Corrections/Updates to "Mathematical Modeling of Transport Phenomena in Polymer Electrolyte and Direct Methanol Fuel Cells"

Erik Birgersson
17.05.2005

Papers


Major revisions

We have redefined the overpotential in the published papers 3 & 4. In the thesis (Paper 3, page 125, Eq. 63; Paper 4, page 172, Eq D.4), the overpotential is taken as

\[ \eta = \phi_s - \phi_m - E_{\text{open}}. \] (1)

However, this approach does not consider the potential drop from the reversible potential, \( E_{\text{rev}} \), to the open circuit potential, \( E_{\text{open}} \). The proper definition is

\[ \eta = \phi_s - \phi_m - E_{\text{rev}}. \] (2)

With this definition of the overpotential, the temperature increase in the PEFC is higher than predicted in the thesis, as illustrated in the published papers 3 and 4.

Minor errata

Unfortunately, a typing error appears in papers 2–4 for the values of \( M_{N_2} \) and \( M_{O_2} \). The correct values are \( M_{N_2} = 2.8 \times 10^{-2} \) kg mol\(^{-1}\) and \( M_{O_2} = 3.2 \times 10^{-2} \) kg mol\(^{-1}\). The simulations have all been run with the proper values for these two molecular masses.

Miscellaneous

In the last paper (7) in the thesis, we used Femlab 2.3 to verify the reduced model. At that time (2003) we were not able to get Femlab to converge for the low relative gas permeability of the net \( (\varepsilon_1 = 6 \times 10^{-3}, \varepsilon_2 = 5, n = 1) \), whence the verification was carried out for a more gas-permeable net \( (\varepsilon_1 = 1, \varepsilon_2 = 2, n = 1) \). Recently (2005), with Femlab 3.1, we obtained convergence even for the low relative gas permeabilities, as depicted in Figure 1 below. This was accomplished by using the general PDE modes for the dependent variables and selecting "Solution form: weak" prior to solving the model. Further, the nonlinear parametric solver for \( \varepsilon_2 \) was invoked to obtain a smooth convergence from the less nonlinear case of \( \varepsilon_2 = 1 \) (initial value) to the final value of \( \varepsilon_2 = 5 \). For very high \( \Delta \)-values \( (\sim O(100)) \), it was sometimes useful to specify the model as a "Highly nonlinear problem". On a final note, we also did not solve for the liquid saturation \( s \) as dependent variable but rather the transformed variable \( S \), similar to the KellerBox approach.
Figure 1. Updated verification of the reduced model for $\varepsilon_1 = 6 \times 10^{-3}$, $\varepsilon_2 = 5$, $n = 1$. (—) corresponds to FEMLAB solutions for $\sim 500$ nodes and the symbols are for the reduced model, with $10^4$ cells: (x) $\Delta = 1.8$, $\Omega_1 = 1.4 \times 10^{-3}$; (□) $\Delta = 4.1$, $\Omega_1 = 3.2 \times 10^{-3}$; ($\forall$) $\Delta = 17$, $\Omega_1 = 1.4 \times 10^{-2}$; (+) $\Delta = 41$, $\Omega_1 = 3.2 \times 10^{-2}$; (★) $\Delta = 179$, $\Omega_1 = 1.4 \times 10^{-1}$. 