

Parameter sensitivity examination and discussion of PEM fuel cell simulation model validation Part II: Results of sensitivity analysis and validation of the model

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Received 22 December 2005; received in revised form 12 January 2006; accepted 25 January 2006
Available online 7 March 2006

Abstract

A three-dimensional, two-phase and non-isothermal numerical model has been developed in Part I of this two-article work. In this article, the parameter sensitivity analysis is performed. The influence of 11 major parameters, including the transfer coefficient, exchange current density multiplied by specific area, porosity, diffusion coefficient, absolute permeability and membrane phase conductivity, were investigated on the effect of the global polarization curve. The results show that the PEMFC global polarization curve is influenced by many parameters and the cathode-side parameters are a stronger influence than those on the anode side. Two different groups of parameters are provided which can result in almost the same global polarization curve, showing that the global polarization curve is not sufficient for the validation. Detailed discussion on the PEMFC model validation is conducted, and it is shown by numerical results that the global polarization curve plus the local current density distribution is still not sufficient for the model validation. A three-step validation approach is then proposed which can be expected to give a unique validation. The three steps are: validation of the global polarization curve; validation of the local current density distribution curve and validation of the cathode overpotential versus current density curve. Four further suggestions are proposed in order to solve the validation issue completely. These include the completeness of the data provided, the accumulation of benchmark data and the necessity for introduction of uncertainty analysis.

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Keywords: PEM fuel cell; Parameter sensitivity; Numerical modeling; Polarization curve; Local current density distribution; Cathode overpotential

1. Introduction

This paper forms the second part of a two-part study of the parameter sensitivity of a PEM fuel cell simulation model. In Part I, a full three-dimensional, two-phase and non-isothermal mathematical model for the PEM fuel cell with a parallel flow field was presented. Computational results such as a PEMFC polarization curve, oxygen mass fraction distribution in the cathode, local current density distribution in the cathode catalyst layer, liquid water saturation distribution in the cathode electrode, cathode and anode overpotentials and temperature distribution in the PEMFC were obtained for the basic case. In

this companion paper, the parameter sensitivity analysis is performed on 11 major parameters such as the transfer coefficient, exchange current density multiply specific area, porosity, diffusion coefficient, absolute permeability and membrane phase conductivity via the developed model. The parameter sensitivity here means how the parameters influence the global performance of a PEM fuel cell represented by the polarization curve ($V-I$ curve). The parameter sensitivity analysis is conducted as follows: the influences of parameters on PEMFC performance are investigated individually by varying one parameter at time, maintaining the remaining parameters at the values of the basic case.

In the following, the sensitivity examination results are first presented, followed by a comprehensive discussion of the model validation issue. Because of the insufficiency of the existing model validation approaches, a three-step validation approach is

DOI of original article: [10.1016/j.jpowsour.2006.01.078](https://doi.org/10.1016/j.jpowsour.2006.01.078).

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Nomenclature

A	area (m^2)
A_s	specific area of catalyst layer (m^{-1})
c	molar concentration (mol m^{-3})
D	diffusion coefficient ($\text{m}^2 \text{s}^{-1}$)
F	Faraday's constant (C mol^{-1})
i	reaction rate (A m^{-3})
i_{ref}	reference exchange current density (A m^{-2})
I	current density (A m^{-2})
K	electrode absolute permeability (m^2)
R	universal gas constant ($8.314 \text{ J mol}^{-1} \text{ K}^{-1}$)
T	temperature (K)

Greek symbols

α	transfer coefficient
ε	porosity
η	overpotential (V)
κ	electrical conductivity (S m^{-1})

Subscripts and superscripts

a	anode
av	average value
c	cathode
ct	catalyst layer
d	diffusion layer
h	hydrogen
m	membrane
o	oxygen
ref	reference values
s	solid; specific
w	water

proposed. Then four further suggestions are proposed in order to solve the validation issue completely. Finally some conclusions are drawn.

2. Parameters selected for sensitivity study

In the following, the physical and electrochemical parameters that influence the PEMFC performance are studied. But those parameters that can be determined with enough accuracy and certainty, such as temperature, pressure, humidity and channel sizes etc., are not included. The parameters for the sensitivity analysis are listed in Table 1, where their values for the basic case are presented, and their variation ranges in the literature are also shown. In addition, the source literature that give the upper or the lower limits of the parameter values are provided.

For the selection of the parameters investigated, the following descriptions are used:

- (1) The PEMFC performance is influenced by the solid phase conductivity, κ_s . In view of its very high value that will lead to a negligible potential loss, which is not included in the influencing parameters. Furthermore, the effect of the mem-

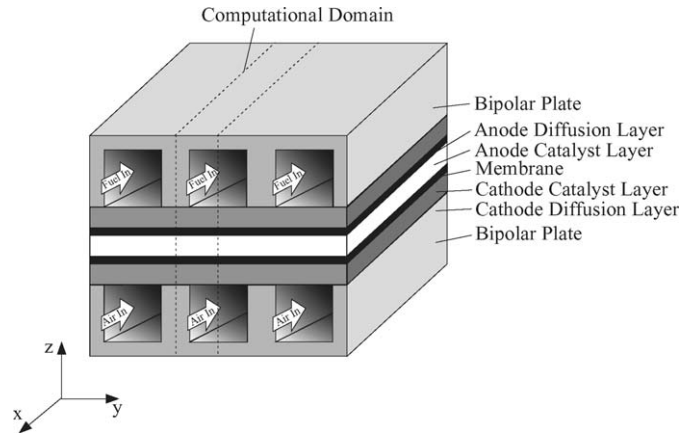


Fig. 1. Schematic view of a PEMFC.

brane phase conductivity κ_m is important [18]; therefore, it is included.

- (2) From the Butler–Volmer equation, we know that $A_s i_{a,\text{ref}}$ and $c_{h,\text{ref}}$ are always related. Hence, they can be united as one parameter. The same discussion applies to $A_s i_{c,\text{ref}}$ and $c_{o,\text{ref}}$. In Table 1, the original variation range of $A_s i_{a,\text{ref}}$ and $A_s i_{c,\text{ref}}$, from 5.0×10^8 to $1.4 \times 10^{11} \text{ A m}^{-3}$ and 10 – $1.0 \times 10^7 \text{ A m}^{-3}$, respectively, are listed. In our numerical simulation, the effect of the variation of $c_{h,\text{ref}}$ and $c_{o,\text{ref}}$ were taken into account via the enlarged variation range of $A_s i_{a,\text{ref}}$ and $A_s i_{c,\text{ref}}$, from 5.0×10^7 to $5 \times 10^{11} \text{ A m}^{-3}$ and 10 – $3 \times 10^7 \text{ A m}^{-3}$, respectively. No individual examination for $c_{h,\text{ref}}$ and $c_{o,\text{ref}}$ was conducted.

Because of the diversity of expressions adopted in the literature, in obtaining the parameter variation range, some transformations were first conducted such that the expressions for the same item were all the same as the ones adopted in this paper, and then some recalculations were performed. Such situations will be mentioned in the related part of the following presentation.

The schematic of the simulated PEMFC model is presented in the companion paper, but for readers' convenience it is re-drawn in Fig. 1 of this paper.

3. Results and discussion for parameter sensitivity study

The 11 parameters involved in the sensitivity analyses fall into six groups: transfer coefficient, exchange current density multiplied by specific area, porosity, diffusion coefficient, absolute permeability and membrane phase conductivity. In the following presentation, the effects of each group of parameters are first discussed in order, and then general features of the influencing parameters are summarized.

