developing materials that meet these performance metrics.
- The project uses simulation and machine learning to pick MOFs to synthesize and hopes to find highperformance, easy-to-make storage materials. The method has been tried for about a decade, and while good MOFs have been made, none have been up to the standards sought; perhaps this will be the time it succeeds.
- The material target of 25 g/L is too low—significantly higher material capacity is needed to achieve that at system level. One of the team members is confusing material with system targets and needs to set the bar higher for volumetric. It is still not convincing that using surface area of MOFs is a useful metric. Higher surface area usually means lots of empty space and lower volumetric densities. The approach presents questions: whether this high-surface-area rule still applies for flexible MOFs, how this is work different from the work done by Don Siegel for many years prior to this project, what added value the machine learning algorithm brings and what it is looking for, and what potential negative effect on the bulk material increasing the defect (to increase active site access) has on the bulk properties of the material.

Question 2: Accomplishments and progress

This project was rated **3.4** for its accomplishments and progress toward overall project and DOE goals.

- The group has shown two examples of viable materials for materials discovery within the useful operating conditions set out for hydrogen storage adsorbents. The accomplishments are of merit, and the understanding gained will contribute to the advancement of the project.
- The project has shown some impressive results, particularly in the modeling and experimental areas. There is excellent agreement between the models and experimental isotherms. The thermal and air stability results are encouraging for several potential applications.
- It is commendable that the project moved from theory to application with the synthesis of materials identified by the modeling. Moving toward significantly higher-capacity materials at room temperature should be focused on the material level.
- The project has shown good progress toward achieving the technical targets for sorption systems. While there is still much to be accomplished to achieve the targets, the approach is meritorious and feasible, and the team is making incremental progress.
- There is roughly 10%-by-mass useful storage with PT swing. The team should look at air stability, looking for no impact over short times (a day) but oxidation over long times (a few weeks). The models suggest copper interaction with less nitrogen in the linker would help. There is no information on the actual performance. The goal, though, was room-temperature MOF, and it seems to have fallen short here.

Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- There are excellent collaborations with leading experts in the field of hydrogen storage/verification of gas adsorption data.
- There is good collaboration and coordination with NIST and the National Renewable Energy Laboratory (NREL), who have both shown a strong impact on validating material performance.
- The collaboration has been active and useful.
- There is good internal collaboration among the computational and experimental efforts at Northwestern, and there is apparent good collaboration on the high-precision sorption measurements at NIST and NREL.
- There is good materials-level collaboration; however, the team needs to use the HyMARC system and cost tools to derive proper material storage targets. The materials proposed do not get out of their own way.

Question 4: Potential impact

This project was rated 3.2 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- This project focus to design "defective" MOFs with open metal sites supports the Program objectives in seeking sorption systems that can operate at higher pressures and at near-room temperatures. If the project succeeds in attaining the technical targets specified, this will have a significant impact on the possibility of such sorbent systems supporting hydrogen storage for a variety of important use cases.
- The potential impact of the research is high and well-aligned to Program goals. The development of a room-temperature MOF would be extremely impactful in a wide range of applications.
- The project aims to make better storage materials at a good price, which aligns well with the roadmap and strategy.
- The discoveries have potential to inform new materials design and further development of hydrogen storage sorbents. The impact will need to be combined with techno-economic analysis to truly verify whether these materials are cost-effective for their proposed use.
- The team needs to provide a credible argument of how these storage targets will result in a significant improvement in performance or cost of current incumbent systems such as liquid hydrogen or compressed hydrogen. It is not yet convincing that these materials can get out of their own way with the current storage targets set by the project.

Question 5: Proposed future work

This project was rated 2.9 for effective and logical planning.

- The proposed future work is a logical extension of the current work and can present opportunities to meet Program goals.
- The future work logically focuses on increasing the number density of the "defect" sites, and hence the open metal sites, to explore whether this drives sorption to higher capacities with higher binding strengths that could result in improved sorption characteristics at near-ambient conditions.
- Chemical design parameters being proposed for future work are based on sound science. However, future work should include leveraging HyMARC's standard for levelized cost analysis to verify the utility of the materials being examined.
- The 77 K targets should be the 233 K targets for these materials to provide significant improvement over incumbent technologies such as compressed hydrogen systems.
- The goals are ambitious but are not really laid out as plans, so this category is hard to evaluate.

Project strengths:

- The methods used have been shown to be incredibly effective. The experimental data have been used well to develop and improve the theoretical models used. The modifications to the materials show good promise in becoming effective and high-performing hydrogen storage materials.
- There is good focus on thermal air and water stability of material—these are practical performance characteristics needed for real-world applications.
- The project strengths are pairing theory with materials discovery and understanding how predicted materials can be further tailored for the goals sought.
- There is a good team of theorists, experimentalists, and collaboration with experimentalists at the labs validating the sorption properties of materials.
- The project has a strong team and theory-guided experiments.

Project weaknesses:

- The material metrics should be further qualified by potential cost analysis.
- The theory is not leading the team to the anticipated ambient temperature results. PT swing gives impressive numbers, but that fails to account for the energy that will be used to re-cool the system and the hydrogen likely to be lost doing so.
- The gravimetric target seems too low to get out of its own way. It is unclear whether the gravimetric target can significantly improve upon a compressed storage system at room-temperature storage performance. It is also unclear whether the lower-pressure operation compensates for poor volumetric capacity from a capital expenditures viewpoint.
- The application area of this project is minimal. Despite the presentation's showing that the project focus is to file down to applications, it is still only at the experimental phase. The use of some targets for applications is useful, but more application focus would be appreciated.

Recommendations for additions/deletions to project scope:

- Perhaps there should be more description and data indicating how many of the "defect" linkers have been incorporated into the "defective" MOFs per unit cell.
- It is unclear what the intended end-use application of this material is or what a proposed system would look like. The team is asked to include a quick summary of how this material performs in the Tankinator and levelized cost model tools.
- When evaluating storage, the team should reduce hydrogen release values obtained when using PT swing by the energy needed to re-cool the MOF and a tank wall, and especially do this when training the machine learning to predict which MOFs to make.

Project #ST-212: Hydrogen Materials Advanced Research Consortium (HyMARC) Seedling: Methane and Hydrogen Storage with Porous Cage-Based Composite Materials

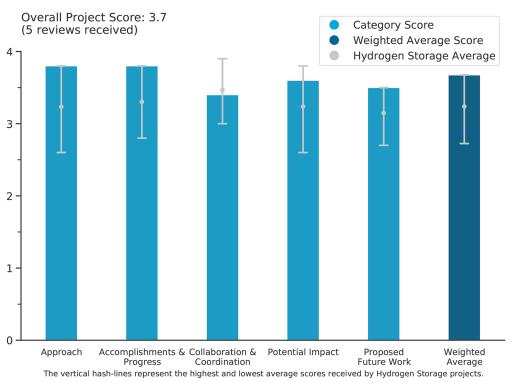
Eric Bloch, Indiana University

DOE Contract #	DE-EE0008813
Start and End Dates	1/15/2019–5/31/2025
Partners/Collaborators	Lawrence Berkeley National Laboratory, National Institute of Standards and Technology, National Renewable Energy Laboratory
Barriers Addressed	Low bulk density and storage capacity of metal–organic frameworks

Project Goal and Brief Summary

Metal–organic frameworks (MOFs) have low bulk densities that present challenges to their use as methane and hydrogen storage materials. This project will attempt to address those shortcomings by preparing high-capacity soluble absorbents that can be placed in the space between MOF crystals, resulting in a porous cage–MOF composite with increased density and volumetric storage capacity.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.8** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

• Identifying new techniques to improve packing density of bulk MOF materials without pelletizing is very much needed because of the well-documented issues with pelletization, such as a disproportionate decrease in gravimetric density for volumetric density gained. The principal investigator's novel solution chemistry

approach provides new techniques that not only increase apparent packing density but could also be used (possibly with other materials) to tune other bulk material characteristics such as enthalpy, sinter stability, catalysis, kinetics, etc.

- This is a nice approach to develop strategies to attempt to maximize the capacity of polycrystalline sorbents by filling the intercrystalline void space with auxiliary molecular or nanoscale sorbent materials. This approach addresses a critical barrier to efficient, useful hydrogen (and methane) storage in sorbents. The project is well-designed, -executed, and -presented.
- The team's approach to maximizing volumetric capacity (and essentially pelletizing simultaneously) by combining MOFs with nanoporous materials is superb. The approach the team has demonstrated is thorough and appropriate.
- This is a novel approach to using the space of a storage tank more completely. The project is responsive to safety review suggestions. In the new method, the nanoscale MOF actually by itself serves as the pellet binder, so there is no waste. Thus, this is highly aimed at key barriers.
- The approach presented in this project is quite novel and exciting. The safety plan is complete and appropriate.

Question 2: Accomplishments and progress

This project was rated **3.8** for its accomplishments and progress toward overall project and DOE goals.

- The project is meeting performance milestones and has passed the go/no-go #2 decision point by improving the methane or hydrogen storage capacity by 50% of baseline, which has been validated by sorption measurements at the National Renewable Energy Laboratory (NREL). The new method of preparation has resulted in materials with improved volumetric uptake and significant mechanical stability. The preparation method is simple and scalable and can be applied to a wide variety of sorbents/cages/nanocluster composites.
- The progress reported is quite incredible. The approach allows for a significant increase in capacity while maintaining the ability to cycle. The rapid screening approach developed for this effort is also quite clever and shows great results.
- The team has made clear progress toward the project's set goals and has established that monoliths can be constructed with MOF crystals and nanoporous materials. The team has shown clear and measurable success and has overcome critical barriers as they appear.
- The project showed an increase of 30%–40% in useable methane (CH₄) with the method and figured how to solubilize almost any MOF. A 50% increase in storage has been demonstrated. The project also made pellets with gain, not loss, in storage. These are important advancements.
- Significant progress has been made in preparing and testing monoliths with demonstrated gains, despite the added complexity of moving to a new university mid-project.
- Question 3: Collaboration and coordination

This project was rated **3.4** for its engagement with and coordination of project partners and interaction with other entities.

