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Optimization of DMFC regulation based on spatial modeling

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ARTICLE INFO

Article history:
Received 17 February 2015
Received in revised form
3 June 2015
Accepted 5 June 2015
Available online 30 June 2015

Keywords:
DMFC
Spatial modeling
System modeling
Dynamic analysis

ABSTRACT

In this work, a spatial model of direct methanol fuel cell (DMFC) is built in Comsol Multiphysics and a system model is built in Matlab Simulink. The peripheral components such as the compressor for the air supply and the pump for the methanol supply are considered in this system model. The dynamic response of the system and the cell internal behavior to fluctuant loads is investigated by connecting the system model and the cell spatial model. During the simulation a series of signals are exchanged between these two models simultaneously such as the flow rate and temperature of the methanol and air, cell voltage, cell power and information about the exhausts. Furthermore, it can be also investigated the power consumption of the peripherals and the efficiency of the cell and system. At the end, the system regulation strategy for a better cell performance is investigated.

Introduction

DMFCs are considered to be a promising energy conversion system for different applications, especially for portable applications due to its high energy density, low working temperature, fast refueling and compact size [1,2]. However, methanol crossover that is methanol molecules move through the electrolyte membrane from the anode to the cathode side and react with oxygen at the cathode side, leads to a decreased cell performance caused by the formation of mixed potentials at the cathode side. Methanol that reacts with oxygen at the cathode does not generate any electrical power. Hence, methanol crossover also results in low fuel efficiency. Dohle [3] investigated a new method to measure the crossover for different current densities. It is reported in Dohle's work that the methanol crossover increases from 200 A m^{-2} to 900 A m^{-2} when the current density decreases from 3000 A m^{-2} to 10 A m^{-2}. Wang's [4] concluded that in high current density case, methanol crossover is dominated by the diffusion and electro-osmotic equally (net methanol crossover 540 A m^{-2}, caused by the diffusion 370 A m^{-2} and caused by the electro-osmotic 170 A m^{-2}). In low current density case, methanol crossover is dominated by the diffusion (net methanol crossover 1020 A m^{-2}, caused by the diffusion 900 A m^{-2} and caused by the electro-osmotic 120 A m^{-2}). Zou [5] compared the

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http://dx.doi.org/10.1016/j.ijhydene.2015.06.030

Nomenclature

Roman symbols

A	Specific surface area, m^{-1}
c	Concentration, mol m^{-3}
C_p	Heat capacity at constant pressure, J $°C^{-1}$]
$C_{p,mass}$	Mass specific heat capacity at constant pressure, J kg^{-1} $°C^{-1}$
D	Multicomponent Fick diffusivities, m^2 s^{-1}
D^T	Thermal diffusion coefficient, kg m^{-1} s^{-1}
E	Electric potential, V
E_{eq}	Equilibrium potential, V
F	Faraday constant, 96,485 A s mol^{-1}
$\mathbf{F}$	Body force vector, N m^{-3}
HHV	Higher heating value, J kg^{-1}
i	Current density, A m^{-2}
$\mathbf{i}$	Current density vector, A m^{-2}
i_0	Exchange current density, A m^{-2}
I	matrix
k	Thermal conductivity, W m^{-1} $°C^{-1}$
k_{br}	Permeability, m^2
$\dot{m}$	Mass flow rate, kg s^{-1}
N	Flux, mol m^{-2} s^{-1}
p	Pressure, Pa
P	Power, W
Q_{br}	Mass source/sink term, kg m^{-3} s^{-1}
Q_h	Heat source/sink term, W m^{-3}
R	Gas constant, 8.314 J $°C^{-1}$ mol^{-1}
R_i	Production/consumption of species i, kg m^{-3} s^{-1}
t	Time, s
T	Temperature, °C
$\mathbf{u}$	Velocity vector, m s^{-1}
x	Mole fraction

Greek symbols

α	Charge transfer coefficient
β	Forchheimer coefficient, m^{-1}
ε	Porosity
η	Overpotential [V], efficiency
λ	Electro-osmotic drag coefficient
μ	Dynamic viscosity, Pa s
ρ	Density, kg m^{-3}
ω	Mass fraction

Subscripts

a	Anode
c	Cathode
i, k	Different species in mixture
j	Joule heating source
l	Electrolyte
mem	Membrane
reac	Reaction
ref	Reference
s	Electrode
sys	System
x	Crossover

methanol crossover under different temperature conditions. The results show that crossover caused by both diffusion and electro-osmotic is higher at high temperature than low temperature. At a temperature of 50 °C the total methanol crossover is 450 A m^{-2}, while at a temperature of 30 °C the total methanol crossover is 270 A m^{-2}.

Furthermore, physical models were proposed in many studies for the detailed cell analysis. The polarization curve was studied for different parameters, including the porosity and permeability of the porous medium in He's [6] and Yang's [7] work. For the same current density, a higher porosity or high permeability leads to high cell voltage and better cell performance. It is suggested in Matar's [8] work that comparing with 8.4 μm and 44 μm, 19 μm is the optimal thickness of the cathode catalyst layer for better cell performance and smaller cathode overpotential. A 3D model was developed by Saarinen [9] for the analysis of the current density distribution. In addition, the temperature distribution was simulated in Argyropoulos's [10] and Cai's [11] work for the purpose of the optimal design of the cell and stack.

Besides this research on the cell level, many works also focused on the analysis of the system. Yang [12] built a system to test the effect of oxygen stoichiometry on the cell potential. The oxygen starvation induces a low cell potential or even a negative potential because of the hydrogen evolution at both half-cells and the hydrogen oxidation at the cathode side. Moreover, the oxygen starvation also elicits highly non-uniform current and temperature distribution in the cell and the Ru (ruthenium) dissolution at the anode side, which is one of the main aging effects in DMFC. The dissolution and unalloyed Ru migrates to the cathode side along with methanol crossover, which also causes the cathode potential reduction [13]. The fluctuation of the cell voltage and power according to the given current profile was studied in Patrabansh's [14] work. An optimal fuel concentration control was proposed by Lian [15], and a maximum power point tracking control was suggested by Zhang [16]. For the portable system, Na [17] reduced the number of components in the system to reduce the system weight and the parasitic power losses.

In the above-mentioned works, either the internal behavior of the cell or the system simulation and optimization were considered. Less research made the detailed analysis of the system and the cell internal behavior during the dynamic operation. Load variations can cause extremely inhomogeneous current distribution, and hence, the cell performance decreases [13]. This irreversible change of catalyst layers shortens the lifetime of the cell. Therefore, in this work a system model is firstly built in Simulink for investigating the dynamic response of the different system components to fluctuant loads. Secondly, a 2D cell spatial model is set up for analyzing its internal behavior. Through the simultaneous communication between the system model and the cell spatial model the system regulation strategy is going to be investigated for better cell performance [18]. Furthermore, the power consumption of the peripherals and the efficiency of the cell and system are investigated.