

DISTRIBUTED PARAMETER MODEL SIMULATION TOOL FOR PEM FUEL CELLS

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RESUMEN: *En este trabajo se ha desarrollado una herramienta de simulación para pilas de combustible tipo PEM, basada en un modelo de parámetros distribuidos. La herramienta está diseñada para realizar estudios de variaciones espaciales y temporales a lo largo de los canales de alimentación de reactantes. El trabajo muestra y analiza los resultados de simulación de una monocelda monocanal. Las variables estudiadas son las concentraciones de los reactantes, presiones, temperaturas, humidificación, contenido de agua de la membrana, corriente, entre otras que influyen significativamente sobre el rendimiento y durabilidad de las pilas PEM.*

ABSTRACT: *In this work, a simulation tool for proton exchange membrane fuel cells (PEMFC) has been developed, based on a distributed parameter model. The tool is designed to perform studies of time and space variations in the direction of the gas channels. Results for steady-state and dynamic simulations for a single cell of one channel are presented and analyzed. Considered variables are concentrations of reactants, pressures, temperatures, humidification, membrane water content, current, among others that have significant effects on the performance and durability of PEMFC.*

Palabras clave: PEMFC, modelado de parámetros distribuidos, simulación dinámica

Keywords: PEMFC, distributed parameter modeling, dynamic simulation

1. INTRODUCTION

In recent years, the proton exchange membrane fuel cells (PEMFC) technology has been incorporated to a wide range of portable, stationary and automotive applications [1]. However, despite current developments, PEMFC are still not accepted as a practical power generator. The key challenge is to reduce the cost and achieve a high performance and long life of the cells.

Variations in the concentrations of hydrogen, water and oxygen, as well as temperature, have significant effects on the performance and durability of PEMFC. All these variables exhibit spatial dependence in the direction of the channels of the anode and cathode and, therefore, it is necessary to introduce partial differential equations (PDE) if they are to be taken into account.

Indeed, distributed parameter first principles modeling allows the detailed study of the fundamental phenomena that occur within a PEMFC. Pioneering one-dimensional distributed parameter models were developed by Bernardi and Verbrugge [2] and Springer et al. [3]. In the last decade, two-dimensional and three-dimensional models have been developed [4-5]. Most recently, a detailed two-dimensional simulation model was presented by Mangold et al. [6] for control purposes.

There are various simulation tools for PEMFC [7], however, very few are flexible enough to manipulate the underlying model equations, which is necessary in order to apply model order reduction techniques and design model-based controllers.

This work is focused on the development of a simulation tool that allows the analysis of variables with important spatial variations, which affect PEMFC performance and durability. The tool is based on a detailed distributed parameter model to be used in model-based controllers.

The paper is organized as follows. Section 2 shows the structure of the modeled system. Section 3 describes the model equations. Section 4 covers the tasks of simulation tool development. Section 5 presents simulation results and Section 6 concludes on the work developed.

2. DESCRIPTION OF THE SYSTEM

This work considers a single cell of one channel (Fig. 1) that includes all the functional parts of the PEMFC: bipolar plates (BP), gas channels (GC), gas diffusion layers (GDL), catalyst electrode layers (CL), a proton exchange membrane and a cooling system. This simple model suits the detailed analysis of spatial variations. The case study selected in the work is a 0.4 m along-the-channel single cell (area

0.4×10^{-3} m) with Nafion 117 membrane. The parameters of the membrane are taken from [8].

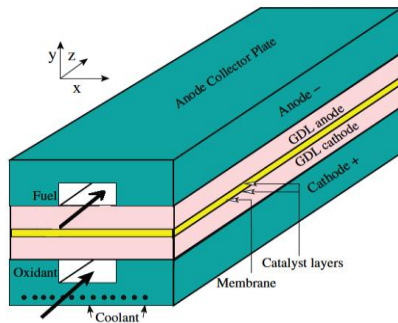


Fig. 1. Structure of the single cell considered in this work.

3. DISTRIBUTED PARAMETER MODEL

The model equations are based on the work by Mangold et al. [6]. This is not only a very recent model, but it is also one of the most detailed set of PEMFC equations in the open literature. The model is 1+1D with approximation of gradients by a fixed number of points in y-direction and partial differential equations along the channel (z-direction) (Fig. 1).

