Research Article

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Responsive Analysis of the Transient Behavior for Computational Biology PEM-FC

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Abstract

All the mathematic models of PEM-FC balanced response have been established according to the Butler-Volmer model of electrode kinetics with numeric approach. To support the interaction between grid side and user side, a PEM-FC controlling device is designed as DSM user agent to provide gird-connected function. The Boost circuit and associated battery energy management system (BEMS) are considered together with temperature effect. It is proved that the porous characteristic of the backing materials facilitates reactant gas diffusion to the catalyst on membrane electrode assembly and it can be regarded as electrical connection between carbon-supported catalyst and the plate during DSM program.

Keywords: fuel cell; demand side management; energy management system; information model

Introduction

With the increasing risk of power outages due to demand fluctuation or large-scale grid malfunctions, the reliability and stability problems of interconnected power grid have become an important issue of modern power system [1]. The Proton Exchange Membrane (PEM) fuel cells are being considered as one of the most competitive back-up battery power source. A fuel cell can generate power without any combustion and thus can be regarded as the clean energy for future power dispatching. Increasing demand of the ice storm, hurricanes and large scale grid malfunctions will always cause unexpected power outage, and the PEM fuel cell have been proved to increase the reliability of power grid by Verizon Cross Functional Team. The oxidant and fuel are stored in the chemical energy without burning directly as traditional energy generating device. Among all types of fuel cells, PEM-FC has many attractive features, i.e., high current density, simple structure, no electrolyte leakage during operation, etc [2][3]. Considering the peak shifting object of power system, fast response characteristics of dispatching instructions are preferred for the PEM-FC that participates DSM project. Rapid power supply from large amount of PEM-FCs will keep the demand level in a certain range and reduce pressure of fossil-fired power plant dispatching[4][5]. However, fast response will easily cause the battery overshoot phenomenon (depend on the working conditions such as humidity, gas flow, pressure, temperature, etc), and it will also affect the performance of battery life to a certain extent [6]. The transient characteristics of each PEM-FC battery cell have close relations with mass transfer in the gas, water, transient transmission, and operating conditions. A typical 2-kW fuel cell stack under different operating conditions and dynamic loads are presented in [7]. The stoichiometric air, humidity, temperature will also change AC impedance. For example, when the stoichiometric air decreases, the PEM-FC stack will significantly increase mass transfer resistance, but it will take very little impact on other resistances [8][9]. By using the fuel cell test system (including high precision oscilloscopes and self-designed switching circuits), the electrical response of PEM-FC is measured under different conditions. Experimental results show that the dynamic response of PEM-FC have close relation with voltage operating conditions of each unit single battery within the electric heap. The electric industry has implemented various methods of demand response [10].

Based on the above discussion, it can be implied that there is no mature information exchanging models and controlling specifications for PEM-FC yet. The motivation of this paper is to present a novel contextual model for the PEM-FC to participate DSM program and also the transient dynamic response performance of PEM-FC will be evaluated by numeric approaches. Information model of the interactive backup power source is examined together with the mathematic model during instantaneous response.

Demand Response Capability Integration of PEM-FC

Problem Statement of PEM-FC within DR System

Since the air pressure and humidity of PEM-FC are controlled by mechanical appliance, the dynamic response characters of the fuel cell are limited by the reaction speed. Therefore, PEM-FC stack can not be used in electrical power system directly due to the lack of unified specification and clear investigation of dynamic response characteristic. Rapid load variation will lead to a sudden power supply shortage, and the output current is always experiencing a relatively long time to establish new steady state. The excessive fuel battery life may be affected by internal battery temperature, pressure, humidity, etc. Hydrogen and oxygen at reference state are diatomic molecules, and the enthalpy of formation is typically changed (It can only be determined by real time monitoring process). Besides, the specific heat values for hydrogen, oxygen, and water have close relation with the temperature. Battery energy management system (BEMS) shall integrate energy controlling function, such as the optimum operation, charging / discharging management, DSM event trigger, etc [11]. Since the PEM-FC can store electrical energy in liquid electrolytes, it can be regarded as a candidate to participate DR program. Figure 1 presents the flow transmission diagram in a PEM-FC. The electrolyte that stored in a tank recycles through the cell and the end plate seal the coolant while the manifold has ports for the hose fittings to connect to the distribution channels in various plates.

