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Multi-objective optimization on multi-layer configuration of cathode electrode for polymer electrolyte fuel cells via computational-intelligence-aided design and engineering framework

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ABSTRACT

Polymer electrolyte fuel cells (PEFCs) have attracted considerable interest within the research community due to the increasing demands for renewable energy. Within the PEFCs' many components, a cathode electrode plays a primary function in the operation of the cell. Here, a computational-intelligence-aided design and engineering (CIAD/CIAE) framework with potential cross-disciplinary applications is proposed to minimize the over-potential difference η and improve the overall efficiency of PEFCs. A newly developed swarm dolphin algorithm is embedded in a computational-intelligence-integrated solver to optimize a triple-layer cathode electrode model. The simulation results demonstrate the potential application of the proposed CIAD/CIAE framework in the design automation and optimization of PEFCs.

1. Introduction

Polymer electrolyte membrane fuel cells (PEFCs) convert chemical energy stored in hydrogen fuels into electrical energy in a direct and efficient manner. Because of their zero-emission nature and increased efficiency, PEFCs have the potential to be used as a primary renewable energy source toward reducing the use of fossil fuels and decreasing pollutant emissions in a sustainable economy. Among the many components of PEFCs, the cathode electrode plays a vital function in the operation of the cell. PEFCs with a multi-layer cathode electrode configuration can increase conductivity by increasing the extent of sulfonation of the polymer. Over the last few decades, a significant amount of research has been conducted to advance PEFC technology.

A number of studies on PEFCs with a multi-layer cathode electrode configuration have been reported in recent years. Wei et al. [1] investigated direct methanol fuel cells consisting of multi-layer electrodes that include a hydrophilic thin film and traditional catalyst layer. Haile [2] reviewed the current status of solid oxides and PEFCs with a focus on the improvements in power densities obtained by reducing the electrolyte thickness and architectural control of composite electrodes. Song et al. [3] performed the optimization analyses on the PEFC cathode catalyst layers using the parameters of the Nafion content, Pt loading, catalyst layer thickness and porosity. In 2004, Grujicic and Chittajallu [4] proposed a model considering the parameters: the air-inlet pressure, cathode thickness and length and the width of the shoulders. Litster and McLean [5] provided an overview of effective fabrication methods and characteristic performances of electrodes; their study also surveyed common components, designs and assembly methods for PEFC electrodes. Tao et al. [6,7] introduced a non-isothermal 3D model for the parameter sensitivity analysis. Wang and Feng [8–10] developed explicit solutions for a triple-layer electrode and found that the layer adjacent to the electrolyte membrane contributes substantially to the production of the electrode Faradic current. Park et al. [11] developed a multi-layer anode electrode to reduce the methanol and water crossover from the anode to the cathode. Ko et al. [12] studied the effects of multi-layer electrode design on direct methanol fuel cells. Fofana et al. [13] proposed a 2D numerical steady state model using a sputtering technique for the design of PEFCs with low platinum loading. Abdollahzadeh et al. [14] investigated the PEFCs' performance by a multi-component mixture model simulating two phase flow. Wang et al. [17,18] proposed a 3D two-phase model to investigate an inverse geometry design optimization of PEFC. Gao et al. [16] investigated the performance of a multi-physical dynamic PEFC stack. Khajeh-Hosseini-Dalasm et al. [15] presented a computational study of f a PEFC with the structural parameters analysis. Jung et al. [19] introduced a model

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to simulate the PEFC stack system. Moein-Jahromi and Kermani [25] carried out a sensitivity study using an agglomerate model to rank the parameters' influence. Considering reaction kinetics and ohmic resistance effects, Pathak and Basu [20] introduced a model to predict the PEFC's performance. Molaeimanesh and Akbari [24] introduced a 3D lattice Boltzmann model to perform the simulations on the catalyst layer's electrochemical reaction. Noorkami et al. [21] investigated the performance and durability of a PEFC with temperature uncertainty. Chen et al. [22] discussed a dual-layer cathode model using a bat swarm algorithm.

Two concerns in the analytical modeling of cathode electrodes have not been addressed in previous studies. (1) The effects of coupling on the performance of PEFCs have not been determined because of the interactions among design variables. (2) Only few effective computational approaches that can be used for quantitative modeling, model analyses, verification, and parameter optimization have been developed.

Thus, a multi-layer cathode electrode modeling technique is proposed for the optimal design of PEFCs via a computational-intelligence-aided design and engineering (CIAD/CIAE) framework, in which a newly developed swarm dolphin algorithm (SDA) is embedded to construct and optimize the quantitative model of a multi-layer cathode electrode configuration. The CIAD/CIAE framework is applied to improve the overall fuel cell performance by varying the design parameters (in the CIAE phase) via selection of proper structural/material parameters (in the CIAD phase).

