ADAPTATION OF MULTI-PHYSICS PEM FUEL CELL MODEL USING SENSITIVITY ANALYSIS

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ABSTRACT
This paper presents the adaption of an existing multi-physics 1D fuel cell model to an existing PEM fuel cell system. The input parameters of the model are separated into system properties, linked to physical values, and running conditions. On the 40 system properties required, a sensitivity analysis was applied in order to identify that only four membrane properties have the most influence on the stack voltage. These parameter values were identified by optimization. The prediction accuracy with the new parameter values decreased to 1.48%.

Keywords: PEM fuel cell, multi-physics 1D model, sensitivity analysis

1. INTRODUCTION
In the pursuit of a sustainable future with regard to energy production and transportation, fuel cells are among the most promising solutions to produce electric energy whenever and wherever needed in an environmentally friendly way. This is due to the fact that most fuel cells can run on hydrogen and hydrogen can be produced from renewable sources without the need of fossil fuel and the emission of greenhouse gases as CO₂. The potential of fuel cells has already been identified, but their commercialization has not yet developed as expected. In order to push the development of PEM fuel cells for different applications, it is very useful to dispose of a complete and viable fuel cell system model that is able to reproduce fuel cell systems precisely. There is a great number of fuel cell models available that respond to different demands (Chrenko, Péra, Hissel, & Geweke, 2008; Grasser & Rüfer, 2006; Rodatz, 2003). There are electro-chemical models, which are able to describe in detail the mechanisms occurring inside a cell allowing to understand and improve electro-chemical processes (Famouri & Gemmen, 2003). There are also system models, providing information about the overall system. Those global models might be zero dimensional (Miotti, Di Domenico, & Guezennec, 2005), which offer little information and are only interesting in cases without faults. One dimensional models consider the propagation of electrons and protons through the cell and offer an interesting compromise between calculation time and accuracy (Gao, Blunier, & Miraoui, 2009) and three dimensional models, which can describe the behaviour at every point of the cell, but need considerable calculation time (Cheddie & Munroe, 2008). The most important output parameter is the cell or system voltage, which is crucial for the utilization of the fuel cell inside a system (Miotti et al., 2005). Moreover it is important to describe the fluidic domain behaviour of the fuel cell, including not only the hydrogen consumption, but also the influence of air stoichiometric ratio and aspects of humidification (Van Nguyen & Knobbe, 2003). Finally, it is important to consider the thermal aspects of the system, because fuel cells have to be kept in a narrow window of acceptable working temperatures and the system behaviour has big influence on the cell temperature.

Among the big number of available fuel cell models, the 1D three domain models of Gao et al. is remarkable, as it provides high accuracy in the three domains of modelling (electric, fluidic and thermal) and furthermore it is capable to provide results in real time (Gao et al., 2009). Unfortunately this model requires a large number of forty system properties, next to twenty different input parameters. Moreover, this model was only trained and validated for one type for fuel cell system. In order to open the model for a wider range of applications, it has to be adapted for different fuel cell systems. This article presents a method to adapt the existing model to a Bahia system, including the identification and evaluation of the most important system properties using sensitivity analysis.

In the following section the Bahia fuel cell system is presented. This system is used as baseline for the new model. Thereafter, basic aspects of the reference model are presented in section 3. The identification of most important system properties and their evaluation is presented in section 4. Results from the initial model, measurement and adapted model are presented in section 5. The article ends with conclusions and perspectives.

2. BAHIA FUEL CELL SYSTEM
The Bahia Fuel Cell System is a complete 1kW fuel cell system for research and education provided by Helion/Areva (Helion/Areva, 2014). This system has been sold widely throughout universities in France and Europe.
It consists of the complete hardware, including not only the fuel cell and its accessories (pumps, valves, cooling system), but also the electric load and the supervision software, installed in a dedicated computer (Figure 1), the package is completed by a software interface module – Bahia Fuel Cell Simulator – which can be used both in testing and simulation mode.

The Bahia fuel cell system is a proton exchange membrane (PEM) fuel cell and contains 24 cells connected in series to provide a maximum power of 1kW. The system is connected to the software module, allowing system control and supervision, offering the possibility to visualize and save a big number of system parameters, like cell and stack voltages, gas flows and temperatures. Figure 2 shows a schematic representation of the system on the Bahia software module.

The fuel cell system was tested for a ramp up polarization curve with a temperature limit of 70°C. Results are shown in Figure 3.

3. **1D, THREE DOMAIN FUEL CELL MODEL**

3.1. **Model Objective**

The multi physics model by F.Gao et al. (Gao et al., 2009; Gao, Blunier, & Miraoui, 2012) contains electrochemical, fluidic and thermal domain respectively. It has been created to run in real time on a fuel cell emulator and to provide the complete set of system parameters of a fuel cell system.

These parameters contain not only the voltage response of the system, but also temperatures at different locations as well as gas and water flows. It is important to know all those parameters as temperature and humidity influence the fuel cell voltage considerably.

3.2. **Model Structure**

The model presented by Gao et al. (Gao et al., 2009, 2012), describes the behaviour of an entire fuel cell stack.
In order to be precise on the entire stack, the system is broken down to the individual cells, all connected in series and linked by temperature and gas flow. Each of the fuel cells is than divided into 10 different layers containing membrane, cathode and anode, gas layers and cooling layers. For every layer the electric, thermal and fluidic behaviour is calculated and the results are linked. The structure is presented in Figure 4.

3.3. Model Parameters
There are two types of inputs to the model, which have to be treated.

3.3.1. System Properties
The system properties include properties of the fuel cell system that have to be known by the model in order to work properly. These parameters include number of cells and their surface, membrane properties, gas diffusion layer properties, bipolar layer properties, cooling system, anode and cathode properties respectively. There are in total 40 system properties that have to be defined.

3.3.2. Running Conditions
The running conditions represent the ambient conditions at the fuel cell, including temperature at different positions of the system, ambient pressure, and pressure at cathode and anode, cooling channel mass flow rate, etc. In total 20 running conditions are required to model the fuel cell system. The parameters are measured from the Bahia fuel cell system and then given as input to replicate the same conditions as in the experiment.

4. IDENTIFICATION OF MAIN SYSTEM PROPERTIES
In order to represent the Bahia fuel cell stack using the same approach that has been used by Gao et al., the system properties and running conditions have to be known. Even though the running conditions can be measured or approximated, the system properties are very specific and partly confidential data, which are not available.

Methods exist to identify parameters for non-linear, multi-input systems, but their calculation time and the complexity to identify parameters increases with the numbers of parameters to identify (Deb, 2001). Therefore, the sensitivity of the result with regard to the system parameters was analysed, before the most important parameters were identified numerically.

4.1. Sensitivity Analysis procedure
The objective of sensitivity analysis is to find system properties that affect the output stack voltage of PEM fuel cell model most. Knowing the most important system properties allows focusing and identifying their accurate values.

The procedure followed is Multi-parametric sensitivity analysis (MPSA) as introduced by Correa et al. (Correa, Farret, Popov, & Simoes, 2005), (Correa, J M, Borello, F. Santarelli, 2011) and used by Gao et al. (Huangfu, Gao, Abbas-Turki, Bouquain, & Miraoui, 2013). The main steps are as follows:

1. Select the set of the parameters to be analysed: 40 parameters (i.e. system properties) selected.
2. Set the numeric variation range of each parameter: This is set to be ±30% from base value for all 40 parameters.
3. For each selected parameter, generate a series of 500 iteration steps.
4. Run the PEM model using the selected series of 500 numbers for each parameter and then calculate the corresponding objective function value using Eq. (1), for different PEM current values.
   \[ f_i = \sum_{k=1}^{500} \left( V_{cell(i),typical} - V_{cell(i),k} \right)^2 \]  
5. Evaluate the relative sensitivity criteria at different SOFC current values of each parameter by using Eq. (2).
   \[ \phi_i = \frac{f_i}{V_{cell(i),typical}} \]  
6. Evaluate the sensitivity index value (overall relative sensitivity criteria) of each parameter by using Eq. (3)
   \[ \theta = \sum_{i=0}^{l^{max}} \phi_i \]  

4.2. Sensitivity Analysis Results
The sensitivity analysis on the given system leads to the conclusion, that a large number of parameters have low influence on the output voltage. The most important parameter is the membrane section area, which seems to be crucial, followed by the membrane dry density and the membrane thickness and to a lesser degree the membrane equivalent mass. It has to be noted, that the most important parameters are all linked to membrane properties. Gas diffusion layer (GDL), anode and cathode seem to have less influence on the output voltage. The result of the analysis is shown in Table 1. In the following we will concentrate on the four most important parameters.