3.1. Transfer coefficients

The investigation of the transfer coefficients involves the anode transfer coefficient and the cathode transfer coefficient, which are the basic kinetic parameters for electrode reactions and are related to the type of electrode reaction, the configu-

Table 1
Influencing parameters for parametric sensitivity analysis

Parameter	Symbol	Value	Range	Reference
Anode transfer coefficient	α_a	0.5	0.25–1.0	[1,2]
Cathode transfer coefficient	α_c	0.5	0.2–0.9375	[3,4]
Anode exchange current density multiply specific area	$A_s i_{a,ref}$	$5.0 \times 10^7 \text{ A m}^{-3}$	5.0×10^8 – 1.4×10^{11}	[5,6]
Cathode exchange current density multiply specific area	$A_s i_{c,ref}$	120 A m^{-3}	10 – 1.0×10^7	[6,7]
Hydrogen reference concentration	$c_{h,ref}$	56.4 mol m^{-3}	26.6–56.4	[8,6]
Oxygen reference concentration	$c_{o,ref}$	3.39 mol m^{-3}	1.2–40.88	[4,9]
Porosity of diffusion layer	ε_d	0.3	0.125–0.7	[10,11]
Porosity of catalyst layer	ε_{ct}	0.28	0.02–0.6	[12]
H ₂ diffusion coefficient at reference state	$D_{h,ref}$	$9.15 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$	2.63×10^{-6} – 1.1×10^{-4}	[13,9]
O ₂ diffusion coefficient at reference state	$D_{o,ref}$	$0.22 \times 10^{-4} \text{ m}^2 \text{ s}^{-1}$	6.5×10^{-7} – 3.2×10^{-5}	[14,9]
Water vapor diffusion coefficient at reference state	$D_{w,ref}$	$2.56 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$	2.56×10^{-5} – 1.1×10^{-4}	[1,9]
Absolute permeability of diffusion layer	K	$1.76 \times 10^{-11} \text{ m}^2$	1.0×10^{-15} – 1.0×10^{-8}	[15,16]
Membrane phase conductivity	κ_m	6 S m^{-1}	0.01–38	[17,6]

ration of the electrode surface and the catalyst properties. The Butler–Volmer equation is often used to describe the electrochemical reactions, but the expressions of the equation are not always the same. Basically there are two types of expressions. One form is:

$$\text{Anode : } i = A_s i_{a,ref} \left(\frac{c_h}{c_{h,ref}} \right)^{1/2} \left(\frac{\alpha_a + \alpha_c}{RT} F \eta_a \right) \quad (1)$$

$$\text{Cathode : } i = A_s i_{c,ref} \frac{c_o}{c_{o,ref}} \left(-\frac{\alpha_c}{RT} F \eta_c \right) \quad (2)$$

Such expressions are adopted, for example, by Ju et al. [9] and Meng and Wang [19]. These kinetic expressions are a simplified form the general Butler–Volmer equation on the assumption that the hydrogen oxidation reaction is facile and hence the surface overpotential is small. The general expressions of the Butler–Volmer equation are [20]:

$$\text{Anode : } i = A_s i_{a,ref} \left(\frac{c_h}{c_{h,ref}} \right)^{1/2} \left[\exp \left(\frac{\alpha_a F}{RT} \eta_a \right) - \exp \left(-\frac{\alpha_c F}{RT} \eta_a \right) \right] \quad (3)$$

$$\text{Cathode : } i = A_s i_{c,ref} \frac{c_o}{c_{o,ref}} \left[\exp \left(\frac{\alpha_a F}{RT} \eta_c \right) - \exp \left(-\frac{\alpha_c F}{RT} \eta_c \right) \right] \quad (4)$$

The difference between these two expressions and Eqs. (20) and (21) in the companion paper (Part I) [21] is that the electron number of the reactions are included in the transfer coefficients of these two expressions. To obtain the variation range of the transfer coefficients, we transformed the expressions in the literature to the expressions adopted in this article and re-calculated the corresponding values.

The effects of the transfer coefficients on the PEMFC polarization curve are shown in Figs. 2 and 3. The results show that the influence of the anode transfer coefficient on the PEMFC performance is small. The polarization curve changes a little with the increasing of the anode transfer coefficient α_a from 0.7 to 1.0.

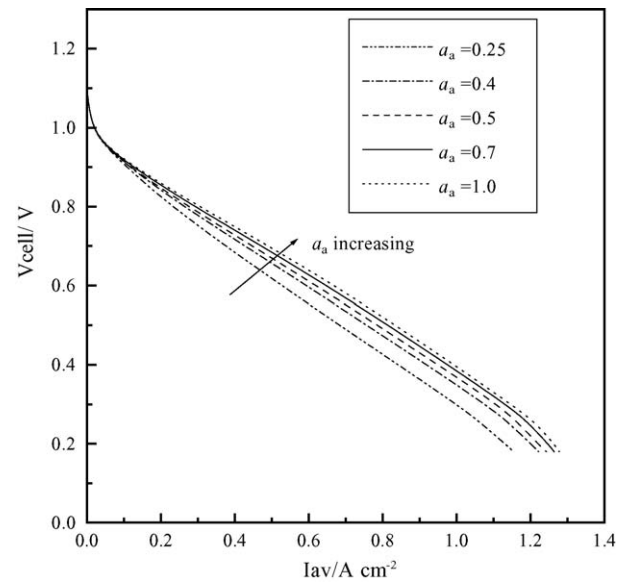


Fig. 2. Effects of anode transfer coefficient.

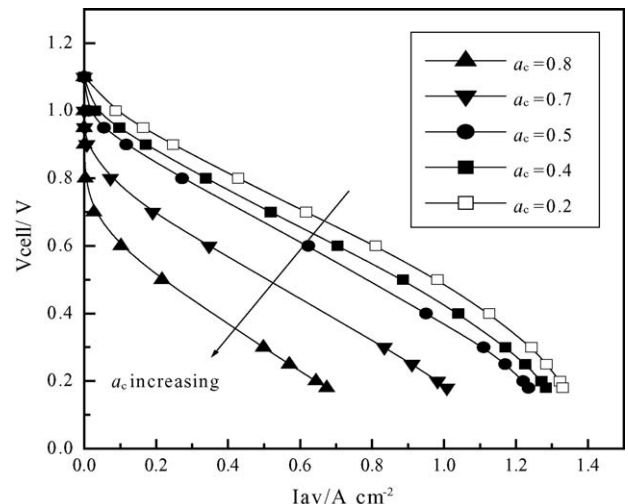


Fig. 3. Effects of cathode transfer coefficient.

While the cathode transfer coefficient significantly affects the polarization curve. The polarization curves for α_c from 0.2 to 0.8 are shown in Fig. 3. It can be seen that the PEMFC performance is very poor when $\alpha_c > 0.8$. In addition, Fig. 3 shows that the cell voltage decreases with the increase of the cathode transfer coefficient for a given current density. This implies that the influence of the cathode transfer coefficient on the PEMFC performance is different from that of the anode transfer coefficient. The reason is that the overpotential of the cathodic electrode is negative, and hence the second exponent term in Eq. (21) (Part I) is the main term to compute the current density through the cathodic overpotential. And, from the structure of Eq. (21) of the first paper, it can be easily observed that for a given electrical current, the reduction of the cathode transfer coefficient causes increase in the cathode overpotential which leads to a decrease in the fuel cell voltage under the given total voltage condition. In the following discussion, the absolute values of the cathode overpotentials are utilized.