By changing the population and maxing the computational speed, this proposed SDA allocates computational resources, which is inspired by the dynamic behaviors of dolphins. Dolphins can respond to changes in the direction and speed of their neighbors quickly during certain activities (e.g. locating roosting crevices, avoiding obstacles, detecting prey) through foraging and searching. The social intelligence, as useful behavioral information, has been passed among dolphin individuals to guide them from one configuration to another as one unit. By employing this type of social intelligence, the SDA is able to achieve a global optimum by deploying parallel and independent dolphin individuals.

The contributions of our work can be highlighted in four aspects. First, a multi-layer model is developed to assess the performance of PEFCs. Second, a new CIAD/CIAE framework with potential cross-disciplinary applications is proposed. Third, the swarm intelligence method of SDA, embedded into the CIAD/CIAE framework, is designed as the optimization engines to determine the optimal parameters for the multi-layer configuration. Fourth, the Pareto reliability index (PRI1) is defined to assess the Pareto-optimal solutions of the multi-objective (MO) optimization procedure.

The remainder of this paper is organized as follows: Section 2 introduces the analytical model of the multi-layer configuration of a cathode electrode; Section 3 introduces the conceptual framework of the CIAD/CIAE and the overall application schematic with a computational-intelligence-integrated solver (CIS); Section 4 describes the SDA algorithm for the multi-layer configuration model optimization; Section 5 defines the fitness function for the optimization of multi-layer configuration model as proposed in Section 2; Section 6 provides the empirical results and validations of the optimal design; and Section 7 concludes the paper and recommends future applications.

2. Analytical model of multi-layer configuration

The membrane electrode assembly (MEA) is the core component of a fuel cell and is composed of a polymer electrolyte membrane (PEM), catalyst layers (CLs) and gas diffusion layers (GDLs) attached to the bipolar plate (BP) layers (Fig. 1).

A PEM has the thin layers ($\leq 10\ \mu$m) of electrodes coated on its surface, which contains a catalyst (typically **Pt**), carbon, an ionomer electrolyte and a void space. Fig. 1 shows the analytical modeling of the triple-layer cathode electrode configuration, three sections are labeled *I*, *II* and *III*.

- Section *I*: A schematic diagram of a PEFC with a triple-layer cathode electrode configuration, which includes three basic components: the anode (aBP, aGDL and aCL), the PEM and the cathode(cBP, cGDL and cCL).
- Section *II*: Assuming that all the CLs have the same oxygen concentrations, temperatures, electronic phase potentials, and equilibrium potentials, which are uniform within each layer [8,9], a triple-layer cathode configuration is depicted in this section, where the triple-layer electrodes have a total thickness of δ. As shown in the circle on the left side, three general phases can be observed when one zooms in on the cCL layer: (1) the void space (for gaseous reactant transport); (2) ionomer content (for proton transfer); and (3) carbon support (for electronic current conduction). Eq. (1) shows the oxygen reduction reaction (ORR), which is essential for all functions.

$$O_2 + 4e^- + 4H^+ \rightarrow 2H_2O + \text{Heat} \tag{1}$$

- Section *III*: Specifically, the cCL layer is composed of three sub-layers, denoted as Layers 1, 2 and 3. The parameters of this model include: σ, the ionic conductivity; a, the catalyst specific area; i, the exchange current density; R_δ, the ionic resistance; I_δ, the current density; δ, the sub-layer thickness; l, the interface location of the three sub-layers; ΔU, a lumped variable, is defined in Eq. (2), where $R_\delta = \delta/\sigma$ is the overall ionic resistance across the cathode electrode. $I_\delta = -j_\delta \delta$ is the current density based on the transfer current density j_δ at the interface of the diffusion media and the electrode.

$$\Delta U = R_\delta I_\delta \tag{2}$$

The relative interface location of the three sub-layers is defined in Eq. (3), where the thickness ratios r_δ of Layers 1, 2 and 3 are given in Eqs. (4)–(6), and δ_1, δ_2 and δ_3 are the thicknesses of the corresponding layers.

$$l = \frac{x}{\delta} \tag{3}$$

$$r_{\delta 12} = \frac{\delta_1}{\delta_2} \tag{4}$$

$$r_{\delta 13} = \frac{\delta_1}{\delta_3} \tag{5}$$

$$r_{\delta 23} = \frac{\delta_2}{\delta_3} \tag{6}$$

As shown in Eq. (7) [10], the factors of the ionic conductivity σ of Layers 1, 2 and 3 are σ_1, σ_2 and σ_3,respectively, which are determined by the electrolyte water content λ [26], as given in Eq. (8); the ionomer tortuosity τ; Nafion content ϵ; temperature T; and local relative humidity μ. The ratios of the ionic conductivity factors of the three layers are given in Eqs. (9)–(11).

$$\sigma = \epsilon^{\tau}(0.5139\lambda - 0.326)\exp\left[1268\left(\frac{1}{303} - \frac{1}{T}\right)\right] \tag{7}$$

$$\lambda = 0.3 + 10.8\mu - 16\mu^2 + 14.1\mu^3 \tag{8}$$

$$r_{\sigma 12} = \frac{\sigma_1}{\sigma_2} \tag{9}$$

$$r_{\sigma 13} = \frac{\sigma_1}{\sigma_3} \tag{10}$$