Physical phenomena occurring within the gas channels is represented by the solution of conservative equations for mass, momentum and energy. The principle of mass conservation is used to model reactant concentrations. A pressure drop relation, similar to Darcy's law, allows the calculation of the flow velocity. The ideal gas law is used to calculate flow pressure. An energy balance is used to determine the flow temperature.

Stefan-Maxwell diffusion equations for a multicomponent gas are used to define the mole fraction gradient in the gas diffusion layers (GDL).

The reaction rates are modeled by Butler-Volmer equations and Faraday's law. Membrane behavior is described by the calculation of membrane water content, water concentration, drag coefficient, net water flux and protonic conductivity. The gas diffusion layers (GDL), catalyst layers (CL) and membrane are considered to be at the same temperature level. These PEMFC components form the solid part.

An energy balance for the solid part, similar to the energy balances of the gas channels (GC), is used to calculate the solid part temperature. Current transport is described by governing equations for conservation of charge and the cell potential is calculated by the polarization curve equation. In this relation activation polarization losses, ohmic losses and concentration losses are considered. The combination of these laws results in a set of PDE and algebraic constraints.

4. MODEL IMPLEMENTATION

The set of PDE and algebraic constraints was discretized spatially along the channel using finite differences. As a result, a set of differential algebraic equations (DAE) was obtained. This new set of model equations was implemented and numerically solved in Matlab®, using a DAE solver.

The simulation model consists of six submodels that are coupled by internal variables. The GC module models reactant concentrations, flow velocity, pressure and temperature in the gas channels. The GDL module studies diffusion in a multicomponent mix of species. The electrochemical reactions and mass fluxes are modeled in the CL submodel. The membrane module consists of a detailed protonic exchange membrane model [8].

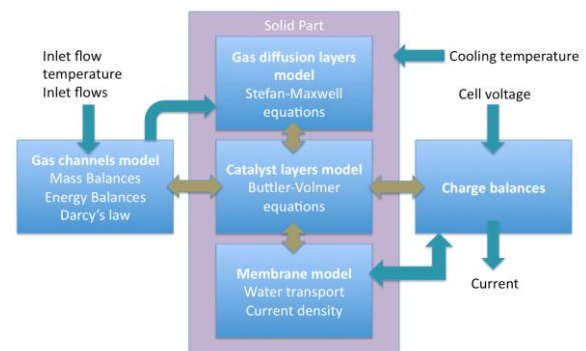


Fig. 2. Scheme of the simulation model.

The solid part module consists of an energy balance to determine the solid part temperature. Finally, cell current and voltage are determined in the charge balances module. The inputs are inlet flows for anode side and cathode side, inlet flows temperatures, cooling temperature and cell voltage. The main output is cell current, but it is possible to have cell current as an input instead of cell voltage. This depends on the operation mode desired. Fig. 2 shows the connections between submodels, inputs and outputs, as well as the phenomena modeled in each module.

5. SIMULATION RESULTS

In order to show the possibilities of the tool, the results of simulations for different variables are shown. Operation conditions are given in Table 1. In order of appearance top-down, left-right, the inputs to the model are: hydrogen and water inflow on anode side, oxygen, water and nitrogen inflow on cathode side, temperature of inflows, cell voltage and coolant temperature.

Table 1. Operation conditions.

Var.	Setpoint	Var.	Setpoint
$\dot{n}_{H_2,in}^A$	3.5 mol m ⁻² s ⁻¹	$\dot{n}_{N_2,in}^C$	35 mol m ⁻² s ⁻¹
$\dot{n}_{H_2O,in}^A$	1 mol m ⁻² s ⁻¹	T_{in}^C, T_{in}^A	350 K
$\dot{n}_{O_2,in}^C$	10 mol m ⁻² s ⁻¹	V	0.8 V
$\dot{n}_{H_2O,in}^C$	5 mol m ⁻² s ⁻¹	T_{cool}	345 K

5.1. Steady-state simulation results

The steady-state results of some important variables considered in the model are presented in this section. Fig. 3 shows spatial profiles of the concentration of reactants (hydrogen and oxygen), nitrogen and water in anode and cathode gas channels. Reactants concentrations are higher at the beginning of the channels, which is the zone of major exothermic reaction rate. In this pressure driven model, nitrogen concentration changes because of flow velocity variation along the channel.