Previous researches are focused on the mathematic models of PEM-FC component. Nevertheless, the auxiliary energy storage aspect of PEM-FC during dynamic response shall be taken into considerations. One of the most efficient ways to keep the stability of the output energy flow is to shunt supper capacitors, and each capacitor voltage is strictly limited. The direct output fuel cell current can be controlled by a transducer with relative complex fabrication. Hence, indirect controlling of the parallel power source is introduced from [12]. The fluctuation of the user load can be absorbed partly by large capacity storage, and the charge/discharge process shall be managed by an energy management system. The internal components of a fuel cell will take quick reaction to the rapid changing loads without involving extra overheating inside, and will improve the dynamic performance. In addition, through the energy management system, the energy flow of the system can be effectively managed with predefined information exchanging model.

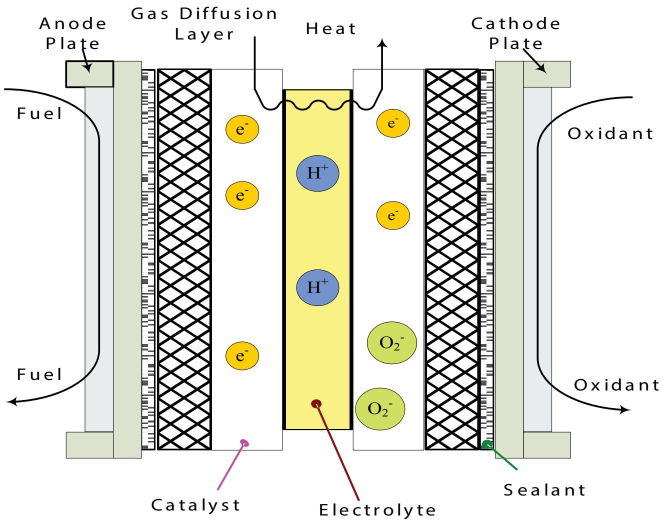

Figure 1: Illustration of the ion exchanging flow transmission of PEM-FC

Mathematic Model of PEM-FC Balanced Response

The kinetics of reactions that occurs on PEM-FC surface are affected by the electrode potential, and the process can be illustrated by the *Butler-Volmer* (*B-V*) model of electrode kinetics [13]. Once the DSM capability of PEM-FC is enabled, the potential and relative energy of the electron may change frequently, and both chemical and electrical energy will also be influenced during response process. Gibbs free energy variation can be used to evaluate the chemical energy released which has close relation with local temperature. The activated complex of Gibbs free energy varies from different transfer coefficient of oxidation and reduction reaction (Figure 2).

According to the geometry curves of energy barrier, the transfer coefficient can be evaluated by the intersection region as,

$$\tan\theta = (1-\alpha)F(E-E_0)/D_x \qquad (1)$$

$$\tan\theta = (1-\alpha)F(E-E_0)/D_x \qquad (2)$$

Where E is the fuel cell potential and E_0 is the associated balanced potential, F is Faraday constant. The transfer coefficient will influence the fuel cell reaction rate together with the activation rate.

The potential of any electrode will influence the reaction kinetics on PEM-FC surface and the reaction rate that is depending on the potential can be controlled by the

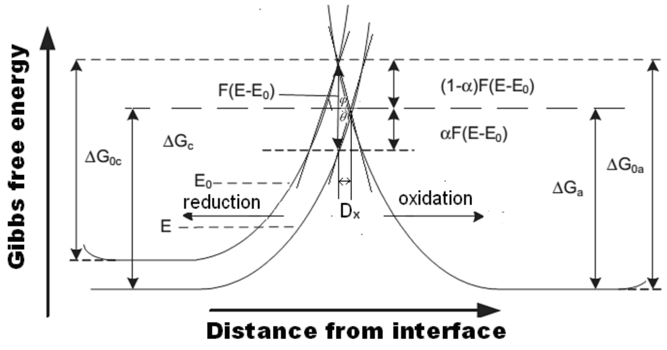

Figure 2: Effect of the potential change on activation energy with the intersection angle and transfer coefficient.

combined backward/forward reaction coefficient. The transfer coefficient can be obtained from *Equ.*(3).

$$\alpha = \tan\varphi / (\tan\theta + \tan\varphi) \qquad (3)$$

The maximum value of Gibbs free energy is identified as the activation energy, and the fluctuation range denotes the standard internal energy of activation during transient state.