- There is good collaboration with key partners such as Jeff Long, Jeff Parilla, and Craig Brown. Given the many directions this project could go, new collaborators may be justified where specialty skills are needed.
- The project has good partners at the National Institute of Standards and Technology (NIST), NREL, and Lawrence Berkeley National Laboratory/University of California, Berkeley. Indeed, given the team's local issues, this collaboration has helped the project move along so that there is progress to report.
- The collaboration in this work is good. It is unfortunate the reactor is down at NIST, but it appears the team has pivoted toward another collaboration.
- There are indications of good collaboration with NREL on sorption measurements and also with NIST.
- The team has found useful collaborations to amplify the work.

Question 4: Potential impact

This project was rated 3.6 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The impact of this is quite significant and aligns well with Hydrogen Program goals. Increasing both the performance and mechanical properties of MOFs is highly desirable and can be used in several applications of interest to DOE. The approach is also incredibly practical, showing promise for use with more developing MOFs.
- This approach tackles the shortcomings of sorption low-bulk-density sorbents (relative to the crystallographic density) of polycrystalline sorbents such as MOFs by utilizing the intercrystalline space. This could result in improvements in the storage capacities of all crystalline porous framework materials. This project is of direct relevance, as it addresses several objectives of the Hydrogen Program.
- There have not been many projects in the past focused primarily on the bulk powder characteristics/ optimization of sorbents. This project has the potential to significantly increase the performance of new materials, reduce/eliminate key barriers in some materials, and likely translate well into new, not-as-of-yetdiscovered materials. Hopefully, lessons learned from this project will provide techniques that make traditional mechanical pelletization obsolete.
- This project would improve the storage medium MOFs in their most challenged physical property, storage density. If successful, this might change the possibilities for light-duty vehicle hydrogen penetration into the market, which would greatly advance DOE goals.
- The work has clear relevance and impact. By maximizing volumetric capacity and overcoming the challenge that many MOF sorbents cannot be pelletized, the project has demonstrated the universality of monolith applicability.

Question 5: Proposed future work

- This project was rated **3.5** for effective and logical planning.
- The project will continue to push the approach to determine the upper limits of sorption enhancement that can be achieved by utilizing the intercrystalline spaces. The team plans to study the effect of this approach on the kinetics of hydrogen sorption/desorption vis-à-vis the "naked" parent framework to examine any impacts from filling the intercrystalline voids. The project is waiting for neutrons to be available once again at NIST such that additional studies of hydrogen sorption in the composite materials can be made.
- A continued focus on thermal property impact of these composites will be interesting (thermal conductivity, enthalpy, etc.). The overall focus should remain on understanding the hydrogen system-relevant impacts of the bulk properties of these composites. In particular, understanding how materials will dust (plug filters, valves, etc.) with cycling will be crucial. The possible next-stage project could include novel techniques to mold these composites into actual tanks and develop novel techniques to integrate them into a small-scale system demonstrator. Also, a deeper understanding on the impact of material surface area could be a useful data point to understand the microscopic impact of these techniques. A further understanding of mechanical properties of the composites is of interest (brittleness, expansion, enthalpy/ adsorption curves, etc.).
- The proposed future work aligns well with the progress so far and continues in a logical manner. Understanding the thermal properties and kinetics of the composites is critical to screening the materials for use beyond the lab.
- The future work is clear and relevant. Specifically, it aims toward scale-up and establishes H₂ adsorption properties after proof of concept with CH₄.
- The project is following the plan, which is an appropriate plan to understand the potential of this approach.

Project strengths:

• Overall, this is the reviewer's favorite project. It is novel and fills a large hole in the portfolio of understanding and engineering bulk properties of materials in the portfolio. There are novel techniques to improve packing density of materials while avoiding traditional tradeoffs. The project could open the door for many novel techniques beyond MOFs and could create tunable materials or provide novel ways to pack sorbents into actual hydrogen storage systems/tanks.

- The approach is innovative and practical. It has shown impressive results so far and holds promise for future development.
- The project has a novel and generally applicable approach to improving storage: a method to make pellets that increases rather than decreases storage.
- The project has a simple yet elegant approach to utilizing the void space of polycrystalline materials. The project is well-executed overall.
- This is an innovative approach to tackling the practical issues of scaling up MOFs for large-scale storage.

Project weaknesses:

- There are no identified weaknesses. The reviewer really liked the project.
- There are no significant weaknesses.
- There are certain materials in the team's study, such as HKUST-1,¹ that still have certain ambiguous synthesis parameters. These issues warrant attention going forward if this material is of major relevance to future work.
- It is understood that the work is upcoming, but the lack of data regarding hydrogen use in the MOF composites is a weakness.

Recommendations for additions/deletions to project scope:

• A potential interesting second phase for the project is to investigate and take advantage of the novel forming techniques of these composites to create practical and cost-effective ways to load them into storage tanks (either traditional small-neck or large-mouth tanks). These materials have potential to be molded in place, etc., and the color change they exhibit could provide valuable quality-control tools.

¹ HKUST-1 is a framework built up of dimeric metal units connected by benzene-1,3,5-tricarboxylate linker molecules.

Project #ST-217: Hydrogen Materials Advanced Research Consortium (HyMARC) Seedling: A Reversible Liquid Hydrogen Carrier System Based on Ammonium Formate and Captured Carbon Dioxide

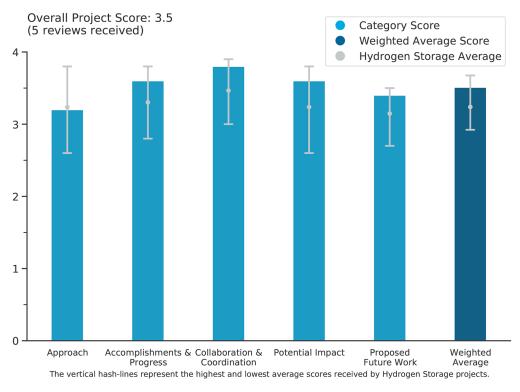
Hongfei Lin, Washington State University

DOE Contract #	DE-EE0008826
Start and End Dates	2/12/2020–9/30/2024
Partners/Collaborators	8 Rivers Capital, Pacific Northwest National Laboratory, Lawrence Livermore National Laboratory
Barriers Addressed	 Catalyst activity and stability Process intensification Process economics

Project Goal and Brief Summary

This project aims to build a prototype ammonium formate-based hydrogen uptake and release system and evaluate its techno-economic potential for commercialization. If successful, this project will develop and demonstrate a new generation of hydrogenation/dehydrogenation catalysts superior to commercially available catalysts. Washington State University is collaborating with 8 Rivers Capital and members of the Hydrogen Materials Advanced Research Consortium (HyMARC) on this project.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.2** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project has identified and addressed critical challenges in the space of liquid organic hydrogen carriers (LOHCs) and catalysis. The approach has several advantages, including using a byproduct of CO₂ capture to develop a hydrogen transport material.
- This project's goal is to make ammonium formate as a solid phase or solution carrier to move hydrogen very safely in bulk and then release hydrogen on site. The project actually uses up CO₂ in the creation step and sequesters it if the CO₂ is recycled into new formate. Developing suitable supports and catalysts is needed in the system to reduce costs. The team is addressing barriers and has a good safety culture and track record. The team also responded to safety suggestions. A real issue, however, is the reverse reaction. Some ammonia release seems inevitable and, in many applications, is entirely intolerable, which is a very serious concern regarding the approach.
- The approach of taking advantage of the superior solubility of ammonium vs. alkali metal formates to provide for increased hydrogen capacity of this potential carrier system is feasible and is a goal in alignment with Hydrogen Program objectives. Where the approach runs into problems is with the relative insolubility of the intermediate ammonium bicarbonate on the hydrogenation of ammonium carbonate to ammonium formate. Operating with slurries may present significant engineering challenges to this approach.
- It is interesting to investigate the ammonium formate liquid carrier. Ideally, we move away from expensive Pd catalysts, though, or provide a pathway for significant reduction in usage of Pd. There is a side benefit of including carbon capture, although the techno-economic analysis (TEA) should be completed to understand market size and feasibility, as well as locations, timing, etc. of capturing CO₂ with other gridbalancing or storage cycles, etc.
- The approach to the project is well-thought-out and is constructed to address project goals on the proposed timeline.

Question 2: Accomplishments and progress

This project was rated **3.6** for its accomplishments and progress toward overall project and DOE goals.

- The project shows very good progress, with the team having:
 - Found metal oxide supports to help stabilize the reaction intermediates, as well as tune the catalyst.
 - Shown that oxygen storage correlates with formate generation rate.
 - Figured out the rate and kinetic parameters of bicarbonate hydrogenation.
 - Shown 20-cycle catalyst stability.
 - \circ Found that a 2.5:1 H₂-to-CO₂ ratio is required for good conversion and is needed to keep the pH below 11.
 - Shown that the project can hydrogenate ammonium bicarbonate to formate in about 72 hours. However, this capture method is about half the price of making formate from formic acid and ammonia.
- The results presented are impressive. A strong understanding of the kinetics was presented, along with great stability data. The optimization of reaction conditions is important to understand. The reaction conditions are extremely favorable, leading to a significantly reduced cost of production compared to the existing commercial process.
- The project is well-executed, making progress, and has demonstrated the feasibility of the reduction of carbonate to formate, albeit with the difficulty of performing heterogeneous catalysis in a rather dense slurry. It would be useful to compare and contrast the carrier properties of ammonium formate and, for example, the sodium salt analog at the same initial concentration to better judge whether the ammonium salts are a help or more of a hindrance in achieving an engineered solution.
- There has been good progress in reaction and catalyst design. The material is stable in the solution and does not leach but may agglomerate (increase in size) after a few cycles.
- The team has met many of the proposed goals, including verification of science, scale-up, long-term cycling considerations, and the economics of the process.

Question 3: Collaboration and coordination

This project was rated **3.8** for its engagement with and coordination of project partners and interaction with other entities.

