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CFD simulation of the transient gas transport in a PEM fuel cell cathode during AC impedance testing considering liquid water effects

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A B S T R A C T

This work presents the application of CFD (Computational Fluid Dynamics) to the unsteady gas transport modelling in the cathode side of a Polymer Electrolyte Membrane (PEM) fuel cell during an AC impedance test. The CFD model development and results during AC impedance experiments for 1D and 2D cases are presented and discussed. The effect of liquid water was considered by modelling scenarios with saturated (according to water profiles obtained experimentally) and dry Gas Diffusion Layers (GDL). It was observed that the magnitude of the transient variations of the oxygen concentration within the GDL is dependent on the frequency of the AC signal during the test, given the differences between the diffusion characteristic time and the oxygen consumption characteristic time. For the 2D model where the differences under-the-rib to under-the-channel can be analysed, it was verified that oxygen concentration is much higher under the channel, however the amplitude of the oscillations during AC testing are significantly higher under the rib. When comparing saturated and dry GDLs for both models, it was verified that oxygen concentrations are higher for dry GDLs, but the amplitude of the oscillations is however higher for saturated GDLs.

1. Introduction

Fuel cells have starting their deployment and initial market penetration over the last years, covering applications such as transport (fuel cell electric vehicles, materials handling vehicles, trucks and buses, rail vehicles) or stationary and portable power generation (back-up power, combined heat and power) [1–5]. It is well known however that there are still many technical and economic barriers to overcome, such as durability and cost [6]. As an example, there is a strong need for increasing the power density (in volume and mass) of the fuel cell stacks. More compact stacks are required to facilitate their integration into efficient automotive powertrains and other transport and portable applications. A higher compactness in terms of stacks with less number of cells highly contributes to the reduction of the total stack and system cost. While this can be achieved by operating the stack at higher current densities, it is well known that advanced designs are required in order to achieve an appropriate water management avoiding the cell flooding and excessive transport or concentration losses [6].

Indeed, reducing mass transport losses by increasing oxygen gas transport in the cathode side of the cell is of major importance for achieving more efficient and compact fuel cells, as gas transport limitations represent the major restriction for the operation at high current densities. Oxygen supplied to the cell must reach the cathode electrode catalyst, diffusing through the porous media of the GDL at the rate required by the electrochemical reaction, which is increasing with the current drawn from the cell according to Faraday's law. In addition to the oxygen diffusion limitations in dry GDLs, the high amount of water produced by the cathode electrode at high current densities is known to block the GDL pores and the electrode reaction sites (and even the flow field channels), causing the cell flooding and preventing oxygen from effectively reaching the catalyst active sites [7,8]. As a consequence, the cell performance will drop significantly and will also lead to an unstable operation. Thus, gas transport and effective transport properties, water management, and cell components specific design to avoid flooding at high current densities are some of the most relevant

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aspects being investigated in PEM fuel cells [7–10]. Powerful techniques such as X-ray imaging or Neutron Radiography [11–13] currently allows for the liquid water visualization in operando fuel cells.

Both CFD (Computational Fluid Dynamics) and AC impedance spectroscopy (or EIS – Electrochemical Impedance Spectroscopy) are also powerful tools for the investigation and design of fuel cells [14–16] and [17–20]. CFD is mainly used for steady-state analysis of the cell such as for the calculation of the polarization curve [21–25] although several transient analyses have been also carried out for the investigation of the cell behaviour under load changes, start-up, or cell purging [26–28]. AC impedance is a transient process, where an AC signal is superimposed to the cell during operation, and the resulting frequencies obtained are analysed in order to investigate different cell phenomena [29–31]. As the current drawn from the cell is not constant during an AC impedance test, but it is the sum of the constant current plus the AC signal imposed, the reactant gases also present a cyclic transient behaviour for their transport and consumption at the electrode, and this behaviour is potentially feasible for its modelling also by means of CFD.

The experimental electrochemical impedance spectra can be modelled by equivalent circuits, such as in Fouquet et al. [32], while also analytical and physics-based models have been derived for the AC impedance spectroscopy of fuel cells. Shamardina et al. [33] developed a pseudo two-dimensional transient model, which is considering the dynamics of the oxygen concentration in the cathode GDL and channel, for the simulation and analysis of electrochemical impedance spectra. Reshetenko and Kulikovsky [34] developed an analytical solution of the physical model for the PEM fuel cell impedance, and analysed physical parameters such as oxygen transport and diffusion coefficients. They found a low value of the oxygen diffusion coefficient in the cathode catalyst layer (4.5e−9 cm^2/s), that was attributed to a large amount of liquid water.

