I. Chemical Subsystem

Governing Equations

- Species Conservation Law

$$\frac{\partial c}{\partial t} = -\nabla \cdot \vec{N} + R_v$$

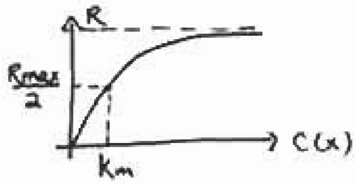
- Constitutive Equation for flux

$$\vec{N} = \underbrace{-D\nabla c_i}_{\text{diffusion}} + \underbrace{\frac{z_i}{|z_i|}\mu_i c_i}_{\text{EE}} + \underbrace{c_i \underline{v}_{fluid}}_{\text{ME}}$$

- D is diffusivity
- μ is mobility
- z_i is valence
- $\underline{v}_{fluid}$ is velocity of fluid

- R_i > '+' for generation
  > '−' for consumption
  > In form of kC_i (conc./time)
  - 0^{th} order: k_0 (conc./time)
  - 1^{st} order: k_1 ($1/$time) $C(x)$
  - 2^{nd} order: k_2 ($1/$conc.·time)·$C(x)$·$a(x)$
  - Michaelis Menten : $R = \dfrac{R_{max}\, C(x)}{K_m + C(x)}$

* Note: only units of K changes



> If only concerned about R:

Ex: $A + B \underset{k_r}{\overset{k_f}{\rightleftharpoons}} C$; $\dfrac{dC_c}{dt} = R = k_{f} AB - k_r C$

$$\frac{dC_A}{dt} = \frac{dC_B}{dt} = -\frac{dC_c}{dt}$$

Boundary Conditions

- flux matching $\hat{n}\cdot(N_1 - N_2) = R_s$

- Concentration matching $C(x_+) = \underset{\substack{\uparrow \\ \text{partition coefficient}}}{k} \cdot C(x_-)$

- Symmetry

Damkohler Number (ratio between reaction & diffusion)

$\alpha^2 = \dfrac{\text{reaction}}{\text{diffusion}}$

- $\alpha^2 \to \infty$, SS profile becomes sharper, "diffusion limited"
- $\alpha^2 \to 0$, SS profile flatens, "reaction limited"

II. Electrical Subsystem

> EQS: • valid because $L^{char} \ll \lambda$

• magnetic field neglected

> Governing Equations

Maxwell Equations

• Faraday: $\nabla \times E = -\cancel{\frac{\partial \mu H}{\partial t}}^{\to 0} \Rightarrow E = -\nabla \Phi$

• Ampère's: $\cancel{\nabla \times H}^{0} = J + \underbrace{\frac{\partial \varepsilon E}{\partial t}}_{\text{Maxwell's contribution}}$

• Gauss: $\nabla \cdot \varepsilon E = \rho$

$\nabla \cdot \cancel{\mu} H = 0$

Conservation of Charge

$$\nabla \cdot J = -\nabla \cdot \frac{\partial \varepsilon E}{\partial t} = -\frac{\partial \rho}{\partial t}$$

$$J = \sum_i z_i F N_i = \sigma \vec{E} + (\quad) \nabla c_i + \rho_r c_i v_{fluid}$$

Lorentz Force Law

$$F = \rho_e(\vec{E} + \cancel{v \times \mu H}^{\to 0}) = \rho_e E$$

Boundary Conditions

$$\hat{n} \times (E_1 - E_2) = 0 \Rightarrow \Phi_1 = \Phi_2$$

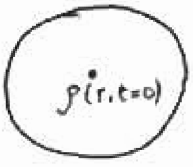
$$\hat{n} \cdot (\varepsilon_1 E_1 - \varepsilon_2 E_2) = \sigma_s$$

$$\hat{n} \cdot (\sigma_1 E_1 - \sigma_2 E_2) + \nabla_s \cdot \underset{\uparrow\ \text{surface current}}{\chi} = -\cancel{\frac{\partial \rho}{\partial t}}^{\to 0} = 0 \quad \text{if SS}$$

> Concepts

Charge Relaxation: $\nabla \cdot J + \frac{\partial \rho}{\partial t} = 0$

Note: charge relaxation is dependent only on time.



