Modeling and Optimization of Hybrid Nafion Membranes Modified with Oxides Based on Artificial Neural Networks and Genetic Algorithms

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ABSTRACT

Recent studies have demonstrated the successful application of artificial intelligence tools in modeling, optimization and design of new materials (Sahoo and Ray 2006.) (Madaeni, Hasankiadeh et al 2010.). This paper describes the application of a Backpropagation Multilayer Perceptron (MLP-BP) neural network based on Levenberg-Marquardt learning algorithm in combination with evolutionary models based on genetic algorithms (GA) to find the optimal operation conditions to provide the highest proton conductivity from a set of hybrid membranes in fuel cell applications. A total of six membranes were analyzed, each one fabricated from a polymer matrix of Nafion and then modified with several oxides (N-HfO2, N-ZrO2, N-La2O3, N-(HfO2, ZrO2), N-(HfO2-La2O3) and N-(ZrO3-La2O3)). The experimental conditions considered for optimization were: temperature of the humidifier (Th) [30-100] ° C, the cell temperature (Tc) [30-120] ° C, voltage [0.05-0.8] (V), relative humidity (RH) [50% -100%] and the membrane thickness (σ). Four-electrode method was employed in fuel cell mode and pulse voltammetry were obtained. The pressure was kept at 15 psi and the nitrogen flow at 500ml/min.

The MLP-BP -GA combination throws the following optimal condition for the Hf-La membrane 1% wt: with 100% of relative humidity and temperatures around 80 ° C in the humidifier and cell. This model also provides the best conditions where the highest conductivity is achieved for every membrane; these estimations were compared against experimental tests obtaining a variation of less than 10%.

Keywords: Artificial Neural Network, Genetic Algorithm, hybrid membranes