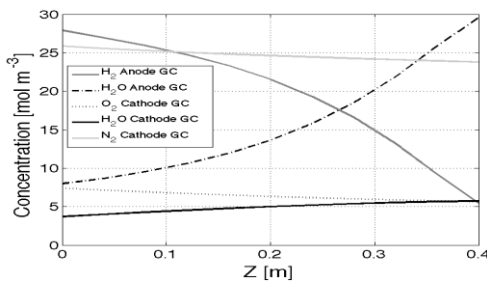


Fig. 3. Spatial profiles of concentration of reactants, nitrogen and water in the gas channels.

Water increases in both sides of the membrane due to water generation on cathode side and back-diffusion on anode side. Fig. 4 shows the current density profile along the channel (right side). It can be seen that the current (and the reaction rate) is higher close to entrance of gasses, where the reactants have higher concentrations. This figure presents flow rates of reactants as well (left side). Major increase of water flow in cathode gas channel is appreciated. Nitrogen flow rate is constant (35 mol m⁻² s⁻¹) because nitrogen is not a reactant.

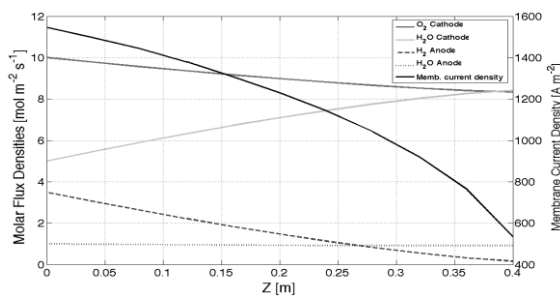


Fig. 4. Spatial profile of membrane current density and flow rates of reactants in gas channels.

Fig. 5 shows spatial profiles of the different temperature levels. As can be seen, temperature rises at the zone of major exothermic reaction rate.

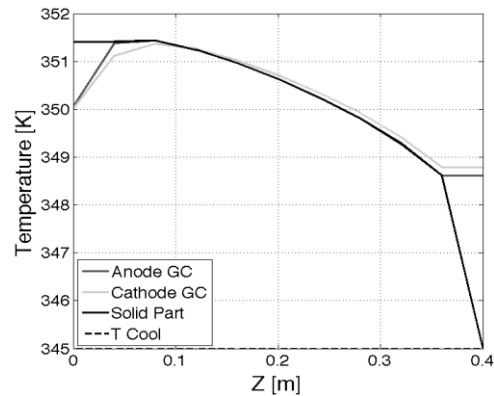


Fig. 5. Spatial profiles of temperature in the gas channels, solid part and cooling level.

Fig. 6 shows spatial profiles for membrane water content, together with spatial profiles of water transport by electroosmotic drag and back-diffusion.

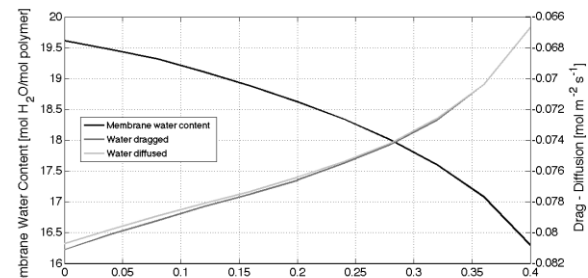


Fig. 6. Spatial profiles of membrane water content, drag (anode to membrane) and back-diffusion (cathode to membrane).

As expected, membrane water content is higher at the zone of major reaction rate and water back-diffusion increases along the channel due to water generated. This agrees with the results shown in Fig. 1, where water concentration increases towards the end of the channel on both sides of the membrane.

