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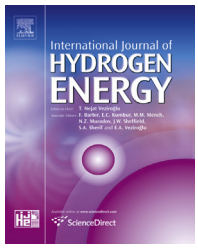

Development of a conceptual design model of a direct ethanol fuel cell (DEFC)

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ABSTRACT

Small fuel cells appear to be appealing solutions to the problem of providing portable energy sources. One promising system is the Direct Ethanol Fuel Cell (DEFC) stacks, which are modular and simple to construct and have certain attributes, such as being a compact and lightweight cell, that make it favorable for portable applications. Nevertheless, there are still many challenges for DEFC commercialization, such as water transport management, EtOH crossover and the sluggish Ethanol Oxidation Reaction (EOR) kinetics on the anode. The phenomena involved with DEFCs are complicated and include transport processes, thermochemical reactions and fluid mechanics that are hard to quantify experimentally. On the other hand, mathematical modeling is a powerful and economical tool that enables us to better understand the physical phenomena that occur during operation. In this study, a conceptual design was developed to obtain a power performance curve. The voltage and current characteristics with the proposed MEA geometry will be used as starting point for more detailed modeling and simulation studies that aim to provide a basic understanding of the internal process of the DEFC. This study is to be used as initial estimations for engineers to design and optimize the DEFC for use in portable applications.

Introduction

Today, parallel to the drastic growth of the portable electronic devices market is a growth in the study of fuel cells (FCs), which are appealing because of their ability to power a device for a longer time compared to conventional batteries. Additionally, the military also requires high-power, long-term devices with silent operation and a low heat signature for use in soldiers' equipment. The safety and environmental issues that are created by the use of metal hydrides in Li-ion instead of nicked-based batteries also create the need for new, green technology power sources. Because we are approaching the energy density limits of rechargeable commercial batteries, small fuel cells are appealing solutions to the problem of

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providing portable energy sources. The main advantages offered by FCs are 1) the flexibility of the device with respect to the power and the capacity achievable with different devices for energy conversion and energy storage, 2) the long lifetime and long service life, 3) the good ecological balance and 4) a very low self-discharge [1,2]. As shown in Table 1, the FCs are simply manufactured with greater power and less weight when compared to other types of power sources rather than Li-ion battery. Nevertheless, the previous findings reported the prolong cost analysis demonstrated the advantages of direct methanol fuel cell over Li-ion battery [3].

Among the different types of FC, the Polymer Electrolyte Membrane Fuel Cell (PEMFC) is suitable for powering portable devices due to its fast start up and use of a solid electrolyte [4]. The storage and distribution of hydrogen remains an obstacle in conventional PEMFC because the fuel need to free of impurities when operated at temperature below 100 °C [5]. Hence, for low temperature FCs, the use of alcohol as energy carrier and its electrochemical oxidation reaction (EOR) in direct alcohol fuel cell (DAFC) seems appealing. The direct alcohol fuel cell (DAFC) stacks are modular and simple to construct and possess favorable attributes, such as containing compact and lightweight cells. Previously, methanol was as utilized as a fuel in DAFCs; however, due to methanol's toxicity, its large-scale use can cause some environmental and safety problems [6,7]. On the other hand, ethanol was chosen as fuel because of several factors: it has a higher energy density, it is less toxic than methanol, it can be produced from agricultural bioprocesses, it is considered to be a renewable energy source, it possesses a lower crossover rate, and it affects cathode performance less severely than methanol [8]. Although DEFCs possess remarkable potential as substitutes for conventional batteries for portable devices, there are still many challenges for researchers to understand. As stated by Brouzgou et al. [9], the key issues that must be overcome for DEFC use to become competitive are water transport management, EtOH crossover and EOR kinetics on the anode. Moreover, in terms of an economical point of view, the higher cost of the membrane and Pt catalyst hinders its entry into the portable power sources market. These obstacles are associated with the complex phenomena involved with the DEFC and can be found in the transport processes, the thermochemical reactions and fluid mechanics.

A fundamental understanding of these complex mechanisms is crucial in order to optimize and manufacture new materials, improve product development, create novel architectures, develop more efficient transport processes, and improve the design optimization and integration, all of which are expected to lead to major gains in performance, efficiency, reliability, manufacturability and cost-effectiveness. Thus, investigations made through experimentation and modeling are greatly needed for quantification of the DEFC complex behavior in order to enhance cell performance. Currently, the focus of the development of DEFCs greatly leans towards the development of catalysts to improve the EOR and crossover effects [10]. Very a few investigations have focused on micro DEFCs and namely among them are Jafri and Ramaprabhu [10] and Aravamudhan et al. [11].

Table 1 – General fuel cell comparison with other power source [21].

	Weight (Kg)	Energy (wh)	Volume (L)
PEMFC	4.3	2190	4.0 L
Li-ion	0.044	2046	0.0191
Zinc-air cell	8.4	2620	9.0
Other battery types	10.9	2200	9.5

However, these experimental studies possess several disadvantages, such as the fact that they are laborious, costly, and inconvenient. Furthermore, the expense of the DEFC system may be detrimental during the experiments. Moreover, the DEFC systems that are composed of complicated physiochemical processes are difficult to understand through experimental investigations. Mathematical modeling is an alternative to experimentation. It is a powerful and economical tool that may play an important role in quantifying and understanding the complicated physicochemical phenomena and performance characteristics of the DEFCs. The DEFC modeling enables us to better understand the physical phenomena occurring during operation. A better understanding of the operation of the DEFCs can lead to improvements in its design (e.g., more compact stacks), performance and life expectancy on the one hand and help us to consider control laws on the other hand [12]. Moreover, a validated mathematical model can predict the performance of the DEFCs under different operating conditions, which can lead to an optimized design of the DEFC system. Very few mathematical models reported for single-cell DEFC either in acidic or alkaline medium [13]. Namely among them are Andreadis et al. [14] pioneer the DEFC modeling works with 1D effects, considering the electrochemical behavior for both anode and cathode. In this study, the DMFC empirical mass transfer coefficient from literature [15] was applied to determine the mass transport from feed stream to diffusion layer. Using the same models, the authors magnify effects of the operating parameters and physical geometry on ethanol crossover across PEM [16]. The ethanol crossover effects significantly influenced the DEFCs performance. Taking into account parasitic current formation at the cathode, the authors have improvised the previous model [17]. The 1D analytical model was developed by Suresh & Jayanti [18] to investigate the ethanol crossover effects. However, the model did not consider the mass concentration losses in cell performance. The recent DEFCs modeling by Meyer et al. [19] by considering the multistep reaction mechanism of ethanol oxidation reaction at anode.

The other analytical model was developed by Heysiattalab [20] considering 2D effects. The neglecting of concentration loss make this model is precise in activation and ohmic loss region only. Sousa et al. [21], developed 2D mechanistic model to characterize the anode of DEFCs. Considering the partial oxidation reaction at anode, the spesies concentration profile was simulated using COMSOL Multiphysics. The soley 3D, CFD model published by Sarris et al. [22] investigated the velocity distribution in the anode flow bed for different Reynolds number.

On the other hand, alkaline direct ethanol fuel cell (AA-DEFCs) modeling are still new and most of the researcher only

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