- The project team received both advice and lab assistance from Pacific Northwest National Laboratory (PNNL), Lawrence Livermore National Laboratory, and 8 Rivers Capital.
- It appears there is good communication and collaboration with the PNNL team, as indicated by several joint publications, and the project has an intellectual property interaction with an engineering/venture capital group at 8 Rivers Capital.
- There is good collaboration with key stakeholders and industry to provide the TEA.
- The project team has a strong group of collaborators, including an industry partner.
- The team has established well-suited collaborations to assist in the project goal.

Question 4: Potential impact

This project was rated 3.6 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The aim is to generate a commercially viable hydrogen carrier cycle, a new way to store and move hydrogen that offers more options to meet roadmap goals, especially in hard-to-decarbonize industries where pipelines may be impractical or unfeasible. The project is well-matched with the U.S. National Clean Hydrogen Strategy and Roadmap goals. The project includes economics, too, which further aligns with needs and goals.
- Developing high-capacity carriers is among the objectives of the Hydrogen Program. The high capacity of ammonium formate therefore makes it of interest in pursuing as a hydrogen carrier. This project is helping to illuminate the pros and cons of the system, which is valuable information to the Hydrogen Program.
- Use of formate carriers as an LOHC is attractive, owing to the low toxicity and cost of the materials. As with all hydrogen on-demand systems, demonstrating stability, purity, and repeatability at an attractive cost will always be the key challenge.
- The project is well-aligned with Hydrogen Program goals, including reducing the cost of hydrogen transmission. The project also has a side benefit of utilizing carbon capture byproducts, transforming captured CO₂ into a useful chemical for energy transmission with very promising economics.
- The project aligns with the Hydrogen Program's goals and objectives. There are numerous reactor considerations that will require further work, but for the most part, the project has a promising outlook for useful impact for a potential hydrogen carrier.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The future work is ambitious but appropriate.
- The next phase will address obtaining a prototype formate-to-power process unit and performing a TEA of the process, benchmarking it against a 700 bar compressed gas system. Perhaps it would be useful as part of the TEA to adjust the compositions of the ammonium salts such that all remain soluble and to explore whether an all-soluble system can be competitive with high-pressure gas storage.
- Focus on the TEA will be key to understanding the proper application for this system. The TEA should also understand the role of CO₂ capture's impact on the system—including whether this will add a supplemental revenue stream.
- The proposed future work is a logical continuation of the work performed and will provide insight into how well this technology compares to the current state of the art.
- The proposed future work is well-thought-out and will work toward the issues the team is currently facing.

Project strengths:

- The technical approach is very innovative and provides a useful path for a chemical waste stream while also reducing the cost of chemical production and hydrogen storage. The approach allows for a more benign, less harmful chemical to be utilized for hydrogen storage and transport. The interest from industry is impressive, as is the tech transfer that has happened thus far.
- The team successfully developed and built a prototype CO₂-to-formate process that integrates CO₂ capture and hydrogenation with aqueous ammonia solutions. The techno-economic considerations indicate this process has potential to reduce ammonium formate cost by a third. The team is well-balanced, with useful collaborations, and is likely to experience continued success.
- The project employs benign materials, with the added benefit of CO₂ capture.
- Chemistry can be driven with low-grade heat.
- There is a good team working on the catalytic/engineering aspects.

Project weaknesses:

- Lower solubility of ammonium formate may be a concern for system design. A full understanding of the solubility of both hydrogenated and dehydrogenated materials is required (including what concentrations at what temperature). Precipitation of material in the wrong area (reactor, valves, etc.) could be an operations and maintenance nightmare. We learned that lesson from the NaNBH₄ Natrium project, which needed to disassemble and rebuild the system multiple times due to crystallization of materials in the lines and reactor. Many reactors were destroyed in the process. Pd in the catalyst is a very expensive material. Eventually, moving away from precious metals will be needed. Demonstrating stability of the catalyst within the solution may prove challenging.
- The reaction rate is a bit slow for most applications. A fast reaction rate would improve throughput, benefiting almost all the possible applications of this technology.
- Dealing with the slurries generated poses a scale-up issue. The team needs to consider large-scale considerations/solutions for whether the process can be adopted by engineers.
- A pathway to mitigating the technological risk surrounding the solubility issues was not presented such as to mitigate the issues surrounding working with rather dense slurries.
- There is likely to be NH₃ release in the H₂ generation stream.

- The team should determine the level of NH₃ (and other impurities) in released H₂.
- A plan for the mitigation of the technical risks surrounding working with slurries in a catalytic system would be beneficial.
- Solubility curves of material should be included in the next review to understand real-world feasibility of the system.

Project #ST-218: Hydrogen Materials Advanced Research Consortium (HyMARC) Seedling: High-Capacity Step-Shaped Hydrogen Adsorption in Robust, Pore-Gating Zeolitic Imidazolate Frameworks

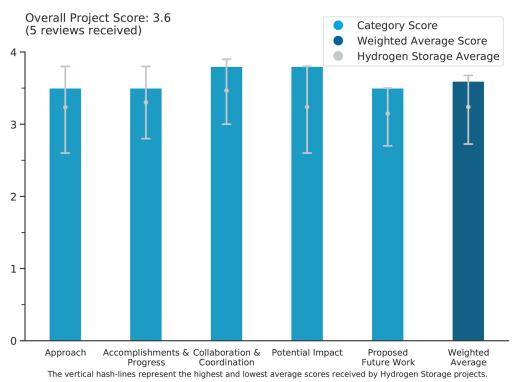
Michael McGuirk, Colorado School of Mines

DOE Contract #	DE-EE0008823
Start and End Dates	2/27/2020–9/30/2024
Partners/Collaborators	National Renewable Energy Laboratory, Lawrence Livermore National Laboratory, National Institute of Standards and Technology, SLAC National Accelerator Laboratory
Barriers Addressed	 Reduce the cost of producing and delivering hydrogen from zero- or near-zero-carbon sources Develop compact, lightweight, and low-cost hydrogen storage systems

Project Goal and Brief Summary

Current approaches to hydrogen transport and delivery entail extreme pressures or cryogenic liquefaction—both energy-intensive processes that increase costs. An alternative is using porous adsorbents that can densify hydrogen under milder conditions by providing enhanced surface area for hydrogen molecular adsorption. However, most porous adsorbents adsorb hydrogen most strongly at low pressures and temperatures. This project is exploring stimulus-responsive porous adsorbents that, through step-shaped adsorption—desorption profiles, can deliver their entire adsorbed capacity with minimal energetic input. These materials could store large quantities of hydrogen under mild conditions, as well as transport and deliver hydrogen with only small swings in pressure and temperature.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.5** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The reviewer is very much in favor of projects that allow tuning of materials and systems. They can improve performance of existing materials and likely be transferable to new materials or reveal new benefits yet to be planned. Methods to manipulate the traditional Langmuir isotherm are needed, and this project uses a novel approach with zeolitic imidazolate frameworks (ZIFs) to improve the controllability of these sorbent systems. From a control perspective, moving to a step curve may improve the energetics but may make the system more difficult to control. The step function provides a very narrow pressure or temperature window in which to release most of the hydrogen from the system. The most ideal curve would be a linear curve in which the system's state of charge (SOC) could easily be tracked by pressure primarily and temperature secondarily. Having a wider operating pressure range will allow for less sensitive (i.e., cheaper) sensors and simpler calculations of SOC. A more linear curve could also reduce the impact of any hysteresis in the system.
- This project directly attacks the lost capacity left at 5 bar in a metal-organic framework (MOF) tank by a morphology change that expels all remaining hydrogen within the pores. The team has made classic MOFs of this type and then modified them to try to achieve the project goals. Thus, the project is aimed at key barriers.
- The project is changing the paradigm of gas adsorption from the typical sorption onto open-framework, high-surface-area materials to an adsorbate-stimulated phase change process that results in a stepwise uptake of gas, which is very innovative and very difficult. This project's approach is well-thought-out and incorporates collaboration on the theoretical treatment of the phase transition.
- The approach is well-aligned to Hydrogen Program goals, and it is very innovative. The unique nature of the materials used shows promise to reduce the energy needed for the use of porous materials in hydrogen storage.
- The approach by the principal investigator (PI) to achieve efficient storage, transport, and delivery of hydrogen under mild conditions by leveraging stimulus-responsive synthetic microporous materials is an effective approach to achieve the project goals. The testing methodology and direction of the project are well-motivated.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals.

- This project's approach is well-directed to provide progress toward providing higher capacities at noncryogenic temperatures. This addresses Hydrogen Program goals in providing for cost and energy reductions of hydrogen storage. The project has made very good progress in accomplishing the replacement of cadmium with aluminum in the ZIF materials, as well as another flexible aluminum-based framework, MIL-53. The project demonstrated the latter has twice the capacity of the project's first material, CdIF-13. The team has explored linker modifications to promote lower energy adsorbate-stimulated pore opening, with promising results to date.
- The project synthesized a family (i.e., 60 different types) of MIL-53 relatives. The team used in situ x-ray diffraction (XRD) to probe the mechanism of opening. The project also provided data for a separate theory team to allow the researchers to better understand the mechanism and thus possibly assist in predicting better linkers to use.
- The PI has achieved excellent progress toward the project's objective, showing a development of understanding of these phase-change materials prior to what has already been discovered about them. The PI has published results and has overcome research barriers sufficiently, especially given limited funding.
- Progress has been steady and shows promise. The move away from cadmium-based systems and toward aluminum-based systems is a challenge—but is for the best. The results of the study show promise to reduce the energy needed by demonstrating performance that approaches a step curve for desorption with minimal hysteresis.

• The project demonstrated the ability to tune the desorption curve with selective ZIF materials. Hysteresis is still a concern for the project, but overall, the team has shown strong, encouraging results toward goals.

Question 3: Collaboration and coordination

This project was rated **3.8** for its engagement with and coordination of project partners and interaction with other entities.

