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PUBLISHER

European Fuel Cell Forum

VERSION

VoR (Version of Record)

PUBLISHER STATEMENT

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Mao, Lei, Lisa M. Jackson, and Sarah J. Dunnett. 2017. "Investigation of PEMFC Parameter Effects on Practical Fuel Cell System Performance". figshare. <https://hdl.handle.net/2134/26404>.

A1205

## Investigation of PEMFC parameter effects on practical fuel cell system performance

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### Abstract

With the fast development of the commercialization of polymer electrolyte membrane fuel cells (PEMFC), especially for stationary power and automotive applications, the overall price of the PEMFC system must be controlled to a reasonable level, and the key is to keep the performance of the PEMFC system stable during its lifetime. Therefore, in the last few decades, the fault diagnosis of fuel cell systems and the prediction of its remaining useful lifetime (RUL) have received much more attention.

Compared to the fault diagnosis of fuel cells, where a set of studies have been devoted to investigating the diagnostic approaches to fuel cell systems under various loading conditions, only limited research has been found into the RUL prediction of these system. Among the studies performed, fuel cells faults are not considered systematically in the prediction analysis, the fault effect is expressed only with collected measurements, thus the prediction is heavily reliant on the quality of measurements. The reason for not including faults in the prediction is that the influences of fuel cell faults in the system performance are not fully understood, especially the performance decay rate due to these faults.

In this study, a parametric study will be performed to investigate the effects of fuel cell faults on the PEMFC system performance using selected parameters representing typical fuel cell faults. Two parameters related to fuel cell membrane faults, including membrane resistance and electrochemical surface area (ECSA) of the catalyst layer, are selected for the analysis. With a developed and validated PEMFC model, the relationship between fuel cell parameters and PEMFC voltage can be evaluated to study their influences on the system performance. Moreover, the evolution of these parameters with time will also be investigated using semi-empirical equations. From the results, the effect of fuel cell faults can be incorporated in the prediction analysis by updating performance decay rate, and RUL of PEMFC system can be determined with occurrence of single or multiple component faults.

## 1. Introduction

In the last few decades, with the fast application of fuel cells in many areas, including stationary power, automotive, and consumer electronics, the reliability and durability of fuel cells during their operation have attracted more attention, and several studies have been devoted to the diagnostics and prognostics of fuel cells.

According to previous research, various approaches have been proposed for the detection and isolation of fuel cell faults. However, compared to studies devoted to the diagnosis of fuel cells, only limited investigations have been performed to predict the performance and remaining useful life (RUL) of fuel cells. Vural et al. (2009), Becker and Karri (2010), Silva et al. (2014) proposed the adaptive neuro-fuzzy inference system (ANFIS) to predict the fuel cell outputs such as voltage and efficiency, which combined the advantages of neural network and fuzzy logic system. Moreover, Jouin et al. (2014a,b,c) employed particle filtering approaches to update the state of the fuel cell system, with updated fuel cell voltage measurements and threshold values, the remaining useful life (RUL) can be predicted.

It should be noted that as it is difficult to develop an accurate fuel cell model due to its complexity, the above methodologies do not employ fuel cell models in the analysis, which makes the performance of proposed approaches depend largely on the quality of collected data. Moreover, among these approaches, the effect of fuel cell faults on its RUL is not considered systematically, thus when the collected data contain high level noise or is not sensitive to the faults, the results may not be reliable when predicting fuel cell RUL with faults. Based on this, it is necessary to further study the effect of fuel cell faults on the fuel cell performance, especially on the RUL predication results. With the results, the influence of corresponding fuel cell faults in predicted RUL can be better clarified.

In this study, a fuel cell model will be developed and used to study the effect of fuel cell faults on its performance. As the membrane is the key element in a fuel cell and most irreversible degradations are related to the membrane, two parameters related to the membrane faults, membrane resistance and electrochemical surface area (ECSA), are selected for the analysis. Moreover, the evolution of these parameters will be investigated using semi-empirical equations. From the results, the effect of fuel cell faults can be incorporated to the analysis when predicting fuel cell RUL.

