Technical and TEA-LCA Consultancy on BoMax H2-Shot Incubator Prize

Cooperative Research and Development Final Report

CRADA Number: CRD-22-23277

NREL Technical Contact: Jamie Kee

NREL is a national laboratory of the U.S. Department of Energy
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Technical Report
NREL/TP-5400-88383
December 2023

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NOTICE

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Cooperative Research and Development Final Report

Report Date: December 4, 2023

In accordance with requirements set forth in the terms of the CRADA agreement, this document is the CRADA final report, including a list of subject inventions, to be forwarded to the DOE Office of Scientific and Technical Information as part of the commitment to the public to demonstrate results of federally funded research.

Parties to the Agreement: BoMax Hydrogen, LLC

CRADA Number: CRD-22-23277

CRADA Title: Technical and TEA-LCA Consultancy on BoMax H2-Shot Incubator Prize

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Sponsoring DOE Program Office(s): Office of Energy Efficiency and Renewable Energy (EERE), Hydrogen and Fuel Cell Technologies Office (HFCT)

Joint Work Statement Funding Table showing DOE commitment:

Estimated Costs	NREL Shared Resources a/k/a Government In-Kind
Year 1	$50,000.00
TOTALS	$50,000.00

Executive Summary of CRADA Work:

NREL has been approached by BoMax Hydrogen, LLC ("BoMax") through the H2-Shot program to provide consultation on the BoMax technology concept. Consultation will include discussions and guidance regarding technical and scale-up considerations, as well as techno-economic and life-cycle analysis (TEA/LCA) implications for the BoMax process.

CRADA benefit to DOE, Participant, and US Taxpayer: Uses the laboratory's core competencies.

Summary of Research Results:

Purpose:

The purpose of this collaboration was for the Contractor to provide technical insights on the BoMax technology and suggestions on developmental directions and technology scale-up considerations. Additionally, the Contractor provided guidance on techno-economic analysis (TEA) and life cycle analysis (LCA) implications, as well as anticipated challenges and drivers, and conducted preliminary TEA/LCA analysis for the technology. The work focused on the core hydrogen generation reactor step (red box in Figure 2 below), in line with a $50,000 national laboratory voucher supporting the Contractor's time for these activities.

Technology description:

The BoMax technology for photocatalytic hydrogen production, as described to the Contractor, is depicted in Figures 1 and 2. In summary, the process concept is an integrated photoreactor system that includes a photocatalytic complex composed of a biologically derived hydrogen production catalyst (FeMo-co and NafY proteins isolated from separate biological synthesis steps) that is bound to CdSe nanoparticles that (when activated by light of a specific wavelength) will catalyze the light-driven production of hydrogen (Figure 1). The hydrogen gas will diffuse from the liquid catalyst slurry and may be collected from the headspace in high purity.

