Electrochemical Potentials in Steady-State Fuel Cell Modeling

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Reaction Potential Equilibrium Sequence

$$\begin{aligned} 2\mu_{\mathrm{H_2}} + 4\mu_{\mathrm{H_2O}} - 4\mu_{\mathrm{e^-}} &= 4\mu_{\mathrm{H_3O^+}} \\ &\neq \mu_{\mathrm{O_2}} - 4\mu_{\mathrm{e^-}} + 6\mu_{\mathrm{H_2O}} \end{aligned}$$

Component Electrochemical Potentials

$$\text{Anode:} \quad u := \begin{cases} u_c := 2\mu_{\mathrm{H_2}} + 4\mu_{\mathrm{H_2O}} - 4\mu_{\mathrm{e^-}} \\ u_m := 4\mu_{\mathrm{H_3O^+}} \end{cases}$$

$$\text{Cathode:} \quad v := \mu_{\mathrm{O_2}} - 4\mu_{\mathrm{e^-}} + 6\mu_{\mathrm{H_2O}}$$

Butler-Volmer Equation

- $i_F = i_0 \left[\exp(\frac{\alpha_a F}{RT}\eta_s) - \exp(-\frac{\alpha_c F}{RT}\eta_s) \right]$
- $F\eta_s := u - v$
- If $|u - v|/RT \ll 1$, then can linearize.
- $i_F = \beta(u - v)$ where $\beta := i_0(\alpha_a + \alpha_c)F/RT$

Diffusivities and Component Conductivities

$$D_k \boldsymbol{\nabla} c_k \cdot \boldsymbol{n} \;=\; s_k i_F / nF$$

$$\begin{aligned}
\varepsilon \boldsymbol{\nabla} u \cdot \boldsymbol{n} &= \varepsilon \sum_k s_k \boldsymbol{\nabla} \mu_k \cdot \boldsymbol{n} \\
&= \varepsilon \sum_k s_k \frac{\partial \mu_k}{\partial c_k} \boldsymbol{\nabla} c_k \cdot \boldsymbol{n} \\
&= \frac{\varepsilon i_F}{nF} \sum_k \frac{(s_k)^2}{D_k} \frac{\partial \mu_k}{\partial c_k} \\
&= i_F F \;=\; \beta(v - u)
\end{aligned}$$

provided

$$\varepsilon := nF^2 \left(\sum_k \frac{(s_k)^2}{D_k} \frac{\partial \mu_k}{\partial c_k} \right)^{-1}$$

and

$$\beta := i_0(\alpha_a + \alpha_c) F / RT$$

What Is Not Included ?

- Time Derivatives: $\dfrac{\partial c_k}{\partial t}$
- Convective, Rotational Flows
- Certain Boundary Conditions