Purdue University DURI Program Research on Two-Phase Fuel Separation in a PEM Fuel Cell

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Abstract

The Discovery Undergraduate Research Program at Purdue University offers approximately 50 students the opportunity to work with faculty running research projects through Purdue's progressive Discovery Park. The internships give students the chance to work directly with faculty and graduate students on exciting interdisciplinary research projects during the school year.

Through the DURI program, a study was conducted on developing a sodium borohydride PEM fuel cell. In this fuel cell, sodium borohydride will be internally reformed, so some method to separate the hydrogen and liquid needs to be developed. This phase separation will be accomplished using layers of different porosities of metal foams. First experimental design uses two layers of metal foam. A catalyst embedded in the high porosity metal foam for NaBH₄'s hydration reaction will produce H₂. Phase separation will occur as the gas diffuses quickly through the low porous metal foam and water is left behind. Eventually, water will completely penetrate the low porosity metal foam, so to prevent "flooding" a low porosity hydrophobic layer is prepared.

The experimental design was modeled with the CFD program Fluent. The calculated velocity vectors showed that the phase separation occurs to some extent, as the velocity vector components change as fluid moves from the high porosity metal foam to the low porosity metal foam. Since the movement of the water wasn't clearly shown in Fluent and the gas distribution at the outlet isn't uniform, research is continued to further investigate these issues. In addition, different variations of the experimental set-up are also being developed and modeled.

Introduction and Research Objectives

A fuel cell is a device that efficiently converts chemical energy into electrical energy. In a typical Proton Exchange Membrane Fuel Cell (PEMFC), hydrogen fuel enters the anode of the fuel cell, where it reacts with a catalyst, releasing electrons. Electrons travel through a circuit while the remaining protons diffuse across an electrolyte membrane. Once through the membrane, protons combine with oxygen at the cathode, producing water, the waste product¹. PEMFCs show a promising future as they have a low operating temperature, are small, have a long stack life and quick start up, and are suitable for discontinuous operation². However, many problems still need to be overcome before these fuel cells become mainstream. One major

problem is the production, storage and transportation of the hydrogen fuel. Traditional methods of producing hydrogen are ineffective. These methods generate hydrogen contaminated with carbon monoxide, which poisons PEMFC electrocatalysts. Producing pure hydrogen, without the carbon monoxide contamination, is an inefficient use of energy. As for hydrogen gas fuel storage, there is no safe, effective way to store gaseous hydrogen that also provides adequate fuel for PEMFC operation.²

One possible solution to the PEMFC fuel problem is to use a liquid form of hydrogen instead of a gaseous form, making the fuel much easier to store and transport. The fuel cell under development uses a sodium borohydride (NaBH₄) solution as fuel. In the anode of the fuel cell, sodium borohydride will react with a catalyst to release the hydrogen that will power a PEMFC. Sodium borohydride is a candidate for a fuel source because it has 10.8% theoretical H₂ efficiency, the bi-products are environmentally safe, the reaction is easily controlled, and the reaction conversion rate is almost 100%²⁻⁵. The one major obstacle with this fuel is the development of an effective means to separate hydrogen from the rest of the solution. Current designs use an external system to reform the NaBH₄ fuel. The goal of this experiment is to eliminate the need for an external system so the fuel cell will be more compact and portable. An experimental design has been developed that uses layers of metal foam of varying porosities as the endplates of the fuel cell. H_2 will be produced when NaBH₄ reacts with a catalyst embedded within a high porosity metal foam. Phase separation should occur as the gas diffuses across a lower porosity metal foam faster than the liquid. To prevent flooding of the endplate, which would inhibit power output, the lower porosity metal foam layer will be coated to make it hydrophobic.

Experimental Design

The objective of the experiment was to see separation of a two phase (liquid and gas) fuel in the endplates of a PEMFC anode. Several possible experimental designs have been developed. Figure 1 shows the first design. On the left is high porosity metal foam; on the right is low porosity metal foam. The two-phase, air-water mixture will enter the metal foam through the inlet on the middle left. It is predicted that most of the water should exit through the outlets on the top and bottom left and most of the gas should exit through the open right side. This design was modeled in Fluent CFD code.



Figure 1: Metal Foam Experimental Design #1

Figure 2: Experimental Design #2

Several variations on this basic design have been created. The design in Figure 2 tests different locations of the inlets and outlets, with one inlet at the top right and one at the top left and outlets at the bottom left and bottom right. Water is injected into the top left inlet and air is injected into the top right inlet. Water should exit at the bottom left outlet and air should exit at the bottom right outlet. If the air and water exited without mixing, it would indicate that the metal foams can maintain phase separation. Another experimental design in development uses three layers of metal foam, rather than two, in hopes of a more even distribution of H_2 outflow. Other designs involve varying the thickness, porosities, and boundary conditions of the metal foams.

Fluent Modeling

Each of the experimental designs was modeled on Fluent. The experimental design was set-up as a mesh file in Gambit. The mesh model was then imported into Fluent, where the grid was checked, the solver formulation and basic equations defined (Eularian, Darcy's Law for Porous Media), material properties and boundary conditions assigned, and the flow field initialized⁷. Once these basic steps were completed, Fluent calculated results.

Results

The following results from Fluent simulations correspond to the experimental design shown in Figure 1. Figure 3 is a diagram of velocity vectors of air colored by pressure. The velocity vector components change as the air moves from high to low porosity, which indicates that the movement of the air is affected by the metal foam's porosity. Since the flow of air is affected by the metal foam's porosity, this could show that phase separation between air and water is taking place. Figure 4 is a diagram of Phase 1 (air) permeability when a permeability value of 1e-8 was used for each metal foam layer.



Figure 3: Velocity Vectors Colored By Pressure

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Figure 4: Velocity Vectors Colored by Pressure

Conclusions

Through the Discovery Undergraduate Research Internship program the following were achieved: (1) Study of the theory behind NaBH₄ PEMFC power systems, (2) Proficient use of Fluent CDF code for simulations, (3) Simulation of metal foam layers from the PEMFC anode section using Fluent with preliminary results on gas and liquid separation, and (4) Limited participation in a catalyst development experiment for the NaBH₄ PEMFC.

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Biography

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