- The team's work with Brian Space has been good for both parties, showing a great example of what collaboration can accomplish and why DOE emphasizes it. Likewise, the team includes very valuable collaborators at the National Institute of Standards and Technology (NIST) and the University of California, Berkeley.
- There appears to be a very excellent collaboration that has formed with another seedling, Brian Space's project, which has used computational tools to illuminate the details of the phase transition from "open" to "closed" porosity in the stepwise transformation. This has allowed McGuirk to make informed decisions on linker modifications. This is a nice collaboration. This project also has an effective collaboration with the NIST structural characterization team (C. Brown et al.), which has been very productive. National Renewable Energy Laboratory (NREL) is assisting with high-pressure sorption measurements, but the high-pressure pressure–composition–temperature (PCT) isotherm system at NREL has surprisingly and unfortunately not produced the data at this time.
- The PI listed collaboration with the HyMARC team, and appropriate connections are listed. Ideally, the PI will also work with HyMARC's Tankinator or levelized cost model to identify potential cost savings of modifying the desorption curve.
- The team is well-integrated with the team at HyMARC labs and has done an excellent job of utilizing the researchers' capabilities to advance the understanding of the materials studied.
- The PI has established reliable structure/theory collaborators that amplify the project's work in key areas.

Question 4: Potential impact

This project was rated **3.8** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- This innovative set of materials, which undergoes a sorbate-induced phase change resulting in a stepwise sorption of gas, has the potential to increase useable hydrogen storage capacity at non-cryogenic temperatures. This potential benefit maps directly onto Hydrogen Program goals and objectives and may have a significant impact on the field of hydrogen sorbents in general.
- This project could make MOFs a suitable hydrogen storage media for transportation, which is a major goal in the Hydrogen Program strategy and part of its roadmap. The project has excellent alignment.
- Reducing the energy demand of existing systems is a way to reduce overall system costs. The learnings from this project could be applied to future sorbents or similar materials. The project's learnings may also be used to tune systems for easier control.
- The project is well-aligned with DOE goals, specifically reducing the cost of hydrogen and providing lightweight storage solutions for hydrogen.
- The project aligns with Hydrogen Program goals, but it has yet to be seen whether the impact of this specific material class will prove cost-effective. The PI is shifting to more earth-abundant metals that comprise the materials, so there is potential for considerable impact if the trends hold through the metal changes. However, the performance seen with more heavy/expensive elements may not hold for the more earth-abundant ones.

Question 5: Proposed future work

This project was rated **3.5** for effective and logical planning.

• The future work is a very logical extension of current activities and outcomes. The work includes a very thorough approach to additional linker modifications supported by a theory collaboration, in situ structural characterization supported by expert x-ray and neutron scattering capabilities, and (hopefully) characterization of high-pressure sorption properties as a function of temperature. As this is a very new

area, there is certainly technical risk involved, but the carefully laid out approach and high level of execution this team has demonstrated mitigates this risk to the degree possible.

- Future work builds on past progress and anticipates potential barriers that face the project.
- Future work is very suitable and will hopefully achieve the project goals.
- Further understanding the phase change mechanisms and developing novel ways to control a system are interesting next steps.

Project strengths:

- Leveraging and interrogating what has been published on this class of MIL materials is important, as the PI believes (and has supporting evidence based on chemical substitution) that there is still much that is unknown about this enticing material class. Given that more earth-abundant metals used in these MOFs could engender more cost-effective materials, this project has numerous strengths toward reaching the goals of the Hydrogen Program.
- The project shows a strong understanding of the material's behavior and the challenges faced with moving from methane to hydrogen storage. The approach is very clever and shows promise to reduce the energy required to utilize this class of hydrogen storage materials.
- The team has experience and agility in making MOFs, and there is a relation to HyMARC. The project is pairing its work with that of Brian Space's team.
- The approach is novel. The team is excellent, and there is very good support from theory and characterization collaborations.
- The project provides new sorbent "tuning" tools.

Project weaknesses:

- This project includes strong hysteresis with initial results. A better understanding and reduction of hysteresis will be critical to providing solutions that have robust control.
- The team's use of other gases may not give a true reading on the best MOFs for use with H₂.

- The team should consider looking to NIST for high-pressure hydrogen sorption studies if the instruments at NREL are unavailable.
- The team should move to hydrogen testing at 5 to 100 bar when possible.
- The reviewer has no extra recommendations.

Project #ST-234: Development of Magnesium Borane Containing Solutions of Furans and Pyrroles as Reversible Liquid Hydrogen Carriers

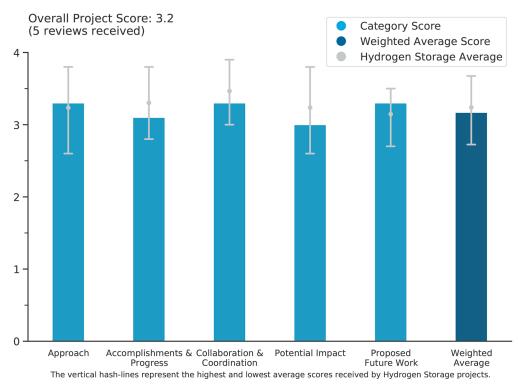
Craig Jensen, University of Hawai'i

DOE Contract #	DE-EE0008824
Start and End Dates	10/1/2019–6/30/2024
Partners/Collaborators	Hawai'i Natural Energy Institute
Barriers Addressed	 Identification of conditions that will enable and maintain the tandem, reversible dehydrogenation of Mg(BH₄)₂ and liquid organic hydrogen carriers catalyzed by pincer complexes
	 Development of high-activity, low-cost catalysts for the reversible, tandem dehydrogenation of Mg(BH₄)₂ and liquid organic hydrogen carriers Cycling stability

Project Goal and Brief Summary

The project goal is to develop hydrogen carriers with high available volumetric densities based on Mg(BH₄)₂ containing liquids and homogeneous pincer catalysts. Through this work, the project aims to demonstrate that liquid organic hydrogen carriers (LOHCs) and complex hydrides can be utilized in tandem to generate advanced hydrogen carriers, as well as showcase the viability of these carriers for reversible hydrogen storage and release through the utilization of homogeneous pincer catalysts to achieve efficient dehydrogenation and dehydrogenation processes. This project would thus allow for the elimination of intrinsic complications associated with gas evolution, greater efficiency of the dehydrogenation process, improved kinetics, and enabling of liquid hydrogen carrier-based hydrogen storage and delivery systems to meet DOE targets.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The novel and technically risky approach of coupling two apparently very disparate storage materials and mechanisms is innovative. If the approach were to work out, it would provide for a potentially interesting hydrogen carrier system. While the approach is high-risk, the Jensen team mitigates much of the risk through a deep understanding of the chemistry and catalysis that is required and experience of radically shifting gears when roadblocks may arise.
- The project followed a variety of trails that were planned but had issues. The team wisely abandoned those trails for more productive alternatives. Eventually, the team recognized that one of the material sinks preventing back reaction was a new and reasonable storage material and developed data on it. Pivoting to a useful output was very good. Goals are aligned with key barriers.
- The attempt to create a hybrid liquid carrier system is applauded. Directionally, this is a good approach to developing a useful sustainable and reusable carrier from metal hydrides and LOHCs. The choice of borohydrides, though, is very thermodynamically taxing. Given the high operating temperatures and pressures for hydrogenation and dehydrogenation, the system would be limited to large-scale grid-related storage. It is unclear if a levelized cost study was included in the original project plan to determine the feasibility of such a system. The development of highly selective nonprecious metal catalysts is also of great importance for practical LOHCs or other carrier systems to significantly reduce side reactions and cleanup (i.e., system complexity). The original target of the project was not to create a new carrier material altogether; rather, it was discovered by mistake.
- The approach is good, making incremental progress toward the goals through experimentation. The approach seems to be rather fluid, moving between compounds until one is found that provides good results. The catalyst used is quite versatile. The safety plan appears appropriate.
- The approach to the project in all its complexities is effective and contributes to overcoming the majority of barriers encountered.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and DOE goals.

- The initial system showed 25.4 kJ/mol enthalpy of dehydrogenation, which is attractive. The project actually attained release at 100°C. However, it is not a reusable system. Pyrrolidine was used at 180°C to reach 50 g/L, a nice density of hydrogen; however, that resulted in a sink of boron nitride bonds that could not be reversed. The project team recognized that the material was a carrier. It became the carrier of interest, B(NC₄H₈)₃, which is reversible at 195°C and 100% reversible at 110 bar. It is very recyclable. There is potential for 87 g/L.
- When the results of the researchers' initial exploration gave them lemons, they made lemonade. The team realized that the chemistry of the combination of the two storage systems was not working out as hoped; however, careful characterization of the products indicated that tris(pyrrolidino)borane was formed. This compound could be reversibly dehydrogenated to the tris(pyranidino)borane. On a material basis alone, this cycles perhaps just 2%–3% hydrogen, and a quick techno-economic analysis (TEA) may have to be done to determine whether this system can achieve DOE goals and objectives for a hydrogen carrier.
- The results provided are great, showing that progress is being made toward identifying an appropriate material that meets project goals. The operating conditions of some of the materials are less than ideal; several are solids at ambient conditions.
- A potential new carrier material was discovered somewhat by accident. The new carrier has many issues to resolve to create a robust system. The project is nearly complete, so developing a system is likely not realistic.
- Significant progress has been made, but there are glaring issues with this material system, given its complex chemistry and limitations on favorable equilibrium for hydrogenation/dehydrogenation. Additionally, the goal of leveraging magnesium borohydride and LOHCs simultaneously has been found

not to be possible; the formation of the B-N bond containing the product will not facilitate $Mg(BH_4)_2$ regeneration. The goal of the project has deviated from the set task.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- The project team worked with Pacific Northwest National Laboratory (PNNL) and the National Renewable Energy Laboratory (NREL) to investigate reactor flows and analysis. That collaboration seems to have greatly helped. The team learned about ways to drive to higher conversion from outside collaboration.
- The project has made good use of Hydrogen Materials Advanced Research Consortium (HyMARC) expertise and capabilities at NREL and PNNL.
- Well-coordinated collaboration among several laboratories is evident.
- Collaborations exist that aid in moving the project forward.