According to the *B-V* equation, the current density per unit catalyst surface areas can be written as,

$$i = i_0\left[\exp\left(\frac{\alpha nFv_{act}}{RT}\right) - \exp\left(\frac{-(1-\alpha)nFv_{act}}{RT}\right)\right] \qquad (4)$$

Where i_0 denote the exchange current density, v_{act} denote the activation polarization, n denote the electrons transferred number during each reaction procedure under temperature T and universal gas constant [8.314J/(mol*K)]. The fuel cell reaction is exothermal, and the generated heat can be used for the heating company rather than a by-product. However, the heat shall be carefully controlled to maintain desired temperature. The heat that dissipates from fuel cell surfaces must be taken away by cooling system. The reactant flow rate for the inlet of PEM-FC should satisfy the basic reactant requirement in each cell.

Experimental Results

As soon as the biological process are turned into equations, the calculation efficiency shall be considered for practical use purpose. It is always usually solved numerically by using modern computer and large-scale tools. One central task for our proposed approach is to find the suitable mathematical model to describe the practical action in network and put them intelligently into different process through system theory. Various numerical solution techniques lend itself excellently to the system theory classification as well. To evaluate the complicated numerical codes, we often use heuristic algorithm instead large amount calculation and storage to accelerate the speed within the boundaries of the system, as well as the interaction between the system and its surrounding environment.

In order to illustrate the contribution of each unit battery, we evaluate the performance from PEM-FC output and Ohmic/Activation loss aspect below. The experimental results are taken with the excitation of step current of 300~700 mA/cm^2 density, the dynamic response performance of PEM-FC experience different trend with different electrode humidification.

Evaluations of PEM-FC Output Variation

There are no obvious relations between PEM-FC dynamic characteristics and the humidity for anode while the humidification takes great impact on cathode. According to the electrode kinetic theories, low humidity on cathode will result in significant ohm impedance changes due to transient water transfer. On the other side, high humidity will lead to water accumulation in the cathode which is caused by the limited density polarization. Detail parameters of the PEM-FC controller is presented in table 1 as follows.

Table 1: Parameters of the PEM-FC controller

Parameters	Values
Switching frequency	25 kHz
Coupled inductor	4.7uH
High-frequency filtering capacitor	50uF
Conductivity	0.1 ohms/cm
Electrolyte area	100cm^2

As the PEM-FC current density increases from 0.01A/cm^2 to 1.4 A/cm^2, the unit battery output voltage keep continuous decreasing from 1.0~1.2V to 0.06V~0.25V as shown in Figure 3. Different current density per unit catalyst surface areas will slightly affect the output voltage of each unit battery. High exchanging current density will improve the output potential level and about 20% increasing for low current density. The *B-V* equation can be applied to both the anode and cathode reaction of PEM-FC to illustrate the exponentially increasing over-potential. The reaction speed will be slower under low current density cases, and with larger activation over-potential for any particular net current. The entropy change of a given reaction is assumed to be the same under all evaluations. However, the reversible fuel cell potential differs from each other under various temperatures. The liquid form of water product under 25□ has 1.23V reversible cell voltage (RCV) and 83% theoretical efficiency while the gas form under 100□ only has 1.17V RCV and 79% efficiency. The corresponding Gibbs free energy changes are -237.2 kJ/mol and -225.2kJ/mol that released from the reaction respectively. The voltage losses in a practical PEM-FC are different under various exchanging current densities. Cell potential decreases as the current density increases from open circuit voltage to activation polarization dominated region. When the current density exceed 0.2~0.3 A/cm^2, the Ohmic polarization become dominate component. After the voltage drops below 30%

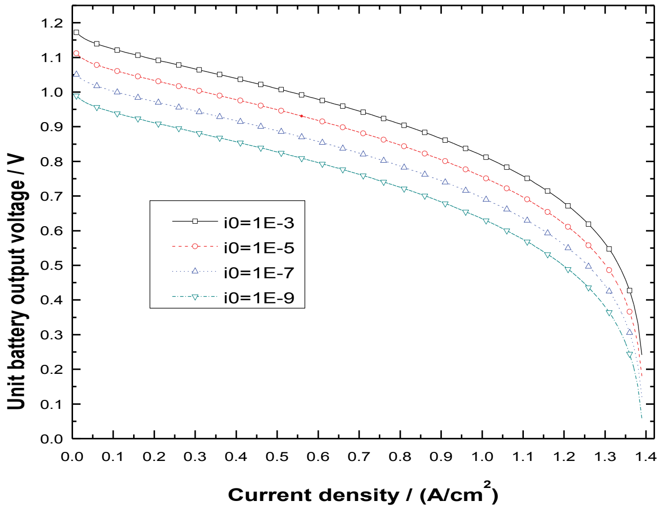

Figure 3: Dynamic response of the unit battery output voltage with different reference exchange current density per unit catalyst surface area

