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An Artificial Neural Network for Capillary Transport Characterization of Fuel Cell Diffusion Media

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This study addresses the development of a design algorithm based on artificial neural network (ANN) that can precisely predict the capillary transport characteristics of fuel cell diffusion media (DM). A three-layered ANN architecture processing the feed-forward error back propagation methodology has been constructed. The designed neural network was systematically trained with the novel benchmark data generated from direct measurements of capillary pressure-saturation of differently engineered DMs under a wide range of conditions [8-10]. Once the trained network learned the complex non-linear relationship between the transport properties and measured parameters of the tested DM samples, it was utilized to predict the capillary pressure of the DM as a function of the hydrophobic additive content and assembly compression pressure at the intermediate conditions, in which the experimental data are not available.

Introduction

Developing a robust, intelligent design tool for multivariate optimization of multi-phase transport in fuel cell diffusion media (DM) is of critical importance. To date, fuel cell manufacturers have been invested considerable resources towards developing advanced DM materials with favorable internal architectures that will provide robust, efficient and durable fuel cell operations under a wide range of operating conditions. However, these efforts generally rely on trial-and-error approaches and require extensive testing programs due to the lack of benchmark data required to improve and expand the existing physical understanding.

Due to the inherent structural complexity and the apparent experimental limitations, most DM characterization attempts are based on modeling studies. An excellent review of the recent modeling efforts is provided by Djilali [1]. Even though these modeling efforts represent a useful starting point to characterize the DM structure, they are mostly intended to provide qualitative connection between the cell performance and the DM material properties rather than providing direct input/output relationships of the relevant design parameters. In terms of design and optimization, the essential goal should be to provide a reliable tool that can precisely correlate the governing input–output relationship of the system. One way to achieve such a tool is to construct an artificial neural network (ANN) trained by actual benchmark data. The key feature of this technique is that ANN is capable of tackling complex and ill-defined problems with its

excellent multi-dimensional mapping capability [2]. More detailed explanation of ANN systems is provided in [3,4]. Recently, a few ANN studies [5-7] related to the fuel cell performance prediction have been reported, but to best of authors' knowledge, no truly direct study focused on developing a design tool for predicting the capillary transport characterization of the fuel cell DM has been reported.

In the present study, a DM design tool using the artificial neural network based on newly available direct benchmark data [8-10] was developed to characterize the capillary transport behavior of the fuel cell DM. The designed neural network was trained with the direct benchmark data of capillary pressure-saturation generated for differently engineered SGL 24 series DMs (5, 10 and 20% PTFE loadings of *wt*.) under various compression loadings (0, 0.6 and 1.4 MPa) [8-10]. The trained network was then utilized to delineate the relative significance of PTFE content of the DM and compression loadings on the capillary pressure of this class of tested DM materials.

Method of Approach

Experimental Approach

SGL 24 series (SIGRACET®) carbon paper DMs coated with micro-porous layer (MPL) were utilized in the experiments. The degree of wettability in these chosen DM samples varies from 5 to 20% PTFE of total weight (*wt*). The capillary transport characteristics (*i.e*. capillary pressure-saturation curves, pore size and distribution, hydrophobic/hydrophilic porosity, *etc*.) were determined under different compression pressures, including 0, 0.6 and 1.4 MPa. The detailed description of the experimental technique and material properties of the tested DM samples have been presented in our previous publications [8-10].

Data Description and ANN Training

A three-layered feed forward error back propagation neural network has been constructed for this study. The tangent-sigmoid and log-sigmoid activation functions in the hidden layers and a linear transfer function in the output layer were used in the current neural framework. The connections between the sub-layers were represented by the specific updated weight functions, which have been calibrated through a set of training data. The measured capillary pressure data were systematically categorized according to the measured saturation, PTFE content of the DM and the assembly compression pressure and then implemented into the constructed neural network.