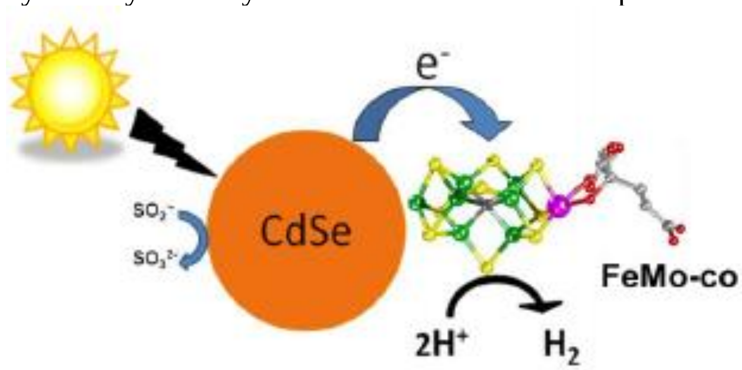

Figure 1. Visual Depiction of the BPH chemical system

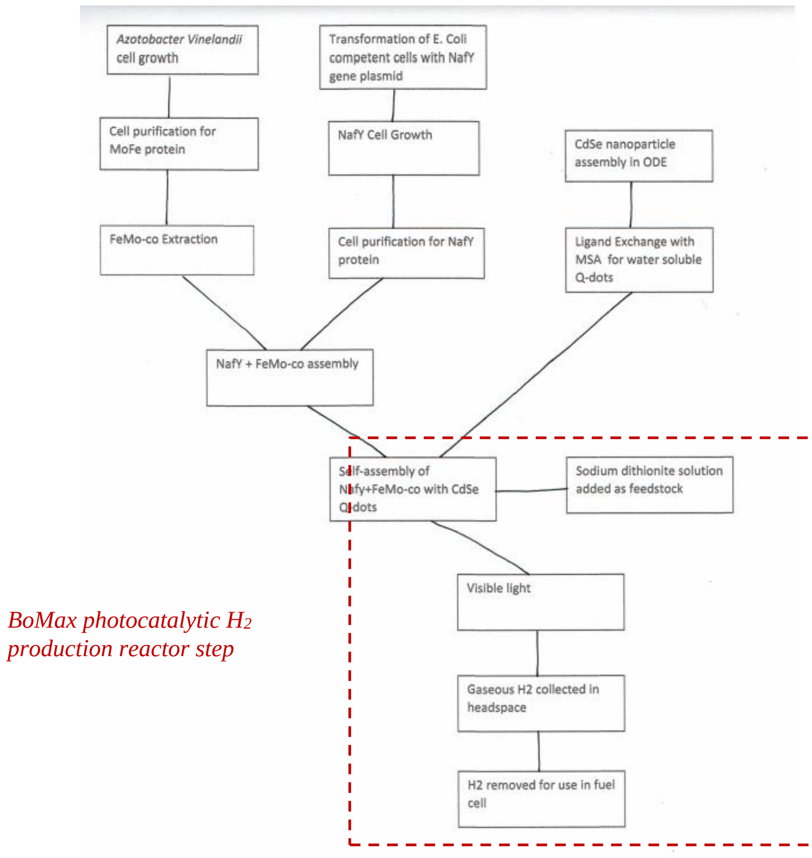

Figure 2: Simplified block diagram schematic of BoMax process for photocatalytic hydrogen (H2) production (provided by BoMax Hydrogen, LLC). Red box denotes key BoMax reactor step, to be the focus of technical/TEA/LCA consultations with Contractor as part of this collaboration. The process for upstream sourcing of NafY + FeMo-co proteins and CdSe nanoparticle catalyst were not included in the scope of work for this CRADA.

Statement of Work:

The work was divided into two tasks – Task 1 focused on TEA/LCA implications for the technology, and Task 2 involved technical consultation regarding experimental and scale-up considerations with Contractor's subject matter expert in the relevant field.

TASK DESCRIPTIONS:

Task 1: TEA/LCA Guidance

In this task, Contractor will work with Participant to provide TEA/LCA guidance around scale-up implications, and other anticipated challenges and drivers for the BoMax technology. TEA focuses on technical evaluation of the technology (applying process and design engineering principles) coupled with economic evaluation (considerations of capital and operating costs for the system as may translate to overall production costs). TEA modeling helps to quantify the economic potential for a technology of interest, while also highlighting key challenges and drivers to achieving this potential. Meanwhile, LCA focuses on similar evaluation of environmental sustainability metrics for the system such as greenhouse gas emissions or fossil energy demands as may be attributed to the production process.

