

### CALIFORNIA STATE SCIENCE FAIR 2017 PROJECT SUMMARY

Name(s)

**Marcus Luebke** 

**Project Number** 

# S0821

#### **Project Title**

## **Running on Water: AI to Design Optimized H2 Production Systems Based on User Priorities of Cost, Efficiency, and Rate**

#### Abstract

**Objectives/Goals** This project is a continuation of a three-year effort to generate hydrogen in real time to power automobiles. To do this effectively, a large design trade space needed to be optimized, with the optimum results depending on a competing set of priorities: namely production rate, efficiency & monetary cost of the chemical system.

My objective was to create a computer simulation of my hydrogen production system and develop an artificial intelligence to identify the optimum solution based on input priorities, to complement my experimental research and enable consideration of exotic materials and geometries that would have been too expensive and complex to test in my garage laboratory.

#### Methods/Materials

For the model, high fidelity conductivity data was required, so I measured conductivity over a series of temperatures and Na2CO3 electrolyte concentrations.

For the code, I created a chemical simulation model (based on known scientific equations, experimental data and mathematical derivations), a utility function (incorporating user input priorities), and an artificial intelligence algorithm (inspired by the biological process of natural selection). The artificial intelligence interacted with the model and utility function, to return optimal designs after tens of thousands of iterations.

#### Results

The AI returns optimum designs based on the priorities placed on hydrogen production rate, efficiency & cost. As an example, for a weighting and threshold of: Production Rate [45%, 0.007 mol/s], Cost [10%, \$100], & Efficiency [45%, 80% efficient] the AI can output a design of 700mm x 460mm x 1mm plates, spaced 0.7mm apart, made of an Aluminum Cathode and Anode, with an electrolyte concentration of 0.6M and a temperature of 82C, at 1.48 Volts.

#### **Conclusions/Discussion**

The results returned by the artificial intelligence (AI) lead to new understandings and new directions to pursue in research and demonstrate that AI is a viable technique for scientific work.

The AI enables rapid identification of optimum designs based on user preferences and trade-offs including but not limited to production rate, efficiency, and cost. It allows researchers to consider a wide range of system options, including exotic materials & geometries, and to test designs and ensure feasibility before investing in experimental systems to validate the performance of these system designs.

#### **Summary Statement**

A computer model of a complex real-time hydrogen generating system and an artificial intelligence algorithm for optimization were created to find the optimal setup based on relative importance of Production Rate, Efficiency & System Costs.

#### **Help Received**

I designed and programmed the code myself. I consulted with the Stanford Graduate Department of Chemical Engineering to validate the science and approach behind my chemical model.