STUDY OF HYDROGEN PURGE EFFECTS ON PERFORMANCE AND EFFICIENCY OF A PEM FUEL CELL SYSTEM

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RESUMEN: *Análisis experimental y modelado CFD se utiliza en este trabajo para analizar la eficiencia del sistema relacionado con la gestión del agua basada en purgas de hidrógeno en un sistema cátodo-abierto de pilas de combustible tipo PEM. El exceso de agua en el ánodo con la salida cerrada disminuye la concentración de hidrógeno en la superficie del catalizador y por lo tanto provoca pérdidas de rendimiento. Purgar el ánodo con hidrógeno elimina el agua y el nitrógeno que difunde a través de la membrana, pero también significa una pérdida de energía y por lo tanto disminuye la eficiencia global del sistema. Experimentos con un stack de 100W han revelado que la necesidad de una purga de hidrógeno depende fuertemente de las condiciones de operación y el estado de salud de la pila de combustible y por lo tanto la decisión de realizar una purga tiene que ser evaluado en línea. Un modelo dinámico CFD de 2 dimensiones de una sola célula dentro de la pila se utiliza para investigar la distribución y el transporte del agua dentro de la célula antes, durante y después de realizar una purga en diferentes condiciones de funcionamiento, ligados al rendimiento de la célula. Por otra parte, el modelo es capaz de estudiar la dinámica de transferencia de agua a través de la membrana y a lo largo del canal, incluyendo la saturación de agua en estado líquido. En total, el trabajo experimental y de modelado ayuda a mejorar la comprensión de transporte de agua en una pila de combustible tipo PEM y por lo tanto facilita el desarrollo de estrategias para aumentar la eficiencia del sistema y la optimización de la gestión del agua para controlar la purga de hidrógeno de manera adecuada.*

ABSTRACT: *Experimental analysis and CFD modeling is used in this work to analyze system efficiency related to hydrogen purge based water management in an open-cathode PEM fuel cell system. Excess water in a dead-ended anode decreases hydrogen concentration at the active catalyst surface and thus causes fuel cell performance losses. Purging the anode with hydrogen removes water and nitrogen that diffused through the membrane but also means wasting energy and thus decreasing overall system efficiency. Experiments with a 100W open-cathode stack have revealed that the need for a hydrogen purge strongly depends on the operation conditions and the state-of-health of the fuel cell and therefore the decision to perform a purge has to be evaluated online. A dynamic 2D CFD model of a single cell within the stack is used to investigate water distribution and transport within the cell before, during and after performing a purge at different operating conditions, linked to cell performance. Moreover, the model is capable of studying water transfer dynamics across the membrane and along the channel, including liquid water saturation. Altogether, the presented experimental and modeling work helps to improve the understanding of water transport in a PEM fuel cell and thus facilitates the development of strategies for increasing system efficiency and optimizing the water management by properly controlling the hydrogen purge.*

Palabras clave: PEMFC, eficiencia, modelado, purga de hidrógeno
Keywords: PEMFC, Efficiency, Modelling, Hydrogen purge

1. INTRODUCTION

Water management in Proton Exchange Membrane (PEM) Fuel Cells is a crucial issue. On the one hand, water is needed to maintain good proton conductivity and therefore has to be kept in the membrane. On the other hand, too much liquid water in the catalyst layers (CL) reduces the electrochemically active surface area and liquid water present in the pores of the gas diffusion layers (GDL) hinders the reactant gases to diffuse to the catalyst surface. Thus, both effects reduce the performance of the system. The goal is to maintain an almost uniform concentration in the membrane by keeping a balance between the two conflicting requirements. To control water transport within a fuel cell system and thereby optimize the membrane hydration at any operation point, proper dynamic water management strategies have to be developed, which has been analyzed recently by [1].

Today most PEM fuel cell systems work with a dead-ended anode which features a hydrogen purge valve located at the anode outlet in order to flush the anode periodically and so remove water. However, purging with hydrogen means wasting energy and thus decreasing overall system efficiency. Therefore the need of a purge has to be evaluated online depending on the actual operating conditions in order to minimize the waste of hydrogen. Feeding the purged hydrogen back into the fuel supply line does not solve the efficiency problem due to the extra power consumption of the necessary hydrogen pump. Moreover, purging is still required in order to remove nitrogen that has diffused through the membrane from the cathode.

