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Sensitivity analysis of uncertain parameters based on an improved proton exchange membrane fuel cell analytical model

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ABSTRACT

In this study, an enhanced non-isothermal, two-phase 1D analytical proton exchange membrane fuel cell (PEMFC) model is developed, which not only considers the water saturation jump, but also proposes a novel method to analytically solve the water phase changes and couple the liquid and vapor transport together. A stringent model validation procedure is used to show good agreement between the simulated results and the experimental data, taking advantage of the "three-step" and "multi-case" validation methods. It is revealed that the uncertain parameters may deteriorate model reliability and credibility, thus demonstrating the necessity to conduct sensitivity analysis. A multi-parametric screening method i.e. the elementary effect (EE) method based on Monte Carlo experiments is implemented to comprehensively analyze the total 22 uncertain parameters (including geometric, physical and electrochemical parameters), which are finally classified into very sensitive ones, rather sensitive ones and insensitive ones. The cathodic parameters are found more sensitive than the anodic ones, and the parameters of different components may have distinct sensitivity. Besides, whether the effect of each parameter is positive or negative on cell performance is also discussed. Furthermore, three cases with different groups of parameters are presented, which show almost the same polarization curve, and the two-sample Kolmogorov-Smirnov (KS) test is applied to verify the stability difference. It is concluded that those uncertain parameters not only influence the cell performance but also affect the model stability, and hence the effects of varying operating conditions should be taken into account in validation work.

1. Introduction

Proton exchange membrane fuel cell (PEMFC) is one of the most promising energy conversion devices with various merits such as high efficiency, zero emission, low-temperature operation, etc. [1–4]. Great efforts have been made to improve the performance, where computational simulation plays an important role [5–7]. In spite of some prominent advantages over experiments such as lower economic cost and time cost, the credibility of simulation results strongly relies on model accuracy. In this regard, a great number of models are developed [1,8,9], which consider more and more physical phenomena to truly reflect the transport processes inside fuel cell.

A PEM fuel cell model involves complicated processes such as electrochemical reaction, mass and heat transfer processes, the scale level of which ranges from microscale to macroscale [10]. Besides, there are over ten empirical parameters that are hard to measure though experiments (such as transfer coefficient), and it is proposed that a model with many degrees of freedom can lead to any desired behaviors with plausible structure and parameter values [11], thus severely reducing the model reliability. Min et al. [12] mentioned that the final outcome of different PEM fuel cell models were almost the same even if the parameters actually took different values, and hence they explicitly discussed the necessity of conducting parameter sensitivity examinations and finally proposed a rigorous "three-step" validation approach in proving the uniqueness and reliability of models.

Sensitivity examination or sensitivity analysis (SA) is usually defined as a study of how the uncertainty of inputs influences the final outcome of mathematical models [13], and it has been performed through various methods, which can be classified by modeling domain and the specific application purposes. The most popular SA method is conducted by varying one parameter at a time while keeping the remaining ones at nominal values, and it is called the "one-factor-at-a-time" (OAT) method. The biggest problem of OAT method is that it is customarily conducted at the baseline point, hence it only reflects the effects of parameters at a given point, not the multi-dimensional parameter space [14]. Therefore, alternatives to OAT method are suggested to promote its general application in SA practices. Bailis et al. [15] and Campbell et al. [16] provided a simple factorial design (FD) in