$$\frac{\partial \rho}{\partial t} + \frac{\sigma}{\varepsilon}\rho(r,t) = 0$$

$$\rho(r,t) = \rho(r,t=0^-)e^{-t/\tau} \quad \text{where } \tau = \frac{\varepsilon}{\sigma} \sim 1\,ns!$$

Double Layer / Debye Length:

Combining $\nabla \cdot \varepsilon E = \rho_e$ & $E = -\nabla \Phi$

$\Downarrow$

$$\frac{d^2\Phi}{dx^2} = \frac{1}{\varepsilon}\sum z_i F c_i(x) \quad \text{- Poisson Equation}$$

For a mono-mono valent species

debye length $\to$ $1/\kappa = \sqrt{\frac{\varepsilon RT}{2 c_0 z^2 F^2}}$

Electro-chemical time scales

$$\tau_{ch.relax} = \frac{\varepsilon}{\sigma} \quad \text{vs} \quad \tau_{diff} = \frac{(L^{char})^2}{D_i}$$

for $1/\kappa \sim L^{char}$ diffusion will compete w/ charge relaxation

$1/\kappa \ll L^{char}$ charge electroneutrality

$1/\kappa \gg L^{char}$ charge needs to be taken into consideration.

Equilibrium $(N_i = 0)$

$$\frac{z_i}{|z_i|}\mu_i c_i E = -D_i \nabla c_i \quad \leftarrow \text{integrate both sides}$$

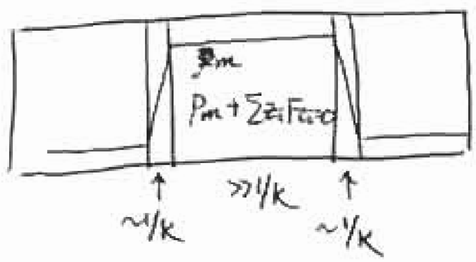
$$\frac{D_i}{\mu_i} = \frac{RT}{|z_i|F} \quad \text{Einstein Relation} \quad \leftarrow \text{use}$$

$$\underbrace{\Phi(x) = -\frac{RT}{z_i F}\ln\left(\frac{c_i(x)}{c_o(x)}\right)}_{\text{Nernst Potential}} \quad \leftarrow \text{find}$$

Solve Nernst Potential Equation

$$c_o e^{-z_i F \Phi(x)/RT} = c_{i\pm}(x) \quad \leftarrow \text{Boltzmann Distribution}$$

Donnan Equilibrium Potential



when ρ_m is constant

$\Phi(x)$ in tissue is constant

$\Rightarrow E(x)$ in tissue $= 0$

$$\underbrace{\Phi_{tissue} - \Phi_{bath}}_{\Phi_{Donnan}} = \text{const} = \left(\frac{c_i(x)}{c_i(0)}\right)^{1/z_i}$$

from Nernst potential equation

Governing Equations

$\nabla \cdot \bar{v} = 0$ incompressible fluid

$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho v = 0$ Conservation of mass

$\rho \frac{Dv}{Dt} = -\nabla p + \rho_e \underline{E} + \mu \nabla^2 \underline{v}$ Navier-Stokes Equation

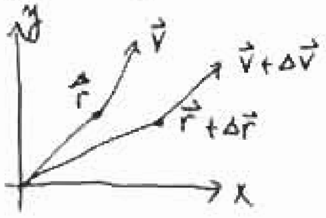
(p: pressure; ρ_e: charge)

$T_{ij} = 2\mu \varepsilon_{ij} + (\lambda - \frac{2}{3}\mu)\delta_{ij} \dot{\varepsilon}_{kk}$ Generalized Hooke's Law

Assumptions

- low Re # $\Rightarrow$ highly viscous
- incompressible
- fully developed flow

Stress - Strain



$\underline{\delta v} = \underline{\underline{D}}\, \underline{\delta r}$

$\underline{\underline{D}} = e + \eta$

$$= \underbrace{\frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)}_{e_{ij}} + \underbrace{\frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i}\right)}_{\eta_{ij}}$$

Please refer to all tutorials & notes for more detailed review.

Work to be looked at:

Full Name: