



## Global parameters sensitivity analysis and development of a two-dimensional real-time model of proton-exchange-membrane fuel cells

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### ABSTRACT

This paper presents a 2-D real-time modeling approach for a proton-exchange-membrane fuel cell (PEMFC). The proposed model covers multi-physical domains for both fluidic and electrochemical features, which considers in particular the flow field geometric form of fuel cell. The characteristics of reactant gas convection in the serpentine gas pipeline and diffusion phenomenon through the gas diffusion layer (GDL) are thoroughly considered in fluidic domain model. In addition, a three levels iterative solver is developed in order to accurately calculate the implicit spatial physical quantities distribution in electrochemical domain. Moreover, the proposed 2-D real-time modeling approach uses a numerical method to achieve a fast execution time, and can thus be further easily applied to any real-time control implementation or online diagnostic system. After experimental validation under different fuel cell operating conditions, an iterative Least Angle Regression (LAR) method is used to efficiently and accurately perform the global parameters sensitivity analysis based on Sobol definition. The online analysis results give an insight into the influences of modeling parameters on fuel cell performance. The effect of interactions between parameters' sensitivities is especially investigated, which can provide useful information for degradation understanding, parameters tuning, re-calibration of the parameters and online prognostic.

### 1. Introduction

During the last few decades, electric vehicles (EVs), and most recently hybrid electric vehicles powered by fuel cells (FCHEVs) have a fast growing interest due to environment pollution and energy crisis. Different from conventional energy device for example thermal machine, fuel cells have been commonly considered as a more suitable energy conversion device for long-range EVs, due to their advantages of compactness, fast fueling time and high conversion efficiency [1–3]. As one type of fuel cell technologies, proton-exchange-membrane fuel cell (PEMFC) has all the above mentioned advantages. In addition, compared to other fuel cell types, PEMFC can provide higher power density for transport and portable applications with relatively lower operation temperature and pressure [4,5].

Nevertheless, before its mass commercialization, there is still much

research to be done. One of the major challenges of PEMFC is the design of appropriate control strategies and auxiliaries to achieve its optimal working modes (cooling circuit, humidifier, air compressor, power converters, etc.) [6]. On the other hand, the fuel cell lifespan should be increased in order to meet the requirements of transportation applications. In addition, as a complicate energy conversion device, fuel cell directly converts electrochemical energy into electricity; it has different inter-coupled nonlinear behaviors in multiple physical domains. In practice, it is very difficult to observe the internal variables and state of fuel cell during its operation. A good understanding of how these parameters impact the fuel cell performance would be very useful for fuel cell system design and control development. Therefore, an accurate multi-physical PEMFC model could greatly help the system control strategy development and the parameters sensitivity analysis. Compared with 1-D models [7–9], a 2-D PEMFC model has the capability to

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provide two-dimensional behavior, which is very useful for spatial non-uniformity and control coupling analysis. This analysis can give detailed and valuable spatial physical quantities information under different fuel cell operating conditions by taking multiple spatial dimensions into consideration.

Many control-oriented PEMFC 2-D models have been previously proposed in the literature [10–17]. However, a common drawback of these works is that the presented fuel cell bipolar plate flow field (gas channels) models are over-simplified (or not even considered). Thus they cannot describe accurately the non-linear and non-uniform pressure distribution characteristics. For example, the gas pressure prediction results of a model without the consideration of channel geometric form, could lead to an inaccurate gas diffusion phenomenon in the serpentine pipeline, which would further impact the accuracy of electrode current density analysis. In these models, the gas supply channel is assumed to be straight and single. In fact, the gas supply pipeline at the anode and cathode sides may have different geometric patterns. For example, the flow field form of Ballard NEXA 1.2 kW fuel cell stack used in this paper includes a single serpentine pipeline in anode side and a parallel serpentine pipeline in cathode side. Therefore, a comprehensive representation of non-homogeneous gas phenomenon by fully taking the geometric form of the fuel cell pipeline into consideration is particularly useful to achieve more confident and reliable spatial distribution information for 2-D model of PEMFC. On the other hand, for the purpose of real-time control implementation and online prognostic, the computational efficiency of a control-oriented PEMFC fuel cell model is crucial for model based control process. The commonly used Computational Fluid Dynamics (CFD) modeling of fuel cell [16,17], who uses complex partial differential equations to describe the gas flow in the flow field, are however not suitable for real-time model-based controller and online diagnostic system since the computational burdens are too heavy.

