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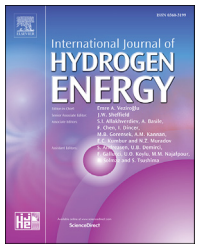

Development of a one-dimensional and semi-empirical model for a high temperature proton exchange membrane fuel cell

Yagmur Nalbant [a], *C. Ozgur Colpan* [a,b,*], *Yilser Devrim* [c]

[a] *Dokuz Eylul University, School of Natural and Applied Sciences, Mechanical Engineering Department, Buca, Izmir, Turkey*

[b] *Dokuz Eylul University, Faculty of Engineering, Mechanical Engineering Department, Buca, Izmir, Turkey*

[c] *Atilim University, Faculty of Engineering, Energy Systems Engineering, Incek, Ankara, Turkey*

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ABSTRACT

High temperature proton exchange membrane fuel cells (HT-PEMFC), which operate between 160 °C and 200 °C, can be generally used in portable and stationary power generation applications. In this study, a one-dimensional, semi-empirical, and steady-state model of a HT-PEMFC fed with a gas mixture consisting of hydrogen and carbon monoxide is developed. Some modeling parameters are adjusted using empirical data, which are obtained conducting experiments on a HT-PEMFC for different values of Pt loading and cell temperature. For adjusting these parameters, the total summation of the square of the difference between the cell voltages found using the experimental and theoretical methods is minimized using genetic algorithm. After finding the values of the adjusted parameters, the effects of different cell temperature, Pt loading, phosphoric acid (PA) percentage, and different binders (PBI and PVDF) on the performance of the fuel cell are examined. It was found that, the performance of the fuel cell using PVDF binder exhibited better performance as compared to that using PBI binder.

Introduction

Fuel cell is an electrochemical device that directly converts chemical energy into electrical energy. Fuel cells have several advantages over conventional power technologies (e.g. internal combustion engines and gas turbines) such as reduced dependence on fossil fuels, high electrical efficiency, and low environmental impact. Fuel cells can be categorized according to the type of electrolyte used, the type of fuel, the type of feeding of fuel (indirect or direct), and the operating temperature (high temperature or low temperature). The most promising technologies currently towards commercialization are Proton Exchange Membrane Fuel Cell (PEMFC) and Solid Oxide Fuel Cell (SOFC).

PEMFC can be classified into two categories according to its operating temperature. The Low Temperature-Proton Exchange Membrane Fuel Cell (LT-PEMFC) operates around 60–80 °C while the High Temperature-Proton Exchange Membrane Fuel Cell (HT-PEMFC) operates between 120 °C and 200 °C [1]. The LT-PEMFC usually uses Nafion® produced by DuPont or another perfluorinated polymer as the membrane.

* *Corresponding author*. Dokuz Eylul University, Faculty of Engineering, Mechanical Engineering Department, Buca, Izmir, Turkey.
E-mail address: ozgur.colpan@deu.edu.tr (C.O. Colpan).

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Water is required for activating the proton conductivity inside the Nafion® membrane. Therefore, the membrane must always be kept in a hydrated condition to maintain optimal performance [2]. When the cell temperature exceeds the boiling temperature of water, water management in the fuel cell becomes more challenging. On the other hand, heat is generated in the electrochemical reaction occurring in the fuel cell. If the heat increases too much, it will cause the membrane to dry up; and the Nafion® membrane will lose its proton conduction capability due to the increases in the proton transport resistance. Thus, water and thermal management issues play a key role in the LT-PEMFCs. In addition, carbon monoxide (CO) tolerance is very low in the PEMFCs operating at low temperatures. Hence, CO poisoning phenomenon causes a significant decrease in the performance of this kind of fuel cells. In order to overcome these problems, research on HT-PEMFC technology has been advanced thanks to the developments in the novel membranes over the last decade. PA doped polybenzimidazole (PBI) membranes, which have good mechanical strength, high proton conductivity, and high thermal and chemical stabilities at high temperatures, have been conventionally used in the HT-PEMFCs without the need for humidification in reactant gases [3]. If they are doped by a strong acid such as PA, sulphuric acid, and nitric acid, their proton conductivity increases. Among the different doping materials, PA is the most promising one because it forms a 3-D hydrogen bonding network with PBI. When the doping level of PA in the membrane increases, the proton conductivity of membrane increases but the mechanical strength of membrane decreases [4]. As compared to LT-PEMFCs, water and thermal management is simpler and CO tolerance is more in HT-PEMFCs. Moreover, waste heat from this fuel cell can be recovered and used to produce other useful forms of energy (e.g. hot water). The major drawbacks of HT-PEMFCs are slow start-up, difficulty in thermal insulation, and higher material degradation rate [1].