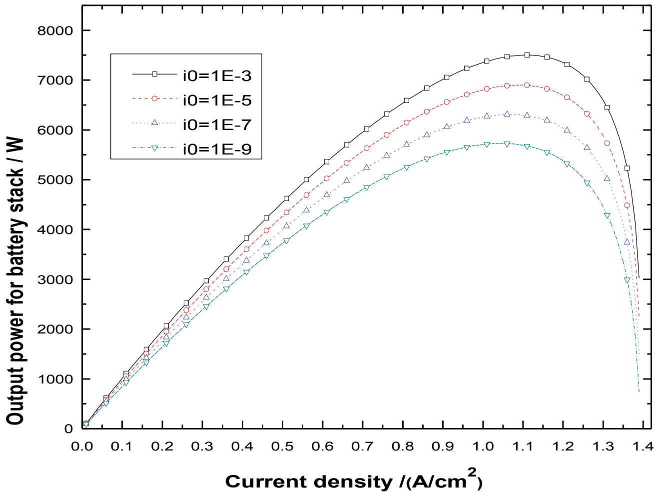

Figure 4: Power output of 90-battery stack output voltage with different reference exchange current density per unit catalyst surface area

reversible cell potential, the concentration polarization becomes dominant.

The change in Gibbs free energy of reaction is the difference between the products and reactants. The reduced value of Gibbs free energy means that there is energy released from the reaction during dynamic response. Based on the principle of electrical and Gibbs free energy transformation of the reversible PEM-FC, the conversion capability can be determined by the thermodynamic potential.

As the electrolyte is not electrically conductive, the hydrogen and electrons will diffuse through the electrolyte and thus reduce the servicing electrons [14][15]. The loss is a quite small part for fuel cell operation but will be significant during low current density cases. Figure 4 present the output power for PEM-FC stack that contains 90 unit batteries. With the increasing current density, the output power of the PEM-FC stack increases rapidly and it experiences a turning point at 1.0~1.2 A/cm^2, this is due to the fact of open circuit voltage decreasing on each PEM-FC cell. The anode electrode potential will move to a more positive value, and will result voltage decrease. The polarization curve presents information on the cell loss and the steady state polarization can be obtained with current recording under operating conditions. The current exchanging density takes the same effect with PEM-FC stack output power as the unit battery voltage is a crucial factor in reducing the activation overvoltage. Increasing current exchanging density i_0 can significant improve the performance of PEM-FC especially for the cathode. The output power of the battery stacks varies from 5.7kW to 7.5kW for different exchanging current density. In practical industrial applications, a higher i_0 can be achieved for by several approaches, i.e., increasing the roughness of electrodes, reactant concentration, etc. Besides, any increase of the PEM-FC temperature, pressure, or catalyst site occupancies will lead to a higher current density. Mass transfer rate can be enhanced by reducing the concentration overvoltage.

The reaction that occurs on PEM-FC catalyst layers are closely related with the activation loss during charging/discharging process. In addition to the activating loss, the production of electronic charge transport movement of the charge electrode shall be considered as a key contribution for energy supply. Bipolar cooling, the contact between the plates is due to the loss of electrons plate, mutual compression of the fuel cell stack degree of contact. Ion transport is more difficult to predict electron transport model fuel cell ratio. The ionic charging loss which is raised by transport resistance occurs in the fuel cell membrane when H+ ions travel through the electrolyte.

Conclusions

In this paper, we have developed a novel information exchanging model for PEM-FC according to IEC PC-118 architecture. To illustrate the dynamic characteristic of PEM-FC that participate demand response program, numeric model is established based on Gibbs free energy model. The transfer coefficient is evaluated by the intersection curves of reaction / oxidation procedure. Experimental results of the Ohmic and activation loss and output power are presented to show the performance of PEM-FC transient response under dynamic pricing model. The performance is evaluated under various environment temperature, thickness of electrolyte layer, current density and also the transfer coefficient. A practical scenario of multiple PEM-FCs are shown under TOU pricing model by using the numeric model of PEM-FC, and the presented mathematic model can be a quite useful tool for further DSM performance evaluation.

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