HW #2 Solutions

(1.) Average charge is

$$\frac{[RH]\,C_p + [R]\,C_d}{[RH] + [R]} = C_p\left(1 + \frac{[R]}{[RH]}\right)^{-1} + C_d\left(1 + \frac{[RH]}{[R]}\right)^{-1}$$

where R is the amino acid side chain,

and C_p and C_d are the charge

in protonated and deprotonated states.

From $pH = pKa + \log_{10}\frac{[R]}{[RH]}$

$$\frac{[R]}{[RH]} = 10^{pH - pKa}$$

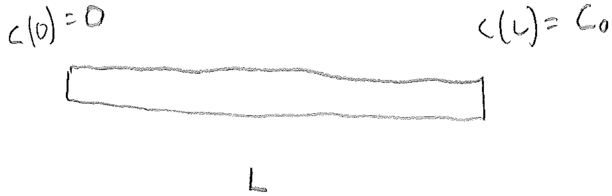
for Asp (D), Glu (E), Cys (C) and Tyr (Y) $C_p = 0$

for Arg (R), Lys (K), His (H) $C_p = 1$

$$C_d = C_p - 1$$

See HW2-1.m for plots.

(2.)



$$400 \ \mathrm{mm/day} = 4.6 \ \mu\mathrm{m/s}$$

$$J_x = -D \frac{\partial c(x,t)}{\partial x}$$

$$\frac{\partial c(x,t)}{\partial t} = D \frac{\partial^2 c(x,t)}{\partial x^2}$$

In steady state $\frac{\partial c(x,t)}{\partial t} = 0$

$$c(x,t) = A + Bx$$

from B.C.

$$c(x,t) = \frac{C_0 x}{L}$$

$$J_x = -\frac{D C_0}{L}$$

for $R = 50$, $D = \frac{K_B T}{6\pi\eta R} = \frac{(1.38 \times 10^{-23} \ \mathrm{J \cdot K^{-1}})(300 \ \mathrm{K})}{6\pi(10^{-3} \ \mathrm{Pa \cdot s})(5 \times 10^{-8} \ \mathrm{m})}$

$$= 4 \times 10^{-12} \ \mathrm{m^2/s} = 4 \ \mu\mathrm{m^2/s}$$

observed flux $J_{obs} = C_0 v$

compare J_x to J_{obs}

$$\frac{J_x}{J_{obs}} = \frac{D C_0}{L} \cdot \frac{1}{C_0 v} = \frac{D}{Lv} = \frac{(4 \times 10^{-12} \ \mathrm{m^2/s})}{(1 \ \mathrm{m})(4.6 \times 10^{-6} \ \mathrm{m/s})} \sim 10^{-6}$$

take $L = 1$ m

The observed flux can't be explained by diffusion. There must be active transport.

(3.) and (4.)

Deybe-Hückel and Poisson Boltzmann

Solutions begin to diverge

around ~ 1 charge per square nm.

see

PB_Shooting Method_Plane.m

PB_Shooting Method_Sphere.m