## 2. Description of fuel cell model

In the analysis, a fuel cell model is developed to study the effect of fuel cell parameters on its performance. In the model, a set of space differential equations are used to express the mass conservation principles, details of these equations can be found in Pukrushpan (2003), Kahn and Lqbal (2005), Rama et al. (2008), Ous and Arcoumanis (2013). The block diagram of the fuel cell model is depicted in Fig.1.

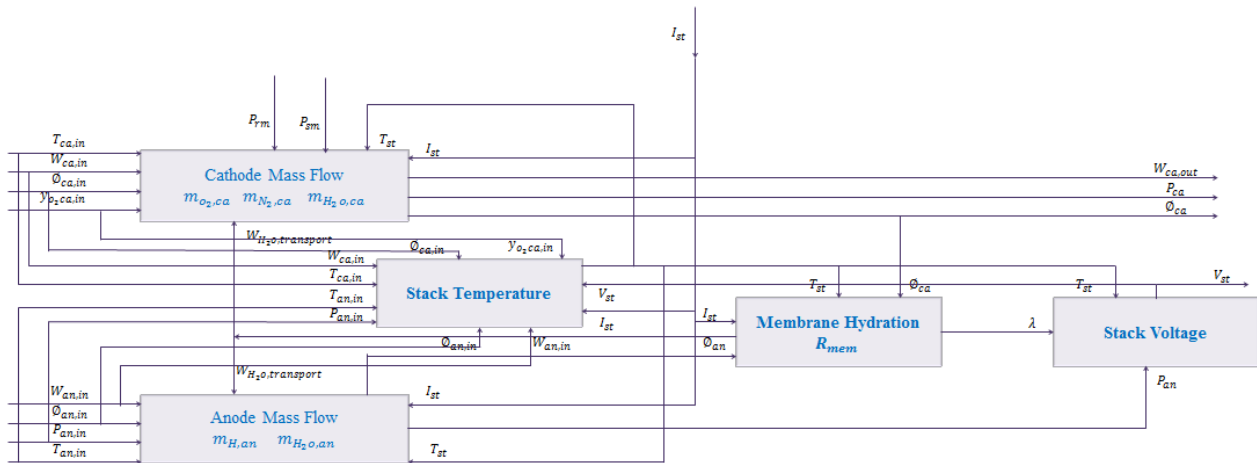


Figure 1 Block diagram of developed fuel cell model

It can be seen from figure 1 that the developed model include modules determining anode and cathode flows, updating fuel cell stack temperature, evaluating membrane condition, and calculating stack voltage.

The performance of the fuel cell model is validated before further analysis. In this study, the polarization curve from a reference paper (Kahn and Lqbal, 2005) was used, and the fuel cell tested in the paper was simulated by configuring model parameters listed in Table 1. With the configured fuel cell model, the polarization curve was obtained and compared to that in the paper, results are shown in Fig.2.

Table 1 Input parameters for fuel cell model from Khan and Lqbal, (2005)

Parameter	Value
Number of fuel cells	54
Active electrode area of single cell	46.5cm <sup>2</sup>
Hydrogen flow rate	1.15 stoich
Air flow rate	2.0 stoich
Hydrogen pressure	3.5 bar
Air pressure	3.5 bar

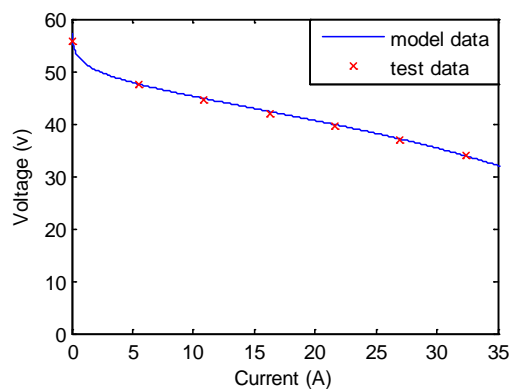


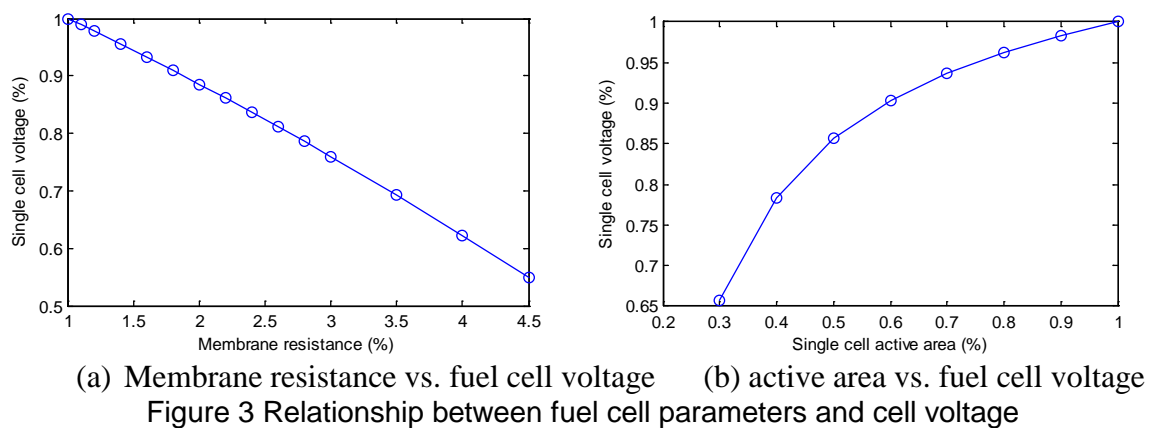
Figure 2 Comparison of polarization curves from the model and test in Khan and Lqbal, (2005)

From comparison of the results, shown in Figure 2, the fuel cell model can simulate the polarization curve with good accuracy, which gives confidence in using the developed model for the following analysis.

### 3. Effect of fuel cell parameters on its performance

With the model described above, the effect of fuel cell parameters on fuel cell performance can be studied. As described in section 1, membrane resistance and ECSA are selected to represent irreversible fuel cell faults, and their effects on the fuel cell performance will be studied.

In the developed model, the ECSA can be changed directly, while the change of membrane resistance can be achieved by modifying membrane thickness. In the analysis, these parameters were reduced gradually and corresponding fuel cell voltage was obtained, the results are depicted in Fig.3. It should be noted that in the results, both parameters and the fuel cell voltage are expressed using percentage change, this can remove the effect due to the consideration of a specific fuel cell, and the results can be used as generic guide after further verification.



From the above results it can be seen that the membrane resistance has an almost linear relationship with the cell voltage, while the relationship between the cell active area and the cell voltage is bi-linear, when reaching a certain value of cell active area (this value may vary for different fuel cell systems), the cell voltage reduction rate will be increased.

As the developed fuel cell model is expected to be used as generic model, these relationships should be valid for other types of fuel cells. For this purpose, the parameters of fuel cell model are modified, including number of cells in the stack, stack outer dimensions and surface area, anode and cathode flow channel parameters, cooling plate dimensions, internal current density, charge and mass transfer coefficients. With these changes, different fuel cells can be simulated, and the relationships between the voltage and the membrane resistance and ECSA determined, these are shown in Fig.4 for 3 different fuel cell configurations, FC1-FC3. It should be noted that the fuel cell parameters have been changed proportionally within reasonable ranges to guarantee the variance of simulated fuel cells (the parameters for FC2 are 0.5 times the parameters for FC1, while parameters for FC3 are randomly selected within the range between 0.5 and 3 times the FC1 parameters). From Fig.4 it can be seen that although the relationships show certain variance, the general trend remains the same, i.e. cell voltage has a linear relation with

membrane resistance, and there is nonlinear relationship between cell voltage and cell active area.

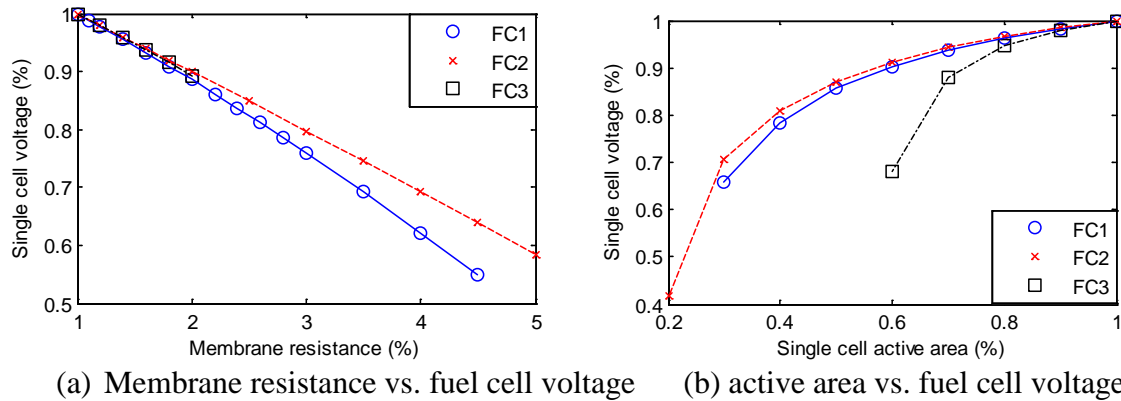


Figure 4 Relationship between fuel cell parameters and cell voltage from different fuel cell systems

During fuel cell operation, fault diagnostic approaches will be performed to identify the occurrence and source of the fault. If a fault is identified, the effect on the fuel cell voltage can be determined using the above results, and the fuel cell RUL can be updated by combining the fault effect in the analysis.

#### 4. Evolution of fuel cell parameters

From the results in section 3, the effects of selected parameters on fuel cell performance have been determined and can be applied in the prognostic analysis to update RUL estimation. However, with these results, the effect of the fault on the fuel cell decay rate can not be evaluated, which may affect the predicted RUL. Therefore, further studies will be performed to study the evolution of fuel cell faults, this can be achieved by studying the evolution of selected parameters.

As an experimental study of fuel cell parameter evolution is complex and time-consuming, semi-empirical equations are used herein for the analysis. The evolution of membrane resistance and ECSA can be expressed by incorporating their effects in the fuel cell voltage calculation (Fowler et al. 2002).

$$V_{\text{cell}} = E_{\text{Nernst}} + \eta_{\text{act,a}} + \eta_{\text{act,c}} + \eta_{\text{ohmic}} + \eta_{\text{concentration}} \quad (1)$$

Where  $E_{\text{Nernst}}$  is the thermodynamic potential (v),  $\eta_{\text{act,a}}$  and  $\eta_{\text{act,c}}$  are anode and cathode activation overvoltage (v),  $\eta_{\text{ohmic}}$  is the ohmic overvoltage (v), and  $\eta_{\text{concentration}}$  is overvoltage due to mass transfer (v).

The ohmic overvoltage can be further expressed as:

$$\eta_{\text{ohmic}} = -iR_{\text{internal}} = -i \frac{rM}{A} \quad (2)$$

Where  $R_{internal}$  is the fuel cell internal resistance ( $\Omega$ ),  $l$  is the membrane thickness (cm),  $A$  is the cell active area ( $cm^2$ ),  $r_M$  is the membrane specific resistivity for the flow of hydrated protons ( $\Omega cm$ ) and can be written as:

$$r_M = \frac{181.6[1 + 0.03(i/A) + 0.062(T/303)^2(i/A)^{2.5}]}{[\lambda_{age} - 0.634 - 3(i/A)]\exp\{3.25[(T - 303)/T]\}} \quad (3)$$

Where  $T$  is fuel cell temperature (K),  $\lambda_{age}$  is the parameter decaying with time, and is a function of relative humidity and stoichiometric ratio of anode and cathode inlet gases, with this parameter, the decay of membrane resistance can be expressed with following equation,

$$\lambda_{age} = \lambda_0 + \alpha \times t \quad (4)$$

Where  $\lambda_0$  is the initial value,  $\alpha$  is decay rate ( $-0.007 h^{-1}$  in Fowler et al.),  $t$  is the fuel cell operating time (h).

It should be noted that the value of  $\alpha$  may be case dependent, and should be determined based on the studied fuel cell. In this study,  $R_{internal}$  can be obtained from the fuel cell model, and  $r_M$  can be determined using Eq.2. With Eq.3,  $\lambda_{age}$  can be calculated, and its evolution can be studied using Eq. 4 to determine the degradation of  $R_{internal}$ .

For degradation of the cell active area, activation overvoltage should be further studied with the following expression (Fowler et al. 2002).

$$\eta_{act} = \xi_1 + \xi_2 T + \xi_3 T [\ln(c_{O_2}^*)] + \xi_4 T [\ln(i)] \quad (5)$$

where  $\xi_1 = -0.948(\pm 0.004)$ ,  
 $\xi_2 = k_{cell} + 0.000197 \ln A + 4.3 \times 10^{-5} \ln c_{H_2}$ ,  $\xi_3 = 6.8 \pm 0.2 \times 10^{-5}$ ,  
 $\xi_4 = -1.97 \pm 0.05 \times 10^{-5}$ ,  $c_{H_2}$  is liquid phase concentration of hydrogen at anode/gas interface ( $mol cm^{-3}$ )

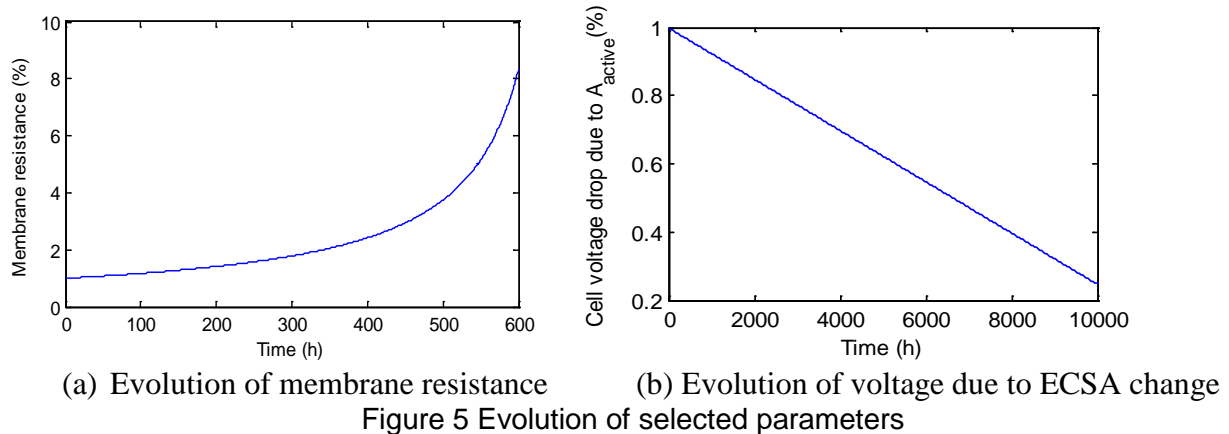
In Eq. 5,  $k_{cell}$  is related to the cell active area and can be used as a measure of ECSA, which will decay with time as follows:

$$k_{cell} = k_0 + \beta \times \frac{t}{T} \quad (6)$$

Where  $k_0$  is initial value,  $\beta$  is the decay rate ( $-0.055 \mu V K h^{-1}$  in the paper), which is also dependent on the investigated fuel cell.

As  $k_{cell}$  can affect activation overvoltage directly, thus its effect on cell voltage can be determined using Eqs.5 and 6.

With above equations, the evolution of  $R_{\text{internal}}$  and voltage drop due to  $k_{\text{cell}}$  can be determined and depicted in Fig. 5.



With above results, the evolution of decay rate due to the selected parameters can be determined. As can be seen, the membrane resistance will change drastically after a certain time (about 500h in this case), which means the fuel cell decay rate due to membrane resistance variation will sudden increase at this time, while the decay rate due to cell active area evolution is increased linearly. Therefore, with these results, an exponential function can be used to express the decay rate due to membrane resistance variation, while decay rate due to ECSA change is a constant value.

The evolution of the membrane resistance was also studied using test data collected from a practical fuel cell system. With polarization curves collected during the system operation, the evolution of Ohmic loss (indicated in Fig.6) can be evaluated, which can be used to indicate variation of the membrane resistance. Fig. 7 depicts the evolution of gradients of Ohmic loss. It should be noted that the x-axis in the figure is the date when the polarization curve is collected, the duration from starting collection point to the point with sudden increase of Ohmic loss gradient is about 3 months, the exact fuel cell system operating time is not available as the system is not under continuous operation. However, the Ohmic loss gradient evolution can be used to configure the coefficients in Eq.4 for the studied fuel cell system.

