

Supplementary Information

A Dynamic Tanks-in-Series Model for High-Temperature PEM Fuel Cell

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Auxiliary equations

The following correlation is suggested for ionic conductivity of the (PBI) membrane [26]

$$k_m = \frac{1}{T} (168x^3 - 6324x^2 + 65750x + 8460)(1 + (0.1432T - 56.89)RH)e^{\left(\frac{-6196x+21750}{RT}\right)} \quad (S.1)$$

where x – the doping level, $x = 0.012m^3 + 0.2111m^2 + 1.2363m + 0.7119$; m – H_3PO_4 concentration; k_m – the proton conductivity. Relative humidity in the membrane is

$$RH = P_{mem}^{H_2O} / P_{sat}^{H_2O} \quad (S.2)$$

Saturation pressure is

$$P_{sat}^{H_2O} = 0.68737 T^3 - 732.39 T^3 + 263390 T - 31919000 \quad (S.3)$$

For a linear concentration profile in the membrane, partial pressure in MEA is calculated as

$$P_{mem}^{H_2O} = 0.5(P_{cat,anode}^{H_2O} + P_{cat,cath}^{H_2O}) \quad (S.4)$$

For the cathode catalyst layer, the concentration of oxygen in the liquid phase is

$$C_{C,cat,L,j}^{O_2} = y_{cat}^{O_2} P / H_{H_3PO_4}^{O_2} \quad (S.5)$$

For the anode catalyst layer, the concentration of hydrogen in the liquid phase is

$$C_{A,cat,L,j}^{H_2} = y_{cat}^{H_2} P / H_{H_3PO_4}^{H_2} \quad (S.6)$$

For oxygen- H_3PO_4 system, Henry constant is

$$H_{H_3PO_4}^{O_2} = \frac{101325}{10132.5 \exp(273.13 m^2 - 431.08m + 178.45 + (-93500m + 156646m - 64288)/T)}$$

For H_2 - H_3PO_4 system, Henry constant is

$$H_{H_3PO_4}^{H_2} = 4H_{H_3PO_4}^{O_2} \quad (S.7)$$

Parasitic current is calculated by equations

$$I_{cross}^{O_2} = \frac{n_e^{O_2}}{\nu^{O_2}} F \frac{K_p^{P_2}}{\delta_m} (P_{cat,C}^{O_2} - 0) \quad (S.8)$$

$$I_{cross}^{H_2} = \frac{n_e^{H_2}}{\nu^{H_2}} F \frac{K_p^{H_2}}{\delta_m} (P_{cat,A}^{H_2} - 0) \quad (S.9)$$

The local mass transfer coefficient in the porous layer is calculated by equation

$$\beta_w^{(k)} = \varepsilon^{1.5} D_m^{(k)} / \delta_{cat} \quad (S.10)$$

The local heat transfer coefficient in the porous layer can be calculated using Chilton-Colborne analogy

$$Nu_w = Sh_w (Pr_w / Sc_w)^{1/3} \quad (S.11)$$

where Nu_w - Nusselt number for catalyst layer; Sh_w - Sherwood number; Sc_w - Schmidt number; Pr_w - Prandtl number.

Equilibrium potential differences

The overall reaction of the anodic hydrogen oxidation in acid solution is given by Kordesch and Simader (Kordesch, K., & Simader, G. (1996). *Fuel cells and their applications* (Vol. 117). Weinheim: VCh.)



The anodic equilibrium potential differences is

$$\eta_{eq}^A = E_{eq}^A + \frac{RT}{n_e F} \ln \left(\frac{(a_{cat}^{H_2})^{0.5} a_{cat}^{H_2O}}{a_{cat}^{H^+}} \right) \quad (S.13)$$

where E_{eq} - the theoretical potential of reaction (S.33); $a_{cat}^{H_2}$ - hydrogen activity in the anode catalyst layer, [mol/L], $a_{cat}^{H_2} = 1000 y_{cat}^{H_2} P / H^{H_2}$; $a_{cat}^{H_2O}$ - water activity in the cathode catalyst layer, [mol/L], $a_{cat}^{H_2O} = 1$.

The overall reaction of the cathodic oxygen reduction in acid solution is (Kordesch, K., & Simader, G. (1996). *Fuel cells and their applications* (Vol. 117). Weinheim: VCh.)



The cathodic equilibrium potential differences is

$$\eta_{eq}^C = E_{eq}^C + \frac{RT}{n_e F} \ln \left(\frac{(a_{cat}^{O_2}) a_{cat}^{H^+}}{a_{cat}^{H_2O}} \right) \quad (S.15)$$

where E_{eq} - the theoretical potential of reaction (S.35); $a_{cat}^{O_2}$ - oxygen activity in the cathode catalyst layer, [mol/L], $a_{cat}^{O_2} = 1000 y_{cat}^{O_2} P / H^{O_2}$; $a_{cat}^{H_2O}$ - water activity in the cathode catalyst layer, [mol/L], $a_{cat}^{H_2O} = 1$.

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