Question 4: Potential impact

This project was rated 3.0 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- Storage materials are needed for many areas of the hydrogen economy, and the storage materials in this project could serve many of them. The project has good alignment with the Hydrogen Program's strategy and roadmap.
- The potential impact is high, given the flexibility of the catalyst and high hydrogen content of the materials investigated.
- The project aims to develop reversible hydrogen carriers. This supports the goals and objectives of the Hydrogen Program; if successful, the project could be impactful.
- Though the principal investigator (PI) has executed commendable chemistry and resolved the mystery of what is occurring in the system, the utility of the trispyrrolidino borane <--> trispryanodino borane recyclable system feels largely cost-prohibitive and too inefficient to suggest great potential impact. The flow reactor that the PI has discussed for future work, however, may change this in some ways, but it is unclear to both the reviewer and the PI what the metrics of such a process would be, based on the provided files.
- As originally planned, this project would have struggled to find relevance because of the high operating temperatures and complexity of the system. It seems that anything using borohydride will always be thermodynamically challenged. It has been worked on for a decade now, and dehydrogenation temperatures remain stubbornly high. The potential new carrier identified is a "goop," as described by the PI. It will be difficult to control—to store and move around—in real-world conditions. Another key concern is preventing premature hydrogen generation while keeping material liquid at ambient conditions.

Question 5: Proposed future work

This project was rated 3.3 for effective and logical planning.

- Future work involves altering the borane moieties to provide a lower-melting liquid system. The plan to move to a continuous flow reactor to remove the equilibrium-limited dehydrogenation in a closed system is a good one, particularly if lower-melting liquid systems can be found.
- The use of a flow reactor is a good way to find the limits of the material performance in more industrial applications. Developing an actual liquid carrier is key to meeting DOE goals.
- Future plans are suitable. The project team will be looking to try the three-carbon version of the rings to help achieve a more useful system, based on thermodynamics.
- It is important to work on keeping the material in liquid state at lower temperatures to create a simple system, preventing side reactions and premature hydrogen evolution.
- Future work will build on the progress of the project and potentially overcome the barrier of an unfavorable equilibrium for hydrogenation/dehydrogenation. The potential impact still appears marginal.

Project strengths:

- The project team has strong chemistry, and the PI and other team members are excellent scientists who have resolved many of the barriers that the project has faced as it has progressed.
- The catalyst is very flexible and well-understood by the project team. The team is very knowledgeable in the chemistry of the materials investigated.
- The project team has world-class expertise and experience in boron chemistry and catalysis.
- Project strengths include chemical insight and the flexibility to follow the possibilities and find a good outcome.
- A project strength is the identification of a potential new class of carrier materials.

Project weaknesses:

- The project would benefit from regular—though infrequent—discussions with an engineering collaborator to help guide efficient exploration of the family of boron tris tris-nitro-pi-bonded ring chemical hydrogen storage "system."
- The hydrogen metrics of the boron adduct appear low and cost-prohibitive, given the complex system chemistry.
- The materials are not ideal for liquid transport. There appear to be significant challenges presented with these materials that may make them difficult to utilize in industrial or commercial applications.
- The project was challenged from the beginning with a thermodynamically challenged class of borohydride materials.

- The project should do what the PI intends to do: search through the options of the nitrogen-substituted ring options for one that has lower enthalpy, good hydrogen content, reasonable cost, and operating conditions in which reactant and product remain liquid at modest pressure.
- Perhaps there is a way to have a cursory TEA to explore where these lower-capacity reversible LOHCs may find a role in hydrogen storage.
- Potentially, the project could pivot to a different LOHC, as propositioned in the project's future work on tris(azacyclopranolidine)borane, TAzacB. The system may encounter similar issues, so alternative LOHC systems should be more intensely examined.
- The following aspects regarding the new carrier are unclear: storage capacity (gravimetric/volumetric), before and after mechanical characteristics, viscosity, thermal conductivity, kinetics, and whether it will precipitate. The final report should include characteristics of the material to better envision the control system required.

Project #ST-235: Hydrogen Storage Cost and Performance Analysis

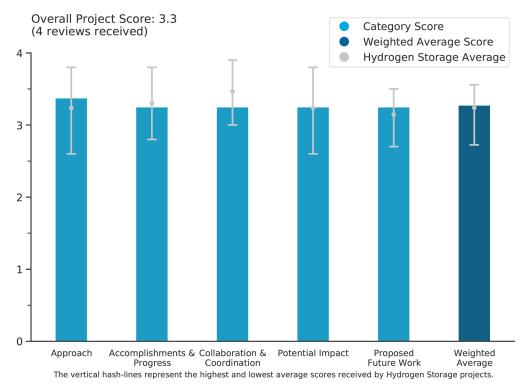
DOE Contract #	DE-EE0009630
Start and End Dates	9/30/2021-9/29/2024
Partners/Collaborators	Pacific Northwest National Laboratory, Argonne National Laboratory
Barriers Addressed	System weight and volumeSystem costSystem life cycle assessment

Cassidy Houchins, Strategic Analysis, Inc.

Project Goal and Brief Summary

This project aims to conduct a comprehensive, independent, and transparent bottom-up techno-economic analysis (TEA) of hydrogen storage systems using Design for Manufacture and Assembly (DFMA). The primary objectives include identifying cost drivers, determining which performance parameters can be improved to have the greatest impact on cost, and providing referenceable reports on the current and future projected costs of hydrogen storage systems for onboard, delivery, and stationary applications. The analyses cover large-scale liquid hydrogen (LH2) storage vessels, helium refrigeration for zero boil-off LH2 storage, bulk LH2 transfer terminals, and utility-scale engineered underground storage. Through this analysis, the project aims to provide insights into cost reduction strategies for hydrogen storage, identify areas with the greatest potential for research and development (R&D) advancements, and provide insights toward meeting DOE cost targets.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The team conducted a detailed TEA of several hydrogen storage-related systems, enabling the community to better understand what the cost drivers are for each system and what targeted research can reduce the cost.
- The project provides an extensive review of factors affecting bulk hydrogen storage. There is much content to analyze in this report, but the cost model bar charts are helpful.
- The team has good expertise in cost modeling, with many years of experience and capable personnel.

Question 2: Accomplishments and progress

This project was rated **3.3** for its accomplishments and progress toward overall project and DOE goals.

- The project conducted several detailed TEAs of hydrogen storage-related systems. The team completed evaluations of large vacuum-insulated spherical storage vessels, a helium refrigeration system, and a novel underground storage system recently proposed by a start-up.
- The project provides a solid and detailed analysis of large LH2 vessel costs. The cost analysis for the engineered underground storage differs drastically from previous calculations by Schmidt, so this difference should be analyzed and explained. Also, the authors should include a full reference to Schmidt, given its importance to this work.
- Extensive cost data are reported and graphed for capital cost and annual operating costs. One potential concern is long-term durability and hydrogen permeability of the large tank storage approaches.

Question 3: Collaboration and coordination

This project was rated **3.3** for its engagement with and coordination of project partners and interaction with other entities.

- There is good collaboration with external companies to determine the manufacturing techniques being used to build the wide range of technologies covered in this work. The work on large-scale hydrogen storage systems diverged from the concept on which the Shell-led project (ST-241) has settled, so it would be good if project ST-241 would share more information to allow a comparison between the vacuum and non-vacuum insulated paths.
- The project has extensive collaboration, considering the narrow field of experts in this project area. The reviewer strongly recommends an ongoing project to capture more data as DOE progresses with the Regional Clean Hydrogen Hubs Program (H2Hubs).
- The project has good collaborations with multiple institutions. However, closer collaboration with Shell is necessary to evaluate the options for LH2 insulation, perhaps under a non-disclosure or similar agreement. It would have been very useful to look at the option of non-vacuum insulation to consider trade-offs between cost and heat transfer performance.

Question 4: Potential impact

This project was rated **3.3** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- This type of modeling is critical so stakeholders can understand how all the different technologies compare to one another economically. This work also helps identify the highest-cost components associated with some systems and where additional R&D is needed to drive down the cost.
- This project provides cost metrics that will be very impactful as the industry moves forward with large hydrogen projects. The use of Perlite insulation is of interest; it would be interesting to know whether it has been used for vehicle tanks as well.
- LH2 storage vessels are obviously important for future hydrogen transport. However, it is not clear whether modeling "engineered underground storage" is the most pressing need for the Hydrogen Program. Perhaps the effort should be invested elsewhere.

Question 5: Proposed future work

This project was rated **3.3** for effective and logical planning.

- The future work proposed seems logical and would improve the analysis of the systems covered by this project.
- The proposed work is meaningful, but consideration should be given to an extended project to track costs associated with H2Hubs and other large capital hydrogen projects.
- There is a future task to model long-term bulk storage. It would be a good idea to conduct a preliminary evaluation of the different options before dedicating so much effort to a particular approach.

Project strengths:

- The project is a detailed economic modeling study that helps the community understand and compare various hydrogen storage technologies. Strategic Analysis, Inc., has good collaboration with external partners to ensure the models are relevant.
- The project provides critical cost review for bulk hydrogen storage. The full report will be very useful to the hydrogen industry.
- The team has good expertise and competent researchers.

Project weaknesses:

- The team did a great job with the available resources. The project should continue as new initiatives are launched to track assumptions and actual results, adjusting the approach as required.
- It would be good to understand the largest sources of uncertainty in the models and how sensitive the results are to these uncertainties. Given the large volume of the underground storage system, the cost of transporting and disposing of the dirt removed during drilling should probably be considered.
- The project did not consider the option selected by Shell researchers. Closer collaboration would have made results more useful. Major differences with previous (old) analyses of Schmidt may reduce the credibility of the results.

- It would be beneficial to investigate non-vacuum-based insulation approaches for large LH2 storage systems and compare them to the vacuum-based insulation systems from this work.
- The project should conduct preliminary evaluation of bulk storage systems before investing significant effort in individual approaches.