The input layer has been configured to include four correlated input parameters based on the non-wetting phase saturation, the compression pressure and the PTFE content of the DM, whereas the output layer is designed for one parameter "the capillary pressure", which is a governing parameter for the capillary transport mechanism in DM. The total numbers of 30 neurons, 10 neurons in each layer, have been found to be most suitable neuron configuration for the present ANN pattern. A total of 340 data sets were utilized in the training and testing phase of the present ANN model. Among this data set, 290 data series were randomly chosen and implemented as a training set, while the remaining 50 data set were utilized as a test set for cross-validation to improve the learning process. After the total number of 3750 training epochs, the present network has been found to achieve the ability to identify the highly non-linear relationship between

the input and output parameters. At the end of this training cycle, the corresponding mean-squared error (relative error between the network output and target values) is converged to a value of 3.4 10^{-7}, which shows the successful completion of the training process. The schematic of the designed neural network architecture is provided in Fig. 1.

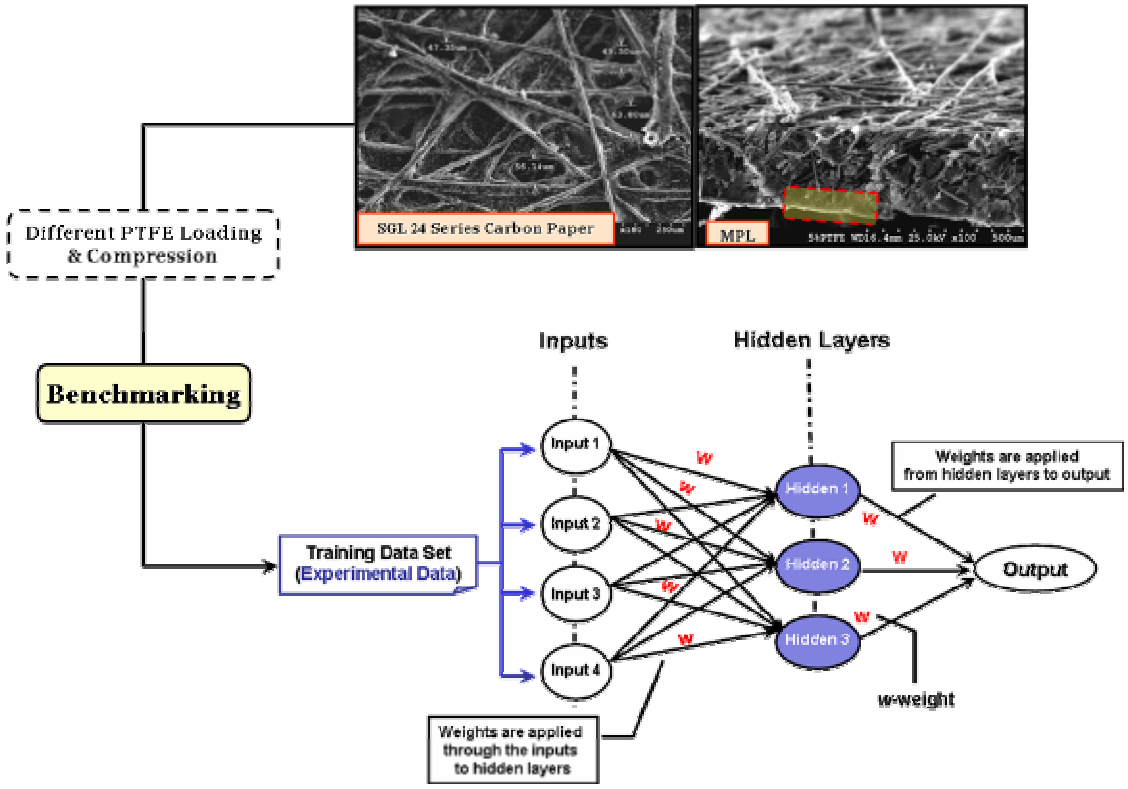

Figure 1: The method of approach and the architecture of the designed ANN

ANN Validation

After the best learning was achieved through supervised training, one to one cross validation of the ANN predictions using discrete input data set (different than the ones used in training process) was performed for all the tested DM samples to evaluate the reliability of the trained network. Figure 2 represents the comparison of measured capillary pressure and the ANN prediction for SGL 24DC (20% PTFE of *wt.*) DM undergoing 1.4 MPa compression (the measurement boundary). The ANN predictions appear to accurately capture the measured capillary pressures in the entire saturation range, even in the high capillary pressure zone (s_{nw}>0.7) which is governed by the micro-porous layer (Fig. 2). This indicates that the present ANN model successfully performs the necessary adjustments in the capillary pressure predictions due to the change in PTFE loading and compression, thus yielding an average uncertainty of ±5.1% of the measured data in overall saturation.

