Machine Learning and Artificial Intelligence
J.-L. Kim (Ed.)

doi:10.3233/FAIA220421

Machine Learning-Based Current Density Simulation for Direct Borohydride Fuel Cell

Amira MOHAMED[a], Hatem IBRAHEM[b], Jung-Hyun LEE[a], and Kibum KIM[a,c,1]
[a] *School of Mechanical Engineering, Chungbuk National University, Korea*
[b] *School of Information and Communication, Chungbuk National University, Korea*
[c] *Physics and Engineering Department, North Park University, United States*

Abstract. Recent studies on fuel cell design have showed that the use of simulation tools is beneficial in terms of saving time and money. Current density management is still a key research problem for several technologies, including Direct Borohydride Fuel Cell (DBFC). This paper describes a systematic machine learning technique for estimating the cell current density for DBFC as a function of various input factors. Artificial Neural Networks (ANN) and Decision Tree Regressor (DTR) are two popular machine learning models that were trained and evaluated for the current density simulation using a conducted fuel cell experiments presented in previous research. The ANN model performed the better than the DTR model in the simulation, with a mean absolute error of 3.00015 for training and 5.57614 for testing. The simulation exhibits very small error values, indicating that the suggested approaches accurately mirror real-world DBFC process.

Keywords. Direct Borohydride Fuel Cell; Machine learning; Artificial Neural Networks

1. Introduction

The development of fuel cells, which transform chemical energy into electrical energy, has attracted research attention due to the growing interest in renewable and sustainable energy generation as a method of achieving net-zero carbon emissions in the future. In recent studies, fuel cell technology has been identified as one of the top possibilities for portable power source batteries [1, 2]. Direct borohydride fuel cells (DBFCs) are gaining attention from researchers because they do not require expensive platinum catalysts, DBFCs might be manufactured at a lower cost than regular fuel cells and they also have a higher power density [3]. DBFCs are a type of alkaline fuel cell that is fed directly with sodium borohydride or potassium borohydride as a fuel and either air/oxygen or hydrogen peroxide as an oxidant as shown in Figure 1. DBFCs are relatively new forms of fuel cells that are currently in development and are appealing owing to their high operational potential in comparison to other types of fuel cells [4, 5]. In more traditional hydrogen fuel cell systems, sodium borohydride may be employed as a hydrogen storage

[1] Corresponding Author; Kibum KIM, School of Mechanical Engineering, Chungbuk National University, Korea/ Physics and Engineering Department, North Park University, United State; E-mail: kbkim@chungbuk.ac.kr.

medium. The borohydride can be catalytically decomposed to regenerate hydrogen for a fuel cell as shown in (1).

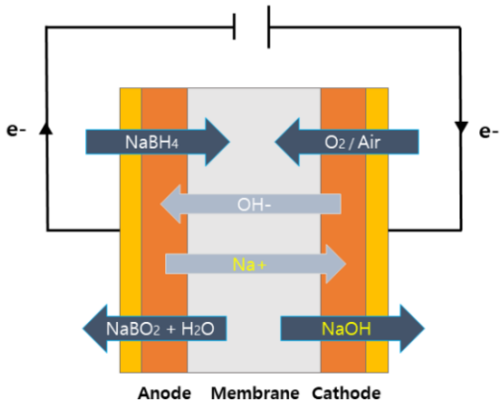

Figure 1. A schematic of a direct borohydride fuel cell that uses oxygen, air as an oxidant.

$$NaBH_4 + 2H_2O \rightarrow NaBO_2 + 4H_2 \quad (1)$$

Direct borohydride fuel cells immediately oxidize the borohydride, avoiding the need for hydrogen generation and even yielding somewhat more energy.

In an aqueous alkaline solution, the borohydride ion may be directly oxidized on a wide range of electrode materials, releasing a minimum of eight electrons. The electro-oxidation of BH4 takes place in the following manner. The anode chemical reaction can be expressed as in (2).

$$NaBH_4 + 8OH^- \rightarrow NaBO_4 + 6H_2O + 8e^- \quad (E^0_{anode} = -1.24\,V) \quad (2)$$

The cathode chemical reaction can be expressed as in (3).

$$2O_2 + 4H_2O + 8e^- \rightarrow 8OH^- \quad (E^0_{cathode} = +0.4V) \quad (3)$$

The simplified reaction of the DPFC is as expressed in (4).

$$NaBH_4 + 2O_2 \rightarrow NaBO_4 + 2H_2O + Electrical\ power \quad (4)$$

Although the current commercial fuel cells have a good design, they need several laboratory tests that cost a lot of money, time, and effort. Instead of costly laboratory trials, we use two popular machine learning models and obtained the best model to overcome the design challenge.

