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Extended criterion for robustness evaluations of energy conversion efficiency in DMFCs

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ABSTRACT

Considering the effects of unpredictable disturbances, a robustness criterion is newly proposed to develop an integrated evaluation with modified efficiency criterion, for comprehensive assessments of energy conversion performances in direct methanol fuel cells. The effectiveness of developed criteria in various situations (including some extreme operating conditions) has been carefully analyzed based on both experimental and numerical results. For undisturbed operations, the modified efficiency criterion could help to avoid potential misinterpretations of energy conversion process in existing criteria. For disturbed operations, the robustness criterion concerning the effects of uncertainty propagations is shown to be an effective guidance for the determination of appropriate operating current densities to design efficiency-stabilized operations. Systematic analysis on its applications in different situations proves that, the integrated efficiency and robustness evaluations can effectively differentiate the effects of operating conditions and membrane types, which is highly beneficial for one's optimal designs of stable and efficient DMFC operations.

1. Introduction

Direct Methanol Fuel Cell (DMFC) is regarded as a prosperous power source for mobile applications attributing to its features of easy handling, rapid charge and high energy density, etc. [1,2]. Lots of efforts have been carried out to improve the DMFC performance for accelerating its commercialization during the past decades [3], such as the optimization of cell structure [4], the improvement of catalyst loading [5] and the amelioration of fuel delivery system [6]. In one's evaluations of those performance-enhanced techniques, how to determine an effective criterion for DMFC operations can be an important problem and therefore deserves further discussions [7,8].

A widely applied assessment of DMFC performance is the relationship of current density (I) and voltage (V) or power density (P), i.e., I-V or I-P curves. Coming very naturally from their definitions, the polarization effects and the output characteristics of DMFC systems can be well depicted [9,10]. However, the I-V and I-P curves mainly concentrate on the system output, rather than the energy conversion process. Under different hypotheses, several criteria were proposed to assess the energy conversion efficiency during the past decade [11,12]. One of the main criteria considers the fact that the energy conversion efficiency is highly relevant with the fuel waste (i.e., methanol crossover effect). It utilized a single-parameter index, the effectiveness of fuel utilization (the ratio between the power-generated fuel amount and the overall fuel consumption), to measure the energy conversion efficiency [11,12]. However, the output characteristics has not been taken into account. Considering the polarization effect, a double-parameter index was proposed to evaluate the overall efficiency by multiplying the potential and Faraday/current efficiencies [13,14]. A very similar criterion was also deduced from the ratio between the output power density and the low heating value of overall fuel consumption [15]. Another type of criterion that was designed to concern about more systematical effects is the triple-parameter index, in which the total efficiency was considered by a product of several parameters accounting for fuel consumption, thermodynamic and voltaic efficiencies [16–18]. Such systematic considerations for global efficiency were also applied to evaluate the DMFC system only at its largest power output [19].

In spite of huge progress has been made, most of the existing criteria have been confined to evaluate DMFC systems with stable operating conditions. However, the environmental disturbances, e.g., the noise of operating parameters or the small variations in load conditions [20,21],

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Nomenclature

ΔG	change in Gibbs free energy
ΔH	enthalpy change in Gibbs free energy
η	energy conversion efficiency
η_F	Faraday efficiency
η_{mod}	system efficiency at undisturbed conditions
η_P	potential efficiency
η_T	thermodynamic efficiency
$\bar{g}$	gibbs free energy in one mole of methanol
C_M	methanol concentration
F	Faraday constant
F_A	air flow rate
F_M	methanol flow rate
F_{MeOHin}	input methanol amount
$F_{MeOHout}$	output methanol amount
F_{MOR}	effective methanol consumption
I	operating current
I_{cross}	crossover current
LHV	lower heating value
N_{cons}	molar flow rate of methanol for effective current generation
N_{cross}	molar flow rate of methanol crossover
R	robustness
T	temperature
V_{cell}	operating voltage
V_{th}	thermodynamic reversible voltage

need to be taken into account in the criteria development for a comprehensive evaluation of the energy conversion performance in DMFCs [22–25]. Systematic robustness has been widely applied to evaluate the ability of a system to resist environmental disturbance without adapting its initial stable configurations in the design, analysis and improvement of energy systems [24,26,27]. For instance, the robustness analysis has been successfully applied to identify the effect of assembly parameters on the pressure distribution inside a stack of proton exchange membrane fuel cells [28]. A robust controller was developed with the consideration of operating condition variations to improve the power output of fuel cells for automotive applications [29]. Robustness analysis has also played an important role in the development of fault diagnosis method for air-feed fuel cell systems [30]. However, to the best of our knowledge, the systematic robustness is not yet applied in the evaluations of DMFC performance in spite of its high potential, which then becomes the initial motivation of the present study.