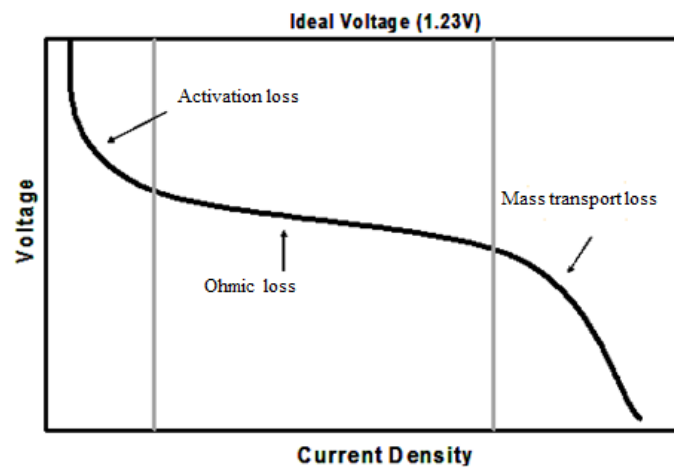


Figure 6 Polarization curve of a fuel cell system

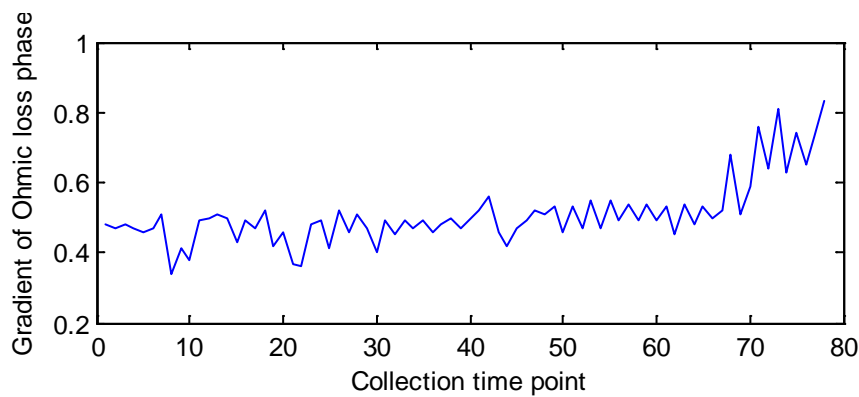


Figure 7 Evolution of Ohmic loss part gradient from collected polarization curve

From above figure, similar evolution trend to results shown in Fig.5(a) can be observed, the Ohmic loss will increase significantly after a certain operation time, which indicate Eqs. 2-4 can be used to express the membrane resistance change with good accuracy after changing  $\alpha$  in Eq.4.

## 5. Conclusions

In this study, the fuel cell model is developed and its performance is validated using test data from references. With the developed fuel cell model, the effect of fuel cell faults on its performance can be evaluated. Two fuel cell parameters are selected in the analysis, membrane resistance and ECSA, as they can be used to represent the membrane faults, which are always irreversible. From the model, the effects of these parameters on fuel cell voltage are determined, which can be considered to update the fuel cell RUL estimation when a corresponding fault is identified. In the study, the percentage change is used to represent the effect and different fuel cell systems are simulated to investigate the effects. Results show that the effects show similar trends, which means the effects are general for these fuel cell systems.

Furthermore, the evolution of fuel cell parameters is determined to update the decay rate in prognostic analysis. The semi-empirical equations are used to study the evolution. From results, bi-value should be used to update the decay rate due to membrane resistance, while decay rate due to ECSA can be updated with a constant value. Moreover, polarization curves collected from a practical fuel cell system are used to investigate the evolution of membrane resistance. Results demonstrate that the membrane resistance from the practical fuel cell system shows similar trend with that from semi-empirical equations.

It should be noted that the coefficients in above results are case-dependent, i.e. their values should be determined from the investigated fuel cells, thus the future work will be performed to apply the proposed approaches in a specific fuel cell system, and the RUL will be estimated to verify its performance.

## Acknowledgement

This work is supported by grant EP/K02101X/1 for Loughborough University, Department of Aeronautical and Automotive Engineering from the UK Engineering and Physical Sciences Research Council (EPSRC).

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