Project #ST-237: Carbon Composite Optimization Reducing Tank Cost

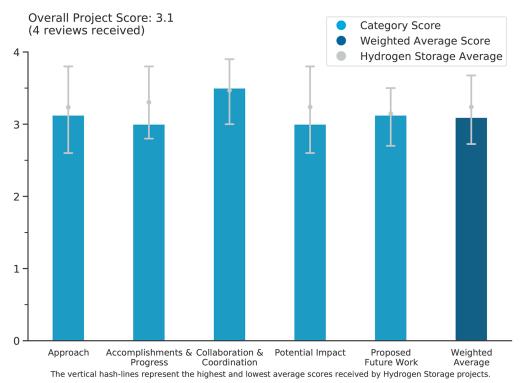
Duane Byer	y, Hexagon R&	D
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DOE Contract #	DE-EE0009240
Start and End Dates	10/1/2021–9/30/2026
Partners/Collaborators	Cytec Engineered Materials, Oak Ridge National Laboratory, Pacific Northwest National Laboratory, Newhouse Technology, Kenworth Research and Development Center
Barriers Addressed	Carbon fiber production costs

Project Goal and Brief Summary

Currently, the cost of high-pressure storage tanks is a significant barrier to the mass deployment of cleaner vehicle fuel sources such as hydrogen and compressed natural gas, and the carbon fiber used in these tanks accounts for approximately half of the total hydrogen storage system cost. This project aims to reduce compressed hydrogen and compressed natural gas storage costs by developing new and optimized technologies to produce low-cost, high-strength carbon fiber with a demonstrated cost of less than \$15/kg, tensile strength of 700 ksi, and tensile modulus of 35 Msi. Carbon fiber technology will be enhanced through controlled fiber morphology using tuned polymer molecular structures and optimal spinning and carbonization conditions. Researchers will use high-throughput fiber manufacturing to increase production capacity, materials characterization to minimize defects, high-performance resin and interfacial engineering to enhance the composite, and modeling to improve pressure vessel design. The project also addresses environmental concerns by exploring new methods to recover the resin and fibers for secondary use.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.1** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- It is great that this project tackles the entire carbon fiber manufacturing process, including recycling. The team is well-suited to reduce the cost of carbon fiber and optimize the entire process.
- The approach may result in modest cost reductions for carbon fiber to be used in hydrogen storage tanks. This project has the highest technology readiness level and least-risk approach; however, it is less innovative in terms of the ability to make substantial cost reductions.
- The team has been researching the proposed tasks (or similar tasks) for several years. It is not clear that large (50%) cost reductions via incremental improvements in different aspects of fiber and vessel manufacturing can be expected.

Question 2: Accomplishments and progress

This project was rated **3.0** for its accomplishments and progress toward overall project and DOE goals.

- The entire team has made good progress toward the project goals.
- The carbon fiber meets the requirements for average strength and stiffness and shows promise for target cost reduction; however, there was no discussion of how exactly the cost would be reduced. A scale-up is planned for the Oak Ridge National Laboratory (ORNL) carbon facility.
- The cost estimate on page 13 seems quite optimistic. The team should specify in detail what needs to be accomplished for this to become a reality.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- This project has a good combination of institutions with long-standing expertise.
- The team is quite large but seems to be well-coordinated; all project partners are making good contributions.
- Project coordination includes multiple supply chain partners—including a polyacrylonitrile (PAN) supplier, ORNL's pilot plant, Solvay, and Hexagon—to make the tanks.

Question 4: Potential impact

This project was rated 3.0 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The project is very relevant to reducing the cost of pressure vessel manufacture. Recycling is important, but it is unclear whether the cost of the recycled carbon fiber will enable large-scale reuse. A preliminary cost estimate would be useful for determining how relevant this is for future carbon fiber utilization.
- It would have been good to see more details about some of the changes made in the carbon fiber manufacturing and utilization process and how the changes have impacted the cost so that others can learn from the steps taken.
- The project shows indications for target cost reduction but does not show a path to reduce embodied energy for carbon fiber production.

Question 5: Proposed future work

This project was rated **3.1** for effective and logical planning.

- Proposed future work is focused on scale-up to large quantities of carbon fiber and assessment of strength distribution where a narrow distribution is desired.
- Future project plans seem in line with the remaining barriers.

• Perhaps it would be most efficient to select one or two of the tasks that are most promising and dedicate all the efforts to these tasks instead of pursuing all possible approaches.

Project strengths:

- It is great that this project tackles the entire carbon fiber manufacturing process, including even recycling. The team is well-suited to reduce the cost of carbon fiber and optimize the entire process.
- The project's strength is the maturity of the approach, which is an incremental cost reduction strategy.
- The project has a good combination of institutions with relevant expertise.

Project weaknesses:

- It would be good to see some of the knowledge from this project transferred to others, considering taxpayers are contributing the bulk of the funding. Progress has been slow.
- Projections are extremely optimistic and need a stronger justification when reported.
- A project weakness is that the project does not address several of the key issues regarding carbon fiber cost and embodied energy.

- It is not clear where the cost reduction comes from and whether it will translate into commercial carbon fiber production.
- Carbon fiber is famous for being responsible for large amounts of carbon dioxide emissions. It is suggested that the project research low-carbon-dioxide manufacturing approaches.

Project #ST-241: First Demonstration of a Commercial-Scale Liquid Hydrogen Storage Tank Design for International Trade Applications

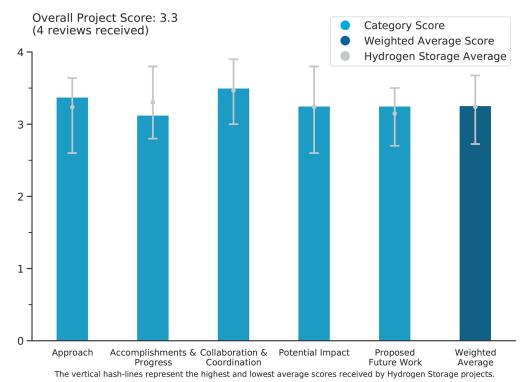
Ed Holgate, Shell

DOE Contract #	DE-EE0009387
Start and End Dates	9/1/2021–8/31/2024
Partners/Collaborators	CB&I Storage Solutions LLC, GenH2 Corporation, NASA Kennedy Space Center, University of Houston
Barriers Addressed	Ultra-low boiling point of hydrogen (20 K)

Project Goal and Brief Summary

One of three priorities in the Hydrogen Program is low-cost, efficient, and safe hydrogen delivery and storage. This project aims to develop a first-of-its-kind affordable, very large-scale liquid hydrogen (LH2) storage tank for international trade applications, primarily for installation at import and export terminals. The project aims to create a large-scale tank design that can be used in the 20,000–100,000 m³ range (1,400–7,100 metric tons of LH2). Key success criteria for the large-scale design include a targeted LH2 boiloff rate of less than 0.1%/day and a capital investment below 150% of liquefied natural gas storage cost. The project will also ensure that the technology meets safety and integrity regulations, codes, and standards.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.4** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project will systematically study applicability of lower-cost solutions to large-scale LH2 insulation. The project utilizes modeling and experiments to determine the missing material properties needed to apply the models to the expected conditions within the storage system. The work results in a subscale demonstration of the design concept to help prove viability.
- The approach is light on details, but the goal of actually building a tank and coordinating at the NASA Marshall Space Flight Center site is impressive.
- Considering alternatives and focusing on the perceived "best" option is a good approach.

Question 2: Accomplishments and progress

This project was rated **3.1** for its accomplishments and progress toward overall project and DOE goals.

- The team has made good progress toward the project goals. Several insulation materials have been tested experimentally, and some did not result in runaway cryopumping. Key progress has been made toward building the subscale storage system. A site to build the subscale system was found, and it is being prepped for construction. The cryostat being built is almost ready for commissioning.
- The presentation is light on details but indicates that the design has been completed and validated with a key focus on insulation and mitigation of cryopumping. It is not clear why an active vacuum pump is not considered to ensure vacuum is maintained.
- The authors are limiting the information presented. While this may be justifiable due to intellectual property (IP) or similar reasons, it makes project evaluation extremely difficult. It seems that the cryopumping issue was solved, but we do not know how. It is unclear whether the project invented a new material or how it is different from materials previously used. There is also a question of whether it would be possible to give a qualitative description without revealing IP. Slide 14 talks about hydrogen and helium in the insulation space. These gases do not condense at the Dewar temperature, so they may be part of the solution, but once again, it is unclear.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- This is a large project with a diverse team. The members seem to be well-coordinated and are all making good contributions to the project.
- The project utilizes key collaborators, most notably the NASA Marshall Space Flight Center.
- There is a good combination of organizations with good, focused expertise.

Question 4: Potential impact

This project was rated **3.3** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- This is an important task for the future of hydrogen production and large-scale delivery.
- This project seems to make good progress toward reducing the cost of large-scale LH2 storage. Given that there is currently not enough LH2 supply to keep local customers satisfied, it is unclear when such systems will be able to play a role in the hydrogen economy. However, such work is needed to demonstrate to investors what is possible. The more information that the team can share with the community, the more relevance and impact the project will have.
- The key impact will come after the tank has been constructed and made operational to ensure the design meets requirements. It would be great to link to the other project cost models.

Question 5: Proposed future work

This project was rated 3.3 for effective and logical planning.

- Testing the materials at LH2 temperatures will begin shortly, as will construction of the subscale storage system, both of which should provide very useful information. These plans are well-aligned with the key barriers the project is addressing.
- This project has a good plan for testing concepts at NASA and demonstrating the validity of the approach.
- The next step is to order the materials and build the tank. Tank performance testing will be critical; a time extension may be required to allow adequate time to report on performance.

Project strengths:

- The project involves a systematic study of using lower-cost insulation and design for large-scale LH2 storage. The team is using fundamental experiments to really understand some of the key barriers. This is a highly skilled team with all the right experience to make this a successful project.
- The project has a strong team, and building and operating the tank is a large and impressive step for the DOE Hydrogen Program.
- There is good project relevance and a good combination of organizations with valuable expertise.

Project weaknesses:

- We know very little of the approach used, and we may not know very much more, as the companies seem very dedicated to communicating as little as possible. There should be a way to explain the approach without revealing IP, and the reviewer would invite the organizations to try it.
- This project has the potential to provide much useful fundamental information and data for others. It is not clear how much of this information will be shared with the community.
- It could take years of monitoring the systems to learn of any deficiencies in the design and capture lessons learned.