Considering the effects of unpredictable disturbances, a robustness criterion is creatively proposed to develop an integrated evaluation with modified efficiency criterion. This integrated evaluations can be applied to comprehensively assess the energy conversion performances in DMFC systems. Methodologies are presented in Section 2, where the efficiency and robustness criteria, as well as the applied numerical and experimental techniques, are all detailedly elaborated. Comparative study between the existing and modified efficiency criteria is firstly presented (Section 3.1), and the applications of efficiency evaluations on disturbed operations are subsequently investigated to study the necessity of robustness evaluations Sections 3.2 and 3.3. Applications of integrated efficiency and robustness evaluation in various situations (including some extreme operating conditions) are then performed and carefully discussed in Section 3.4. Conclusions are summarized in Section 4.

2. Materials and methods

Systematic analysis on the efficiency and extended robustness evaluations in DMFC systems is performed based on the collaborations of experimental and numerical techniques. In this section, the applied experimental and numerical techniques, as well as the evaluation criteria are described. Firstly, the experimental platform is presented, and then some preliminary experimental works based on DMFCs with different Membrane Electrolyte Assemblies (MEAs) are carried out to generate reference data for numerical validations. Numerical models about the energy conversion process inside DMFCs are then validated and presented. Subsequently, the existing classical criteria of efficiency evaluations are comprehensively described, and thereafter, a newly modified efficiency criteria as well as the extended robustness evaluation are both proposed in details.

2.1. Experimental setup

Fig. 1 shows the experimental set-up of DMFC testing system. The peristaltic pump (BT300LC) is used to transport the methanol solution composed by deionized water and pure methanol, while an air compressor (OUTSTANDING OTS-550) regulated by a mass flow controller (OMEGA FMA-2605A) is applied to pump the air into the cathode side. A supplementary heating apparatus controlled by a temperature controller (Omega CSC32) is used to regulate the operating temperature. During operations, the DMFC performance is monitored by an electrochemical workstation (CHI660E), and the production of CO_2 is measured by a CO_2 concentration detector (JA500-CO2-IR1). The current density is regulated by an electronic load device (ITECH it8211) to different levels, and the corresponding voltage is thus measured.

Several DMFCs with different MEAs have been applied in experiments for different research purposes (Fig. 1, bottom). In order to study the effects of operating conditions, a specific single-cell DMFC consisting of a five-layer MEA with an effective active area of 25 cm^2 sandwiched by graphite end plates with serpentine channels of 30 passes. The five-layer MEA is composed by a Nafion 212 membrane, an anode catalyst layer with 4.0 mg/cm^2 Pt loading, a cathode catalyst layer with 0.03 mg/cm^2 Pt loading and two gas diffusion layers. Besides, the effects of membrane types are also investigated by introducing Nafion 115 and 117 membranes, for which the catalyst loading and active area are kept to be the same with those of Nafion 212. It is important to notice that the thicknesses of Nafion 115, 117 and 212 membranes are 127, 183 and 50.8 μm, respectively.

2.2. Numerical model

Considering the integrations of the governing equations of continuity, momentum conservation, species transport and electrochemical phenomena, we have developed a three-dimensional numerical model to investigate the energy conversion process in DMFC systems [31]. The overpotential effects including concentration, activation and ohmic ones are accounted by a semi-empirical model which has been well embedded inside this numerical model. It has shown a good agreement with experimental results in our previous studies, and has been successfully applied to study the underlying mechanisms of energy conversion process, the combined effects of different operating parameters and the operation strategy to enhance the voltage stability in different DMFC systems [31,32]. We have applied this well-constructed numerical model in the present study. For simplicity and concision, more details are not contained here but can be available in Refs. [31,32].

Numerical simulations were performed using a Computational Fluid Dynamics (CFD) code known as Fluent 16.0 which is based on the finite volume method. The manually defined parameters/conditions are all coded by User Defined Functions (UDFs) and then integrated into the CFD model. Flow domains are discretized into structured grids,