Given the limited budget available to the Contractor for this phase of work, coupled with the technology reflective of an early-conceptual stage of research and uncertainties regarding commercial scale-up of the process, comprehensive TEA/LCA modeling is not planned to be conducted for this award phase (though such models may be built in subsequent phases with expanded budget allowances). Instead, the Contractor will engage with the Participant to provide more general guidance on likely pinch-points or other envisioned challenges/drivers that may influence TEA/LCA potential, based on further details of the technology to be furnished by the Participant. This will include any available preliminary cost analyses performed previously, as well as schematic diagrams of the photocatalytic reactor system as envisioned for commercial scale. If sufficient information can be furnished by Participant regarding prior cost analysis calculations, Contractor will assist in reviewing this information and providing insights on potential areas of further cost savings or refinements that could be applied to the analysis, as well as associated impacts on contributions to $/kg hydrogen production costs. Likewise, if sufficient information can be provided by Participant regarding mass and energy inputs/outputs (primarily around the key photocatalytic reactor step), a preliminary estimate of associated greenhouse gas emissions burdens may be furnished by Contractor on a kg-CO2/kg hydrogen basis. These TEA/LCA considerations may also be used to highlight key drivers or contributors to overall costs or greenhouse gas emissions that may be envisioned for the technology at scale, to provide guidance to the Participant on key areas of research which may provide the greatest impact in working to progress the technology to a higher stage of maturity.

Task 1 Results:

Preliminary/feasibility-level TEA/LCA was performed on the Participant's technology, including the balance of plant components. The targeted BoMax system, as modeled for a localized scale unit, is a 32-panel installment capable of producing hydrogen to power a 4-kW fuel cell for use at a residence. The hydrogen is assumed to be produced at atmospheric pressure. As the hydrogen evolves from the reactor, it is compressed and stored. The storage tanks provide hydrogen for use as a fuel to generate power for a residential unit. A simplified process diagram is illustrated in Figure 3. Due to solar heating in the panel array, a refrigeration loop is required to maintain the reactor temperature. Both the refrigeration and compressor require electrical loads.

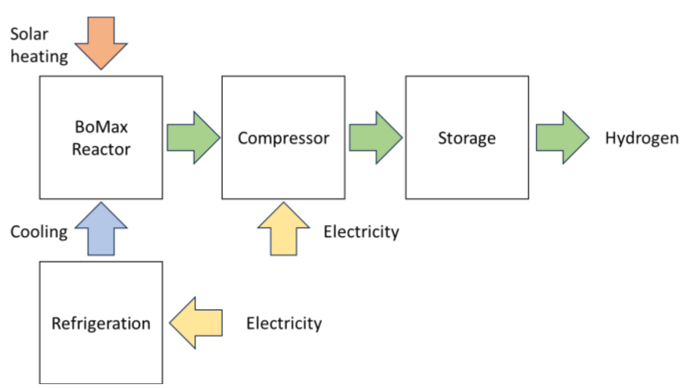

Figure 3: Illustration of BoMax system as modeled for TEA/LCA including balance of plant components.

The TEA included sizing and costing each of the downstream components, as well as the BoMax reactor, which was sourced from design/cost information provided by the Participant (NREL did not attempt to estimate costs for the reactor itself within the scope of this effort). Hydrogen is produced in the reactor using a nanoparticle photocatalyst. The protein enzymes on the nanoparticles combine the electrons with available hydrogen ions to produce hydrogen gas. The protein-catalyst complex is soluble in water and containerized in 1 m x 1m x 7.5 cm square panels as illustrated in Figure 4. To produce the hydrogen for a 4-kW fuel cell for residential operation, 32 panels are required based on a target maximum hydrogen productivity of roughly 3 g/L-day furnished by BoMax (envisioned to be achievable as a future goal). The reactor system is estimated to cost $15,000-$20,000 based on initial estimates provided by BoMax. The estimate includes just the frame. The catalyst is expected to be active for 90 days and thus will be replaced every 90 days. The operating costs associated with replacing the catalyst are expected to be $4,650 per 90-day replacement, or $18,600 annually for producing hydrogen continuously. As noted above, manufacturing and cost details for this specific protein-catalyst complex were outside the scope of this study; instead, the catalyst cost was supplied by BoMax, and applies cost reductions anticipated to be achievable through bulk pricing at scale and bringing catalyst fabrication in-house.