3.2. Product of exchange current density and specific area

The effects of the anode exchange current density multiplied by the specific area and the cathode exchange current density multiplied by the specific area are shown in Figs. 4 and 5. The extended range of $A_s i_{a,ref}$ is 5.0×10^7 to $5.0 \times 10^{11} \text{ A m}^{-3}$, but only three curves corresponding to $A_s i_{a,ref} = 5.0 \times 10^7$, 5.0×10^8 and 5.0×10^9 are shown in Fig. 4. It is found in our simulations that when the value of $A_s i_{a,ref}$ is increased to beyond the value of $5.0 \times 10^9 \text{ A m}^{-3}$, there is no detectable affect on the PEMFC polarization curve. The curves in Fig. 4 are relatively parallel in the ohmic and the concentration polarization zones. Fig. 5 shows the effects of the cathode-side parameter. It can be clearly observed that the effect of $A_s i_{c,ref}$ on the PEMFC polarization curve is more significant than that of $A_s i_{a,ref}$. The results of the effect of the cathode exchange current density on the PEMFC

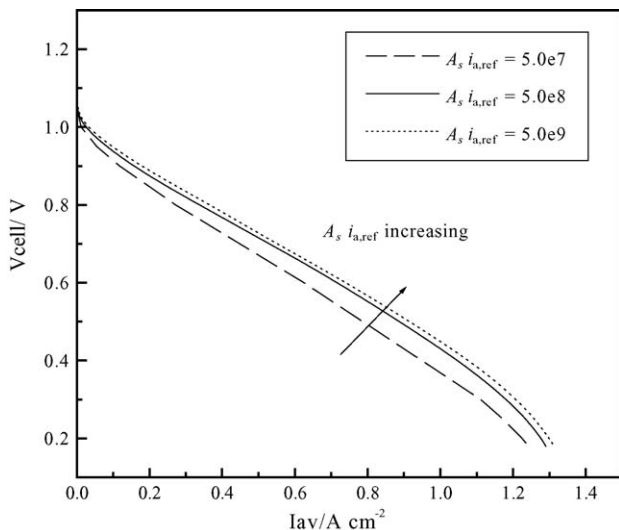


Fig. 4. Effects of anode exchange current density \times specific area for catalyst layer.

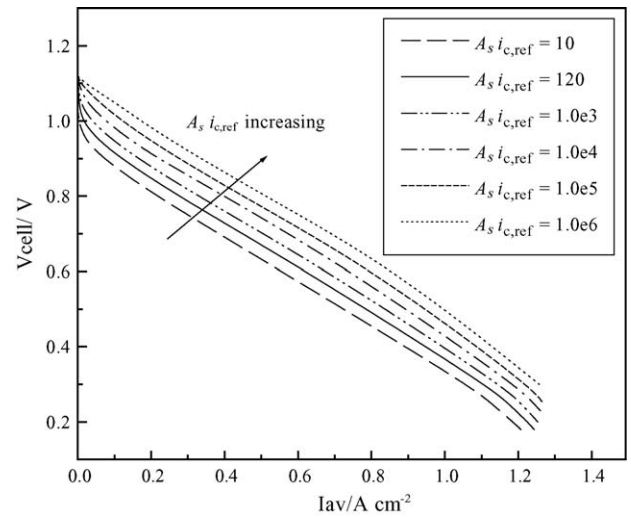


Fig. 5. Effects of cathode exchange current density \times specific area for catalyst layer.

performance given by Wöhr et al. [7] are quite similar to the ones presented in Fig. 5.

3.3. Porosities

The effects of the diffusion layer porosity and the catalyst layer porosity on the performance of PEMFC are shown in Figs. 6 and 7. The simulation results show that the effect of the diffusion layer porosity on the PEMFC performance is significant when the porosity is in the low value region ranging from 0.125 to 0.3. With increase of the diffusion layer porosity, its effect becomes weaker and weaker. When the diffusion layer porosity reaches 0.6, its further increase will not affect the polarization curve.

The effect of the catalyst layer porosity from the present model is quite different. Theoretically, the catalyst layer is porous, and the variation of its porosity may change the specific area of the electrode. Hence, the variation of the catalyst layer porosity should affect the PEMFC performance. How-

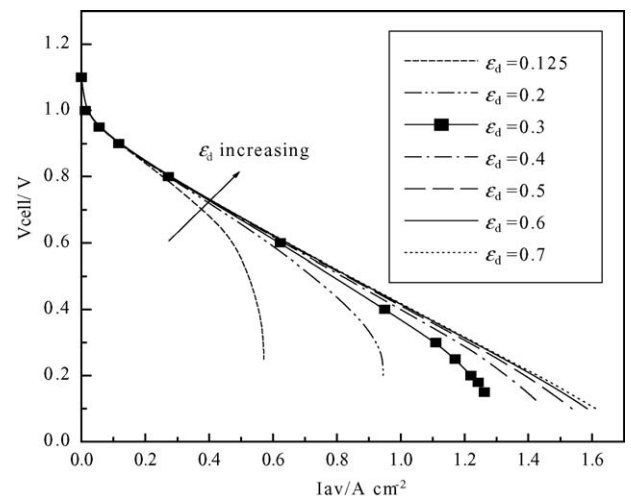


Fig. 6. Effects of diffusion layer porosity.

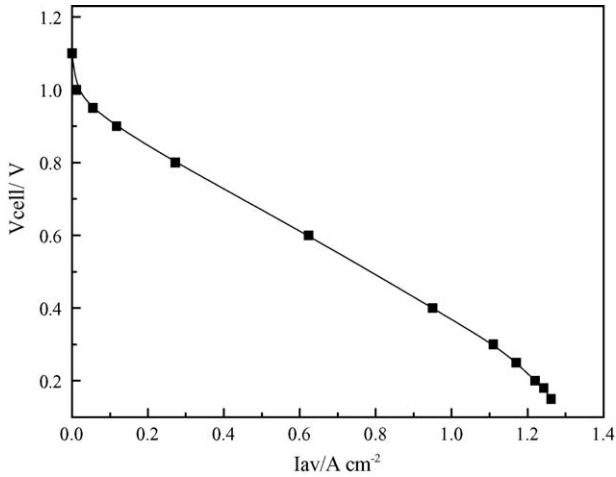
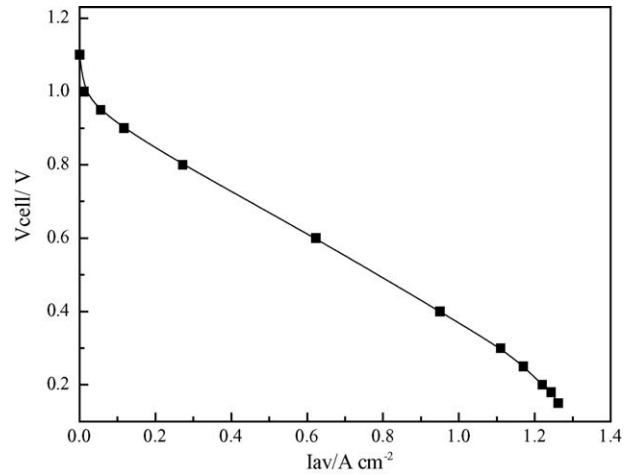


Fig. 7. Effects of catalyst layer porosity.

Fig. 8. Effects of H₂ diffusion coefficient.

ever, the simulated results of the catalyst porosity by the present model show that the variation of the catalyst layer porosity (from 0.02 to 0.6) actually does not affect the PEMFC polarization curve. This resulted from the process simplification in the catalyst layer adopted in the present model. Chan and Tun [22] adopted an agglomerate model for the catalyst layer and their results show a significant effect of the catalyst porosity on the PEMFC performance. Their results indicated that the limiting current of the cell reduces significantly with the decreasing of the catalyst layer porosity. More recently, Yin [12] simulated the effect of the catalyst layer porosity by using an agglomerate model. He found that an overall enhancement of performance of PEMFC was obtained as the catalyst layer porosity is increased from 0.02 to 0.1, and a further increase of porosity renders a decline of performance of PEMFC. These results are opposite to those given by [22]. From the above discussion, we know that the catalyst porosity does affect the PEMFC performance, but an appropriate description of its effect has not been reached yet in the literature. Therefore, the simulation model for the catalyst layer needs to be further improved in order to predict its effect on the PEMFC performance at least qualitatively.