2. EXPERIMENTAL ANALYSIS

As explained, it has to be evaluated if and when a purge is necessary in order to avoid an exaggerated waste of energy. To be able to decide on the need of a purge, it has to be detected when the anode is flooding and thus has to be flushed. In order to analyze the need for a purge, the anode inlet pressure difference before and during a purge has been recorded at different stack currents and ambient conditions with a 100W open-cathode stack set up in an environmental chamber. This system by default operates in a constant purge period mode (10s), which has to be optimized, as explained in section 1. In order to flood the stack the ambient conditions are set to 10ºC and 95% relative humidity. The anode is dead-ended and purges are performed every 60s with a duration of 500ms. The monitored variables have been measured continuously throughout the whole test, which is shown plotted in Fig 1. The cathode inlet conditions are controlled via the environmental chamber of the test station.

By changing the operation point from 2 to 5 A the cathode outlet dew point temperature increases because more water is produced in the fuel cell. At this operation point and wet ambient conditions the effect of a purge on the cathode outlet humidity can be noticed as oscillations of the purge frequency appear in this signal, as shown in Fig 1. (dashed red circle).
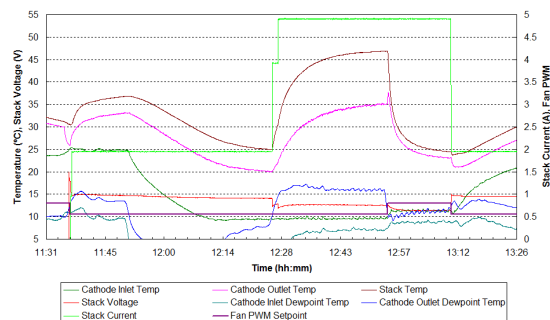

Fig. 1. Monitored variables during the purge test.

The cathode outlet dew point decreases during a purge because water diffuses from the cathode through the membrane and leaves at the anode outlet, which cannot be observed at non-flooded operating conditions since there is not as much water available within the stack. Thus, these oscillations are an indicator for cell flooding.

Increasing the fan flow rate leads to a voltage drop since flooding gets worse due to the reduction in temperature of about 20ºC, which causes condensation in the stack. However, this effect can only be observed at low ambient temperatures and high relative humidity where the effect of stack cooling and condensation overbalances the antithetic effect of water removal from the stack, which leads to drying out of the stack at high temperatures.

The measured anode inlet pressure curves during purges at different operating conditions are compared in Fig 2. The inlet pressure decreases during the change in stack current from 2 to 5A due to increasing hydrogen flow rate and the nature of the non-controlled, mechanical pressure regulator. The effect of flooding on the anode inlet pressure during a purge can be noticed. The maximum pressure difference during a purge is defined as the difference between the highest and the lowest point of the curve. It can be seen that the pressure difference decreases with cell flooding compared to dry conditions because water in the GDL impedes hydrogen from passing through the anode and thus the low pressure part of the curve increases due to the interdigitated flow field geometry on the anode. Hence, both the pressure difference and the oscillations in the cathode outlet humidity during a purge are indicators of cell flooding. If a controlled pressure regulator would be used, the pressure of hydrogen could be increased by a small amount within the allowed operating range of 0.4 to 0.6 bars, according to the manufacturer specifications, in order to push the extra water out. However this would not only increase the cost/complexity of the system but could as well increase the amount of hydrogen wasted during a purge due to the higher inlet pressure.
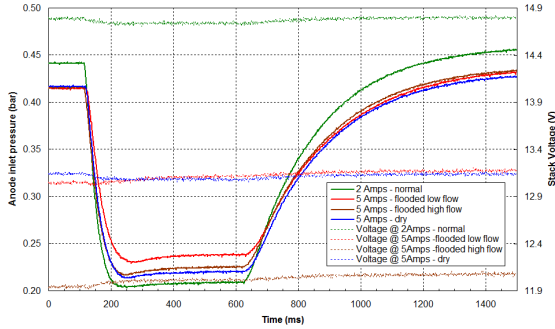
Fig. 2. Anode inlet pressure during purge at different stack currents and operating conditions.