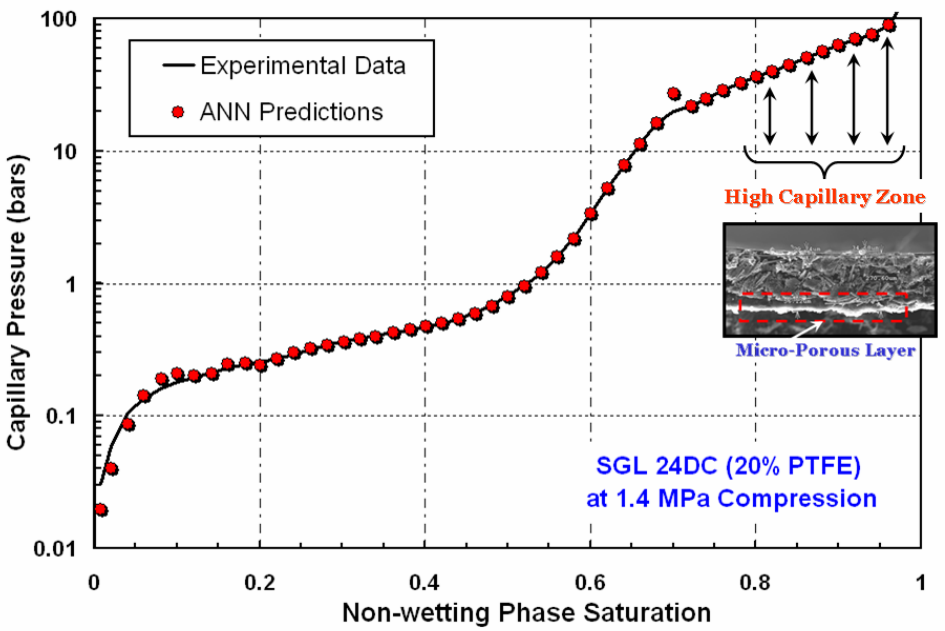

Figure 2: Comparison of experimental data and the present ANN predictions for SGL 24DC carbon paper DM treated with 20% PTFE of *wt*. at 1.4 MPa compression.

Results and Discussions

The well-known limitation of the ANN system is its insufficient capability of performing extrapolations [4], since the designed network is only suitable for representing the characteristic patterns of the system within the range of original training data set. Recalling that the experiments described herein were performed at 0, 0.6 and 1.4 MPa for the DM samples treated with different PTFE content (5, 10 and 20% of *wt*.), the main focus in this study is placed on evaluating the relative significance of PTFE content and the compression pressure on the capillary pressure of the tested DM samples at the intermediate testing conditions within the range of tested parameters, in which the experimental data are not available.

Degree of Wettability

Figure 3 shows the predicted capillary pressure versus % PTFE content of the DM at different saturations (*i.e*. 0.1, 0.2, 0.3 and 0.4) at a compression of 0.3 MPa (*i.e*. intermediate condition for which the experimental data are not available). The ANN capillary pressure predictions follows an increasing trend with an increase in PTFE content for all saturations, however exhibits relatively higher sensitivity (high capillary pressure) at high saturations (*i.e*. s_{nw}=0.3 and 0.4). This can be attributed to the strong dependence of capillary pressure on the local water content of the pore and the hydrophobicity of the pore matrix. The degree of PTFE loading in DM increases the imbalance at the line of contact, yielding a higher capillary pressure. The increase in capillary pressure is amplified with an increase in the liquid saturation, which leads to enhance the increase in the molecular imbalance at the interface [11].