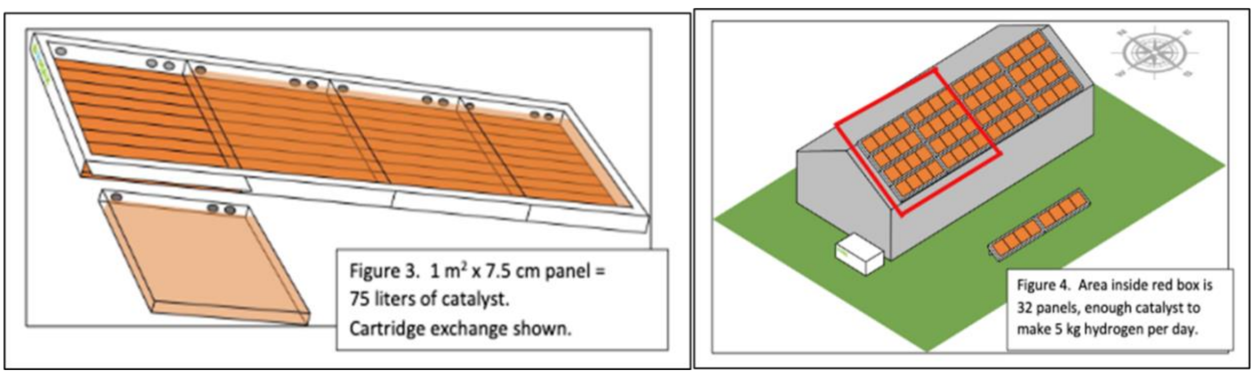

Figure 4: Visual representation of BoMax system for approximately 5 kg hydrogen production per day. Adapted from figures provided by BoMax.

Under this study, the hydrogen produced by the BoMax unit is intended to power a 4-kW fuel cell. The fuel cell supplies power to a residential unit. Due to the daily and seasonal changes in solar irradiance and therefore hydrogen production potential, hydrogen storage must be used to satisfy the fuel cell hydrogen demand at a fixed hourly rate. A residential load profile from Florida is assumed as the representative load profile using the ResStock tool [1]. ResStock is a tool by NREL that provides annual energy consumption rates on an hourly basis. The ResStock tool provided an hourly demand profile, and on the other hand, the variable hydrogen generation supply was determined by the solar profile. The hourly direct normal irradiance (DNI) was taken from NREL's System Advisory Model (SAM https://sam.nrel.gov/) for Sanford, Florida. The DNI was used to calculate the hourly generation of hydrogen attributed to the available solar irradiance. Based on the data provided from experiments in a lab setting (which remains to be confirmed in an outdoor environment), 14% of the input irradiance is converted into hydrogen on a kWh basis. The balance of supply and demand equated to 54.62 kg of required hydrogen storage capacity to accommodate an entire year.

Hydrogen must be stored at elevated pressures to achieve any reasonable storage footprint, especially in a residential area. Geologic storage is a common option for bulk storage of hydrogen. However, due to the scale of this operation, above-ground storage tanks would be more site appropriate. Three storage options were considered for storing the 54.62 kg of hydrogen, the first being “low-pressure” storage tanks, the second being “high-pressure” storage tanks, and the final option being metal hydride storage, which is at the lowest pressure, but requires high material costs. The low-pressure tanks required the lowest installed cost, while metal hydride tanks were approximately double the installed cost.

Each storage option (low pressure, high pressure, and metal hydride) required different pressures, and therefore required different compressor configurations. The compressor sizing and costing is performed using the methodology described in HDSAM3.1 [2]. In addition to capital expense, the compressors have electricity usage, which is input as an operating expense to the TEA. The high-pressure tanks required the highest pressure, which correlated to the largest capital expense and electricity usage. However, relative to the differences in storage cost, the differences in compressor cost were small.

Active cooling is needed to maintain optimal reaction temperature (targeted temperature of 25 ^{o}C). The nature of the reactor requires exposure to sunlight, which will result in solar heating. The refrigeration load is estimated based on the expected solar exposure. The maximum DNI in Sanford, Florida was taken as 1026 W/m^2. The BoMax system assumes a 32 m^2 area, which equates to a maximum 32,832 W (32.832 kW) of solar heating. Based on [3], 54% of the solar irradiance is assumed to contribute to heating, netting 17.7 kW. This heating amount is balanced by a refrigeration loop sized to handle 17.7 kW of cooling. A cost correlation was used and sourced from HDSAM3.1.