- Hopefully, the basic materials measurements at LH2 temperatures will be published, as the information would be very useful for the community. Maybe more materials can be added to the test matrix to help anonymize the materials that will be used and protect the proprietary design information.
- The team should consider adding some minimal level of post-project reporting to better document lessons learned.
- It seems adequate either to demonstrate the approach or to give up on it and return to standard vacuum insulation.

Project #ST-242: Dimethyl Ether as a Renewable Hydrogen Carrier: Innovative Approach to Renewable Hydrogen Production

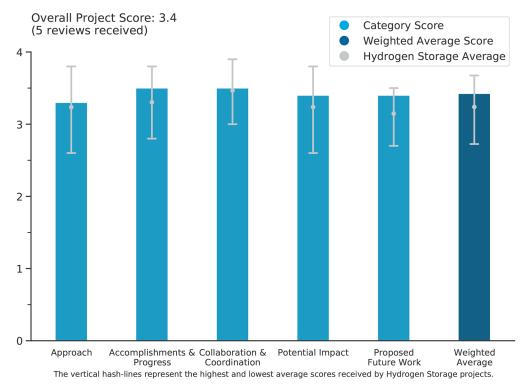
DOE Contract #	WBS 4.5.0.405
Start and End Dates	4/5/2022–4/5/2025
Partners/Collaborators	Los Alamos National Laboratory, Oberon Fuels, Inc.
Barriers Addressed	 Renewable hydrogen production scale-up Transportation and distribution costs Renewable hydrogen process commercialization

Michael Heidlage, Los Alamos National Laboratory

Project Goal and Brief Summary

The project aims to commercialize renewable dimethyl ether (DME) as a fuel-cell-grade hydrogen carrier capable of storing and transporting hydrogen on a global scale. The team is designing, building, and demonstrating the process using Los Alamos National Laboratory's (LANL's) novel dual catalyst bed to produce 25 kg per day fuel-cell-grade hydrogen. The quality of the generated hydrogen will be validated via fuel cell performance and testing. The project will then provide project partner Oberon Fuels, Inc. (Oberon) with full documentation to support Oberon's commercialization plan.

Project Scoring



Question 1: Approach to performing the work

This project was rated **3.3** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

- The project approach to utilizing DME as a hydrogen carrier through construction of a modular reactor setup is excellent. Most major barriers to utilization have been overcome.
- The approach was well-explained and justified, taking advantage of the industrial partner's access to "green" DME and LANL's history and knowledge of developing onboard DME-to-hydrogen reformers for fuel cell applications. As described, this project potentially will be the springboard to an Oberon 1,000 kg/day unit. The discussion indicated that detailed attention was given to conducting this work safely. The project builds on well-described chemistry and catalysis and is developing a small-scale reactor system using solid chemical process engineering approaches. The project is well-designed and feasible.
- The approach addresses several challenges, including the safe transport of hydrogen and renewable hydrogen transport.
- The project approach includes using DME as a carrier of hydrogen and using existing data on steam reforming DME to hydrogen and CO₂ (i.e., no return material) to accelerate reactor design. The project includes significant safety analysis and planning. The industrial partner will implement the technology. There is some concern about impurities, unconsumed DME, and by-products fouling the pressure swing adsorption (PSA) system and thus the fuel cell that uses the hydrogen. So the project addresses relevant barriers.
- The reviewer is not a big fan of using electric heat to drive the endothermic reaction. The 134 kJ/mol requirement will drive a large energy demand, which may not be available from the grid when/where needed. It will limit the autonomous potential of this technology to areas where a reliable electrical hookup is provided or drain valuable electricity from the grid at a time when this system might be used to supplement the grid with power. The reviewer would rather see sacrificial hydrogen used to provide heat to increase the autonomy of the system. Furthermore, a reaction temperature of 205°C for full conversion yields precludes the use of low-grade heat or cogeneration possibilities that could be used to further improve the efficiency of the system. It is unclear if a lower-temperature, lower-yield system could be operated in parallel with an exhaust gas recirculation system to get the yield improved back to approximately 100% (i.e., it is unclear if the yield curve is entirely dependent on temperature or if it is also a function of kinetics). If high yield can be achieved at a low temperature, though a larger system may be needed. It would be interesting to investigate the tradeoffs.

Question 2: Accomplishments and progress

This project was rated **3.5** for its accomplishments and progress toward overall project and DOE goals.

- There is excellent progress on design/modeling and small-scale proto buildup.
- The project has made strong progress, including the design and delivery of the reactor as well as the full development of the piping and instrumentation diagram.
- The project is making steady progress in modeling, refining, designing, and constructing a DME reformer capable of generating 25 kg per day hydrogen. A significant discussion of operational safety for this project at LANL was provided.
- The project team designed a small footprint reactor and worked out heat transfer issues in the reactor, reducing the temperature difference across the catalyst from nearly 100°C initially to approximately 30°C. The team built the reactor and created a modular design for easy expansion and less overcapacity. The team completely designed the full process model, started building it, and developed controls.
- The accomplishments are clear and progress toward scale-up is very impressive; however, there is a misrepresentation of the process being of "low or negative carbon intensity" (slide 4). Specifically, in the generation of hydrogen through the project's process, as was inquired about during the presentation and is documented in the team's supporting information, the project's schematics indicate there is no attempt of CO₂ capture; the process is simply emitting CO₂ generated (alongside hydrogen) from the steam-reformed DME into the atmosphere. "DME Steam Reforming: (CH₃)₂O + 3H₂O ↔ 6H₂ + 2CO₂" is on slide 6. This

project's goal, to the reviewer's understanding, is centered on the creation of a hydrogen carrier process for offsetting CO_2 emissions. It feels disingenuous to the reviewer to suggest there is low to negative carbon intensity if no attempt at CO_2 capture is made, regardless of where the CO_2 is initially sourced from in the creation of DME.

Question 3: Collaboration and coordination

This project was rated **3.5** for its engagement with and coordination of project partners and interaction with other entities.

- Oberon and LANL are interacting closely on the project. Oberon has raised its ante, which can be taken as a sign that it sees promise with the approach and direction that the LANL team is taking.
- The project has a heavily involved industrial partner, Oberon, that may build a 1,000 kg/day pilot.
- Great collaboration between LANL and Oberon is evident.
- There is clear and effective collaboration within the project.
- The project has good collaboration with appropriate laboratory and industry contacts.

Question 4: Potential impact

This project was rated **3.4** for supporting and advancing progress toward Hydrogen Program goals and objectives.

- The project allows for the transport of hydrogen at greater density with lower pressure at a modest temperature. The hydrogen can come from negative carbon pathways. This aligns well with several DOE goals and with DOE's strategy.
- Converting DME derived from biomass/renewables to hydrogen of suitable purity for fuel cell applications is of high relevance to DOE's Hydrogen Program goals but likely also for the goals of the Bioenergy Technologies Office.
- Finding practical liquid hydrogen carriers can tremendously simplify and expand use case opportunities for large-scale deployment of hydrogen for production/delivery and grid balancing activities.
- The project has the potential to provide hydrogen from renewable sources using a carrier that is easily transported and less harmful than several other liquid organic hydrogen carriers (LOHCs) that are under investigation.
- There is a clear impact for DME steam reforming to be an excellent hydrogen carrier. CO₂ capture needs to be included in the final process.

Question 5: Proposed future work

This project was rated **3.4** for effective and logical planning.

- The project is well-planned and has a very engineering-oriented progression of decision points and milestones, all of which seem quite reasonable and feasible.
- The proposed plans build upon the completed work and should demonstrate hydrogen production at scale.
- The project has clear and well-thought-out future work that builds upon past progress.
- A shakedown of the test system and controls is planned. The system is planned to operate at 12 kg/day hydrogen. The project team is finishing the planned work, as they should.
- An appropriately sized demonstrator is planned. For the next review, it would be good to provide more information about the reactor kinetics and capital expenditure requirements for a large-scale system. The reviewer does not have a good feel for how big a reactor is for a 12.5 kg/day or 25 kg/day system. It is unclear what output could be anticipated from an International Organization for Standardization (ISO) trailer-sized portable system, for example.

Project strengths:

• The reactor and system designs are very well done. The material used is safer to transport than several other LOHCs and comes from a low-carbon-intensity process.

- The project has a strong engineering-oriented team to develop an engineering solution for a DME-tohydrogen process that is supported by a significant industrial entity, Oberon.
- The project uses agriculture waste to generate DME and then DME to make hydrogen. This could be a benefit to rural America.
- DME as a hydrogen carrier is an attractive proposition. A cost-effective and reliable reformer design will be key to large-scale deployment.
- There is compelling scale-up potential for a reliable hydrogen carrier.

Project weaknesses:

- The use of electricity and high temperatures for dehydration will limit the locations where systems can be deployed or cogeneration opportunities for increased efficiencies.
- No CO₂ waste mediation steps are mentioned or considered.
- It is not clear if the clean-up section is sufficient for removing the variety of impurities from CO (from low freezing point toxic gas to unused DME, a volatile liquid). The PSA unit will doubtlessly yield a cleaner hydrogen stream, but it is not clear if the hydrogen will be clean enough and the system durable so that later in use, the PSA will not be swamped with byproducts on its surface, reducing its effectiveness.
- The challenging development of a control system seems like an oversight in the program planning. The process seems rather intensive for hydrogen release, requiring post processing like water gas shift and PSA. The process is almost twice as energy intensive as methanol reforming. It is unclear if the advantages of DME outweigh the significant energy premium needed in comparison to straight methanol steam reforming. The process is also water intensive, requiring more water on a mass flow basis than DME.

- Although not a requirement, this would be a much more compelling case, and thus more likely to be a saleable product, if the CO₂ was captured and used or in some way sequestered or trapped so that the large-scale user could then get carbon credits.
- CO₂ waste mediation steps should be included at the back end of the process.
- It is unclear where in the hydrogen ecosystem these systems will be used and at what scale. It is unclear if this will be used for large-scale grid balancing and/or delivering fuel to forecourt stations. Appropriate system tradeoffs and analysis should be made to adjust for the intended use case. Depending on the end use application, the project team should investigate hydrogen offtake/burn if the system is portable/remote and reliable electricity hookup is not available or the system is intended for use in grid balancing.
- If low-temperature cogeneration opportunities exist to provide the heat, consider developing a lower temperature system.