2. Related work

Many current findings have offered machine learning-based fuel cell modeling methods. Hossain et al. [6] have proposed a machine learning algorithm namely Support Vector Machine (SVM) regression, Regression Trees, and Gaussian Process Regression (GPR) for modeling the effect of palladium supported on carbon nanotube used for formic acid

electro-oxidation for DBFC. In previous research, we also have developed an artificial neural network-based fuel cell design approach for proton exchange membranes, the most prevalent and commonly used fuel cell type [7]. Kheirandish et al. [8-9] have studied the SVM, ANN, and Hebbian learning models' performances using their own dataset for stack voltage. They demonstrated that SVM was better than ANN in small datasets, whereas ANN performs better on bigger datasets. In this research, we used a public dataset on DBFC [10] that investigates the relationship between the various fuel cell characteristics to simulate the current density depending on four different parameters.

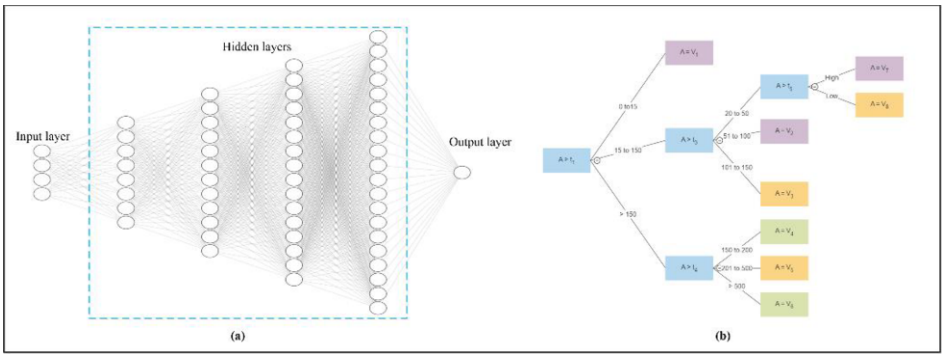

Figure 2. (a) A sample artificial neural network architecture. The input layer has four neurons, the 4 hidden layers have a sequential increase in the number of neurons. The output layer has one neuron for the current density prediction. (b) A sample decision tree regression model with learnable thresholds (t1).

3. Proposed method

We compare the performance of two popular machine learning algorithms, which are the artificial neural network (ANN) and the decision trees regression (DTR), to simulate the performance of DBFC. We employ a public dataset of single DBFC experiments [10] for training and test of the proposed models. This dataset contains results from tests on the Direct Borohydride Fuel Cell (DBFC) anode's impedance and polarization using catalysts with Pd/C, Pt/C, and Pd decorations. In fact, varied anode catalyst loadings, applied voltages, and concentrations of Sodium Borohydride (SBH) are considered in the results along with an explanation of the experimental specifics of the electrochemical investigation. Voltage, power density, and resistance of DBFC are assessed by polarization and impedance curves using the suitable equivalent fuel cell circuit, which depend on the weight percentage of SBH, applied voltage, and quantity of anode catalyst loading. This dataset is helpful for modeling, power source research, and in-depth analysis in DB fuel cell studies. In the proposed models, we employ the data of DBDC with Pd/C catalyst. The input parameters to the machine learning model are cell voltage, SBH weight percent, Pd/C anode catalyst loading, and solution type while the output parameter (the parameter to be predicted by the machine learning model) is the cell current density. There are fixed parameters which is excluded from input parameters (as they are fixed) over all the dataset such as anode catalyst (which is Pd/C), anode support (which is Nickel foam), cathode catalyst (which is HypermecTM k14 with a loading of 5 mg/cm2), cathode support (which is Carbon cloth) and the surface area (4.5 cm2), all experiments are done under an electrolyte condition of 2 Moles of KOH with a different

concentrations of SBH (1, 3, 5, 8 wt% SBH). The dataset contains 250 sample for training and 30 samples for validation.