3.4. Diffusion coefficients

The effect of the hydrogen diffusion coefficient, oxygen diffusion coefficient and the water vapor diffusion coefficient in their reference states were investigated and the results are shown in Figs. 8–10. The values of $D_{h,ref}$ range from 2.63×10^{-6} to 1.1×10^{-4} . But only one polarization curve is shown in Fig. 8, which implies that the hydrogen diffusion coefficient hardly affects the PEMFC polarization curve. The effect of $D_{o,ref}$ on the PEMFC polarization curve is significant. Especially in the lower value region, the influence will decline with the increasing value of $D_{h,ref}$. When $D_{h,ref} > 5.0 \times 10^{-5}$, its influence can be neglected. For the investigation of $D_{w,ref}$, the lower limit is reduced to $1.0 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$. From Fig. 10, it can be seen that in the variation range studied, the value of $D_{w,ref}$ does have some effect, but this effect is not as strong as that of

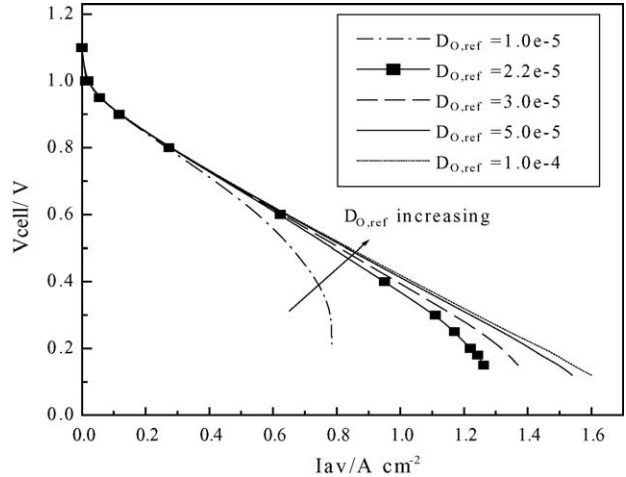
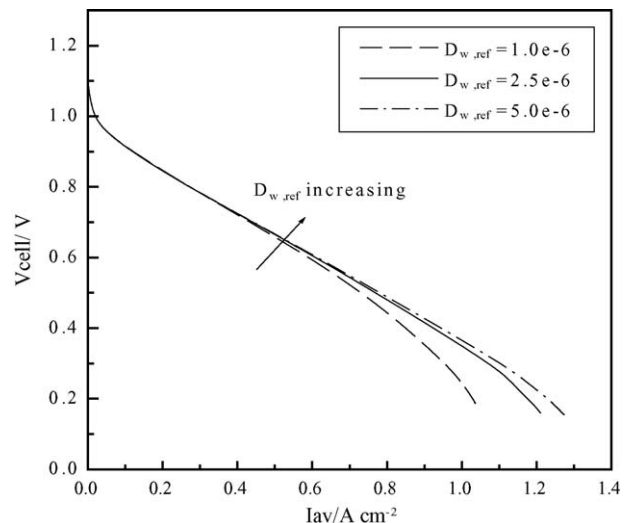
Fig. 9. Effects of O₂ diffusion coefficient.

Fig. 10. Effects of water vapor diffusion coefficient.

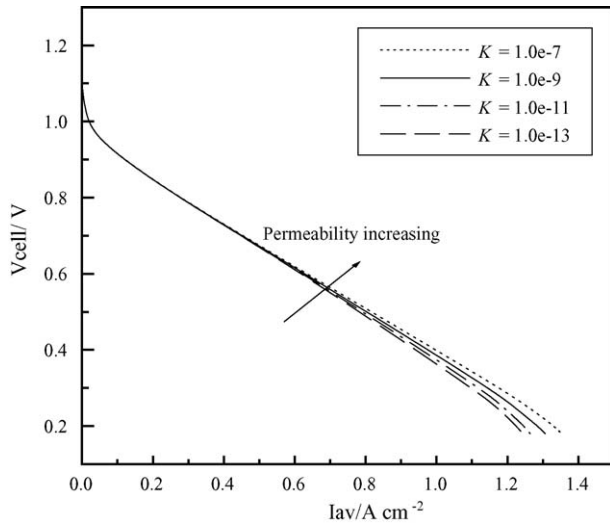


Fig. 11. Effects of diffusion layer permeability.

$D_{o,ref}$. Our numerical simulation practices have shown that when $D_{o,ref} > 1.0 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$, the influence can be neglected.

3.5. The diffusion layer absolute permeability

The effect of the diffusion layer absolute permeability on the PEMFC polarization curve is shown in Fig. 11. In the literature, the variation range of the diffusion layer absolute permeability is extremely wide. Accordingly, in our simulation, a variation range of 1.0×10^{-13} to $1.0 \times 10^{-7} \text{ m}^2$ was selected. As can be seen in Fig. 11, the decrease of permeability will reduce the PEMFC performance a bit, and the “limiting” permeability value is $1.0 \times 10^{-13} \text{ m}^2$, below which the permeability does not affect the performance any more. Qualitatively, these results agree with the simulations reported in literature, but there is some discrepancy. Lum and McGuirk [16] found that the “limiting” permeability value was $1.0 \times 10^{-9} \text{ m}^2$. Kulikovskiy [23] obtained similar results for the direct methanol fuel cell. This discrepancy may have mainly resulted from different models.

3.6. The membrane phase conductivity

In this part of study, two kinds of simulations were conducted. One with a constant membrane phase conductivity, ranging from 3.4 to 17, and the other with a variable phase conductivity, determined by Eq. (22) in the companion paper [21].

The effect of constant membrane phase conductivity on the PEMFC polarization curve is shown in Figs. 12. It can be seen that the PEMFC polarization curve is improved with increasing membrane phase conductivity, and in the lower value region, this improvement is more significant. When the variable membrane phase conductivity is adopted, the polarization curve crosses the curves of the constant membrane phase conductivity, whose membrane phase conductivity ranges from 9 to 15. From Eq. (22) of [21], it can be found that the variable phase conductivity increases with the increase in water content. A small current density leads to a small membrane water content, and hence the membrane phase conductivity is small. This variation trend of

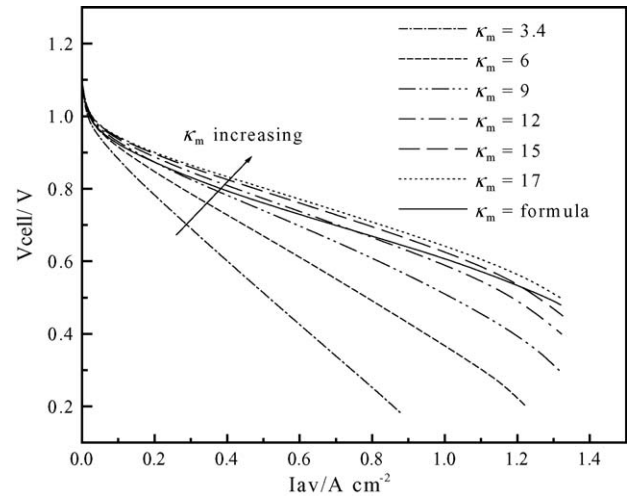


Fig. 12. Effects of membrane phase conductivity.

the membrane phase conductivity with water content leads to the intersection of the polarization curve of a variable membrane phase conductivity with that of constant conductivity. From physical intuition, the polarization curve with a variable membrane conductivity is more reasonable, even though the polarization curves of a constant phase conductivity qualitatively exhibit the phase conductivity effect.

From the above presentation, the following features may be noted. Firstly, the effects of the cathode-side parameters such as cathode transfer coefficient, cathode exchange current density multiplied by specific area and oxygen diffusion coefficient are more significant than those of the anode-side parameters, such as the anode transfer coefficient, anode exchange current density multiplied by specific area, hydrogen diffusion coefficient and diffusion layer absolute permeability. Hence, many researchers focus their interests on the cathode side investigation [9,24,25]. Secondly, the parameters investigated can be classified according to their influence on the polarization curve as: insensitive (ε_{ct} , $D_{h,ref}$ and K); sensitive (α_a , $A_s i_{a,ref}$ and $D_{w,ref}$); and highly sensitive (α_c , $A_s i_{c,ref}$, ε_d , $D_{o,ref}$ and κ_m), such a classification was adopted in [26] for the fuel cell stack parameters. Thirdly, some parameters are actually a function of electrical current, such as the membrane phase conductivity. However, in order to examine its effect on the polarization curve, usually a constant value is assumed during the simulation of each case. Such simulated results can only give qualitative descriptions. For the fuel cell design of optimization, such parameters are better treated as variables.

