Energy Conversion and Management 103 (2015) 623–638

Contents lists available at ScienceDirect

Energy Conversion and Management

journal homepage: www.elsevier.com/locate/enconman

Numerical simulations of a full-scale polymer electrolyte fuel cell with analysing systematic performance in an automotive application

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ARTICLE INFO

Article history:
Received 20 March 2015
Accepted 4 July 2015
Available online 14 July 2015

Keywords:
Computational simulation
Polymer electrolyte fuel cell
Systematic analysis

ABSTRACT

In fuel cell powered electric vehicles, the net power efficiency is a critical factor in terms of fuel economy and commercialization. Although the fuel cell stack produces enough power to drive the vehicles, the transferred power to the power train could be significantly reduced due to the power consumption to operate the system components of air blower and cooling module. Thus the systematic analysis on the operating condition of the fuel cell stack is essential to predict the net power generation. In this paper numerical simulation is conducted to characterize the fuel cell performance under various operating conditions. Three dimensional and full-scale fuel cell of the active area of 355 cm^2 is numerically modelled with 47.3 million grids to capture the complexities of the fluid dynamics, heat transfer and electrochemical reactions. The proposed numerical model requires large computational time and cost, however, it can be powerful to reasonably predict the fuel cell system performance at the early stage of conceptual design without requiring prototypes. Based on the model, it has been shown that the net power is reduced down to 90% of the gross power due to the power consumption of air blower and cooling module.

1. Introduction

Polymer electrolyte fuel cell (PEFC) generates electric current from the chemical reaction between hydrogen and oxygen. It constitutes of polymer membrane coated with catalyst layers at anode and cathode sides, gas diffusion medium, bipolar plates. One of the attractive applications of PEFC is an automotive because it offers higher efficiency, lower fuel cost, and emission-free energy source with high power density. In this regard, recent studies have made a good technological progress of PEFC performance by enhancing the electrochemical reactions and lowering the electrical resistance. Perng et al. [1] showed 8% higher PEFC performance with modifying the flow field to improve reactant transport at the catalyst layers. Tian and Qin [2] suggested that $Zr_{55}Cu_{30}Al_{10}Ni_5$ could be used as a potential bipolar plate for PEFCs attributed to its significantly lower electrical resistance than conventional material of 316L. A new nano-composite membrane was developed in order to increase proton conductivity under the high temperature condition of 100 °C [3]. Nonetheless, there remain many challenging issues of cost reduction [4,5], long-term durability [6,7] and fuel economy [8,9] for commercialization. For the automotive application, an increase in the operating temperature of PEFC is essential to keep the cost of the cooling fan and radiator within economically sensible limits [10]. Therefore, all the aforementioned issues should be addressed at higher temperature with considering operating conditions of pressure, stoichiometry ratio (SR), and humidity [11].

The PEFC system is designed to achieve a specified maximum power and the operation is optimized around the nominal operating design-point in order to maximize the overall system efficiency [12]. To this end, a large number of studies have been conducted to model the PEFC system, optimize the operating conditions, and simulate fuel cell vehicle [12,13]. Performance analysis has been developed based on a single fuel cell by using zero dimensional [14], one dimensional [15], two dimensional [16], and multidimensional [17] models. Chen et al. [14] optimized the operating conditions in terms of operating cost with the predicted PEFC performances from a zero dimensional model. The operating parameters of temperature, pressure, SR, and relative humidity were optimized with one dimensional and non-isothermal model by Mawardi et al. [15]. They showed how the optimal operating conditions could be found in accordance with the various design constraints and different power requirements. Ahluwalia et al. [16] presented the stack performance as a function of PEFC system

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http://dx.doi.org/10.1016/j.enconman.2015.07.011
0196-8904/

Nomenclature

a	water activity
A	projected area of radiator, m^2
c_p	specific heat, J kg K^{-1}
C_r	condensation rate, s^{-1}
C_i	molar concentration of species i, kmol m^{-3}
D_i	diffusivity of species i, m^2 s^{-1}
F	Faraday constant, 96,485 C mol^{-1}
I^{tr}	volumetric transfer current, A m^{-3}
$\dot{m}$	mass flow rate, kg s^{-1}
P	pressure, Pa
P_c	capillary pressure, Pa
R_{ohm}	ohmic resistivity, Ω m
s	liquid water saturation
S	source term
T	temperature, K
$\vec{u}$	fluid velocity vector, m s^{-1}
$\dot{W}$	power, W