The first proposed model is an artificial neural network (ANN) with the architecture shown in figure 2. The ANN can be trained on large enough data to form a relationship between the input and output parameters through learnable weights. An optimization method was used to optimize the training method, which is Adam's optimizer [11]. The basic form of the learnable parameters is as follows:

$$F = ACT(\sum_{i=1}^{N} w_i X + b) \quad (1)$$

where ACT is an activation function in our case, we used Gaussian error linear unit (GELU) [12] as an activation for all hidden layer as it produced better results than the commonly known rectified linear unit (RELU). w_i is the learnable weight parameters vector and bi is the biases vector. The optimizer updates the weights vector w_i following the gradient descent equation as follows:

$$Wi = \frac{\partial F}{\partial wi} - \beta \quad (2)$$

where $\frac{\partial F}{\partial wi}$ is the gradient of F with regard to w_i vector. function an input layer with four neurons was designed to receive the four input parameters, four hidden layers were designed to model the relation between the input and the output parameters with gradual increasing in the number of neurons in the following order 32 → 64 → 128 → 256, while the output layer has a single neuron for current density prediction.

Several numbers of layers were tested to find the best architecture which corresponds to the lowest error value of the prediction as it will be shown in the experimental results section.

The second proposed model is the decision tree regression (DTR) model which is a well-known machine learning algorithm with the shape of a tree with nested branches. A decision tree has the structure of flowchart in which each leaf node represents a class label, each internal node represents a "test" on an attribute and each branch indicates the result of the test (decision taken after computing all attributes). Classification or regression rules are represented by the routes from root to leaf. The main hyper parameter in DTR algorithm is the tree depth which defines the splitting branches of the regression tree. DTR aims to learn the splitting thresholds for the nested conditions in the training process. A block diagram of the DTR model is shown in figure 3-(b). Least squares/standard deviation reduction is used as a metric to choose features in the regression tree [13].

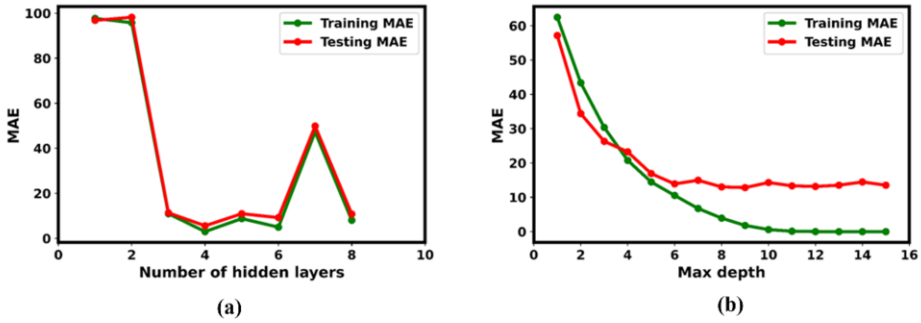

Figure 3. (a) MAE training and testing as function of the various hidden layer counts for the ANN model. (b) MAE training and testing as a function of maximum depth for the DTR model.

4. Experimental results

To choose the best model performance in case of the ANN, we trained ANN models with an increase in the depth of the network (the number of the neurons in each layer is twice that for the previous layer e.g. 32 → 64 → 128 →…→4096). Each time we evaluate the trained ANN configuration on the validation set and measure the mean absolute error (MAE) between the ground truth values of the current density and the predicted values. Figure 3-(a) shows the MAE attained for each configuration (from one hidden layer to 8 hidden layers). The ANN configuration of 4 hidden layers produced the lowest test MAE value (5.57614) showing that the more increase in the network depth does not improve the model's performance anymore. For the DTR model, we trained the DTR model while varying the max depth each time (from max depth of 1 to 15) to find the best max-depth corresponding to the best model's performance. Figure 3-(b) shows the test MAE value for each max depth from 1 to 15 showing that a max-depth of 6 is the best one and produces the lowest MAE value (13.), noting that other max-depth values seems to have the same performance, but we choose the lowest max-depth that gives the best performance and also the lowest DTR complexity, so 6 is the best value.

We also compare the performance of the ANN to that for the DTR. The ANN achieves a lower test MAE value than that for the DTR model. Table 1 shows a comparison between the ANN and the DTR model on the DBFC dataset in terms of the training and test MAE values showing that the ANN can efficiently learn the DBFC simulation problem and more accurately than the DTR model.