Fig 2. also shows the stack voltage during a purge. The anode purge prevents the stack from flooding and thus improves performance, as it is depicted by the increasing stack voltage during a purge at flooded conditions. However, at 2A and 5A at dry conditions, the stack voltage actually decreases during a purge and thus, hydrogen and energy is wasted, which has to be avoided in order to improve efficiency.

3. MODELING APPROACH

To develop a proper strategy for purging the anode, CFD modelling is an important tool. By dynamic simulation of water and temperature distribution during and between purges, linked to the cell performance, insights can be gained on how to control purge durations and intervals. Once the voltage is decaying due to reduced reactant transport, which is indicated by a current dependent voltage threshold or gradient, a purge has to be performed. However, the goal of an effective purge strategy would be to increase the interval between purges by changing operation conditions like fuel cell temperature or flow rates and thus minimizing the purge frequency during operation. In order to investigate the relations between performance, temperature, water distribution and liquid water saturation a complete CFD model of the fuel cell is used. Based on the simulation results the necessary control strategies can be derived and finally applied to the system via a model-based controller.

The CFD model used in this work is an extension of the work presented by [2]. The extended model takes into account experimentally validated reaction kinects described by a Butler-Volmer approach and the transport and distribution of liquid water saturation in the membrane-electrode-assembly (MEA). Since the hydrogen oxidation reaction kinetics are fast compared to the oxygen reduction reaction kinetics the anode kinetics are neglected [3]. The local current density at this boundary is computed based on the operating conditions (temperature, pressure, reactant

concentrations) and the cell voltage $V_{(fc)}$, which is equal to the thermodynamic reversible potential $\left(E_{th(T,P)}\right)$ of a PEM fuel cell minus the three major losses: activation $\left(\eta_{act}\right)$, mass transport $\left(\eta_{mt}\right)$ and ohmic $\left(\eta_{ohm}\right)$.

$$V_{fc} = E_{th(T,P)} - \eta_{act} - \eta_{mt} - \eta_{ohm} [V] \qquad (1)$$

Thus, the reaction kinetics dependent local current density at the catalyst boundary can be described as:

$$\eta_{kin} = E_{th(T,P)} - V_{fc} - \eta_{ohm} [V] \qquad (2)$$

$$i_{loc} = i_0 \cdot 10^{\left(\frac{\eta_{kin}}{A_c} - k_{mt} \ln\left(\frac{c_{O2}}{c_{O20}}\right)\right)} [A \, cm^{-2}] \qquad (3)$$

On the right-hand-side of equation (3) i_0 represents the exchange current density, A_c is the cathode Tafel slope, k_{mt} is the empirical mass transport constant [3], c_{O2} is the local concentration of oxygen at the catalyst boundary and c_{O20} is the reference concentration of oxygen.

The effects of liquid water in the GDL on performance are modelled by the incorporation of the approach presented in [4]. Here the increased activation losses due to liquid water blockage of active sites are taken into account by correcting the active area with the liquid water saturation s.

$$A_{act}(s) = (1-s) A_{act} \grave{c}_{s=0} [cm^2] \qquad (4)$$

In a similar way the reduced oxygen transport rate through the GDL is considered by using a liquid water saturation dependent porosity in the Bruggemann-corrected diffusion equations.

$$\varepsilon_{GDL/MPL}(s) = (1-s) \varepsilon_{GDL/MPL} \grave{c}_{s=0} \qquad (5)$$

The model was experimentally validated with a 100W open-cathode PEM fuel cell stack and compared to the voltage loss dissection presented in [5]. The model coincides well with the experimental data, as shown for example for a steady state operation point at 0.266 Acm^{-2} in Fig 3. It shows that the model is capable of predicting the three major voltage losses in accordance with the experimental results of [5].
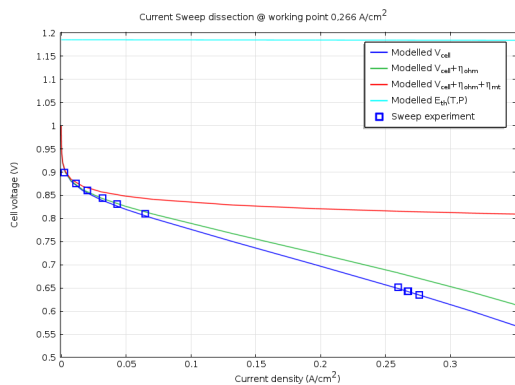
Fig. 3. Modelled voltage loss dissection at 0.266 Acm^{-2} operating point

