IMPORTANT EQUATIONS

Thermodynamics

$$dU = dQ - dW = dQ - p\,dV$$

$$dS = k \ln \Omega = \frac{dQ}{T}$$

$$H = U + pV$$

$$G = H - TS$$

$$\Delta G = \Delta H - T\Delta S \text{ (isothermal process)}$$

$$\Delta G = -nFE$$

$$\mu = \mu^0 + RT \ln a$$

$$E = E^0 + \frac{\Delta S}{nF}(T - T_0) - \frac{RT}{nF} \ln \frac{\prod a_{\text{prod}}^{v_i}}{\prod a_{\text{react}}^{v_i}}$$

$$\varepsilon_{\text{real}} = \varepsilon_{\text{thermo}}\, \varepsilon_{\text{voltage}}\, \varepsilon_{\text{fuel}}$$

$$\varepsilon_{\text{thermo, fc}} = \frac{\Delta G}{\Delta H}$$

$$\varepsilon_{\text{voltage}} = \frac{V}{E}$$

$$\varepsilon_{\text{fuel}} = \frac{i/nF}{v_{\text{fuel}}}$$

$$\varepsilon_{\text{thermo,electrolyzer}} = \frac{\Delta H}{\Delta G}$$

$$\Delta \hat{h}_f = \Delta \hat{h}_f^0 + \int_{T_0}^{T} c_p(T)\, dT$$

$$\hat{s} = \hat{s}^0 + \int_{T_0}^{T} \frac{c_p(T)}{T} dT$$

Modeling

$$V = E_{\text{thermo}} - \eta_{\text{act}} - \eta_{\text{ohmic}} - \eta_{\text{conc}}$$

$$V = E_{\text{thermo}} - [a_A + b_A \ln(j + j_{\text{leak}})] - [a_C + b_C \ln(j + j_{\text{leak}})] - (jASR_{\text{ohmic}}) - \left(c \ln \frac{j_L}{j_L - (j + j_{\text{leak}})}\right)$$

Reaction Kinetics

$$j_0 = nFC^* f e^{-\Delta G^{\ddagger}/(RT)}$$

$$j = j_0^0 \left(\frac{C_R^*}{C_R^{0*}} e^{\alpha nF\eta/(RT)} - \frac{C_P^*}{C_P^{0*}} e^{-(1-\alpha)nF\eta/(RT)} \right)$$

$$j = j_0 \frac{nF\eta_{\text{act}}}{RT} \quad \text{(small overpotential/current)}$$

$$\eta_{\text{act}} = \frac{RT}{\alpha nF} \ln \frac{j}{j_0} \quad \text{(large overpotential/current)}$$

Charge Transport

$$\eta_{\text{ohmic}} = j(ASR_{\text{ohmic}}) = j\frac{L}{\sigma}$$

$$ASR_{\text{ohmic}} = A_{\text{fuelcell}} R_{\text{ohmic}} = \frac{L}{\sigma}$$

$$\sigma = |z|Fcu$$

$$u = \frac{|z|FD}{RT}$$

$$D = D_0 e^{-\Delta G/(RT)}$$

$$\sigma T = A_{\text{SOFC}} e^{-\Delta G_{\text{act}}/RT} = A_{\text{SOFC}} e^{-E_a/kT}$$

Mass Transport

$$j_L = nFD^{\text{eff}} \frac{c_R^0}{\delta}$$

$$\eta_{\text{conc}} = \frac{RT}{\alpha nF} \ln \frac{j_L}{j_L - j} = c \ln \frac{j_L}{j_L - j}$$

Fuel Cell Systems

$$\varepsilon_0 = \varepsilon_R + \varepsilon_H$$

$$\varepsilon_R = \varepsilon_{FP} \times \varepsilon_{R,\text{ SUB}} \times \varepsilon_{R,\text{ PE}} = \frac{\Delta \dot{H}_{(\text{HHV}),\text{ H}_2}}{\Delta \dot{H}_{(\text{HHV}),\text{ fuel}}} \times \frac{P_{e,\text{ SUB}}}{\Delta \dot{H}_{(\text{HHV}),\text{ H}_2}} \times \frac{P_{e,\text{ SYS}}}{P_{e,\text{ SUB}}}$$

$$\text{Gravimetric energy storage density} = \frac{\text{stored enthalpy of fuel}}{\text{system mass}}$$

$$\text{Volumetric energy storage density} = \frac{\text{stored enthalpy of fuel}}{\text{system volume}}$$

$$\text{Carrier system effectiveness} = \frac{\%\text{ conversion of carrier to electricity}}{\%\text{ conversion of neat H}_2\text{ to electricity}}$$

Fuel Cell Fundamentals: Third Edition. Ryan O'Hayre, Suk-Won Cha, Whitney G. Colella and Fritz B. Prinz