The capital expenditures are summarized in Table 1. The total capital expense is $121,628, which is made up of the reactor, compressor, storage, and refrigeration components. The largest cost is the storage, making up nearly half the total cost. For the base case scenario, the low-pressure storage case was used as it incurs the lowest capital and power costs. The hydrogen production reactor makes up approximately 12% of the cost, while the balance of plant components makes up the remaining 88% of the total cost. Each component is assumed to follow a 5-year MACRS depreciation schedule.

Table 1: Capital expenditure inputs for techno-economic analysis

Capital expenditure	Value	Depreciation schedule
Reactor	$15,000	5 yr MACRS
Compressor	$24,866	5 yr MACRS
Storage	$65,471	5 yr MACRS
Refrigeration	$16,291	5 yr MACRS
Total	$121,628	

The variable operating cost or feedstocks considered in this analysis are the electricity required for both the compression and refrigeration and the catalyst replacement cost. The electricity feedstock is represented on a kWh/kg basis, normalized to the production rate of hydrogen. Table 2 summarizes the two electricity demands. Based on average residential electricity prices [4] the electricity price was taken as 0.16 $/kWh (based on the local grid mix) and escalating annually at the assumed inflation rate of 1.9%.

Table 2: Feedstock usage inputs

Feedstock	Usage (kWh/kg hydrogen product)
Compressor electricity	3.35
Refrigeration electricity	6.00
Total	9.35

The catalyst replacement cost is structured as a fixed annual cost. Every 90 days, $4,650 must be spent to replace the catalyst (based on cost inputs furnished from BoMax), which equates to $18,600 per year, assuming continuous hydrogen production. However, when operating in sunlight, the catalyst will not be operating continuously through the day. Therefore, the replacement cost was scaled by the long-term utilization (22%), assuming that the catalyst replacements would be less frequent if not under constant use.

Table 3: Fixed operating expense inputs

Fixed operating expense	Cost ($)	Escalation
Catalyst replacement	4,092	1.9%

Table 4 outlines the sales specification and financing information parameters for H2FAST to be used in the techno-economic analysis. The commodity being sold is hydrogen and is produced at a maximum nameplate capacity of 7 kg/day, which is the maximum flowrate needed to flow to a 4-kW fuel cell. The long-term utilization is 22% based on the expected production relative to the nameplate production, which provides an expected 1.5 kg/day observed over the year. The hydrogen price is modeled to escalate at an inflation rate of 1.9%. The operating life of the unit is set to 20 years and an installation period of 1 year. There is no assumed demand ramp-up time. The tax structure assumes a total tax rate of 21%, which includes state, federal, and local taxes combined. The capital gains tax was set to 15%. A general inflation rate over the plant lifetime is taken as 1.9%. The leveraged after-tax nominal discount rate is set to 10%; consequently, the expected internal rate of return (IRR) is also set to 10% at an NPV of zero. The initial debt-to-equity ratio is set to 3, where at project initiation, 75% is debt and 25% is equity. The debt structure is a bond debt or a revolving debt, where the project is in constant debt over the project lifetime and any remaining debt is paid in the final year. The interest rate is set to 4%, and 200% of monthly expenses are kept as cash on hand.