4. Discussion on model validation approach

4.1. Is the polarization curve sufficient for model validation?

From the above analyses, it can be seen that the PEMFC polarization curve is affected by many parameters, and the effects may be qualitatively different. That is, one parameter may have a pos-

Table 2
Two groups of parameters

	α_a	α_c	$A_s i_{a,ref}$	$A_s i_{c,ref}$	ε_d	ε_{ct}	$D_{h,ref}$	$D_{o,ref}$	$D_{w,ref}$	K	κ_m
Group 1	0.5	0.4	5.0×10^7	120	0.3	0.28	9.15×10^{-5}	2.2×10^{-5}	2.56×10^{-5}	1.2×10^{-12}	6
Group 2	0.4	0.5	5.0×10^8	120	0.3	0.28	9.15×10^{-5}	2.2×10^{-5}	2.56×10^{-5}	1.2×10^{-12}	6

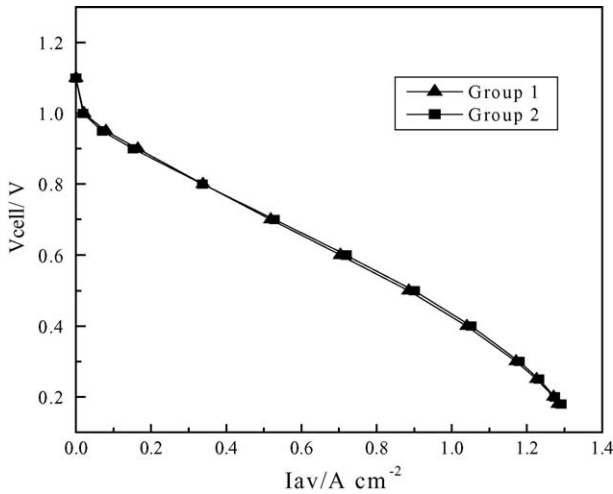


Fig. 13. Two nearly identical polarization curves from two groups of parameters.

itive effect (the cell voltage increases with the parameter) while another has a negative effect. Thus, a question may arise as to whether the polarization curve only can uniquely and reliably demonstrate the validity of a physical and numerical model? In order to answer this question in a very definite way, we have worked out two such groups of given parameter conditions for a PEMFC which can result in almost the same $V-I$ curves.

Such two groups of parameters are listed in Table 2 and the corresponding polarization curves are shown in Fig. 13. For the exactness of the presentation, the one-to-one correspondence of the $V-I$ data are listed in Table 3. It can be seen that the two polarization curves are almost the same, and from the uncertainty allowed from engineering view of point, they may be regarded as the same. So, we can definitely conclude that the polarization curve only is not sufficient for the validation of PEMFC models from an engineering point of view.

As summarized in our previous paper [21], very recently this validation issue has been attracting the interest of more and more authors and several improved approaches have been proposed. These can be classified two types. One type of improved validation approach is the comparison with the polarization curve for three operational conditions (multi-case comparison) proposed by Hu et al. [27], and the other is the multi-step validation

approach adopted in [16,28,29]. The two types of improved validation approach are now further reviewed as follows.

The major idea of the multi-case comparison approach [27] is as follows: (1) for a model to be validated first assuming a set of geometric parameters, the stoichiometric ratios and other operational conditions which are not specified in the test data source, say the one presented in [30], such as $A_s i_{a,ref}$ and $A_s i_{c,ref}$ are adjusted to make the predicted $V-I$ curve match the selected experimental polarization curve; (2) from the data source, another set of $V-I$ curves is chosen which are obtained at different operational pressures. If the same values of $A_s i_{a,ref}$ and $A_s i_{c,ref}$ can also lead to a good agreement between the predicted curve and the test data, then the second level validation is regarded as successful; (3) from the data source another set of $V-I$ curves are obtained at different operational temperatures. Take A_s a constant for a certain electrode [31]. Modify the value of $i_{c,ref}$ according to following equation provided in [32]:

$$\log_{10}(i_{c,ref}) = 3.507 - \frac{4001}{T} \quad (5)$$

If the newly predicted $V-I$ curve obtained with the modified values of $A_s i_{c,ref}$ can still give good agreement with the new set of $V-I$ test data at different operational temperatures, then the validation is considered to be completed with enough accuracy and uniqueness.

It should be admitted that this validation approach seems more rigorous than the conventional one in which only one global polarization curve is compared. However, there still is a large room for uncertainty. As indicated above, the $V-I$ curve is a synthesized outcome resulting from many influencing factors among which some have a positive effect while others have a negative influence. Thus, the reliability and uniqueness of such a validation approach is questionable.

Hakenjos et al. [28] and Ju and Wang [29] pointed out that the polarization curves are not sufficient for the validation of PEMFC models, and they validated their models with the current density distribution. Furthermore, Lum and McGuirk [16] also validated their model with the current density distribution along the channel length and oxygen species distributions in the PEMFC. These researchers believe that apart from the global polarization curve, if the current density distribution or oxygen species distributions in the cell agree well with the correspond-

Table 3
 $V-I$ properties for two groups of parameters

V	0.18	0.2	0.3	0.5	0.6	0.7	0.8	0.9	0.95	1.0	1.1
Group 1 I_{av}	1.283	1.271	1.171	0.886	0.704	0.518	0.338	0.165	0.08	0.0213	7.8×10^{-5}
Group 2 I_{av}	1.291	1.274	1.179	0.9	0.719	0.528	0.337	0.152	0.07	0.019	7.7×10^{-5}

ing experimental data, the model validation can be considered complete and unique.

Theoretically speaking, a full validation approach should include the polarization curve, the local current density distribution and the distributions of all species. However, as indicated in our previous paper [21], difficulties in measurements do not allow us to take such a theoretical validation approach. Thus, our task is to find such a validation approach which includes as few as possible indices while can validate a model with enough engineering certainty. Because of the difficulty involved in the measurement of species distribution, we focus our attention on the global polarization-local density distribution approach, and will call it the “two-step validation approach”. Based on our numerous numerical simulations, we have found that the two-step validation approach is still not enough for a unique and reliable validation. After trying many possible methods, we finally found an appropriate third validation index: the cathode and anode over-potentials.

In the following, the validation approaches proposed in [16,28,29] are applied to our examples to check feasibility.

Fig. 14 shows the current density distribution in the cell for the cell voltage of 0.6 V. The current density data in Fig. 14a are taken at the right side along the channel length, and in Fig. 14b at the half-length of the channel shown in Fig. 1. Fig. 15 shows the

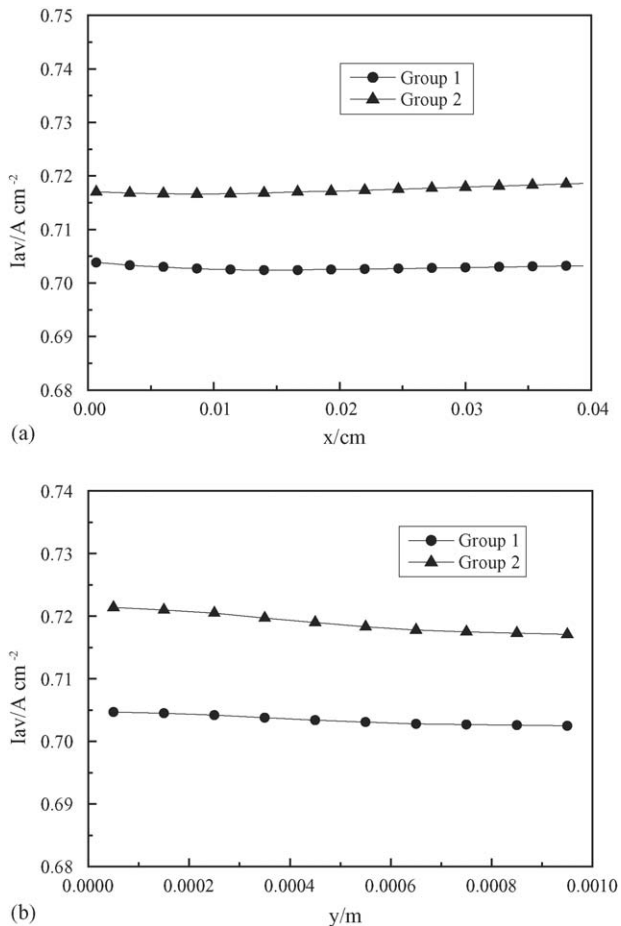


Fig. 14. Current density distributions of the two groups of parameters ($V_{cell}=0.6\ V$). (a) Along the channel length, (b) at the half-length of the channel.