Project #ST-243: FueL Additives for Solid Hydrogen (FLASH) Carriers for Electric Aviation

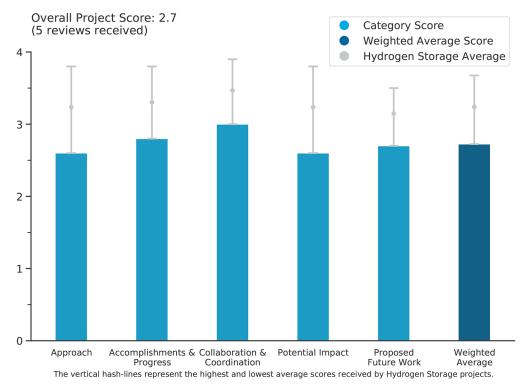
Noemi Leick, National Renewable Energy Laboratory

DOE Contract #	WBS 4.1.0.504, DE-EE0001647
Start and End Dates	11/1/2022 (NREL), 3/15/2023 (Honeywell) - 6/14/2024
Partners/Collaborators	Honeywell, SLAC National Accelerator Laboratory, Colorado School of Mines
Barriers Addressed	 Cost of borohydride fuel too high Lacking assessment matrix for fuels is preventing efficient material screening Impurities in H₂ stream: detrimental to fuel cells and toxic to living organisms

Project Goal and Brief Summary

The project focuses on optimizing fuel formulation for hydrogen-powered unmanned aerial vehicles (UAVs). Currently, most UAV technologies rely on non-renewable electric power. The project aims to develop cost-effective fuel cells with materials-based hydrogen storage. The team will develop a FueL Additives for Solid Hydrogen Carriers (FLASH) formulation that can deliver 6 g $H_2/100$ g fuel and design, build, and test a fuel cell cartridge compatible with FLASH. The formulation with be tested with a 600 W fuel cell system, and the team will quantify the specific energy of the cartridge and system.

Project Scoring



Question 1: Approach to performing the work

This project was rated **2.6** for identifying and addressing objectives and barriers and for project design, feasibility, and integration with other relevant efforts.

• The project approach is novel and demonstrates a path to cost effective hydrogen storage materials.

- The team's approach to the project is effective and contributes to overcoming most scientific barriers.
- The project team is using material for generating hydrogen for a drone with 600 W fuel cells. The material is used as a one-way carrier, which greatly reduces constraints on chemistry options. The project includes a significant safety effort since the material is pretty reactive. The team uses a salt mix with NaBH₄:N₂H₅Cl to keep costs reasonable. All these points add up to a good approach, and one aimed at some important barriers, but the extreme needs of the platform may push the team to a niche solution. The current project plan has reactive material either premixed or layered, which, as the team is aware, could lead to stability issues.
- A weakness of the project approach is the lack of discussion as to what the UAV system requirements and fuel configurations must be to inform the choice of hydrogen release mechanisms, how the release would be initiated onboard, and the list of candidate materials that have a chance of meeting all of the criteria for the UAV application. Discussion such as this was lacking. One criterion that was discussed was shelf life, which this reviewer guesses is a critical requirement for the application; however, the mixture of hydrazinium chloride and sodium borohydride was demonstrated to evolve hydrogen at room temperature upon mixing, indicating, as expected, that there is no useful shelf life for this material. One might anticipate moving on to other candidate material(s) at that point.
- NaBH₄ is a very difficult material to work with in a small package. Significant thermal and post processing hydrogen cleanup work often results in bulky, complex, and unreliable systems that may not improve upon conventional/incumbent systems such as 350/700 bar tanks. This project will struggle to provide a stable system that will survive the rigors of drone duty cycles. Limiting this cartridge to a one-way use system will significantly narrow the useful applications to specialty or military applications; it may not have broad appeal for civilian applications.

Question 2: Accomplishments and progress

This project was rated 2.8 for its accomplishments and progress toward overall project and DOE goals.

- The cost of the material is attractive and is approaching targeted values. The performance of the material is good, showing stable hydrogen release under operating conditions.
- The project team found that the speed of delivery is a tradeoff with even delivery rate. The project has not yet achieved the desired properties, but the team is close. The team considered or tested a variety of materials for fuel and salt.
- The project team's choice of an acid-base reaction of hydrazinium salts and borohydride salts generates hydrogen spontaneously, as was demonstrated. Thus, the shelf-life requirement cannot be met by this approach. While some hydrogen is released on mixing, the mixtures need to be heated to above 50°C to initiate further hydrogen loss. The team did not discuss how this heat would be delivered onboard a UAV. The results that were obtained were not discussed in relation to how they might impact the onboard requirements of the UAV system.
- Critical to the success of this project is the selection of the control system that will be used to create a system that (1) is stable, i.e., does not generate hydrogen when not in use or when perturbed heavily by hard landings, etc.; (2) provides pure hydrogen without the weight and complexity of significant clean-up systems; and (3) provides load-following hydrogen supply without complex system auxiliaries. Thus far, such a control mechanism has not been proposed. At this stage, with 1/4 of DOE funds spent, at least a design concept should have been proposed this year.
- Significant progress has been made, but there are glaring weaknesses that need to be addressed to improve the viability of this system. However, given the high reactivity/dangerous materials and the toxic products potentially formed with routine use, there are numerous barriers facing this project that may not be easily overcome.

Question 3: Collaboration and coordination

This project was rated **3.0** for its engagement with and coordination of project partners and interaction with other entities.

- The National Renewable Energy Laboratory (NREL) team has good collaboration with the team at Honeywell, who study bigger samples and do fuel cell compatibility.
- Very close collaboration between NREL and Honeywell is evident.
- The project has good collaboration; the project partners participate and are well-coordinated.
- It was not clear if at this stage of the work the collaboration with Honeywell was well-established. The team noted the future involvement of Metropolitan State University of Denver.
- Overall, the team selected good partners; however, experienced partners in system design and control are needed to bring this concept to fruition. The principal investigator did not clarify if the HyMARC tankinator and levelized cost model tools will be used in the early stages of the project. While the reviewer assumes this will be the case, the collaboration and next steps for using these tools should be called out specifically in proposed future work.

Question 4: Potential impact

This project was rated 2.6 for supporting and advancing progress toward Hydrogen Program goals and objectives.

- Borohydrides are not yet a viable storage material. If the reversibility and byproducts could be addressed, it could be a valuable storage material. The project has a reasonable alignment to the Program's strategy. However, this is planned as a one-way carrier.
- The project team has made good progress towards the FLASH materials' use, but the system is incredibly reactive and has high potential for inadvertent runaway reactions. It is unclear if there is a large potential impact of such materials for hydrogen storage.
- As currently configured, the project is not poised to advance the onboard fuel for the UAV concept. The materials being studied do not advance what is already well-known to the Hydrogen Program.
- The UAV market is rapidly growing, and the use of hydrogen opens up new possibilities for this segment. The allocation of resources to this segment is certainly warranted, but it is doubtful that all the system considerations needed to control NaBH₄ will be successfully contained in a cartridge application.
- The performance of the material is advancing, but this is a niche application that may work for a few applications but is not applicable to a majority of commercial use cases.

Question 5: Proposed future work

This project was rated 2.7 for effective and logical planning.

- The project team will work on stability and maybe better materials. All of the future work listed is appropriate.
- The team's discussion on future work indicated that the rather extensive literature of the hydrazine/hydrazido borane/borohydride compounds has been appreciated. This is indicated by the future plan of replacing hydrazinium salts with ammonia borane, an approach that may solve some problems but create others, e.g., in the purity of the hydrogen delivered as these mixtures are well-known to generate copious quantities of volatile borazine, which interacts deleteriously with platinum on fuel cell catalysts.
- The proposed future work builds on the previous work well, but there are still significant challenges that remain regarding the operation and packaging of the material.
- The project's future plans generally build on the past progress, and the principal investigators are working to overcome the major barriers. This chemistry may work against the team's best intentions, however.
- The project team needs to propose a robust and realistic control mechanism for the reaction before any scaleup work. There may be more innovative opportunities in the control mechanism than in the material itself (properties of NaBH₄ are relatively well known).

Project strengths:

- The project team has shown great flexibility and innovation in the development of stacking the reactants. The material costs are approaching the desired targets, and the material shows promise to provide the needed amount of hydrogen per unit weight. The safe handling and testing of these materials is impressive and laudable.
- The principal investigator and project team are excellent scientists who are considering how best to utilize the chemical system for their goals. It is complicated, but progress is being made.
- This project is opening a new frontier for hydrogen systems in the rapidly expanding UAV industry. Novel methods are needed here, and there are potentially many opportunities.
- This is a very innovative project with a strong team.

Project weaknesses:

- The materials investigated present several hazards and seem quite dangerous. The engineering mitigations required to make the system safe for use may negate the benefits of the materials themselves (e.g., adding a water reservoir to mitigate any environmental leak concerns is going to impact the storage capacity of the system). There is no clear reasoning behind why such aggressive and hazardous chemicals are being investigated, beyond reducing the cost compared to the current technology. Advances have been made in physical hydrogen storage that may be more appropriate for this application than the materials presented.
- One project weakness is the stability of current fuel configurations.
- The lack of focus on control mechanisms is a weakness for the project.
- The proposed chemistry has fundamental issues that work against foreseeable progress.

- The project team should use a liquid reactive with a solid with little or no mechanical mixing. Then, the two parts of the fuel delivery system can be kept separate for safety and stability, and the liquid can be metered into the solid to control hydrogen flow. The team should consider a water-based delivery system so that fuel cell water can be a reactant and, if acceptable, the spent fuel material can be simply washed away as it is used, thus lightening the vehicle.
- The project team should provide a more thorough explanation of key performance criteria that UAV systems will need. This hasn't been explored much up until now and will certainly become an important factor. A better understanding of the needs of a hydrogen storage system, particularly regarding duty cycle and environmental factors, will be valuable in itself regardless of the technical success of this particular project.
- The project team needs to gain a more thorough understanding of what the options are for initiating onboard hydrogen release from a solids-containing cartridge system within the constraints of a UAV system.