Table 1. Comparison between the ANN and the DTR model on the DBFC dataset in terms of the training and test MAE values.

Model	Hidden layers or Max depth	Training MAE	Test MAE
ANN	4	3.00015	5.57614
DTR	6	10.544853	13.90037

5. Future work

The achieved results from the experiments are quite encouraging and may result in more broadly applicable simulation results in further studies. Future research will concentrate on expanding the model's design parameters to include various electrode materials and catalysts that are outside the subject of the current study, however this step requires a more comprehensive dataset that is gathered through various designs and tests. The optimization of ANN on the more generic fuel cell datasets is also a part of the future study.

6. Conclusion

Two machine learning models, neural networks (ANN) and decision tree regression (DTR) were developed and assessed for current density modeling utilizing Direct Borohydride Fuel Cell experiments published in a previous article. The ANN model had the best simulation results, with mean absolute errors for training and testing of 5.57614 and 3.00015, respectively. The suggested approaches effectively simulate the real DBFC

performance based on the ANN simulation's very low error levels. The entire research provides an accurate modeling tool for the DBFC output current density depending on other design parameters.

Acknowledgement

This research was funded by the National Research Foundation of Korea (NRF), grant number (2019R1D1A3A03103616).

References

[1] Eftekhari A, Fang B 2017, Electrochemical hydrogen storage: opportunities for fuel storage, batteries, fuel cells, and supercapacitors. International Journal of Hydrogen Energy, 40 (2017), pp.25143-25165.
[2] Tan WC, Lip Huat S, Hui ST, Jin X, Cai ZS, Ming CY. Overview of porous media/metal foam application in fuel cells and solar power systems. Renewable and Sustainable Energy Reviews, 96 (2018), pp. 181-197.
[3] S. Colominas J, McLafferty DD. Macdonald, Electrochemical studies of sodium borohydride in alkaline aqueous solutions using a gold electrode, J Electrochim Acta. 2009; pp. 3575-3579.
[4] Amendola SC, Onnerud P, Kelly M, Petillo P, Sharp-Goldman SL, Binder M. A novel high power density borohydride-air cell. J. Power Sources, 84(1999), pp. 130–133.
[5] Choudhury NA, Raman RK, Sampath S, Shukla AK. An alkaline direct borohydride fuel cell with hydrogen peroxide as oxidant, J. Power Sources, 143(2005), pp.1-8.
[6] Hossain SS, Ali SS, Rushd S, Ayodele BV, Cheng CK. Interaction effect of process parameters and Pd-electrocatalyst in formic acid electro-oxidation for fuel cell applications: Implementing supervised machine learning algorithms, International Journal of Energy Research. 2022.
[7] Mohamed A, Ibrahem H, Kim KB. PEM fuel cell design simulation for electric vehicles using artificial neural networks. IEEE International Conference on Consumer Electronics (ICCE). IEEE, 2022: 1-4.
[8] Kheirandish A, Motlagh F, Shafiabady N, Dahari M. Dynamic modelling of PEM fuel cell of power electric bicycle system, International Journal of Hydrogen Energy, 41(2016), pp.9585-9594.
[9] Kheirandish A, Shafiabady N, Dahari M, Kazemi MS, Isa D. Modeling of commercial proton exchange membrane fuel cell using support vector machine. International Journal of Hydrogen Energy, 41(2016), pp.11351-11358.
[10] Hamidi S, Sabouri S, Haghighi S, Askari K. Experimental dataset of electrochemical efficiency of a Direct Borohydride Fuel Cell (DBFC) with Pd/C Pt/C and Pd decorated Ni-Co/rGO anode catalysts. in Chem-Rxiv, Cambridge: Cambridge Open Engage, 2020.
[11] Diederik PK, Jimmy BA. A method for stochastic optimization. 3rd International Conference on Learning Representations, ICLR 2015, San Diego, CA, USA, May 7-9, 2015, Conference Track Proceedings. 2015
[12] Dan H, Kevin G. Gaussian Error Linear Units (GELUs), arXiv preprint arXiv, (2016), pp.1606.08415.
[13] Lewis RJ, An Introduction to Classification and Regression Tree (CART) Analysis. In Annual Meeting of the Society of Academic Emergency Medicine. 2000.