Table 4: Sales specification and financing information parameters

Parameter	Value	Unit
Nameplate capacity	7.12	kg/day
Commodity	Hydrogen	
Commodity escalation	1.9	%
Operating life	20	Years
Installation months	12	Months
Demand ramp-up	0	Years
Long-term utilization	22	%
Total tax rate	21	%
Capital gains tax	15	%
General inflation rate	1.9	%
Leveraged after-tax nominal discount rate	10	%
Initial debt/equity financing ratio	3	
Debt type	Bond debt/revolving debt	
Debt interest	4	%
Working capital	200	%

Based on the above parameters, the base case H2FAST techno-economic analysis results estimated the levelized cost of hydrogen as $21.30/kg. This levelized cost includes both the compressor and storage components, which are not standard when comparing production pathways. Without the compressor CapEx, storage CapEx, and compressor operating cost, the levelized cost drops to $11.55/kg. Figure 5 shows the cost breakdown when including both compression and storage. Figure 6 shows the levelized cost breakdown for just the production of hydrogen directly from the reactor system, which does not include compressor or storage.

For the cost breakdown in Figure 5 when compression and storage are included, the capital expenditures and financing contribute heavily to increasing the levelized cost. The largest contributors are the dividends paid, storage capital expenditure, interest expense, and the repayment of debt. Dividends paid are included here because the model identifies all project cash generated in excess of reserve requirements as dividends and does not speculate on the treatments of any retained earnings. The figure presents four categories labeled operating revenue, financing cash inflow, operating expense, and financing cash outflow. The summation of inflow streams, operating revenue and financing cash inflow, is equal to the summation of the outflow streams, operating expenses and financing cash outflow. The hydrogen sales price point that provides a net present value of zero while achieving the desired rate of return, is labeled as the levelized cost. The catalyst replacement contributes $7.25/kg to the levelized cost. The electricity input required for the compressor and the refrigeration contributes $1.49/kg to the levelized cost. A significant portion of the levelized cost is attributed to initial capital investment and debt, which is where most of the cost reductions could be made. In Figure 6, the compression and storage are not included in the levelized cost. In this scenario, the catalyst replacement cost is the largest operating expense at $7.25/kg. Increasing the duration of the catalyst or achieving further bulk pricing cost reduction could have a large impact on the levelized cost. In addition, the electricity contribution decreases to \$0.96/kg by removing the compression power.

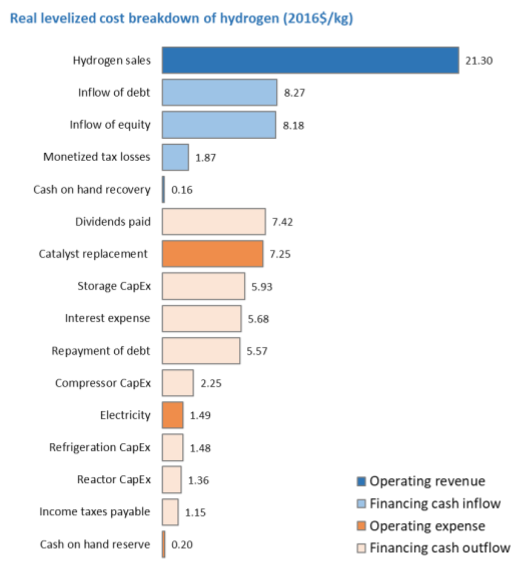

Figure 5: Levelized cost breakdown including compression and storage

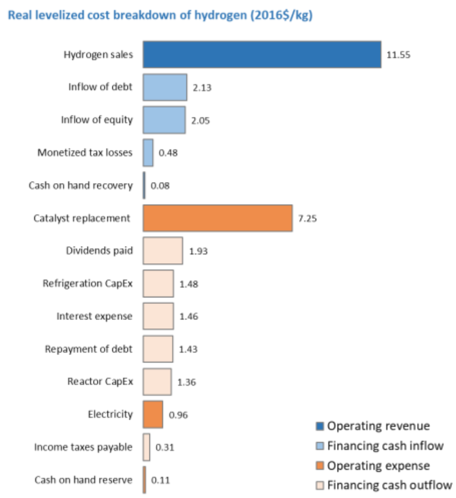

Figure 6: Levelized cost breakdown for production of hydrogen directly from the reactor system (excluding compression/storage)

