

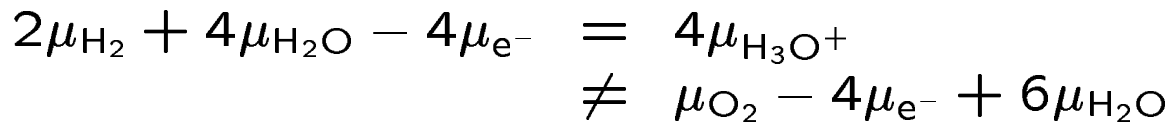
# Electrochemical Potentials in Steady-State Fuel Cell Modeling

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## Reaction Potential Equilibrium Sequence



## Component Electrochemical Potentials

$$\text{Anode: } u := \begin{cases} u_c & := 2\mu_{\text{H}_2} + 4\mu_{\text{H}_2\text{O}} - 4\mu_{\text{e}^-} \\ u_m & := 4\mu_{\text{H}_3\text{O}^+} \end{cases}$$

$$\text{Cathode: } v := \mu_{\text{O}_2} - 4\mu_{\text{e}^-} + 6\mu_{\text{H}_2\text{O}}$$



## Butler-Volmer Equation

- $i_F = i_0 \left[ \exp\left(\frac{\alpha_a F}{RT} \eta_s\right) - \exp\left(-\frac{\alpha_c F}{RT} \eta_s\right) \right]$
- $F \eta_s := u - v$
- 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

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

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

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