This work presents the CFD modelling of the gas transport within the GDL at the cathode side during the execution of an AC impedance test. Although many CFD modelling of PEM fuel cells have been presented in the literature during the last 10–20 years [14,15], to the best of the knowledge of the authors very few CFD models of an EIS test have been developed. Hinaje et al. [35] developed a 2D model in COMSOL software to represent an EIS experiment of both a healthy and defective cell, whereas Chevalier et al. [36] also used COMSOL to model different scenarios of EIS aiming at identifying degradation modes and cell properties. Both works show the potential value of AC impedance test simulation for investigating degradation phenomena, cell properties, characterize state of health. However, none of the models were taking into account the impact of liquid water (single phase gas mixtures were considered) and the detailed analysis of the gas transport and concentration profiles were out of the objectives of both works. In the present work, gas transport during an AC impedance test is modelled by means of CFD, considering the impact of liquid water within the GDL. Both 1D and 2D approaches will be presented.

2. Model development

The models are based on the developments presented in a previous work [37] where a modelling approach coupling CFD and Neutron Imaging data was carried out. In brief, the model resolves the gas species mass transport in the cathode side, with a pre-defined distribution of liquid water within GDL/MPL which locally affects the effective diffusion coefficient and therefore the gas transport. In Ref. [37], the pre-defined distribution of liquid water was obtained by means of Neutron Imaging experiments. This modelling approach has been used for the transient gas transport during AC testing. It must be however stated that in the most general approach it would not be strictly required to pre-define the distribution of liquid water, as long as the model used is able to calculate and provide the liquid water distributions. As the characteristic times of the dynamic AC testing are milliseconds, the liquid water transport and distribution is not affected by the test, being therefore constant and stationary during the experiment. This means that a conventional CFD multi-phase model accounting for liquid water transport can be also used, where the liquid water distribution should be maintained constant and stationary during the transient simulation. Results for both a 1D model and a 2D model will be presented, representing different “1D” and a “2D” experimental cells respectively as discussed in Ref. [38]. The aim of this is to provide first the modelling framework in a simple 1D geometry, and later apply this for a more realistic 2D scenario. The same methods can be also applied for extending future studies to 3D CFD models.

2.1. Cell description

The physical model developed corresponds to a cell aimed at achieving a 1D behaviour [38] in the through-plane direction (direction normal to the membrane plane), which was built at Paul Scherrer Institut (PSI, Laboratory for Electrochemistry). The 1D behaviour is enforced in the cell by using very thin ribs, a thick GDL medium, and also high stoichiometric factors. The cell is having 10 channels of 1.0 mm wide and 0.55 mm depth, with 1.0 mm ribs. The active area is 1 cm^2. In order to enforce the 1D behaviour of the oxygen transport (in the normal direction with respect to the MEA), four GDLs were placed in the cathode side of the cell, 3 x Sigracet 24BA (5%PTFE, 190 μm thickness when uncompressed) and 1 x Sigracet 24BC (5%PTFE, with Micro Porous Layer, 235 μm thickness when uncompressed). The porosity of the GDLs is 84% according to manufacturer (after compression the porosity is reduced to 78.6%, as 30% compression was applied). A stacked set of GDLs would ensure this one-dimensional behaviour, because of the longer oxygen pathway from channel to electrode that minimizes the heterogeneities introduced by the channel-rib effect (longer gas pathway existing for oxygen under the ribs than under the channels in the GDL, which results in a two-dimensional gradient of oxygen concentration). For this reason, the rib width was reduced as much as possible and the oxygen path was incremented by using the four stacked GDLs. Finally, a Gore Primea 57 series catalyst coated membrane with 0.1 mgPt/cm^2 in anode and 0.4 mgPt/cm^2 in cathode was used.

A second cell featuring a single GDL (SGL 24BC, 0.235 mm thickness and 0.84 porosity uncompressed, 0.200 mm thickness and 0.817 porosity under 15% compression) is the base for the development of the 2D model.

2.2. Model development

For the particular cell enforcing to have a 1D (through plane) behaviour, the model developed can be also defined as 1D. The model of the cathode side of the cell has been developed in ANSYS-CFX [39]. The mesh consists of 40 hexahedral cell elements, as depicted in Fig. 1.

A gas mixture with oxygen, nitrogen, water vapour and helium (to reduce the oxygen concentration to 5%) were considered, with ideal gas properties, where the cell conditions were set to 70 °C and 2.1 bar(g). A CFD framework generally resolves the Navier-Stokes transport equations (momentum, mass conservation, energy and species transport). However, in this particular case only the species transport is resolved, as in the GDL the fluid convection can be neglected and the cell is considered isothermal. The model