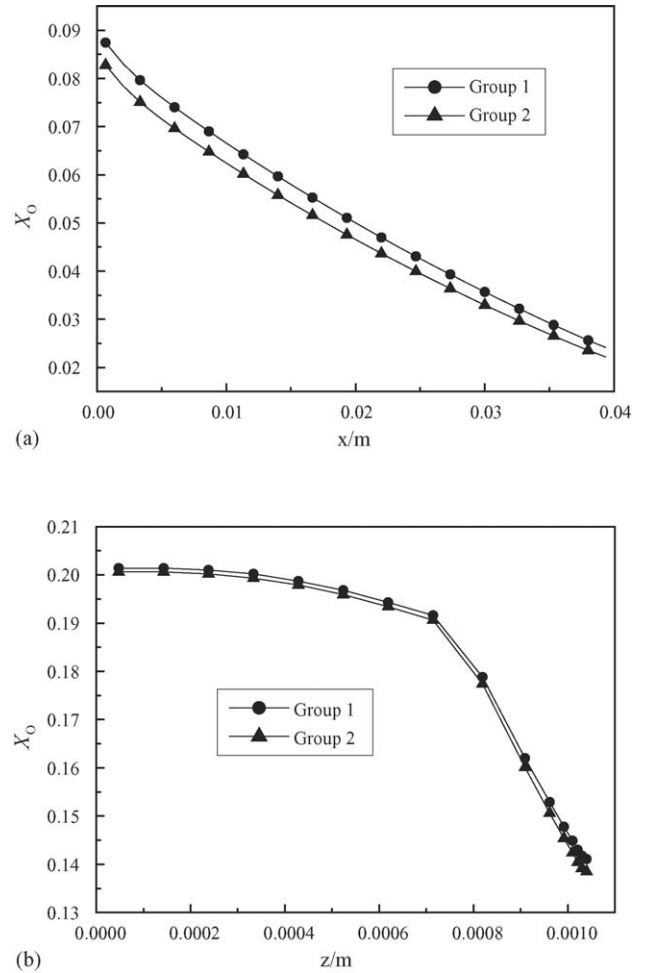


Fig. 15. Oxygen concentration distributions of the two groups of parameters ($V_{cell}=0.6\ V$). (a) Along the channel length, (b) along the through-plane direction.

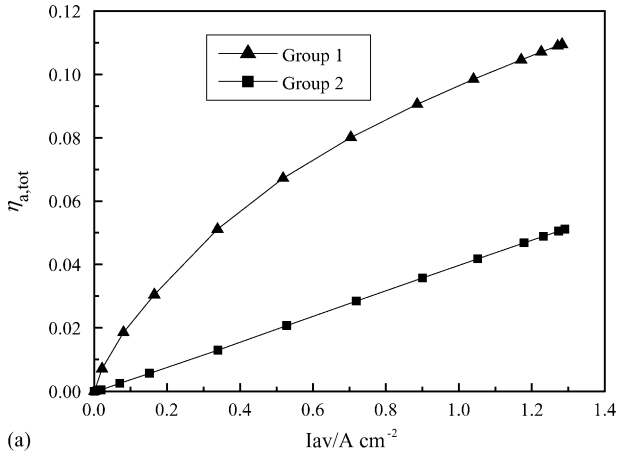
oxygen concentration distributions on the cathode side when the cell voltage is 0.6 V. The oxygen concentration data for Fig. 15a are taken at the catalyst layer adjacent to the membrane on the left side along the channel length, and for Fig. 15b at the half-length of the channel in the through-plane direction. It can be seen that the difference of the current density distributions in the cell for the solutions of the two groups of parameters are not significant. The maximum difference is only about 2%. So, the current density distributions are not sufficient to uniquely validate the PEMFC model. The difference of the oxygen concentration distribution on the cathode side is more significant than that of the current density distribution. The oxygen concentration distribution is taken from the outlet surface of the catalyst layer adjacent to the membrane, and the maximum difference of the solutions for the two groups of parameters is about 8.8%, which may be regarded as large enough to differentiate the two solutions. Thus, the species distributions in the cell can be used as an additional index to uniquely validate the PEMFC models. However, as it has been pointed out, it is very difficult to examine experimentally the species distributions in the channel. It is almost impossible to measure the species distributions in the catalyst layers. Therefore, from a practical point

of view, it is necessary to look for other additional indices by combination of which with the global and local current density validation of a PEMFC model can be conducted completely and uniquely.

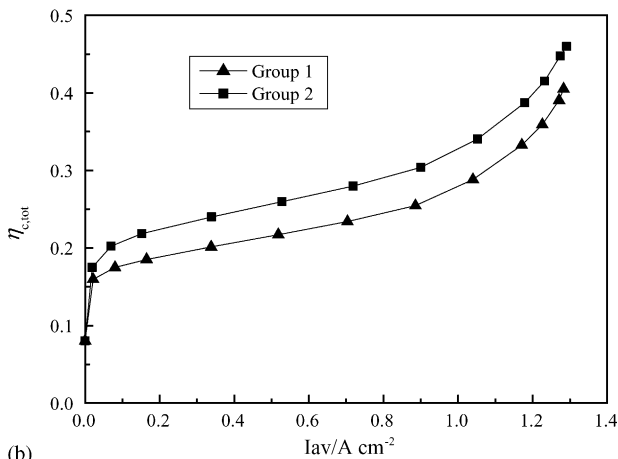
After many numerical practices, we found such an additional index for a reliable and unique validation, i.e. the anode over-potential and the cathode over-potentials. This implies that apart from the global and local current density comparison,

comparison of the numerical anode over-potential and cathode over-potential with the corresponding experimental data can make the validation reliable and unique. Historically, we found that Singh et al. [33] gave the numerical results of anode and cathode overpotential versus electrical current, but they focused on which potential loss was the dominant and did not focus on the validation issue. As far as the feasibility of the cathode and anode over-potentials is concerned, Han et al. [34] recently presented an experimental method to determine the anode over-potential and cathode over-potential. Even though the obtained over-potential data needs special design of the test fuel cell equipment, generally speaking, the measurement of the over-potential is easier than the measurement of the species concentration distributions. Thus, these two over-potentials, especially the cathode over-potential, are proposed as the third validation index.