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Nomenclature

A	area (m^2)
a	water activity
C_i	gas species molar concentration ($mol\,m^{-3}$)
d_h	hydraulic diameter (m)
D_i	gas species diffusion coefficient ($m^2\,s^{-1}$)
E	voltage (V)
EW	equivalent weight of membrane
F	the Faraday's constant ($C\,mol^{-1}$)
ΔG	molar gibbs free energy change ($J\,mol^{-1}\,K^{-1}$)
I	current density ($A\,m^{-2}$)
J	molar flux rate ($mol\,m^{-2}\,s^{-1}$)
K	permeability (m^2)
k	thermal conductivity ($W\,m^{-1}\,K^{-1}$)
l	volume fraction
M	molecular weight ($kg\,mol^{-1}$)
n_d	electro-osmotic drag coefficient
Ω	area specific resistance (Ωm^2)
P	pressure (Pa)
P_c	capillary pressure (Pa)
Q	heat source ($W\,m^{-3}$)
R	universal gas constant ($J\,mol^{-1}\,K^{-1}$)/reaction rate ($A\,m^{-3}$)
$R^a_{0,ref}$	anodic reference reaction rate ($A\,m^{-3}$)
$R^c_{0,ref}$	cathodic reference reaction rate ($A\,m^{-3}$)
RH	relative humidity
s	liquid saturation in porous electrodes
Sh	Sherwood number
ST	stoichiometry ratio
ΔS	entropy change ($J\,mol^{-1}\,K^{-1}$)
T	temperature (K)
X	mole fraction

Greek symbols

δ	thickness (m)
σ	conductivity ($S\,m^{-1}$)
ε	porosity
η	overpotential (V)
λ	membrane water content
α	transfer coefficient
θ	contact angle °
μ	dynamic viscosity (Pa s)
ρ	density ($kg\,m^{-3}$)

Subscripts and superscripts

0	standard state
a	anode
act	activation
back	back diffusion
c	cathode/channel
ch	channel
CL/cl	catalyst layer
eff	effective
EOD	electro-osmotic drag effect
evap	evaporation
g	gas
GDL/gdl	gas diffusion layer
H^+	proton
H_2	hydrogen
H_2O	water
hyd	hydraulic permeation
i	gas species or layers/inner
in	inlet
l	liquid phase
m	membrane or membrane electrolyte
MPL/mpl	micro-porous layer
Nafion	Nafion
o	outer
O_2	oxygen
ohm	ohmic
out	output/outlet
P	bipolar plate
por	porous material
ref	reference state
rev	reversible
s	solid substrate
sat	saturation state
vap	water vapor
w	wall

analysis, which estimated the factors' main effects and interactions as well. In addition, regression analysis was adopted to do sensitivity analysis especially for linear models or additive models [17]. Furthermore, Sobol [18–20] proposed a variance based method and it was a precise quantitative approach in determining factor sensitivity with multi-order indexes in nonlinear models. Due to its drawback of large computational expense, this variance based method is not well applicable when involving a large number of uncertain parameters. Another good implementation called regionalized sensitivity analysis (RSA) method based on Monte Carlo filtering is seen [11,21], and it isolates critical parameters by classifying results of an objective function as "acceptable" or "unacceptable". The disadvantage of RSA is that it needs a threshold in classification of the results, which is a subjective process that may influence the final conclusions [22]. Moreover, Morris [23] and Campolongo et al. [24] extended the OAT method by randomly selecting some trajectories to cover the whole space of input factors. This approach is generally known as "elementary effects" (EE), and it is an ideal SA alternative because of its high calculation efficiency and simple operating procedure.

Although SA is a sophisticated research tool in diverse scientific domains, there are not many relevant studies towards fuel cells [25]. Min et al. [12] have systematically analyzed 11 major uncertain parameters of the fuel cell model by individually varying one parameter at a time and they have advocated that the uncertainty analysis should be an indispensable part in simulation work. Laoun et al. [26] explained the effects of several parameters by the variance based method, but they used a relatively simple empirical PEM fuel cell model, which neglected some significant physical phenomena. Srinivasulu et al. [27] have identified the relative importance of parameters in a PEMFC electrochemical model based on a multi-parametric sensitivity analysis (MPSA) approach [28], but the work did not present a complete fuel cell model for analysis.

There are two major deficiencies in the previous studies: they are based on an empirical or an incomplete fuel cell model that simplifies certain physical and electrochemical processes; or they are practiced by a simple qualitative OAT method which in fact neglects the whole space of input parameters. The biggest obstacle to do sensitivity analysis in a complete fuel cell model is its high computational expense, since a single case is likely to take large amount of time (especially for multi-dimensional models), making it impossible to fulfil a systematic sensitivity analysis.

To tackle the aforementioned problems, a non-isothermal two-phase