Fig 4. shows the comparison to the experimental data at different operation points and cell temperatures and thus shows the good model representation over a wide range of operating conditions. The validated model is now used to study the hydrogen purge effects on fuel cell performance, as explained above. Fig. 5 shows a representative simulation where the saturated, dead-ended anode is driven into hydrogen starvation, which decreases the average current density at the catalyst layer significantly.
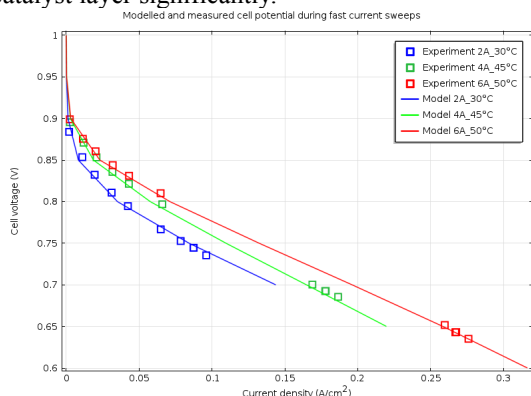

Fig. 4. Comparison of modelling results and experimental data at different operating conditions

By performing a hydrogen purge at 9s for 200ms water is removed from the anode and the hydrogen concentration at the active layer as well as the current density recovers.
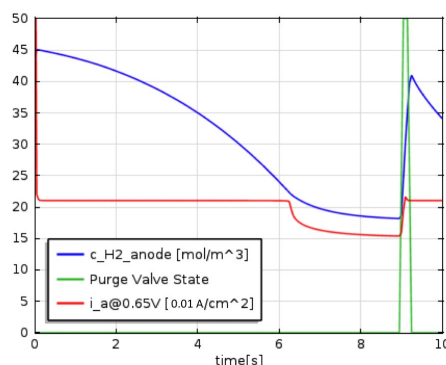

Fig. 5. Representative simulation of hydrogen starvation due to flooding operation conditions (0.2A/cm^2, T_{FC}=45ºC, RH$_{cat}$=100%)

Besides studying the hydrogen purge phenomena the model gives also the possibility to investigate water transfer dynamics across the membrane and along the channel. Fig. 6 shows the mass flow rates of water across the membrane from anode to cathode and vice versa. The initial conditions are 65%RH @ 25ºC at the cathode inlet and a dry anode supplied with pure, dry hydrogen. The operation point is 0.2Acm^{-2}. The plot of water mass flow rates along the channel at different times shows that the diffusive fluxes through the membrane switch their direction once the anode gets filled with water. Together with the electro-osmotic drag (EOD) water is now driven also by diffusion from anode to cathode and gets removed from the system by the forced convection in the cathode flow channels. However, as dry hydrogen is supplied in a counter-flow system, the end of the channel (cathode-outlet, anode-inlet) shows another change in the flow direction, dominated by back diffusion of water from the cathode.
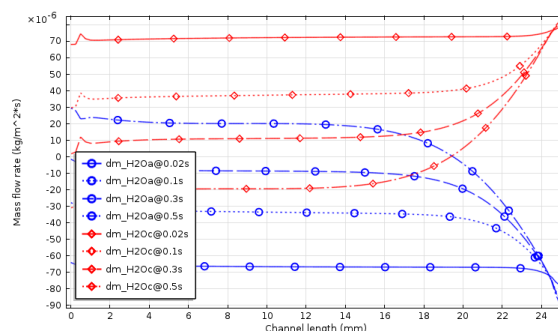

Fig. 6. Water mass flow rates across the membrane from 0 to 0.5s (0.2A/cm^2, T_{FC}=60ºC, RH$_{cat}$=65%@25ºC)

4. CONCLUSIONES

Based on experimental observations a 2D CFD model for investigating performance and efficiency related phenomena of hydrogen purges has been developed and validated. The model is now used to study strategies for increasing system efficiency and

optimizing the water management of the fuel cell by properly controlling the hydrogen purge.

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