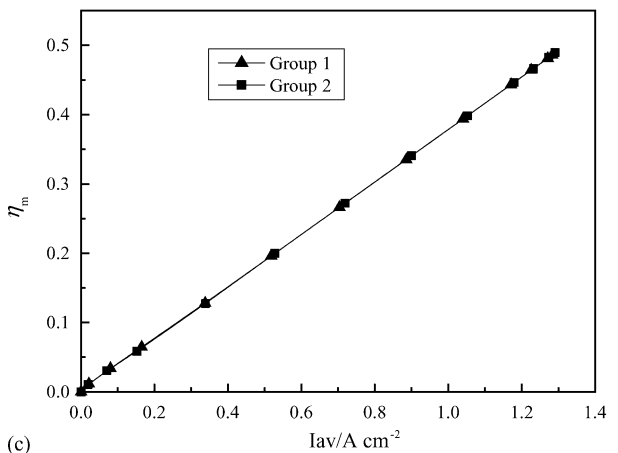
The differences of the over-potential curves for the two groups of parameters are presented in Fig. 16. The results show that the anode over-potential and the cathode over-potential curves are very different for the two groups of parameters. Whereas, the difference between the membrane over-potential curves is trivial. Thus, we propose that a reliable and unique validation approach should include the comparison of the polar-



(a)

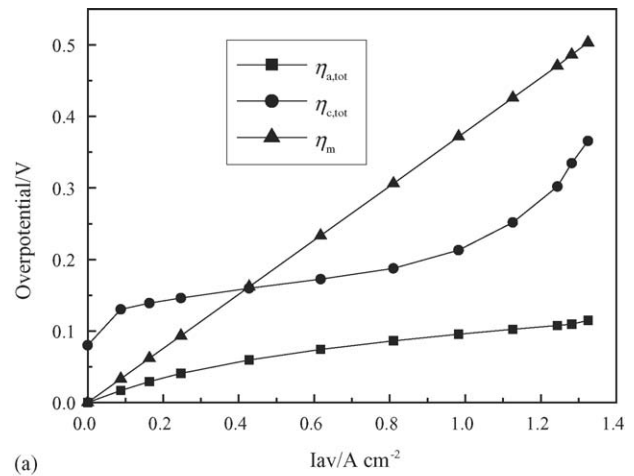


(b)

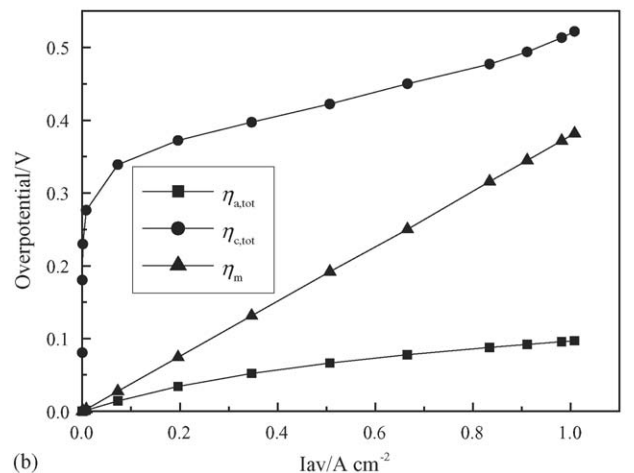


(c)

Fig. 16. Overpotential curves of the two groups of parameters. (a) Anode over-potential, (b) cathode overpotential, (c) membrane overpotential.



(a)



(b)

Fig. 17. Effect of cathode transfer coefficient on the overpotentials. (a) $\alpha_c = 0.2$, (b) $\alpha_c = 0.7$.

ization curve, local current density distribution and the cathode over-potential distributions.

In addition to the third validation index, it should be highly sensitive to the variation of the major influencing factors. Our numerical practices do demonstrate such character for the cathode over-potentials. The following are our numerical results.

The effects of the five major sensitive parameters on the anode, cathode and membrane over-potential curves are shown in Figs. 17–21. From Fig. 17, it can be clearly observed that the cathode and membrane over-potentials change a lot when the cathode transfer coefficient was varied from 0.2 to 0.7. In addition, at these two values of α_c , the dominance of the three losses is different: for a lower cathode transfer coefficient, the membrane loss is the major one with the cathode loss secondary. These results are similar to the numerical results of Singh et al. [33]. Whereas at higher cathode transfer coefficients, the cathode over-potential is higher than the membrane over-potential. From Figs. 18–21, the effects of diffusion layer porosity, the product of cathode exchange current density and specific area, the diffusion coefficient at reference state and the membrane phase conductivity are shown, respectively. The above-mentioned fig-

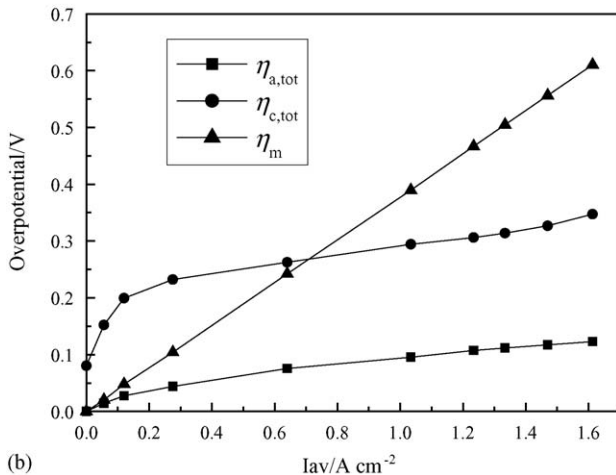
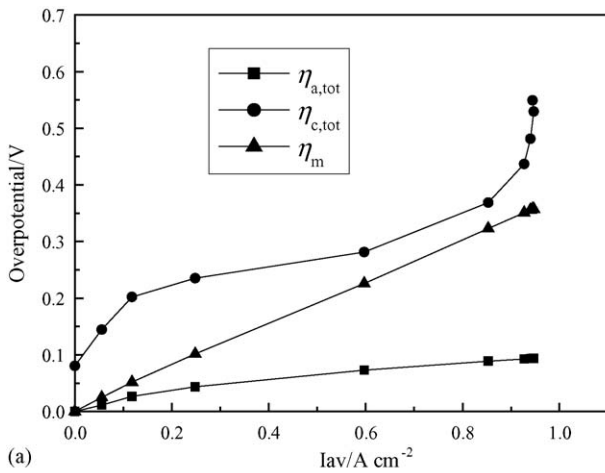


Fig. 18. Effect of diffusion layer porosity on overpotentials. (a) $\epsilon_{diff}=0.2$, (b) $\epsilon_{diff}=0.7$.

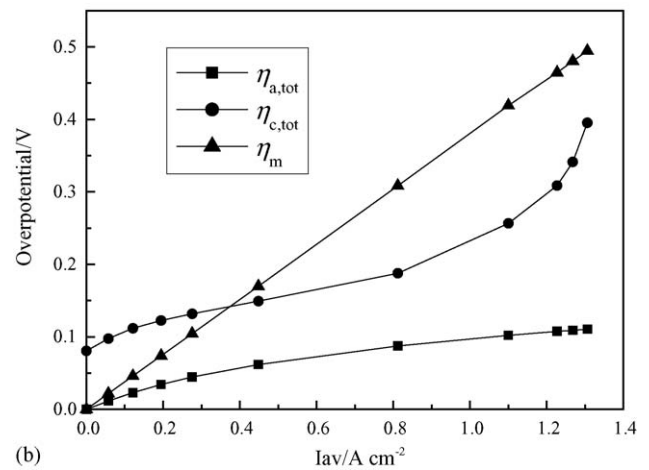
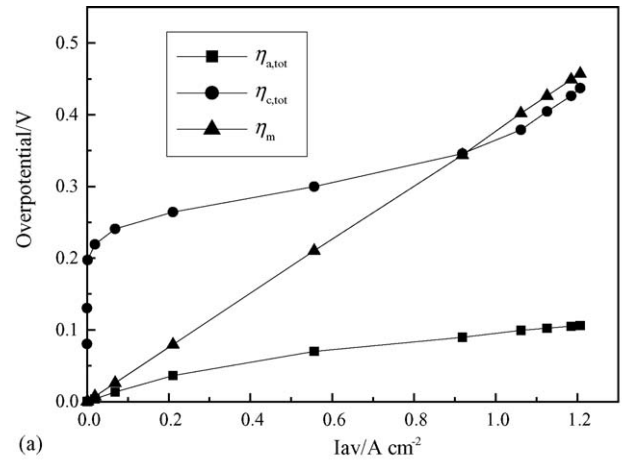


Fig. 19. Effect of cathode exchange current density multiplied by specific area on overpotentials. (a) $A_s i_{c,ref} = 10$, (b) $A_s i_{c,ref} = 1.0 \times 10^5$.

