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Review

Modeling and simulation of a direct ethanol fuel cell: An overview

S. Abdullah [a,c], S.K. Kamarudin [a,b,*], U.A. Hasran [a], M.S. Masdar [b], W.R.W. Daud [a]

[a] Fuel Cell Institute, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia
[b] Department of Chemical and Process Engineering, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia
[c] TATIUC, Telok Kalong, 24000 Kemaman, Terengganu, Malaysia

HIGHLIGHTS

- Fundamental scientific research is required to understand the complex electrochemical behavior.
- Modeling and simulation play an important role in examining the DEFC system.
- Not many work presented the fundamental issue of DEFC.
- This paper presents current progress as well as the current problem in DEFC in term of modeling and simulation.

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ABSTRACT

The commercialization of Direct Ethanol Fuel Cells (DEFCs) is still hindered because of economic and technical reasons. Fundamental scientific research is required to more completely understanding the complex electrochemical behavior and engineering technology of DEFCs. To use the DEFC system in real-world applications, fast, reliable, and cost-effective methods are needed to explore this complex phenomenon and to predict the performance of different system designs. Thus, modeling and simulation play an important role in examining the DEFC system as well as in designing an optimized DEFC system. The current DEFC literature shows that modeling studies on DEFCs are still in their early stages and are not able to describe the DEFC system as a whole. Potential DEFC applications and their current status are also presented.

1. Introduction

Currently, the demand for power sources for applications of less than 250 W is increasing significantly in parallel with the rapid development of wireless digital communication and advanced computing technologies. Fuel cell (FC) systems with higher energy density are seen as a potential candidate to fill the growing gap between energy demand and supply for mobile applications. The FC energy density for such devices is increasing 3 to 10 times more quickly than the energy density of the lithium batteries currently in use [1]. Additionally, they offer advantages such as not requiring recharging, being more environmentally friendly and having more flexibility in system design [2,3]. For portable electronic applications, the size, volume, energy density and power density are more important features than efficiency. Thus, the direct alcohol fuel cell (DAFC), which is a sub category of the Proton Exchange Membrane Fuel Cell (PEMFC), has garnered much attention from researchers and manufacturers, especially for mobile and stationary applications, due to its low operating temperatures, solid state electrolyte and low efficiency compared to other types of FCs. Other DAFC advantages include easier handling and transportation, an energy-dense yet reasonably stable reaction liquid at all environmental conditions, a lack of complex steam reformers, the capability to use the traditional fuel infrastructure, and simple start up [4–7]. Foremost, the alcohol energy density is comparable to that of the current fuels, gasoline and diesel, as shown in Fig. 1. Proven to that, MTI, Toshiba, Motorola, Samsung are targeting Direct Methanol Fuel Cell (DMFC) stack for portable electrical appliances power source [8]. Instead of performance, economic viable is another important factors that contributes to better energy suppliers for portable devices. Besides, this small FC require an economically viable fuel [7,9,10] as fuel source. A few types of

* Corresponding author. Department of Chemical and Process Engineering, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, Malaysia. Tel.: +60 389216422; fax: +60 389216148.
E-mail addresses: ctie@vlsi.eng.ukm.my, ctie@eng.ukm.my (S.K. Kamarudin).

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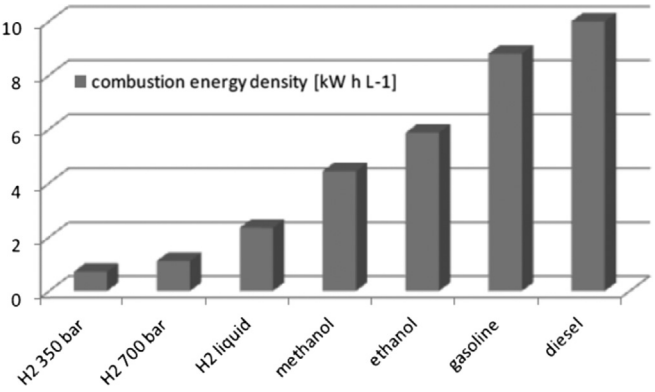

Fig. 1. Energy density comparisons of alcohols and other types of fuels [79].

substance commonly used as fuel in FC such as alcohols and hydrogen including the price were presented in Table 1. In terms of price, methanol wins over ethanol that makes it is the most widely chosen as fuel in DAFC for researches and future commercialization. However, a significant drawback of methanol such as low boiling point, inflammability, toxicity are harmful to end user if leakage during applications [4,8]. As alternative, ethanol is a potential fuel for operating FC due to fuel higher energy density, less toxicity [11–16]. Ethanol's technical features are strong due to it is an energy-dense liquid so it stores compactly and it contains 35% oxygen, so it aids in clean combustion make it appealing as fuel in FC specially for portable device. Moreover, ethanol is renewable energy and it is domestically produced, via hydration of ethane and fermentation of sugars and yeasts as shown in Fig. 2. This can directly displace imported oil and petroleum products, and it provides economic support and alternative markets for agricultural crops. Previous studies have demonstrated ethanol to be a promising alternative fuel with an electrochemical activity comparable to methanol and ethanol and a crossover less severe than methanol [11–13,17–20].