In recent years, several studies have focused on mathematical modeling of HT-PEMFCs to have a better understanding of the transport phenomena occurring inside the fuel cell that cannot be easily measured by experimental methods. These models provide more insights compared to experimental studies in the design and optimization of the fuel cells [5]. There are several modeling studies for PA doped HT-PEMFCs in the literature. For example, Cheddie and Munroe [6] developed a parametric model for a HT-PEMFC based on PBI membrane, which predicts the polarization curve for different porous media characteristics and compared the results of this model with experimental data. Scott et al. [7] developed a one dimensional model of a HT-PEMFC that incorporates the effects of cell temperature and pressure on the diffusion coefficients, the exchange current density, the cell voltage, and the power density, and the effect of water transport on the proton conductivity of the PBI membrane. Ubong et al. [8] investigated the effects of air stoichiometry, operation temperature, and pressure on the HT-PEMFC performance through developing a 3-D model of a fuel cell having triple serpentine flow channels. Mamlouk et al. [9] developed a one-dimensional model of a HT-PEMFC based on PBI membranes using the principles of thermodynamics, transport phenomena and chemical kinetics and applied the thin film assumption technique. Their model exhibited very good agreement with experimental data and was used as a tool that provides in understanding the reasons behind the performance limitations for optimizing the electrode performance. Shamardina et al. [10] developed a simple analytical model of a HT-PEMFC for investigating the crossover of reactant gases through the membrane. Chippar and Ju [11] developed a gas crossover model for a HT-PEMFC having a PA-doped PBI membrane. In their study, numerical simulations were conducted varying three critical parameters (temperature, current density, and gas crossover diffusivity) to investigate the effect of gas crossover on the HT-PEMFC performance. Sun et al. [12] developed a two-dimensional and single-phase model and investigated the effects of cell temperature and the properties of mass transfer on the performance of the HT-PEMFC. Moreover, the numerical model was used to analyze the effects of the cell temperature, the gas diffusion layer (GDL) porosity, and the GDL thickness on the current density. Sezgin et al. [13] developed a three-dimensional HT-PEMFC model by using COMSOL Multiphysics for investigating the effect of some important design and operating parameters (inlet velocity of hydrogen and oxygen and proton conductivity of the PBI membrane). Caglayan et al. [3] developed a three-dimensional model of a HT-PEMFC made of PA doped PBI membrane. This model was used to investigate the effect of the cell temperature (between 100 °C and 180 °C) on the performance of the fuel cell. The results showed that when the temperature increases, the performance of fuel cell increases.

Catalyst layer of a HT-PEMFC consists of the catalyst (e.g. carbon supported platinum [Pt/C]), the binder (e.g. PBI, polyvinylidene difluoride [PVDF], polytetrafluoroethylene [PTFE], and Nafion®), the solvent, and the PA. The selection of the binder is a critical factor affecting the performance of the fuel cell. The binder material used in catalyst layer affects the mechanical properties, gas permeability, Pt utilization, the impregnation of PA, and oxygen oxidation reaction rate in the catalyst layer of a HT-PEMFC [14]. In the literature, several studies are found related to the effect of the binder on the performance of the HT-PEMFC. For example, Su et al. [14] investigated the gas diffusion electrodes (GDEs) which were prepared with five different binders (Nafion®, PBI, PTFE, PVDF, and PBI-PVDF), to optimize the performance of PA doped PBI based HT-PEMFCs. The results of their study showed that PVDF and PTFE binders yielded higher performance compared to Nafion® and PBI binders due to their superior electrochemical properties and CL structure. In another study by Su et al. [15], they studied the effect of different membrane and binder types on the performance of the gas diffusion electrode (GDE), and these GDEs were analyzed using cyclic voltammetry (CV), polarization curve, durability test, and electrochemical impedance spectroscopy (EIS). The results of their study showed that the GDEs prepared with PTFE and PVDF provide better performance than those prepared with the Nafion® and PBI GDEs for all domains of the polarization curve. Ergun et al. [4] studied the effect of two electrode preparation methods (PBI and PBI-PVDF as the binder in the catalyst ink) to determine the optimum electrode structure. Their study showed that the power output of fuel cell increases from 0.015 to 0.072 W/cm^2 when the binder is changed