Greek symbols

η	overpotential, V
λ	membrane water content
μ	dynamic viscosity, kg s^{-1} m^{-1}
ξ	efficiency
ρ	density, kg m^{-3}
τ	shear stress, N m^{-2}
φ	electric potential, V
ψ	consumed power ratio

Superscripts and subscripts

an	anode
cat	cathode
eff	effective value
l	liquid water
mem	membrane
ref	reference value
sat	saturation
sol	solid

efficiency to analyse the relationship between the cost and performance of automotive fuel cell systems by solving the two dimensional stack model. They suggested that the reduced platinum and system cost were comparable with the lowered design-point efficiency from 40% to 35%. Wu et al. [17] proposed a multidimensional model to optimize operating conditions. The proposed model was developed by employing one and two dimensional model for catalyst layer while the gas diffusion layer was three dimensionally modelled. They reported that the optimal operating condition of temperature, SR, pressure and humidity were significantly changed by the required power consumption. In addition, the semi-empirical models have also been used to conduct the performance analysis of PEFC stack [18–20]. The performance of the PEFC system with water and thermal management subsystems has been investigated by developing the dynamic and semi-empirical models [12,21–27]. Under various drive cycles of the vehicle, the transient dynamic PEFC system models were developed to optimize the control strategy [21–25], and maximize the net system power [12,26] and the fuel economy of the vehicle [27].

Although the previous works provided better understanding of the PEFC system performance and proposed good control strategies under various operating conditions, however, the model to describe PEFC were still limited to zero or one dimensional, analytical, or semi-empirical bases. Since the different designs of gas diffusion layers and flow channels can cause significant changes in PEFC performance [28–30], the analytical or semi-empirical models are difficult to capture the effects of nonlinear and three dimensional phenomena. The existing three dimensional numerical simulations have been well developed and vigorously used to predict the PEFC performance with good accuracy [31–33]. Raj and Shamim [34] showed that significant influence of three dimensional effects on the species concentrations in PEFCs. Nonetheless, full-scale three dimensional numerical simulations have not been often reported due to computational time and cost. To the author's knowledge, only two papers have been published so far to demonstrate the feasibility of full-scale cell simulation [35,36]. The numerical simulation is beneficial to reduce the experimental tasks of performing parametric study in order to optimize the performance. At the early stage of conceptual design, the numerical simulation becomes a powerful tool to predict the performance for the given design constraints without prototypes.

In this paper, a PEFC system including air blower and cooling module with desired net power above 75 kW is specified in the application of commercial vehicles. To this end, a PEFC stack with 400 cells is conceptually designed where the active area and current density of a single PEFC are 355 cm^2 and 1 A cm^{-2}, respectively. The efficiencies and capacities of the air blower and cooling module are predetermined with considering the layout limitation. Numerical approach is applied to simulate the performance of the conceptual PEFC vehicle. Firstly, three-dimensional numerical simulation for the full-scale PEFC is conducted under a reference operating condition. And then, the electrochemical, fluid dynamic and thermodynamic characteristics are described to analyse various relevant physical parameters of pressure, voltage, temperature, oxygen concentration, and water content. Additional simulations are carried out under various operating conditions of temperature, coolant flow rate, air SR, and pressure. The effects of operating conditions on the PEFC stack are demonstrated in terms of net power which accounts for the generated and consumed power in the PEFC system. The results show that the three dimensional numerical simulations for the full-scale PEFC reasonably predict the performances by successfully describing the combined phenomena of fluid dynamics, heat transfer and electrochemical reaction. It is also shown how the limited cooling capacity constrains the operating temperature range and that the net power of PEFC system is affected by the different operating conditions.

2. Numerical simulation for a full-scale single PEFC

2.1. Numerical model

In this numerical simulation, three dimensional computational domain for a single PEFC is depicted in Fig. 1(a). The single PEFC is designed to have three compartments of one reaction zone and two flow distributors. The flow distributors are designed to uniformly supply the hydrogen, air and coolant to the respective multiple channels while the reaction zone is constituted of the plural layers for electrochemical reaction. The cross sectional diagram