MF22 Equation Sheet

Calculating the thermodynamics of fuel cells

$$\Delta G = -nFE_{OC}$$

Nernst Equation

$$E_{OC} = E_{OC}^{o} - \frac{nF}{RT}\ln\left(\frac{[products]}{[reactants]}\right)$$

$$\textit{for fuel cell} \quad \left(\frac{[products]}{[reactants]}\right) = \quad \left(\frac{[H_2O]}{[H_2]\sqrt{[O_2]}}\right)$$

Temperature dependence of E_{OC}

$$E_{OC} = E_{OC}^{o} + \frac{\Delta S}{nF}(T - T^{o})$$

Butler-Volmer Kinetics

$$i = i_o\left([O_2]^{*}e^{\frac{\alpha F}{RT}\eta} - [H_2O]^{*2}e^{-\frac{(1-\alpha)F}{RT}\eta}\right)$$

Potential Losses

$$E_{loss} = \eta^{a} + \eta^{c} + jR_{mt} \qquad E_{cell} = E_{OC} - E_{loss}$$

Activation Polarisation

$$\Delta V_{act} = \eta = E - E_{EQM} = \frac{RT}{\alpha F}\ln\left(\frac{i}{i_o}\right)$$

Concentration Polarisation

$$\Delta V_{c} = E - E_{EQM} = \frac{RT}{nF}\ln\left(\frac{[C^{*}]}{[C_o]}\right)$$

Ohmic Resitive Losses

$$V_{Ohm} = i\ x\ R_{total}$$

Fuel Cell Efficiency

$$\xi = \Delta H\frac{V}{nF} = \frac{V}{1.482}\ for\ hydrogen$$

Linear Approximation of IV Curves

$$i = \frac{V_{OC} - V_{cell}}{k}$$

$$W = V_{cell}\ x\ i$$

$$W_{max} = \frac{V_{OC}^{2}}{4k}\ and\ is\ reached\ when\ V_{cell,W_{max}} = \frac{V_{OC}}{2}$$

Stoichiometry Factor

$$\lambda = \frac{nFNHw}{I}$$

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Efficiency of Thermoelectric Devices

$$ZT = \frac{S^2 \sigma T}{\kappa}$$

Kinetic of Nucleation

$$\Delta G = 4\pi r^2 \gamma + \frac{4}{3}\pi r^3 \Delta g_v$$

$$r_c = -\frac{2\gamma}{\Delta g_v}$$

$$\Delta G_c = \frac{16\pi\gamma^3}{3(\Delta g_v)^2}$$

Nucleation Rate

$$k_n = Ae^{-\left(\frac{\Delta G_c}{kT}\right)}$$

Gibbs-Thomson Relationship

$$lnS = \frac{2\gamma v}{kTr}$$

DVLO Theory (Attractive Van der Waals and Electrical Repulsion)

$$V_A = \frac{Aa}{12}H$$

$$V_R = \varepsilon a \psi_o^2 \ln(1 + e^{-\kappa H})$$

$$\kappa^{-1} = \sqrt{\frac{\varepsilon_o \varepsilon_r kT}{2N_A e^2 I}}$$

Brus Equation

$$E_{QD} = E_B + \frac{\pi^2 \bar{h}}{2R^2}\left(\frac{1}{m_e^*} + \frac{1}{m_h^*}\right)$$

Dynamic Light Scattering

$$D = \frac{kT}{6\pi\alpha\eta}$$

X-Ray Photoelectron Spectroscopy

$$KE = hv - BE - \phi$$

$$BE_F = hv - KE - \phi_{spec}$$

MF22 Equation Sheet

Optical Resolution

$$D = \frac{\lambda}{2Sin\theta}$$

Probe Sample Convolution

$$L = \sqrt{4Rr}$$

Bell Evans Model

$$< f^* > = \frac{k_b T}{x_t} \ln\left(\frac{r x_t}{k_{off} k_b T}\right)$$

Friddle-Noy Model

$$< f^* > = f_{eq} + \frac{k_b T}{x_t} \ln\left(1 + e^{-g} \frac{r x_t}{k_{u(f)} k_b T}\right)$$

FRET

$$\phi_f = \frac{photons\ emmitted}{photons\ absorbed}$$

$$I = I_o e^{-\left(\frac{t}{\tau}\right)}$$