Influence of nature and concentration of iron ions on the degradation of PEMFCs: a modeling study

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Polymer Electrolyte Membrane (PEM) Fuel Cells represent a promising technology for high-efficiency energy conversion as an alternative to fossil energies. However, under practical operating conditions, the durability of the current technology is not yet high enough to be economically viable. Modeling is becoming a more and more important tool for understanding degradation mechanisms and predicting the lifetime of fuel cells (1). To this goal, we apply multiphysics elementary kinetic models that describe electrochemical reactions and transport processes in a highly detailed way (2,3,4). This allows a reliable prediction of the long-time behavior of the cell, which always involves temporal extrapolation away from short-term measurements (5).

This study presents a 1D model of the PEM chemical aging, which represents one of the major mechanisms inducing irreversible PEMFC performance decay. The model describes water, gas and ion transport across the PEM, production of hydrogen peroxide in the anode CL, transport of peroxide into the PEM, its decomposition, and chemical degradation of the PEM through radicals attack (Fig. 1). Parameter identification and model validation is performed using published experimental work from several groups (Figs. 2 and 3) (6,7).

It has been observed experimentally by Kodama *et al.* (8) that the degradation rate depends nonlinearly on the concentration of iron ions in the membrane. Particularly, under very aggressive conditions the membrane degradation is not as high as expected. This study shows a model-based analysis of the influence of ion concentration on the degradation rate. The different effects of Fe²⁺ and Fe³⁺ are quantified.



Fig.1: Schematic of the degradation mechanism that is modeled in the present study.



Fig. 2: Simulated and experimental (from Liu and Zuckerbrod (6)) water peroxide concentration as a function of membrane thickness.



Fig. 3: Simulated and experimental (from Young & al (7)) fluoride emission over time.

References

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