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Correction to “Understanding Multi-Ion Transport Mechanisms in Bipolar Membranes”

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Article Recommendations

In the original version of this article, when equations were referenced within the main text, the numbering was offset by 2. For instance, when eq 1 was referenced, it was incorrectly referred to as eq 3. When eq 16 was referenced, it was incorrectly referenced as eq 18, and so on and so forth for all other references to the equations in the main text. The correct equation referencing is shown below for all instances:

Page 52512. “...where $\beta = \frac{I_0 F}{RT}$ as per comparison with eq 4. We note that the form of eq 5 is consistent with the Butler–Volmer equation for describing the electrochemical kinetics of Faradaic charge-transfer reactions at solid electrodes.^{46,47}”

Page 52512. “...where α is defined to be 1 in all regions outside of the water-dissociation catalyst layer, preserving the proposed kinetics of the non-catalytically assisted water dissociation (eq 5).”

Page 52514. “...which are nontrivial and quite complicated, the concentration of water in the BPM is assumed to follow a complementary functional form to that for the fixed charge (eq 11).”

Page 52520. “As the membrane potential is increased, hydroxide anions form within the catalyst layer and are transported into the AEL, thereby shifting the equilibrium between hydrogen phosphate and dihydrogen phosphate toward hydrogen phosphate (eq 8).”

Page 52521. “Therefore, by fitting a value for the hydration of the AEL and CEL when completely exchanged with salt ions ($\lambda_{\text{H}_3\text{O}^+} = 0$, $\lambda_{\text{OH}^-} = 0$), the linear profile (eqs 32–33) defining local ionomer hydration...”

In the original version of this article on page 52513, the equations in Table 2 (12–14) and Table 3 (17–19) are missing their equation numbering. These tables are shown

Table 2. Chemical and Electrochemical Potentials of Species Present in Model

species	potential
H_3O^+	$\tilde{\mu}_{\text{H}_3\text{O}^+} = \tilde{\mu}_{\text{H}_3\text{O}^+}^0 + RT \ln \left(\frac{c_{\text{H}_3\text{O}^+} c_{\text{H}_2\text{O}}^0}{c_{\text{H}_3\text{O}^+}^0 c_{\text{H}_2\text{O}}} \right) + F\Phi + RT \ln(\gamma_{\pm}^E) \quad (12)$
OH^-	$\tilde{\mu}_{\text{OH}^-} = \tilde{\mu}_{\text{OH}^-}^0 + RT \ln \left(\frac{c_{\text{OH}^-} c_{\text{H}_2\text{O}}^0}{c_{\text{OH}^-}^0 c_{\text{H}_2\text{O}}} \right) - F\Phi + RT \ln(\gamma_{\pm}^E) \quad (13)$
co- and counterions	$\tilde{\mu}_i = \tilde{\mu}_i^0 + RT \ln \left(\frac{c_i c_{\text{H}_2\text{O}}^0}{c_i^0 c_{\text{H}_2\text{O}}} \right) + z_i F\Phi \quad (14)$

Page 52512. “Both buffer reactions are considered in their bimolecular form for consistency with the bimolecular water dissociation mechanism employed in the present study (see eq 1). The equilibrium constants, K_i , for eqs 8 and 9...”

Page 52513. “Equation 11 allows for smooth, differentiable transitions (i.e., a smoothed step function) at the interface between the electrolyte and ionomer phases as well as between the AEL and CEL.”

Page 52513. “...where N_i is the molar flux of species i , and D_i is the diffusivity of species i . The Nernst–Einstein relationship is used to relate mobilities and diffusivities. Substitution of eqs 12–14 into eq 16 yields the flux of each individual ionic species, as shown in Table 3.”

below with their proper equation numbering to facilitate easier understanding of the derivations presented in the work.

In the original article on page 52514, eqs 32 and 33 are missing a factor of $(1 - f_{\text{H}_3\text{O}^+})$ and $(1 - f_{\text{OH}^-})$, respectively, from the first term in each equation. They should read as follows:

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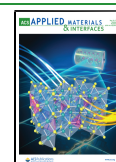


Table 3. Flux of Ionic Species in Model

species	flux
H_3O^+	$N_{\text{H}_3\text{O}^+} = -D_{\text{H}_3\text{O}^+} \frac{dc_{\text{H}_3\text{O}^+}}{dx} + D_{\text{H}_3\text{O}^+} c_{\text{H}_3\text{O}^+} \frac{d(\ln(c_{\text{H}_2\text{O}}))}{dx} + D_{\text{H}_3\text{O}^+} c_{\text{H}_3\text{O}^+} \frac{FE}{RT}$ $- D_{\text{H}_3\text{O}^+} c_{\text{H}_3\text{O}^+} \frac{d(\ln(\gamma_{\pm}^E))}{dx} \quad (17)$
OH^-	$N_{\text{OH}^-} = -D_{\text{OH}^-} \frac{dc_{\text{OH}^-}}{dx} + D_{\text{OH}^-} c_{\text{OH}^-} \frac{d(\ln(c_{\text{H}_2\text{O}}))}{dx} - D_{\text{OH}^-} c_{\text{OH}^-} \frac{FE}{RT}$ $- D_{\text{OH}^-} c_{\text{OH}^-} \frac{d(\ln(\gamma_{\pm}^E))}{dx} \quad (18)$
co- and counterions	$N_i = -D_i \frac{dc_i}{dx} + D_i c_i \frac{d(\ln(c_{\text{H}_2\text{O}}))}{dx} + z_i D_i c_i \frac{FE}{RT} \quad (19)$

$$\lambda_{\text{CEL}} = (1 - f_{\text{H}_3\text{O}^+}) \lambda_{f_{\text{H}_3\text{O}^+}=0} + f_{\text{H}_3\text{O}^+} \lambda_{f_{\text{H}_3\text{O}^+}=1} \quad (32)$$

$$\lambda_{\text{AEL}} = (1 - f_{\text{OH}^-}) \lambda_{f_{\text{OH}^-}=0} + f_{\text{OH}^-} \lambda_{f_{\text{OH}^-}=1} \quad (33)$$

Additionally, in the following sentence it is stated that “ $\lambda_{f_{\text{H}_3\text{O}^+}=1}$ and $\lambda_{f_{\text{OH}^-}=0}$ are both taken from measurements of BPM water uptake in DI water ($\lambda = 9$).⁵” This should read, “ $\lambda_{f_{\text{H}_3\text{O}^+}=1}$ and $\lambda_{f_{\text{OH}^-}=1}$ are both taken from measurements of BPM water uptake in DI water ($\lambda = 9$).⁵”

In the original version of the manuscript, on page S2514, it is stated that $M_{i,M} = \left(\frac{1}{M_i} + \frac{1}{M_M}\right)$ is the reduced molar mass. This equation is missing a negative exponent and should instead be written as $M_{i,M} = \left(\frac{1}{M_i} + \frac{1}{M_M}\right)^{-1}$ to properly model the ionomer-phase diffusion coefficients.

In the conclusions section on page S2524, it is stated that “The simulations show that an optimal BPM should have a thin dissociation catalyst layer, and a thinner AEM than CEM layer...”, despite this statement being contrary to what is demonstrated in the discussion section. The trend is correct as depicted and examined within the discussion, and the conclusions should instead read: “The simulations show that an optimal BPM should have a thin dissociation catalyst layer, and a thinner CEM than AEM layer...”

None of the errors presented above change any of the analysis or major conclusions presented in the work.

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