5.2. Simulation results for step changes

At $t = 10$ s the inflow of oxygen is increased up to 10.5 mol/m²s for 100 s, then at $t = 210$ s, inflow of hydrogen is changed up to 4 mol/m²s for 100 s and finally, water inflow in the cathode is changed down to 4.5 mol/m²s. Fig. 7 shows the results of time variation of reactant concentrations for three specific points along the channel. It is important to notice the different response of the system depending on the channel point. Changes at the first point of the channel are almost immediate, whereas there is a slower time constant further along the channel.

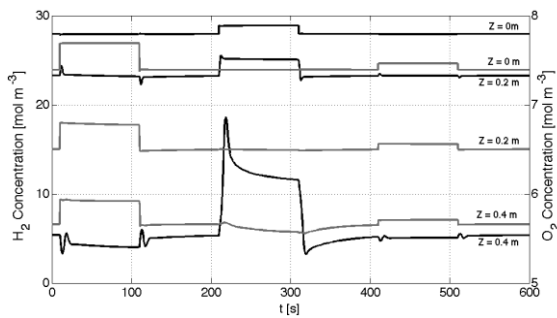


Fig. 7 Time evolution of reactants concentration at the beginning point, middle point and channel end. Black lines correspond to hydrogen concentration.

Fig. 8 shows similar results for time variation of water concentration.

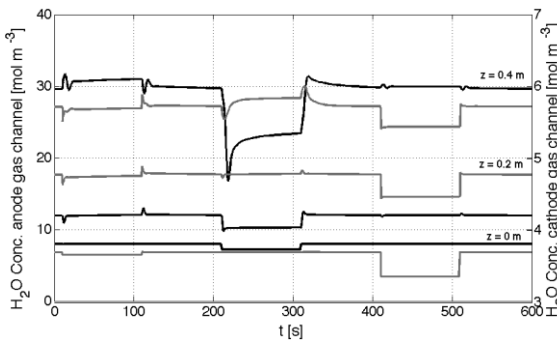


Fig. 8 Time evolution of water concentration for anode and cathode gas channel at the beginning point, middle point and channel end. Black lines correspond to water concentration in the anode side.

Fig. 9 shows the same type of diagram for membrane current density and membrane water content. The increase in reactants concentrations effectively increases membrane current density and water content.

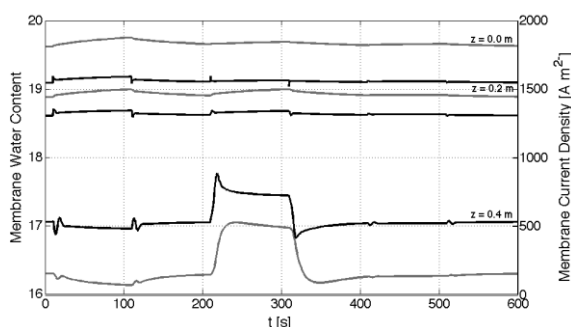


Fig. 9 Time evolution of membrane water content and current density at the beginning point, middle point and channel end. Black lines correspond to membrane current density.

Finally, Fig. 10 presents the results of time evolution for the solid part temperature. The slow dynamics of temperature can be appreciated in this diagram. Changes in concentration of reactants and water cause a decrease in the solid part temperature due to the entrance of lower temperature gasses.

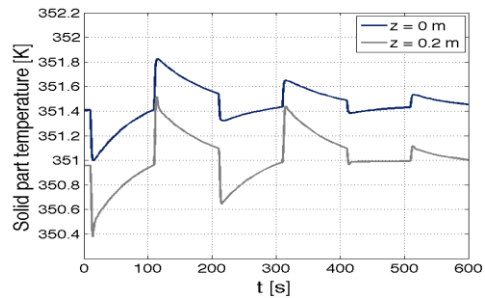


Fig. 10 Time evolution of solid part temperature at the beginning point and middle point.

6. CONCLUSIONS

A two-dimensional PEMFC simulation tool, suitable for along-the-channel studies, has been developed in Matlab®. The tool is flexible enough to apply order reduction techniques and to be used in model-based control design. Simulation results show the importance of considering, and therefore, controlling aspects of spatial profiles, especially for PEMFC performance and durability issues. It is the intention of the authors to make the source code publicly available.

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