Effects of Nitrogen and Water Accumulation in the Dead-Ended-Anode Operation of PEM Fuel Cells

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Dead-ended-anode operation of PEMFC can achieve high hydrogen utilization and self-humidification with low component complexity, which yields a promising configuration for mobile and portable power systems. This operating mode offers insight into severe flooding and hydrogen starvation conditions. Experimental and modeling efforts that explain the effects of dead-ended anode operation and associated hydrogen starvation on voltage measurements and fuel cell life are scarce in the literature. Once properly calibrated, models can be used for fuel cell diagnostic and anode purge scheduling based on voltage measurements.

In this work, we present a two-dimensional transient model and simulations of a PEMFC operating with a dead-ended anode. The model is qualitatively validated with pressure, temperature, flow and liquid water accumulation measurements using neutron imaging of a 53 cm^2 PEMFC[1]. The data and model both show reversible voltage degradation, which can be recovered by purging the anode.

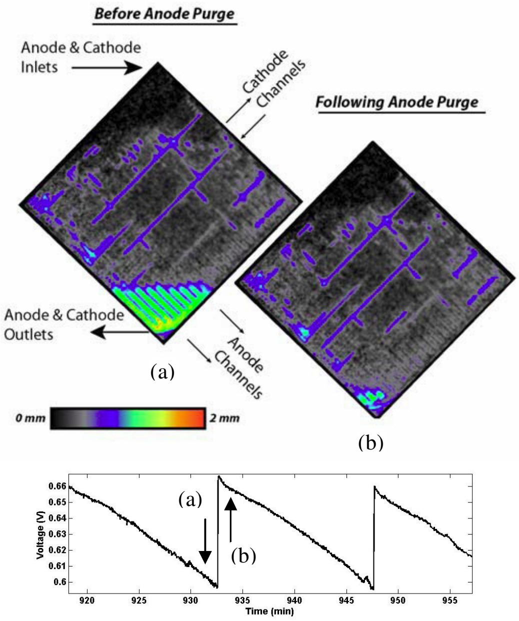

Figure 1. Neutron images showing liquid water thickness (mm) in a dead-ended PEMFC before and after an anode purge and recoverable voltage loss.

The model geometry is simplified considering that the anode side of the cell consists of parallel straight channels, and cathode side has parallel serpentine channels in which the average flow is in the same direction as the anode flow, and therefore can be approximated well by a co-flow model. Thus along the channel and through the membrane-electrode-assembly directions are considered in the 2D model.

Other salient features of our model are listed as follows:
(a) Transport of gas species in flow channels and gas diffusion layers is modeled by Maxwell-Stefan equations.
(b) Convection of gaseous species in the flow channels is modeled by laminarized Navier-Stokes equations, where the inertial terms are dropped from the force balance, but buoyancy effects due to composition of gas mixtures are included.
(c) Gas convection in the gas diffusion layers is modeled by Darcy's Law.
(d) Only permeation of nitrogen in the membrane is considered since it can accumulate in the anode as opposed to instant reaction of oxygen (hydrogen) at the anode (cathode) catalyst layer(s).
(e) Charge transport (electrons in the electrodes and flow plates, and protons in the membrane) is subject to conservation of charge and Ohm's Law.
(f) Water transport in the membrane is modeled as advection-diffusion, in which the electroosmotic drag of water is considered as ionic current driven advection effect.
(g) Darcy's Law is used for saturated liquid flow in the GDLs for which van Genuchten's saturation model is used with the parameters obtained by Gostick et al[2] for the GDL material used in the experiments[1].
(h) Butler-Volmer equations are used for reaction kinetics at the anode and cathode catalyst layers. Cathode-side is modified to include proton concentration, which is assumed to be in equilibrium with the anode-side in kinetic equations.
(i) Anode and cathode catalyst layers are assumed to be very thin and projected onto the anode and cathode-side membrane-GDL interfaces.

A finite-element representation of the governing equations subject to boundary conditions mimicking experimental conditions is solved using a commercial multiphysics package, COMSOL.

According to our preliminary results most of the reversible voltage degradation observed in experiments can be attributed to accumulation of nitrogen and water vapor in the anode, which displaces hydrogen. Hydrogen depletion in the anode side leads to a proton deficiency on the cathode side and increased proton-concentration losses at the cathode. The effect of gravity is important and leads to the 'stratification' of gasses in the anode channels with a smooth profile subject to short height of the anode channels and relatively large diffusion coefficient of hydrogen. Following the purge, depletion of hydrogen near the exit (bottom) of anode channels is more severe than the inlet (top), where a pressure regulator keeps the total pressure constant in the anode chamber and replenish hydrogen as it is consumed. The current density distribution is highly non-uniform, reaching its maximum (2-5 times of the average) near the anode inlet and approaches zero near the outlet due to hydrogen starvation. Cathode-side water production and back diffusion is largest where the current density reaches to its maximum. However, the experimental data indicate that additional water transport mechanisms should be considered to explain liquid water accumulation in the anode-side.

References
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2. Gostick, J.T., Fowler, M.W., Ioannidis, M.A., Pritzker, M.D., Volfkovich, Y.M., and Sakars, A. (2006), Journal of Power Sources, 156, pp 375-387.