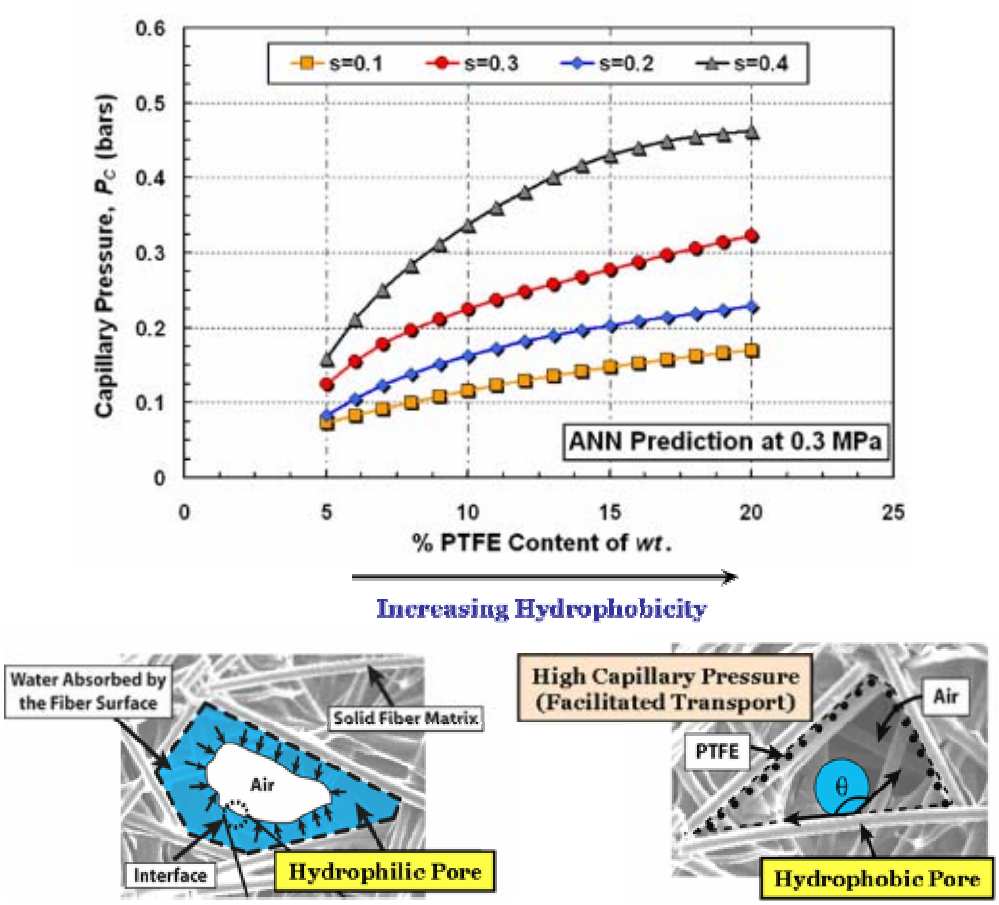

Figure 3: The predicted capillary pressure versus % PTFE content of the DM for different saturations (0.1, 0.2, 0.3 and 0.4) at 0.3 MPa compression (*i.e.* intermediate conditions for which the experimental data are not available).

Compression and Pore Size Effect:

In order to delineate the effects of compression and corresponding reduction in pore size, the response (prediction) of ANN model under different compressions were analyzed. Figure 4 shows the predicted capillary pressure versus % PTFE content of *wt.* of the DM at constant saturation (s_{nw}=0.3) under different compression conditions, ranging from 0 MPa to 1.4 MPa with an increment of 0.3 MPa (*i.e.* intermediate conditions for which the experimental data are not available).

