

Today: I. Recap EQS

10/13

Flux, Current, Constitutive Laws

⇒ Coupled Electrochemical Transport

II. Laplace; Poisson: Formulation of Boundary Value Problems & Bound. Conditions for EQS

III. Methods of Solution (Separation of Variables. good again)
→ Examples

I Coupled Electrochem Transport

$$\textcircled{1} \underline{N}_i = -D_i \nabla C_i + (z_i) \underline{E} + (1) C_i \underline{v}_{se}$$

$\left(\frac{\text{mol}}{\text{m}^2 \cdot \text{s}}\right) \left(\frac{\text{m}}{\text{s}}\right)$
 ↑
 for units to match

$$\textcircled{2} \frac{\partial C_i}{\partial t} = -\nabla \cdot \underline{N}_i + R_i$$

$$\textcircled{3} \nabla \cdot \underline{\epsilon E} = \rho_e(r, t) = \sum_i z_i F C_i$$

↑ ↑
 valence $10^5 \frac{\text{Coul}}{\text{mol}}$

$$\textcircled{4} \nabla \times \underline{E} \simeq 0 \Rightarrow \underline{E} = -\nabla \Phi \quad \text{--- } \Phi = \text{potential (volts)}$$

• because $\nabla \times (-\nabla \Phi) = 0$ for conservative field.

• '-' because Electric field flows down the potential gradient

$$\textcircled{5} \nabla \cdot \underline{J} = -\frac{\partial \rho_e}{\partial t}$$

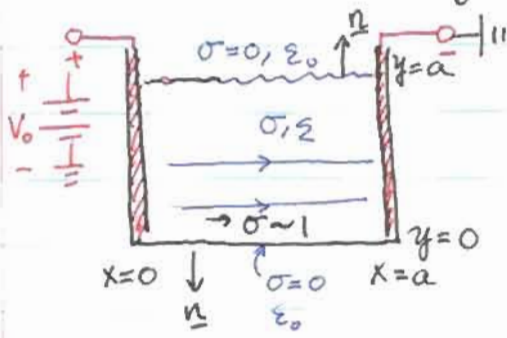
$$\textcircled{6} \underline{J} = \sum_i z_i F \underline{N}_i = (\sigma) \underline{E} + () \nabla C_i + () \underline{v}_{se}$$

↑
 $\frac{\text{Coul}}{\text{m}^2 \cdot \text{s}}$

↑
 $\frac{\text{mol}}{\text{m}^2 \cdot \text{s}}$

for + charge, + current, moving to the right
- charge, + current, moving to the right

Last Time: Demo



Find: $\Phi(x,y) + \underline{E}(x,y)$ in R given approp.

B.C.'s on $\Phi(x,y)$

B.C.'s: $x=0, \Phi=V_0$

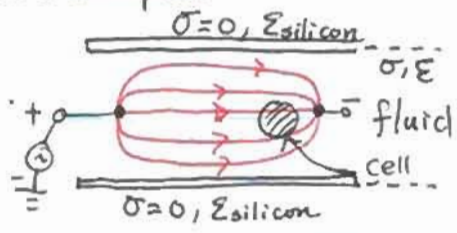
$x=a, \Phi=0$

$y=0, \left. \begin{matrix} n \cdot \nabla \Phi = 0 \\ E_y(x, y=0) = 0 \end{matrix} \right\}$

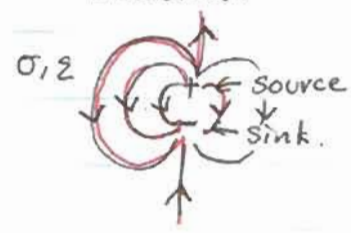
$y=a, \left. \begin{matrix} n \cdot \nabla \Phi = 0 \\ E_y(x, y=a) = 0 \end{matrix} \right\}$

Note: Boundary Conditions on Φ or E

More Examples:



Boundary: between conducting & insulating material.



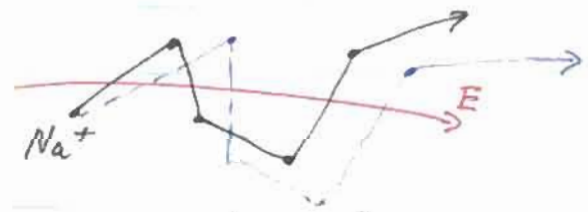
current dipole



Constitutive Law for $\underline{J} (\Rightarrow \underline{N}!)$ in Ionic Media (Physiologic)

"ions in thermal equilibrium w/ solvent @ temp T"

"Thought Model"



Einstein Relation

$$\frac{D_i}{u_i} = \frac{kT}{z_i F} = \frac{RT}{z_i F}$$

Water: $\left(\frac{1000 \text{ gm}}{\text{l}}\right) \left(\frac{\text{mol}}{18 \text{ gm}}\right) \sim 55 \text{ M}$

$$\cancel{\frac{m dv}{dt}} + \frac{m v}{\tau_{col}} = q E \rightarrow \underline{v}_{ion \pm} = \pm \left(\frac{|q| \tau}{m}\right) E$$

$\left(\frac{\text{m}^2}{\text{v.s}}\right) u_i \equiv$ mobility of species

$$\underline{J} = \sum z_i F (c_i \underline{v}_{particle})$$

$$\underline{J} = \underbrace{F(z_+ c_+ u_+ + z_- c_- u_-)}_{\text{"ohmic"}} E + \underbrace{(\quad)}_{\text{diff.}} \nabla c + \text{convection.}$$

σ . elec cond. $\left(\frac{\text{mho}}{\text{m}}\right) = \left(\frac{\text{S}}{\text{m}}\right)$

Note: charge not changing the E_{total} .