Under calculation efficiency premise, an accurate mathematical PEMFC model generally incorporates both semi-empirical and physical parameters in different physical domains. However, many semi-empirical parameters, such as electrode charge transfer coefficient or electrode porosity, are very difficult or even impossible to be theoretically determined. On the other hand, the physical parameters in membrane electrode assembly (MEA) (for example the thickness of GDL) are very difficult to determine by measurement due to the thickness in micrometer range. Moreover, it should also be noted that, all the parameters values may change during the fuel cell degradation, as well as their sensitivities. Therefore, as an important step during the fuel cell model development, performing a parameter sensitivity study can provide us useful information for parameters tuning, modeling assumptions and aging parameters recalibration. In the literature, Corrêa et al. [18] investigated the effects of ten parameters on the fuel cell performance, using multi-parametric sensitivity analysis (MPSA). Dalsam et al. [19] presented the fuel cell cathode catalyst layer parameters sensitivities study based on a mathematical model in a steady-state condition. The proposed model covers different physical domains. Zhou et al. [20] presented a parameters sensitivity study based on a lithium-ion battery model using MPSA method. However, most of these analyses are based on 1-D models, and their sensitivity analyses are investigated only on a single parameter.

In addition, these sensitivity analyses only evaluate the effect of a single parameter on the model performance. The main drawback of this local sensitivity analysis is that the evaluation of simultaneous effects of all parameters on the model is ignored. In reality, the fuel cell is an inter-coupled nonlinear multi-physical system, lots of model parameter variables are coupled, and the variation of one parameter may influence the others. Therefore, in addition to the single parameter sensitivity, the interactions between parameters have to be evaluated using a more systematic and comprehensive analysis method.

The global sensitivity analysis method is a satisfactory solution for this problem [21,22]. In the global sensitivity analysis method, all the

model parameters are varied simultaneously over a certain parameter range. By using this method, not only the local influence of each individual parameter, but also the interactions between different parameters on the fuel cell model performance can be effectively measured. However, such global parameters sensitivity study for fuel cell applications has not been reported so far in the literature.

A 2-D multi-physical real-time model of PEMFC is fully developed in this paper. The major contributions of this paper can be summarized as follows:

- (1) A novel non-uniform control volume mesh grid is defined in fluidic domain model based on channel geometric form, in order to thoroughly describe the under-rib convection between neighboring channels by fully considering the flow field geometric patterns of fuel cell.
- (2) An iterative solver has been developed to solve the implicit spatial physical quantities distribution in electrochemical domain. This original iterative solver algorithm is composed by three interactive computational loops and uses a robust convergence method for real-time computation.
- (3) An iterative Least Angle Regression (LAR) method is used to efficiently and accurately perform the global parameters sensitivity study based on Sobol definition. The analysis results provide an insight into the influence of each individual parameter on the fuel cell performance, and further analyze the significance of the interactions between each parameter of fuel cell in real-time. Such online analysis allows model-based controller or diagnostic system to take fast decisions and actions.

The paper is organized as follows: a 2-D PEMFC model, which covers two multi-physical domains: fluidic and electrochemical, is proposed in Section 2. Section 3 gives the model implementation and experimental validation. Section 4 uses an iterative least angle regression method to provide online global parameters sensitivity analysis results. Section 5 presents final conclusions and future works.

## 2. Multi-physic 2-D PEM fuel cell model

In this section, a full 2-D, multi-physical PEMFC model is presented. Different from the previously developed PEMFC models [23–25], the proposed model fully considers two-dimensional convection and diffusion phenomenon in fluidic domain, and spatial physical quantities in electrochemical domain. Moreover, the proposed model is oriented to the real-time calculation, in order to effectively perform the global parameters sensitivity analysis.

Fig. 1 shows the basis of individual layers in a single cell of the proposed fuel cell stack. From Fig. 1, a single cell model consists of 7 individual layers: (1) cathode gas supply channel; (2) cathode gas diffusion layer (GDL); (3) cathode catalyst layer; (4) membrane; (5) anode catalyst layer; (6) anode gas diffusion layer (GDL); and (7) anode gas supply channel. Moreover, the fuel cell operation temperature is considered as an input in each individual layer.

### 2.1. Electrochemical domain model

The total output voltage  $V_{cell}$  of a single-cell can be calculated by the following equation:

$$V_{cell} = E_{cell} - V_{ohmic} - V_{act} \quad (1)$$

where  $E_{cell}$  is the single fuel cell thermodynamic voltage (V),  $V_{ohmic}$  is the Ohmic voltage drop (V),  $V_{act}$  is voltage drop due to activation (V).

The following Nernst equation is used to calculate thermodynamic voltage  $E_{cell}$  [26]:

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