The DOE H-Shot program's $1/kg cost target for hydrogen production is ambitious but can be potentially realized through multiple improvements in the process. Figure 7 illustrates tiered improvements that may be made to the BoMax system and the resultant sequential improvements to the levelized cost of hydrogen production in $/kg. The starting point for the waterfall chart is the current estimate for the production cost of $11.55/kg as discussed in Figure 6 (excluding compression and storage). The first improvement is increasing the lifetime of the process from 20 to 40 years, which decreases the levelized cost by $0.94/kg. The subsequent improvement decreases the catalyst cost by 50% relative to the basis furnished by BoMax, which decreases the levelized cost by $3.7/kg. The annual catalyst replacement category relates to the lifetime of the catalyst, where instead of replacing the catalyst every 90 days, it is instead replaced only once per year, which decreases the levelized cost by another $2.6/kg. Another improvement target would be to decrease the cost of the reactor, where a 50% reduction would decrease the levelized cost by $0.72/kg. The preliminary TEA assumed residential electricity prices in Florida, however, if the electricity price can be purchased at the industrial price point near $0.07/kWh, the levelized cost would decrease by $0.55/kg. Increasing the utilization by 50% would require identifying a location that increases the availability of solar irradiance. This utilization lies outside the realm of theoretically possible values for solar irradiance in the United States, but if such a location were available or an artificial light source was used (without consideration of added costs for artificial lighting), this would decrease the levelized cost by $1.31/kg. Decreasing the heating load required by the refrigeration by 50% would decrease the levelized cost by $0.43/kg. Finally, if the catalyst could achieve a 25% higher hydrogen productivity (leading to 25% fewer panels and associated catalyst required for the same hydrogen output), then levelized cost would decrease by another $0.24/kg to finally achieve $1.06/kg. It is important to note that individual $/kg savings illustrated here would vary based on the order of these sequential improvements but would ultimately land at the same final value inclusive of all improvements taken together. Regardless, the greatest opportunities to improve the levelized hydrogen cost could be realized through reducing the catalyst costs and extending the catalyst lifetime.

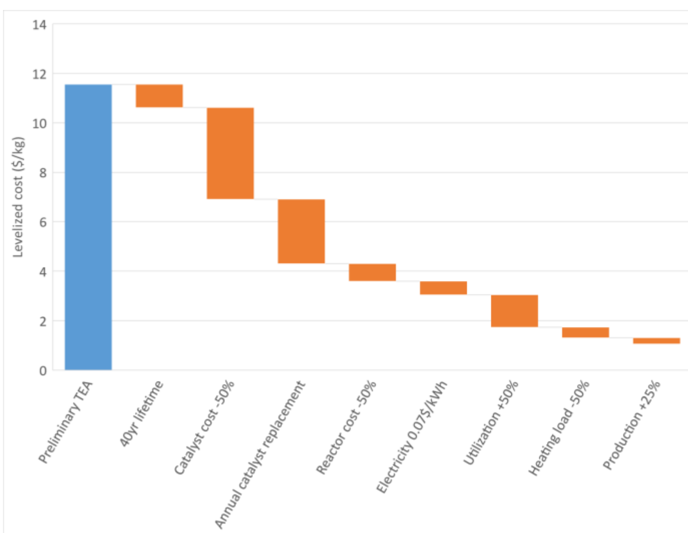

Figure 7: Waterfall chart on plausible paths to achieve $1/kg H-shot target (excluding compression/storage costs)

This preliminary TEA is intended to provide insights into the largest cost contributors and guide R&D efforts toward future priority focus areas. This work identified the largest cost in the process to be the catalyst replacement cost. Some of the most valuable efforts by BoMax in late 2022 and 2023 have been to bring all these catalyst components' production in-house to the BoMax lab. First this contributes to the quality control of the production process. This move guarantees more robust catalyst performance with each replacement every 90 days. Furthermore, with the scaling up of the production process, scaling factors will be employed to further decrease catalyst production costs. Improving catalyst hydrogen production efficiency and extending the life of the catalyst will further reduce overall costs. BoMax has already started efforts to make progress on reducing the catalyst cost and improving reliability in the production line, which will make large strides in reducing the levelized cost.