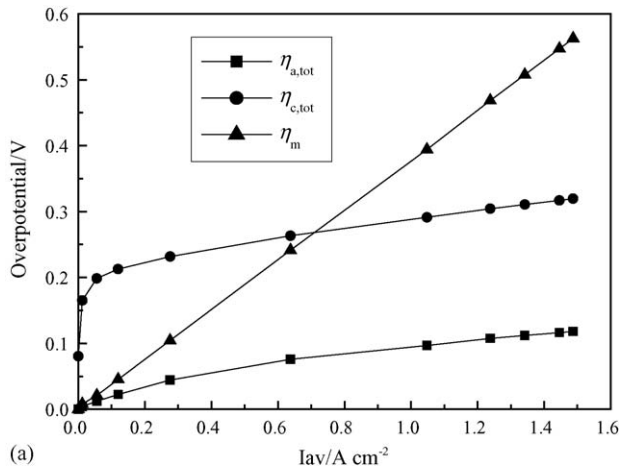
ures all show that the cathode over-potentials are sensitive to these parameters.

4.2. Our suggestions for model validation and presentation of simulation and test results

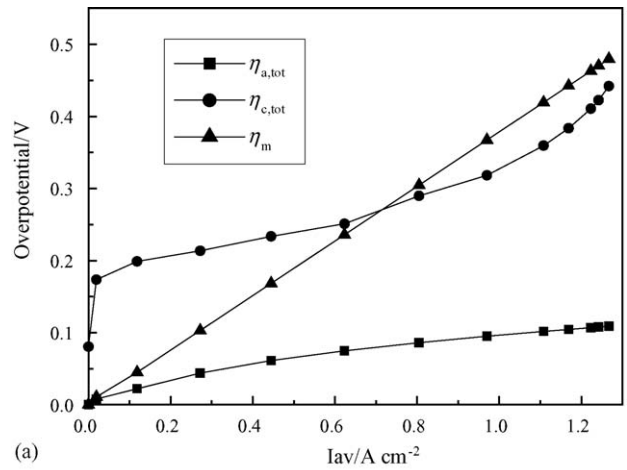
For a reliable and unique validation of a PEMFC simulation model, we propose the following three-step validation approach:

- (1) The test data for a global polarization curve are compared;
- (2) The test data for local current density distribution are compared;
- (3) The test data for the cathode over-potential versus current density curves are compared.

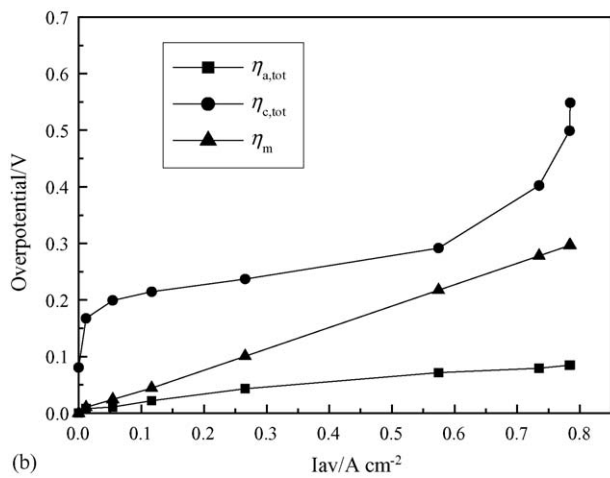
Because of the extreme complexity of the internal process in a fuel cell and the difficulties involved in reliable measurement of the fuel cell parameters, the present authors are fully aware that the model validation issue is far from being solved, and we further propose the following suggestions to the international community of fuel cell researchers in order to accelerate the process.



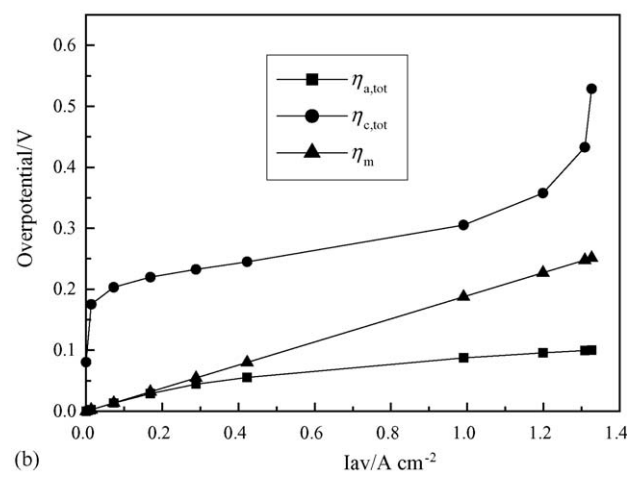
(a)



(a)



(b)



(b)

Fig. 20. Effect of diffusion coefficient at reference state on overpotentials. (a) $D_{o,ref} = 1.0 \times 10^{-4}$, (b) $D_{o,ref} = 1.0 \times 10^{-5}$.

Fig. 21. Effect of membrane phase conductivity on overpotentials. (a) $\kappa_m = 6$, (b) $\kappa_m = 12$.

- (1) When a new model and numerical results are presented, all the simulation parameters involved in the calculation should be clearly provided, so that any other authors can re-compute the presented cases in order to make some comparison.
- (2) When some test data of fuel cell performance, either the global polarization results or the distribution of some species are reported, the test conditions should be provided as much as possible, so that any other researcher can use the data with full confidence.
- (3) Accumulation of reliable test data is extremely important to finally solve the validation issue. Those research groups in the world who possess sophisticated measurement facilities should provide benchmark data for the international community. This situation is quite similar to that when CFD appeared some 30 or 40 years ago and benchmark test data were gradually gathered via the efforts of different research groups in the world. The same discussion also applies to the numerical simulation results.
- (4) Uncertainty analysis for either experimental measurement or numerical simulation is suggested for fuel cell studies so that for any test data or numerical results, we can have a certain confidence. In the mechanical engineering and

CFD/NHT community, uncertainty analysis has long been a necessary condition for the publication of research results [35–37]. In order to apply simulation models to engineering applications, such analysis is indispensable.

5. Conclusions

Based on a three-dimensional, two-phase, and non-isothermal model developed in Part I of this two-article work, the parametric sensitivity analyses of 11 parameters and model validation discussion are provided in this paper. The following conclusions are drawn:

- (1) The performance of a PEMFC is affected by many parameters. The influences of the cathode-side parameters and the membrane phase conductivity are more significant than that of the anode-side parameters, diffusion layer absolute permeability and water vapor diffusion coefficient. The parameters can be classified according to their influence on the polarization curve as: insensitive (ϵ_{ct} , $D_{h,ref}$ and K), sensitive (α_a , $A_s i_{a,ref}$ and $D_{w,ref}$) and highly sensitive (α_c , $A_s i_{c,ref}$, ϵ_d , $D_{o,ref}$ and κ_m).

- (2) The parameters that affect the performance of a PEMFC are many, so that different parameters can lead to the same polarization curves. Hence, the polarization curve only is not sufficient for a reliable and unique validation of a PEMFC model. Two groups of parameters are provided which can result in almost the same polarization curve.
- (3) A three-step validation approach is proposed for a complete and unique validation. These three steps are: (1) validation by the global polarization curve, (2) validation of the local current density distribution curve, and (3) validation by the cathode over-potentials versus current density curve.
- (4) In order to finally solve the validation issue, four further suggestions are proposed to the international fuel cell community. These include the completeness of the data provided, the accumulation of benchmark data and the necessity of introduction of uncertainty analysis.

Acknowledgement

This work is supported by the National Natural Science Foundation of China (No. 50236010, 50425620).

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