However, the current Direct Ethanol Fuel Cell (DEFC) technologies are able to meet the two important features yet that is efficiency and total operation cost [21], in order to realize the DEFC commercialization. The well-known sluggish anode electro catalyst activities are at relatively low temperature (20°C–120 °C) due to problem in C–C bond breaking which lead to the low performance remains as the major technological problem [22,23]. This slow kinetics of ethanol electro-oxidation (EOR) produces unwanted intermediate products such as acetic acid and acetaldehyde. Additionally, acetic acid is a dead-end for EOR, when occurring in DEFC, as it cannot be further oxidized in the potential range typical for a working fuel cell [24]. Another major issues facing by DEFC is ethanol permeated through membrane caused mixed potential effects at cathode which lead to reduce cathode performance and fuel utilizations [25]. Besides, the DEFC system cost is still unfavorable due to expensive Pt-based catalyst and nafion based membrane [26].

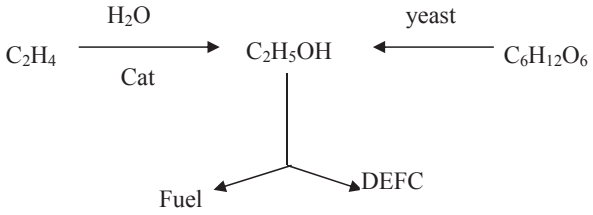

Fig. 2. Production routes of ethanol from hydration of ethane or from fermentation of sugars.

2. The applications of modeling in DEFC

Basically, the model is developed according to the specific purpose as 1) scientific understanding 2) technological development and 3) system control. As DEFC modeling still at early stages, most of the previous model was developed for scientific understanding. The scientific understanding model enables us to investigate the coupling phenomena inside DEFC towards efficiency. The DEFC efficiencies were determined from power peak density and current density. According to Heysiattalab et al. [27], these two main performance indicators are primarily influenced by design parameters such as temperature, pressure, and fuel concentration. These parameters are difficult to precisely quantify due to the complex physico-chemical processes occurring in the DEFC and involve transport processes, thermodynamics, and fluid mechanics. Fundamental scientific research is required to elucidate this complex phenomena and engineering technology. Breakthroughs in material development, the acquisition of fundamental knowledge, and the development of mathematical models and experimental tools are particularly important in current DEFC research [28].

Many experimental studies have been carried out to investigate complex phenomena in the DEFC [29–41], and a comprehensive review including DEFC developments and applications was compiled by Ref. [10]. However, experimental works have several disadvantages; for example, they are time consuming, costly, and limit the number of FC designs that could be tested. Thus, modeling and simulation are appealing as useful tools in the study of complex DEFC systems. They enable the determination of the impact of a great variety of conditions and variables on the DEFC system's global or local operating point. Furthermore, the user of the model can test various hypotheses without the risk of deterioration or destruction of the real system. Moreover, to our knowledge, no optimization work has been performed for the DEFC; and this is essential to improving the design and performance of the cell.

There are a few requirements in building a DEFC model as tabulated in Table 2. The spatial dimension which ranging from one dimensional to three dimensional as shown in Fig. 3 is important to describe FC phenomena when mass transport limitations taken into account. The higher dimensional model involved multiple complex equations that required computational solver such Computational Fluid Dynamics (CFD), Comsol Multiphysics, etc. The

Table 1
Common Fuels with properties and prices used in Direct Fuel Cells [20].

Fuels	Energy density (Wh L^{-1})	Standard theoretical potential, E^0	$-\Delta G$ (kJ mol^{-1})	$-\Delta H$ (kJ mol^{-1})	Reversible energy efficiency	Price (USD gal^{-1})
Methanol	4820(100%wt)	1.213	702	726	0.967	1.13
Ethanol	6280(100%wt)	1.145	1325	1367	0.969	2.04
Formic acid	1750(88%wt)	1.4	270	254.3	1.062	72.00
2-propanol	7080(100%wt)	1.122	1948	2005.6	0.971	39.1
Hydrazine	5400(100%wt)	1.615	623.4	622.2	1.002	179
Ethylene glycol	5870(100% wt)	1.220	1176.7	1189.5	0.99	37.09