<table>
<thead>
<tr>
<th>Rank</th>
<th>Parameters (System Properties)</th>
<th>Sensitivity Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Membrane Section Area</td>
<td>1416.3177</td>
</tr>
<tr>
<td>2</td>
<td>Membrane Dry Density</td>
<td>476.1759</td>
</tr>
<tr>
<td>3</td>
<td>Membrane Thickness</td>
<td>223.0769</td>
</tr>
<tr>
<td>4</td>
<td>Membrane Equivalent Mass</td>
<td>77.4765</td>
</tr>
<tr>
<td>5</td>
<td>Catalyst Section Area</td>
<td>10.0850</td>
</tr>
<tr>
<td>6</td>
<td>GDL Porosity</td>
<td>9.7113</td>
</tr>
</tbody>
</table>

Figure 4 Structure of FC stack, cell & layers model presented by Gao et al. (Gao et al., 2009) (Gao et al., 2012).
5. COMPARISON OF RESULTS

Figure 5 shows the results of the model with default, improved model and measurement results, it can be seen, that the identification of the four most influencing parameters leads to a significant improvement of the model with regard to measurement values. The mean error for a polarization curve dropped from 9.58% to 1.48%.

![Figure 5 Modelling and Experimental Results](image)

In order to validate the solution, the optimized system properties were used on a more dynamic current profile. This profile is based on the power demand that might occur in a fuel cell vehicle (based on Renault Zoé vehicle) on the new European driving cycle (NEDC).

This power demand was scaled down so that the peak power demand is within the working limits of the Bahia fuel system. Figure 6 shows the measured and simulated voltage profile. It can be seen that improvements have to be made with regard to the open cell voltage. As seen from figure 5 at low currents the open cell voltage is higher than experimental voltage and in NEDC there many idling / no load and low load phases, the same effect is reflected on the NEDC.

![Figure 6 Comparison of Experimental and Simulated voltage in NEDC](image)

### 4.3. Parameter Identification

As shown before, there is a strong difference with regard to the sensitivity for different parameters. Unfortunately very little information is available for the system, neither from system manufacturer nor from other researchers. Therefore the parameters have to be identified numerically (Laffly, Pera, & Hissel, 2007). Hence, a non-linear, constrained approach based on least-squares method is applied in Matlab Software (Deb, 2001). The initial and optimized parameter values are presented in Table 2.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Default Value</th>
<th>Final Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Membrane Section Area</td>
<td>[m²]</td>
<td>0.1476</td>
<td>0.01</td>
</tr>
<tr>
<td>Membrane Dry Density</td>
<td>[kg/m²]</td>
<td>1970</td>
<td>858.596</td>
</tr>
<tr>
<td>Membrane Thickness</td>
<td>[mm]</td>
<td>0.1279</td>
<td>0.0517</td>
</tr>
<tr>
<td>Membrane Equivalent Mass</td>
<td>[kg/mol]</td>
<td>1.0</td>
<td>0.5055</td>
</tr>
</tbody>
</table>
The parameter identification is done with initial temperature of cathode, anode and cooling channels at 60.8°C. However, for NEDC the same was 30.5°C. The difference in initial temperature reflects on the NEDC simulation. Thus at the beginning of NEDC the experimental voltage is higher and towards the end the theoretical voltage is higher than experimental voltage. This can be attributed to warming up the Bahia Fuel System as the whole driving cycle lasts 1220 seconds.

6. CONCLUSION AND PERSPECTIVES
A precise model is a very important tool in order to complete the research portfolio of a fuel cell system. Even though the Bahia fuel cell system is useful for experiments with regard to different applications, it does only provide a very limited number of technical data. In order to use a physical model, instead of a black box model, an existing multi-physics model - capable of doing real time evaluation - was chosen and its forty system properties were analysed with regard to their sensitivity on the model result. The sensitivity analysis showed that only few system properties have a big influence on the stack voltage and that all the most influencing parameters are linked to membrane. Afterwards, the four most influencing parameters are identified with the help of a non-linear constrained parameter identification based on least squares method. Those results are re-injected into the model and show considerable improvement of the model results in comparison to the measurement values.

In the following the four most important system properties have to be identified more accurately, for different working temperatures. With improved parameters, the model will be used for different applications, which may contain real time application.

REFERENCES


AUTHORS BIOGRAPHIES

Raaj Ganesh SAMIKANNU RAMESH was born in Tamil Nadu, India in 1988. He received Bachelor of Engineering degree in Automobile Engineering in 2005 at PSG college of Technology affiliated to Anna University, Chennai, India. He worked in Automotive Transmission engineering, research, design and development division of Maruti Suzuki India Limited, New Delhi India for 3 years. He is currently pursuing Masters in Automotive Engineering for Sustainable Mobility jointly conducted by École d'ingénieurs Polytech Orléans affiliated to University of Orleans, Orleans, France and Institut Supérieur de l’Automobile et des Transports (ISAT) affiliated to University of Franche Comté in Belfort, France in 2008. His research is linked to technologies for automotive applications, namely hybridization, battery technology and fuel cell systems. He is now working as a research intern at Laboratory DRIVE, affiliated to ISAT & University of Burgundy. He is currently working on the modelling of low temperature fuel cell systems.

El-Hassane AGLZIM was born in Morocco February 13, 1981. AGLZIM received in 2004 the “DESS” degree (specialized graduate degree) degree in embedded electronics systems from the University of Metz, France. In 2005, AGLZIM received the M.Sc. degree science engineering, from the University of Nancy, France. After that, he joined the Instrumentation and microelectronics Group of the LIEN Laboratory LIEN), University of Nancy, France, in October 2009 AGLZIM obtained the Ph.D. degree in the Instrumentation and Microelectronics (IM) Science at the University of Nancy. His Ph.D. thesis was entitled ‘Characterization by electrochemical impedance spectroscopy method of the complex impedance of a fuel cell - evaluation of the influence of humidity’. From 2009 to 2010, he completed a Postdoc in the System and Transportation Laboratory (SeT) in Belfort, France. He joined the Energetic team of the ISAT in September 2010 as an associate professor. He works in the field of fuel cells and has published several articles in the domain. His current research interests the diagnosis of fuel cells by using the Impedance Spectroscopy method. In parallel to his research works, he teaches electrical engineering, signal acquisition, electrical motors and hybrid vehicles.

Daniela Chrenko was born in Germany in June 1978. She received the Dipl-Ing. FH degree in applied physics of the university of applied sciences in Wedel, Germany in 2002, the MSc of process engineering at the university of applied sciences in Hamburg Germany in 2006 and the PhD for the study of on-board hydrogen production for low temperature fuel cell systems at the university of Franche Comité in Belfort, France in 2008. Her research is linked to technologies for automotive applications, namely hybridization, battery technology and fuel cell systems. She worked on Stirling engines in combination with high temperature fuel cell systems. The aim of her current research is to increase energy efficiency in transportation applications, including studies of energy demand, energy management and main system components as batteries and fuel cell systems. She is now working as associate professor at the University of Burgundy and teaching electrical engineering, signal acquisition, electrical motors and hybrid vehicles.

Luis Le Moyne was born in Mexico City, on April 24, 1969. He received in 1992 the Engineer degree from the Ecole Nationale Supérieure d’Arts et Métiers (Paris tech), in 1993 the D.E.A degree in Energy Conversion, from the University of Paris 6, France. He developed advanced modelling of Diesel engines for airborne. After that, he joined the Physics & Mechanics lab, University Pierre and Marie Curie (Paris VI), France, where he started his Ph.D. thesis under the supervision of Pr. J. Jullien. In 1997 he obtained the Ph.D. degree in the Energy Conversion Science at the Ecole Nationale Supérieure des Arts et Métiers (Paris Tech). His Ph.D. thesis was entitled ‘Air/Fuel excursions reduction in transient functioning of S.I Engines’). From 1998 to 2008, he was an associate lecturer in the University Pierre and Marie Curie (Paris VI). In September 2007, he was awarded the «Habilitation à Diriger des Recherches» (HDR) from University Pierre and Marie Curie (Paris VI). For his research on ‘Reactive mixture formation studies in internal combustion engines’. In September 2008 he joined ISAT University of Burgundy where he founded the energy, propulsion, electronics and environment department, and in February 2011 was nominated director of institute.