The life cycle analysis in this study is represented as emissions in units of $kgCO_2e/kgH_2$. The well-to-gate (WTG) emissions are used to quantify green hydrogen production and are used in determining clean hydrogen production tax credit brackets in the Inflation Reduction Act (i.e., 45V tax credit). The WTG emissions encompass Scope 1, 2, and 3 emissions. Scope 1 emissions are direct emissions from within the process. Scope 2 emissions are embedded emissions associated with sourcing feedstocks. Scope 3 emissions are indirect emissions that occur both upstream and downstream. The WTG emissions are analyzed using the GREET tool [5] and grid emission rates from the EPA eGRID tool [6].

The GREET model evaluates energy and emission impacts for hydrogen production pathways. For solar applications, as would be observed in the BoMax reactor, the Scope 1 emissions would be zero because there are no direct emissions coming from the process. The Scope 2 and 3 emissions are modified from the electricity to hydrogen production route. Regarding Scope 2 emissions, the only feedstock considered in the analysis is the electricity used in the compressor and refrigeration. The combined electricity usage for the low-pressure storage case is 9.342 kWh/kg of hydrogen. Both the Scope 2 and 3 emissions are scaled in proportion to the electricity usage in this analysis.

Using the GREET values for Scope 1, 2, and 3 emissions scaled to the grid emissions and the electricity usage, the WTG emissions were determined to be approximately 1.41 $kgCO_2e/kgH_2$ as shown in Table 5. This value uses the Florida 2021 grid mix as reported by the eGRID tool and the 9.34 kWh/kgH_2 electricity usage noted above. Alternatively, if solar or wind power were used instead, the net GHG emissions would be near zero. In addition to the WTG emissions, there could also be embodied emissions regarding the production and sourcing of the catalyst. While this specific protein-catalyst complex represents a very specialized material and is not reported in the literature, a value of approximately 200 kg CO_2e per kg catalyst was identified in the literature based on a CdSe nanoparticle proxy [7].

Table 5: Emissions using Florida 2021 electrical grid

Scope	kgCO2e/kgH2
1	0.00
2	1.20
3	0.15
Catalyst embodied emissions	0.06
Total	1.41

Task 2: Scientific/Technical Consultation with Subject Matter Expert

Task 2 will support a mechanism to encourage open dialogue and feedback from Contractor's subject matter expert(s) with research experience in this domain. Under this task, the Contractor will engage both with the Participant as well as the Contractor's TEA/LCA staff to provide insights on key advantages and challenges for the BoMax technology, and any potential solutions that may help mitigate the challenges or improve the TEA/LCA drivers highlighted in Task 1. Contractor may also comment on related experimental work they have tried and what worked or did not work, to help provide guidance to the Participant in framing future experimental plans.

Task 2 Results:

In addition to the engineering and analysis staff who provided guidance on process design and associated TEA/LCA implications, members of the NREL team served in a scientific/technical consulting role given the focus of related research similar to the topic of the CRADA. Over the course of the project, the NREL team participated in phone calls and email exchanges with the BoMax/NREL team to provide advice and guidance regarding technical hurdles and R&D priorities for future consideration as BoMax continues developing this technology. These discussions with the NREL team also focused on addressing issues when scaling up the system, especially regarding the balance of plant. The NREL/BoMax team conducted monthly meetings to provide feedback on the technology and share new progress on the models. The iterative process allowed the Participant to refine TEA and LCA inputs as new design considerations came to light.

Task 3: Additional Tasks

Other work at the direction of the Participant, consistent with the scope and subject to the availability of funding. As part of Task 3, the Contractor will prepare a CRADA Final Report. Preparation and submission will be in accordance with the terms of this agreement.

Task 3 Results:

This report serves to meet the requirement for the CRADA Final Report with preparation and submission in accordance with the agreement's Article X.

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Subject Inventions Listing: None.

ROI #: None.