II.E.4 High-Performance, Low-Cost Hydrogen Generation from Renewable Energy

Technical Targets

<table>
<thead>
<tr>
<th>Characteristics</th>
<th>Units</th>
<th>2012 Target</th>
<th>2017 Target</th>
<th>Proton Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen Cost</td>
<td>$/gge</td>
<td>&lt;3.70</td>
<td>&lt;3.00</td>
<td>3.64</td>
</tr>
<tr>
<td>Electrolyzer Capital Cost</td>
<td>$/gge</td>
<td>0.70</td>
<td>0.30</td>
<td>0.67</td>
</tr>
<tr>
<td>Electrolyzer Energy Efficiency</td>
<td>% (LHV)</td>
<td>69</td>
<td>74</td>
<td>65</td>
</tr>
</tbody>
</table>

Note: Estimates are based on H2A v2.1, for electrolysis only (compression-storage-delivery not included). Model assumes $0.05/kWh.

Accomplishments

- A new flow field design resulted in a 20% cost savings, reductions in part count and assembly time, improved cell robustness and is ready for production validation and commercial release.
- Additional alternative flow field materials are being evaluated to provide an additional 15 to 20% cost reduction in the near future.
- Demonstrated a new catalyst formulation and application technique through the successful operation of prototype electrolyzer cells containing 55% less precious metal in the catalyst layers.
- A comprehensive electrolyzer cell model has been created at Penn State and is currently being validated against physical test data.

Introduction

This project addresses the DOE Hydrogen Program objective for distributed production of hydrogen from proton exchange membrane (PEM) water electrolysis. The DOE technical targets for hydrogen cost as well as electrolyzer efficiency and capital cost will be directly addressed through the advancement of key components and design parameters. Currently, a significant portion of the electrolyzer system capital cost comes from the cell stack(s). When added together, the flow fields and membrane electrode assemblies (MEAs) constitute over half of the total cell stack cost (Figure 1). Significant cost reductions of these components as demonstrated with this research are required in order to reach the targets. Further optimization of cell stack components
results in efficiency gains at the system level and ultimately a reduction in the cost to produce hydrogen.

**Approach**

The scope of work for this project allowed for research and development in several key areas relating to cell stack cost reduction. Topics included: 1) flow field design, 2) catalyst formulation, and 3) computational performance modeling. Advancements in flow field design are intended to be advantageous for low-cost, high-volume manufacturing. Alternatives to the current flow field design include composite bipolar plates or unitized flow fields which consolidate parts and reduce the amount of required precious metal plating. Material testing samples and prototype flow fields will be fabricated and tested for compatibility with the corrosive environment known to exist within operating electrolyzer cells. Higher efficiency oxygen evolution catalysts are of interest because the oxygen evolution reaction is inefficient and therefore requires high catalyst loadings to achieve reasonable operational voltages at the desired current densities. Improving catalyst utilization can substantially reduce the cost of the MEA by reducing the noble metal content in the catalyst layers. Novel electrode structures will be constructed using alternate synthesis techniques and characterized for performance and durability. Computational modeling of an electrolyzer cell will allow for optimization studies to be performed around flow field material and architecture. Cell performance can be quantified in ways not typically possible with standard physical test experiments. Validation of all of the previously mentions design changes will be achieved through cost analysis based on the H2A model.

**Results**

During this project, significant near-term electrolyzer cell cost reductions were identified through the testing of non-metal flow field components (Figure 2). The use of alternative conductive materials has been shown to provide comparable electrochemical performance when compared to legacy designs while allowing for the consolidation of components and the use of manufacturing methods more suitable for high volume production. Additional materials are still being evaluated that could present a further cost reduction thanks to their ability to be injection-molded in a full-scale production scenario. It should be noted that the operating potential of electrolyzer cells is typically above 2.0 V while water, oxygen and hydrogen gasses are also present at various pressures and temperatures. The challenge with alternative materials is to ensure that they can withstand these highly corrosive conditions contained within an operational electrolyzer cell while also maintaining low electrical resistance.

Specially developed emersion tests have allowed for the evaluation of several materials and coating options within the described environment. These tests indicate that while coatings can effectively protect materials from corrosion, small cracks or discontinuities in the coating may be allowing a gradual corrosion of the substrate material. Completed test runs have been limited to 500 hours, therefore, it will be necessary to perform additional longer term tests in order to better quantify the rate of corrosion. If the rate of corrosion is significant, process improvements will be required in order to ensure continuous coverage of the substrate material. Remaining testing of alternative materials will be focused on evaluating the impact of the electrical resistivity of prototype flow fields on cell potential during operation.

Significant advancements have been made in the development of an optimized catalyst formulation and application technique. This work has demonstrated a 55% reduction in the amount of precious metal used in the catalyst layers of the MEA. As a result, the cost of the MEA can be reduced and will in turn create cost savings at the cell stack and total system level. These improvements save cost and improve quality.
while maintaining cell potential performance when compared to existing commercial cell stacks operating at standard conditions (Figure 3). In order to achieve this, a mathematical model was developed and refined to accurately predict the final catalyst loading from the beginning of the formulation and application process. Using the model, it was possible to perform a concise matrix of experiments and quickly determine the lower limits of catalyst loading with respect to desired cell performance. The selected application technique represents an improvement over existing production techniques in that it allows for improved accuracy and uniformity while also enabling higher speed throughput.

A comprehensive computational model of an electrolyzer cell has been developed at Penn State and is capable of predicting performance parameters based on the geometry of the flow fields and specified operating conditions. Calculated parameters include overall cell potential, distribution of potential and current density distribution, as well as, volume fractions of water, oxygen and hydrogen in various regions of the cell. Results can be plotted in as colored gradients superimposed over three-dimensional models or as more traditional plots such as polarization curves (Figure 4). This custom-developed code merges traditional two phase flow modeling with a specialized electrochemical model. Variables common to both sets of governing equations create linkages between the sections of the model and improve the accuracy of the results.

Design parameters and operational data from a baseline design have been provided to Penn State for the purpose of validating the model. Once the predicted results are confirmed to be consistent with actual data over a larger range of conditions, the model can reliably be used for parametric analysis of electrolyzer cell designs. Cell component architecture can be refined in light of model performance predictions and the relative impact of design parameters on overall efficiency can be understood. It is anticipated that improved water distribution within the cell will allow for better thermal management. The minimization of coolant flow could reduce demands on the system such as the pump flow and pressure head requirements which can lead to reductions in capital cost and gains in system efficiency.

**Conclusions and Future Directions**

- Tests have shown that alternative conductive materials can remain stable in the corrosive environment of operational electrolyzer cells for tests up to 500 hours, however, much longer term testing is required to ensure stability beyond the 30,000 hour minimum operational life of Proton Energy Systems cell stacks.
- Cost reductions can be made by controlling the catalyst formulation process and through advanced application techniques. The next step is to implement the formulation and application processes developed during this project into Proton’s commercial production design.
- Electrolyzer cell performance can be predicted with the use of a comprehensive computational model. No future work is planned at this time but the next step would be for Penn State to develop an executable program which could interface directly with computer aided drafting and design models and provide upfront electrolyzer simulation capability.