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Letter to the Editor

There is a mistake in Farhat's model published in volume 138

There is a mistake in Farhat's model and results [1]. The primary goal of this letter is to disprove his model and results. In his model, wrong expression of Eqs. (3) and (4) induced the mistake of the modified Butler–Volmer equation. According to the article, k_f and k_b are rate constants ($cm^{-1}\,s^{-1}$), C_R and C_p are concentrations ($mol\,cm^{-3}$), S is active surface area (cm^2). Then the units of $k_f C_R S$ and $k_b C_P S$ are $mol\,cm^{-4}\,s^{-1}$, but the units of v_f and v_b are $mol\,cm^{-2}\,s^{-1}$. Therefore, Eqs. (3) and (4) [1] is wrong. Now, we give the corrected equations and deduction, and definitions of symbol are held as the same of Farhat's model.

According to the half cell electrode reaction Eq. (2) [1], the forward and backward reactions rates, respectively, are as follows:

$$v_f = k_f C_R = \frac{I_f}{nFS} \tag{1}$$

$$v_b = k_b C_P = \frac{I_b}{nFS} \tag{2}$$

The net reaction rate is, therefore, the difference between forward and backward reaction rates, i.e.:

$$v_{net} = v_f - v_b = k_f C_R - k_b C_P = \frac{I_f - I_b}{nFS} \tag{3}$$

rearranging:

$$I_{net} = I_f - I_b = nFS(k_f C_R - k_b C_P) \tag{4}$$

According to Eqs. (7) and (8) of Farhat's model [1], we get:

$$I_{net} = I_0 \exp\left[\frac{-\alpha n F(E - E_{eq})}{RT}\right] \tag{5}$$

where:

$$I_0 = nFSk^0 C_R^{*(1-\alpha)} C_P^{*\alpha} \tag{6}$$

Dividing by the nominal area A and rearranging, then the activation polarization for the oxygen reduction reaction at the cathode will become:

$$\eta_{c,act} = \left(\frac{RT}{n\alpha_c F}\right) \ln\left(\frac{i_{0,c}}{i}\right) \tag{7}$$

where:

$$i_{0,c} = \frac{nFSk^0 C_R^{*(1-\alpha)} C_P^{*\alpha}}{A} \tag{8}$$

As can be seen, Eq. (8) is quite different from Eq. (13) in Farhat's article. According to Eqs. (14)–(17) in Section 3.1 in Farhat's article, we get:

$$\eta_{c,act} = \left(\frac{RT}{n\alpha_c F}\right) \ln\left(\frac{3\gamma \frac{m_c}{A} nFk C_{O_2}^{*(1-\alpha_c)} C_{H^+}^{*(1-\alpha_c)} C_{H_2O}^{*\alpha_c}}{i r_c \rho_c}\right) \tag{9}$$

where m_c/A is the catalyst loading ($g\,cm^{-2}$), which is a important parameter of PEMFC catalyst layer. The main control equation should be changed into:

$$E_{cell} = E_{eq} - (i + i_n)R + \left(\frac{RT}{n\alpha_c F}\right) \ln \times \left(\frac{3\gamma \frac{m_c}{A} nFk C_{O_2}^{*(1-\alpha_c)} C_{H^+}^{*(1-\alpha_c)} C_{H_2O}^{*\alpha_c}}{(i + i_n) r_c \rho_c}\right) + \left(\frac{RT}{nF}\right) \ln\left[1 - \left(\frac{i + i_n}{i_1}\right)\right] \tag{10}$$

In conclusion, the influence of different microstructural parameters in a catalyst layer should be studied by examining model predictions given by Eq. (10) but not Eq (24) of Farhat's model.

Reference

[1] Z.N. Farhat, Modeling of catalyst layer microstructural refinement and catalyst utilization in a PEM fuel cell, J. Power Sources 138 (2004) 68–78.

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