Title

Understanding Water and Thermal Management in Polymer-Electrolyte Fuel Cells

Author
Weber, A

Publication Date
2023-12-12

Peer reviewed

CRADA Final Report **Date 4/27/18**
April 2018

PI _Adam Weber__________

CRADA No. LB08003874

LBNL Report Number:__________

OSTI Number __________________

1. Parties: Toyota Motor Company

2. Title of the Project: Understanding Water and Thermal Management in Polymer-Electrolyte Fuel Cells

3. Summary of the specific research and project accomplishments:
(Were the goals of the CRADA achieved? Include relevant information but do not include proprietary or protected CRADA information.)

Overall the goals were achieved in that improvements in cell performance were realized that were related to water and thermal management. Diagnostic and cell models were made and key limiting phenomena elucidated.

We operated according to the statement of work. In terms of tasks:

- **Task 1: Water drain mechanism understanding from CL to FF**
  - 1.1: Water management in GDL
  - 1.2: Visualize water in GDL
- **Task 2: Model update for MEGA phenomenon understanding**
  - 2.1 Diffusion-media and Interface Modeling
  - 2.2 Reaction modeling
  - 2.3 Cell modeling
- **Task 3: High temperature operation**
  - 3.1. Analysis of ionomer thin films
  - 3.2 Catalyst-layer resistance analysis

For Task 1, work involved mainly 1.1 and the GDL / Flowfield interface. Using the custom goniometer and different materials, we visualized how droplets detached and different flow regimes within the channels (i.e., droplet, thin-fil, and plug). This was accomplished for different material sets including GDLs, Kapton, and Teflon in order to provide data and comparisons with different wettabilities. The data was used to develop more rigorous 3-D droplet models in the channel that can be averaged to be used in the overall 2-D continuum model. Both micro and nano computed x-ray tomography was used to explore the impact of water in the GDL, MPL, and CL including under operation.

For Task 2, the main focus was on 2.3 and the understanding of transport phenomena and specifically the use of different models that correlate to the above issues examined in the GDL in Task 1. We conducted modeling studies to examine whether representative elementary volumes exist in GDLs, where we found using the imaging from Task 1 and direct numerical models that they do not. This has implications in that macrohomogeneous approaches will not capture the specific distributions of reactant concentrations, temperature, etc. They only demonstrate general results, which will not be sufficient for durability and related studies. We also used the model to match experimental differential-cell data under less than fully humidified conditions. The model demonstrated good agreement with the data. This was further verified by utilizing the previously developed 1+2-D model and comparing the simulation predictions with integral and segmented cell data. In association with UTRC, we also demonstrated how the model can be used for quick diagnostics and interpretation of different limiting cases when examining a delta-V plot and oxygen gain in terms of initial and final polarization performance.

For Task 3, we have worked a lot with thin films as well as different CLs to determine the CL resistance and possible correlation to thin-film structure and properties. In Task 3.1, we have continued our analysis of different PFSA thin films in terms of their structure/function relationships, where we have seen that multi-acid side chains show promise for lower transport resistance due to their inherently different morphology when in thin-film form. We also further confirmed that the impact of gaseous environment and specifically reduced and oxidaed Pt surfaces cause changes in the underlying ionomer structure and hence its water uptake. In terms of Task 3.2, we characterized the local resistance of the provided MEAs using the H2-limiting current setup. We have developed an analysis that demonstrated that the impact of local resistance is linear as a function of I/C ratio for the same loading, wherein the intercept is related to the amount of sulfonate adsorption by the ionomer. This interfacial resistance represents about 20% of the total local transport resistance and is expected to change as the ionomer nature and equivalent weight changes. In addition, we also refined the separation of the various resistances with the aid of more detailed analytical and numerical models including the impact of anisotropic diffusion, as expected for ionomer thin films.

Deliverables:

Deliverable Achieved	Party (LBNL, Participant, Both)	Delivered to Other Party?
Quarterly Reports	LBNL	Yes
Final Report	LBNL	Yes
Training of Company employee	LBNL	Yes

5. Identify publications or presentations at conferences directly related to the CRADA?

6. List of Subject Inventions and software developed under the CRADA: None
(Please provide identifying numbers or other information.)

7. A final abstract suitable for public release:
The Parties developed understanding of water and thermal management in fuel cells using a detailed 1-D model for the through-plane direction, a gas-channel relation model for the flow-channel direction, and a method to account for the rib/channel direction. The model simulates and predicts the water transport phenomena occurring within the fuel-cell sandwich, including the complex interplay among the various phases. This model enables optimum designs, operating conditions, and material properties for use in commercial PEFCs for automotive applications. In addition, novel advanced diagnostic methods and submodels were developed to determine the critical properties and model parameters and explore specific phenomena (e.g., ionomer thin films).

8. Benefits to DOE, LBNL, Participant and/or the U.S. economy.

The research proposed in this CRADA is aimed at improving the existing LBNL fuel-cell model and fuel-cell understanding. Validation and refinement of this model will enable work that LBNL is conducting on fuel cells for DOE to be enhanced and of greater impact. Subsequently, the improved models will better enable energy-security for the United States and help meet the 2020 technical targets for fuel-cell technology adoption as laid out by the Department of Energy. The work will also allow for the development of knowledge and experience in fuel-cell modeling for the engineers at TMC. In addition, specific simulations will help to optimize TMC fuel-cell performance. Overall, increased understanding will enable key gaps for technology realization in the marketplace to be identified and overcome, thus enabling the hydrogen economy.

9. Financial Contributions to the CRADA:

DOE Funding to LBNL	$0
Participant Funding to LBNL	$ 1,219,600.00
Participant In-Kind Contribution Value	$ 552,000.00
Total of all Contributions	$ 1,771,600.00