The ANN simulations reveal that for a given PTFE loading, the capillary pressure is prone to increase in parallel with compression pressure within the compression range of 0 to 0.6 MPa. The increase in capillary pressure with compression can be attributed to the corresponding reduction in pore size, which in turn, leads to an increase in the liquid water resistance of the pore matrix. In order to overcome the enhanced resistance, a higher capillary pressure is needed. One other observation that can be drawn from Fig. 3 is such that within the compression range from 0.6 to1.4 MPa, ANN predictions reveal that the compression seems to have relatively less effect on the capillary pressure, especially for DMs having % PTFE content higher than 10%, consistent with the experimental observations [8-10]. As seen in Fig. 4, the DM coated with 15% PTFE is found to exhibit a 26% increase of capillary pressure as the compression is increased 0 to

0.6 MPa, whereas 7% increase of capillary pressure is observed with an increase in compression from 0.6 to 1.4 MPa. This behavior can be attributed to the relatively higher increase of hydrophilic sites compared to the hydrophobic sites. Any further increase in compression from 0.6 MPa seems to promote the dispersion of more hydrophilic sites, producing higher hydrophilic surface area, which in turn, hindering the increase in capillary pressure. The increase in the hydrophilic characteristics of the DM is also observed by Bazylak *et al*. [12].

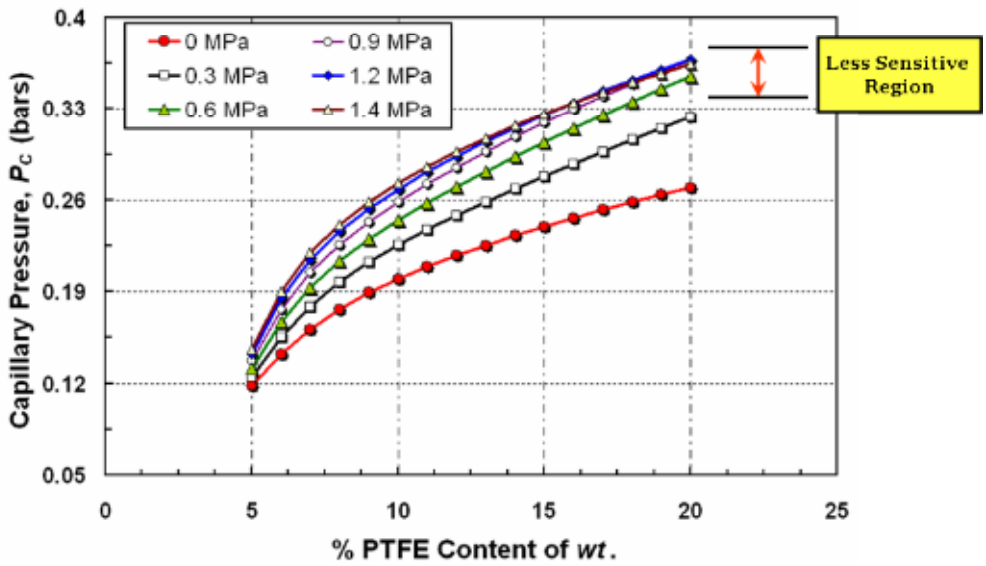

Figure 4: ANN prediction of the capillary pressure versus % PTFE content of the DM under different compressions (intermediate conditions) for a given saturation of 0.3.

Conclusions

A three-layered feed forward artificial neural network was designed and trained with the benchmark data generated from capillary pressure-saturation measurements of the differently engineered DMs [8-10]. The trained network was then utilized to predict the capillary transport characteristics of the fuel DM at intermediate conditions, where the experimental data are not available. The current results confirm that ANN predictions are consistent with those obtained from experimental analysis [3-5], yielding an average uncertainty of ±5.1% of the measured data The ANN simulations reveal that tailoring the DM with high PTFE loading and applying high compression pressure lead to higher capillary pressure, therefore promoting the liquid water transport within the pores of the DM. The compression of the DM leads to an increase in capillary pressure, especially within the compression range from 0 to 0.6 MPa due to the corresponding reduction in effective porosity. Any further increase in compression above 0.6 MPa appears to have relatively less effect on the capillary pressure possibly due to the relatively higher increase of the hydrophilic characteristics of the tested DMs.

The artificial intelligence model presented herein can be further extended into a more detailed design algorithm that couples the DM internal architecture with the cell performance. The development of such an advanced design tool based on this framework is ongoing work in our laboratory and will be reported in subsequent publications.

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