NPRE 470 HW # 6 Solutions

3.1 (a) Forward

(b) Forward

(c) The voltage drops

3.13
$$j_0(T) = j_0(T_0)\, e^{-\frac{\Delta G_1^{\ddagger}}{R}\left(\frac{1}{T}-\frac{1}{T_0}\right)}$$

$$\frac{j_0(600k)}{j_0(300k)} = \frac{e^{-\frac{\Delta G_1^{\ddagger}}{R}\left(\frac{1}{600}-\frac{1}{300}\right)}}{e^{-\frac{\Delta G_1^{\ddagger}}{R}\cdot 0}} = e^{+\frac{\Delta G^{\ddagger}}{R\cdot 600k}} = 10^4$$

$$\Rightarrow \frac{\Delta G^{\ddagger}}{4986} = 9.21 \qquad \Rightarrow \Delta G^{\ddagger} = 45.9\ kJ/mol$$

9.9

Concentration loss

$$\eta_{conc} = \frac{RT}{nF} Ln \frac{j_L}{j_L - j} \qquad \text{where } j_L = nFD^{eff}\frac{C_R^0}{\delta}$$

↳ Let it be $j_L = a/\delta$

Activation loss

$$\eta_{act} = \frac{RT}{\alpha nF} \log \frac{j}{j_0^0 \delta} \qquad \text{Let } j_0^0\delta = b\delta \text{ for simple notation.}$$

Neglect the nonessential difference between Ln and Log.

The total loss of V is

$$\eta_{conc.} + \eta_{act} = \frac{RT}{nF}\left(Ln \frac{a/\delta}{a/\delta - j} + \frac{1}{\alpha} Ln \frac{j}{b\delta} \right) \qquad ①$$

We want to minimize ① WRT. δ or the term.

$$Ln \frac{a}{a - j\delta} + \frac{1}{\alpha} Ln \frac{j}{b\delta} \qquad ②$$

Differentiate ② WRT δ

$$\frac{a-j\delta}{a} \cdot \frac{-a}{(a-j\delta)^2} \cdot (-j) + \frac{1}{\alpha} \cdot \frac{b\delta}{j} \cdot \frac{-j}{(b\delta)^2} \cdot b = 0$$

$$\frac{-1}{a-j\delta} \cdot (-j) + \frac{1}{\alpha} \frac{-b}{b\delta} = 0$$

$$\frac{j}{a-j\delta} + \frac{1}{\alpha} \frac{-1}{\delta} = 0$$

$$\frac{j}{a-j\delta} = \frac{1}{\alpha\delta}$$

$$j\alpha\delta = a - j\delta$$

$$(\alpha+1)j\delta = a$$

$$\delta = \frac{a}{(\alpha+1)j} \qquad \text{where } a = nFD^{eff}C_R^0$$

The End!