II. Poisson / Laplace (• No ∇C ; $v_{fl} = 0$) • $L^{char} \ll \lambda$

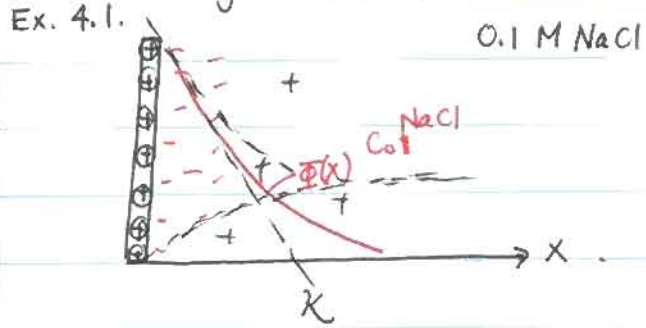
?? Maxwell	EQS.
$\nabla \cdot \epsilon E = \rho$	$\nabla \cdot \epsilon E = \rho$
$\nabla \times E = -\frac{\partial \mu H}{\partial t}$	$\nabla \times E = 0$
$\nabla \times H = J + \frac{\partial \epsilon E}{\partial t}$	$(E = -\nabla \Phi)$
$\nabla \cdot \mu H = 0$	$\nabla \cdot J = -\frac{\partial \rho}{\partial t}$
$\nabla \cdot J = -\frac{\partial \rho}{\partial t}$	$J = \sigma E$

"Static" (steady cardiac) vs time varying-non equal

From EQS In general: ① + ②

$\nabla \cdot \epsilon (-\nabla \Phi) = \rho_e(r, t)$ Gauss.
 $\nabla^2 \Phi = -\frac{\rho_e}{\epsilon}$ Poisson's Eq.

Find $\Phi \rightarrow$ get $E = -\nabla \Phi$



Ex. 4.1.

Find $\Phi(x)$ given $C_+(x)$
 $C_+(x) = C_0 e^{-zF\Phi/RT}$

$\frac{1}{\lambda} \sim$ Debye Length

Class of Problems: Steady Conduction ($\frac{\partial}{\partial t} \rightarrow 0$) "static"

$\nabla \cdot \epsilon E = \rho_e$ (ohmic medium)
 $\left[\begin{array}{l} \checkmark E = -\nabla \Phi \\ \checkmark \nabla \cdot \sigma E = 0 \end{array} \right]$

$\nabla^2 \Phi = 0$ Laplace's Equation

$\frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} + \frac{\partial^2 \Phi}{\partial z^2} = 0.$

Find $\Phi(r, t)$ in region R given boundary conditions on Φ or $n \cdot \nabla \Phi$ on S surrounding R .

Remember B.C's.

Law

$$\nabla \cdot \epsilon E = \rho_e$$

$$\nabla \times E = 0$$

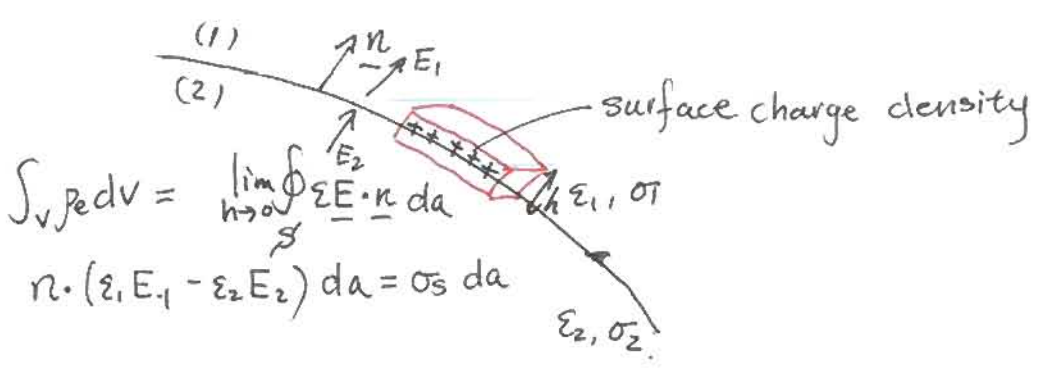
$$\nabla \cdot J = -\frac{\partial \rho_e}{\partial t}$$

Boundary Conditions

$$\underline{n} \cdot (\epsilon_1 E_1 - \epsilon_2 E_2) = \sigma_s$$

E_{tan} = continuous
 $\Phi_1 = \Phi_2$ @ interface.

$$\underline{n} \cdot (\sigma_1 E_1 - \sigma_2 E_2) = \frac{\partial \sigma_s}{\partial t}$$



$$\int_V \rho_e dv = \lim_{h \rightarrow 0} \oint_S \epsilon E \cdot \underline{n} da$$

$$\underline{n} \cdot (\epsilon_1 E_1 - \epsilon_2 E_2) da = \sigma_s da$$