H2NEW Hydrogen (H2) from Next-generation Electrolyzers of Water:
H2NEW LTE: Performance and Benchmarking

Nemanja Danilovic, LBNL; Guido Bender, NREL; Adam Weber, LBNL

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DOE Hydrogen Program
2021 Annual Merit Review and Peer Evaluation Meeting

Project ID # P196b
Project Goals

Goal: H2NEW will address components, materials integration, and manufacturing R&D to enable manufacturable electrolyzers that meet required cost, durability, and performance targets, simultaneously, in order to enable $2/kg hydrogen.

H2NEW has a clear target of establishing and utilizing experimental, analytical, and modeling tools needed to provide the scientific understanding of electrolysis cell performance, cost, and durability tradeoffs of electrolysis systems under predicted future operating modes.
H2NEW Task 2: Performance and Benchmarking Overview

Timeline and Budget

- Start date (launch): **October 1, 2020**
- Awarded through September 30, 2025
- FY21 DOE funding: **$1.45M**
- Annual budget adjustments anticipated

Barriers

- Capital Cost
- Performance

National Lab Consortium Task Team

Deputy Director: Nemanja Danilovic (LBNL)
Task Liaisons:
Guido Bender (NREL)
Adam Weber (LBNL)
Subtask Leads:
Rajesh Ahluwlia (ANL)
Siddharth Komini Babu (LANL)
James Young (NREL)
Dave Cullen (ORNL)
Ethan Crumlin (LBNL)
Daniel Hussey (NIST)
Relevance and Impact

<table>
<thead>
<tr>
<th>Electrolyzer Stack Goals by 2025</th>
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<td>LTE PEM</td>
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<td><strong>Capital Cost</strong></td>
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- Task 2 “performance” activities specifically focus on the capital cost and efficiency targets:
  - Membrane selection and crossover characterization to improve efficiency and reduce capital cost
  - Catalyst selection and screening to reduce capital cost and help improve lifetime
- Modeling and characterization work within Task 2 cross cuts with Tasks 1 and 3 and help address the durability/lifetime target.
Approach: Task 2 Breakdown

Task 2a: Performance benchmarking, baselining, validation
i. Coordination with domestic (HydroGEN Topic 2b) and international partners (IEA)
   1. Development of protocols, reference cells, round robin
   2. Development of reference materials and standardized tests for cell material evaluation

Task 2b: Cell performance testing in support of electrode development
i. In-situ cell testing independent of durability testing
   1. Advanced diagnostics, operating condition studies, seg cell.
ii. In-operando (beam-line) testing of cells for performance enhancement & degradation studies

Task 2c: Ex-situ studies focused on performance factors
i. Advanced characterization of structure, morphology and properties of inks and electrodes

Task 2d: Cell level model development
### Approach: Task 2

<table>
<thead>
<tr>
<th>Milestone Name/Description</th>
<th>Due Date</th>
<th>Type</th>
<th>Status</th>
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<tbody>
<tr>
<td>Finalize standard, state-of-the-art MEA material set, fabrication process, and/or source to be utilized in baseline studies including those for durability, performance, and scale-up/integration – All Labs</td>
<td>12/31/2020</td>
<td>QPM</td>
<td>Complete</td>
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<td>Identify parameter space and experimental matrix that support the model needs of the consortium with regards to in-situ, ex-situ, and in-operando experiments. Labs – NREL, LBNL, ANL.</td>
<td>3/30/2021</td>
<td>QPM</td>
<td>Complete</td>
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<td>Complete cell design and validation of a neutron imaging cell to be used with the high-resolution imaging detector at NIST. Cell performance in imaging hardware within ±10% of performance in a 25cm² cell. Labs – LANL, NIST.</td>
<td>3/30/2021</td>
<td>QPM</td>
<td>Complete</td>
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<td>Identify and prioritize needed in-situ, ex-situ, and in-operando diagnostic methods of interest to be developed in subsequent quarters potentially in future discretionary supported projects. Labs – NREL, LBNL, ANL, ORNL.</td>
<td>6/30/2021</td>
<td>QPM</td>
<td>On Track</td>
</tr>
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<td>Assess the impact of the stress tests on electrode, membrane, and PTL through voltage loss breakdown and use ex-situ characterization to identify degradation mechanisms and support AST development. Determine initial stressors to be investigated in detail for potential to accelerate specific degradation mechanisms. Labs – NREL, LBNL, ANL, LANL.</td>
<td>6/30/2021</td>
<td>QPM</td>
<td>On Track</td>
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<td>Establish and validate single cell performance testing protocols on SOA MEAs with PGM loading of &lt;0.8 mg/cm² and membranes &lt;100 µm demonstrating a minimum performance of 2 A/cm² at 1.8 V and demonstrate ability to perform voltage loss breakdown modeling as verified by agreement within 10% across at least 3 labs.</td>
<td>9/30/2021</td>
<td>Milestone</td>
<td>On Track</td>
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Approach in a Nut-Shell

Use H2NEW capabilities to perform
- In-situ diagnostics
  - Performance, CV, EIS, ...
- Ex-situ diagnostics
  - Microscopy, In-plane/Through plane conductivity, corrosion tests, CT-scan ...
- In-operando testing
  - X-ray & Neutron imaging
- Modeling
  - Voltage Breakdown Analysis, Transport phenomena...

... to investigate
- Material
- Layers
- Components
- Devices
- Interfaces

... and understand & improve
- Properties
- Interactions
- Phenomena
- Degradation
- Performance
Approach for LTE Performance in Detail

**Circumvent Edisonian Approach**

- Commercial MEAs are “overdesigned” with high catalyst loadings and thick membranes
- Poor understanding of structure, interfaces and performance impacts

**Commercial materials:**
- 0.4 mgIr/cm²
- 2 mil membrane
- Ti PTL and Pt coating

**Spray coated CCM Status 2020**

- Academic MEAs have demonstrated loadings as low as 0.05 mg/cm²
- Translation to high-throughput MEAs is not feasible without an understanding of underlying properties and function

**Understanding Structure Property Relationships**

**Performance & In-Situ Characterization**

- N. Danilovic, ECS Transactions, 75 (2016) 395

Utilize in situ characterization techniques to evaluate materials and components. Establish protocols and benchmark across institutions.

**Advanced In-Situ Characterization**

- Z. Taie, ACS AM&I, 12 (2020) 52701

Develop and utilize advanced electrochemical diagnostics.

**Ex-Situ Diagnostics**

- Develop and utilize ex-situ diagnostic techniques to extract component level parameters and to determine performance impacting characteristics.

**In-Operando Characterization**

- Develop and utilize operando techniques to identify performance and durability limiting phenomena in operating cells.

**Cell Level Modeling**

- Utilize cell level modeling to understand underlying mechanisms and to guide in design and optimization of cells and components

**Spray coated CCM Status 2020**

- 2025
  - 77% LHV @ 3 A/cm²
  - 0.5 mg PGM/cm²

- Utilize cell level modeling to understand underlying mechanisms and to guide in design and optimization of cells and components
Accomplishment – Future Gen MEA Definition

Pathway to Future Gen MEA
- Membrane
  - Thin PFSA material approaching ~2mil
  - Evaluate novel membranes
- Anode Electrode
  - Ultrasonic Spray Coating
  - 0.4 mgIr/cm² Alfa Aesar IrO₂
  - Evaluate new electrodes
  - Porous Transport Layers
    - Critical component
    - Ti sinter (Mott) vs Ti fiber (Bekaert)
    - Coatings: Model (sputtered) vs e-plated (commercial)
- Cathode Electrode
  - Ultrasonic Spray Coating
  - 0.1 mgPt/cm², 46 wt% Pt/Vulcan C
  - Evaluate new materials
  - Gas Diffusion Layer
    - Carbon Paper, no MPL

H₂ crossover challenges
- Integration
- Durability

Unsupported Catalyst Distribution
- Meet Baseline Performance
- Durability

Minimize PGM loading
- Durability Impacts

Emerging Degradation Phenomena
- Durability

Hydrophobicity vs hydrophilicity
- Catalyst interface
- Anode/cathode current distribution
Approach: State-of-Art Performance Diagnostics

- Utilize and establish measurement methods and test procedures
- Develop reproducible analysis pathways for community

- Apply methods to H2NEW
- Study phenomena at interfaces, coatings, materials and operating conditions
- Iterate between models and experiment

![Conditioning / Break In](chart1)

![VI-Curves](chart2)

![HFR free Performance](chart3)

![Detailed HFR & Impedance Information](chart4)

![Kinetic Performance](chart5)

![Voltage Loss Breakdown](chart6)
Approach: Development & Utilization of Advanced Diagnostics

- Enable and conduct the detailed study of phenomena at interfaces, coatings, materials and operating conditions.

Examples:

- High throughput degradation studies using segmented cell or rainbow stack.
- Combinatorial material testing.
- Through plane voltage distribution and potential measurements.
- Transport and crossover processes.

Segmented Cell
- High throughput
- Combinatorial Research

Internal Voltage Sensor Cell
- Separation of losses in-situ
- EIS tool to study interfaces

Hydrogen Crossover Sensing
- Application of novel Ex-situ & In-operando methods
Approach: Development & Utilization of Ex-Situ Diagnostics

- Enable and conduct the detailed study of material properties and degradation phenomena
- Characterize interfaces, material composition and morphology

Examples:
- Structure impact on conductivity and transport
- Coating defects & oxide thickness
- Coating penetration
- Pore structure & pore size distribution
- Nanoscale morphology

- Inform and exchange info between capabilities and with all tasks
- Support holistic understanding
Approach: Development & Utilization of Advanced Characterization Techniques

- Operando study of reaction, transport and flow phenomena in cell & at interfaces
- Characterization of impact of material choice, composition and morphology

Examples:
- Water & oxygen transport through cell components and their impacts on performance
- Real time water dynamics & degradation phenomena
- Hydrophobicity loss tracked locally
- Catalyst-ionomer interaction across length scales
Approach: Multi-physics electrolyzer model

2-D Cell Level Multiphysics Models

- Provide relevant parametric component level properties
- Use operando studies to obtain phenomenological data to guide the modeling analysis
- Validate models by generating physical phenomena at the component level, diffusivity shown
- Cell diagnostics to validate predictive cell optimization and mitigation strategies

In/ex-situ Diagnostics

- Properties
- Methods
- Component properties

Operando Studies

- Cell performance
- Explain
- Validate

Component phenomena

- Submodels
- Optimization/Mitigation

Cell diagnostics

- Validate
- Validate

Optimization/Mitigation
Accomplishment – Operando Diagnostics

• Q2 QPM: Complete cell design and validation of a neutron imaging cell to be used with the high-resolution imaging detector at NIST. Cell performance in imaging hardware within ±10% of performance in a 25 cm² cell

⇒ Performance validated to be within 10%
⇒ Some HFR differences seen due to differences in balance of cell components
Accomplishment – Baseline Materials Selection

- Evaluation of Anode PTL materials underway with
  - “state-of-the-art” MEAs
  - “Future Generation” MEAs (FuGeMEA)
- Two distinct PTL architectures
  - Felt material
  - Sintered material
- Various PTL parameters
  - Coating/uncoated
    - In-house
    - At supplier
  - Thickness
  - Porosity

- Interplay between MEA loading and PTL confirmed
- MEAs with low loadings have higher sensitivity towards functionality of PTL / catalyst layer interface
- Coatings significantly improve cell resistance
  - Improvement of interfacial resistance
  - Improvement of thermal conduction within cell
• Not Applicable, first year of project
Collaboration and Coordination

NREL Team Members: Shaun Alia, Guido Bender, Allen Kang, Bryan Pivovar, Tobias Schuler, James Young, Jason Zack


ANL Team Members: Rajesh Ahluwalia, C. Firt Cetinbas, Nancy Kariuki, Debbie Myers, Jaehyung Park, Nancy Kariuki, Andrew Star, Xiaohua Wang.

LANL Team Members: Siddharth Komini Babu, Rangachary Mukundan, Xiaoxiao Qiao

ORNL Team Members: Jefferey Baxter, Dave Cullen, Harry Meyer, Shawn Reeves, Alexey Serov, Haoran Yu.
Proposed Future Work

Task 2a: Performance benchmarking, baselining, validation
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Any proposed future work is subject to change based on funding levels
Summary—Task 2

• The task 2 effort focuses on cell performance and characterization with the goal of achieving higher cell efficiency

• Task 2 work areas includes electrochemical, structure and functional characterization as well as cell level modeling
  – Understand the performance impacts of different commercially available iridium based electrocatalysts, membranes and PTLs
  – Understand interfacial phenomena responsible for performance and durability limitations
  – Determine underlying mechanistic phenomena using modeling
  – These efforts will be highly integrated with the Task 1 durability and Task 3 scale-up efforts

• Early accomplishments include
  – Sourcing and evaluation of PTLs with and without coatings from two commercial suppliers
  – Identifying components and make up of spray coating fabricated MEAs for consortium baseline use
  – Definition of requirements of experimental parameters for modeling inputs
Technology Transfer Activities

- No current patent or licensing sought
- H2NEW website and marketing material being developed
- Interactions with the following OEMs:
  - Mott
  - Bekaert
  - JM
  - Heraeus
  - Chemours
  - Pajarito Powder
  - 3M
- IP generation mechanism through CRADAs with industry to be sought during the course of the project
Progress Towards DOE Targets or Milestones

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*Table 3.1.4 in MYRD&D
Publications and Presentations


- Park J., Kang Z., Bender G., Ulsh M., Mauger S.A. “Direct roll-to-roll coating of catalyst-coated membranes for low-cost PEM water electrolysers.” Oral presentation at the Fall ESC Meeting (virtual); October 2020.

Special Recognitions and Awards

• Bryan Pivovar was awarded the 2021 Energy Technology Division Research Award of the Electrochemical Society and the 2021 US Department of Energy Secretary’s Honor Award.