Assign 5 - Biophys2019

May 16, 2019

1

(a) pH = [7.6, 7.8]

$$pH = -log\big[H^+\big] \tag{1}$$

We can rearange 1 to obtain $\big[H^+\big] = 10^{-pH}$ and use this to find the concentrations of H^+ for the pH's.

$$\big[H^+\big] = 10^{-7.6} = 2.51\text{x}10^{-8}\text{M} \tag{2}$$

$$\big[H^+\big] = 10^{-7.8} = 1.58\text{x}10^{-8}\text{M} \tag{3}$$

Using $V_{Ecoli} \approx 6.7\text{x}10^{-16}\text{L/cell}$ we calculate $N_{H+} = [H^+]$ x N_A x V_{Cell} and find $N_{H+}^{7.6} = 10.12\ \frac{\text{ions}}{\text{cell}}$ and $N_{H+}^{7.8} = 6.37\ \frac{\text{ions}}{\text{cell}}$.

(b) Periplasmic space $\approx 0.4\text{x}V_{Ecoli}$ with $\text{pH}^{Peri} \approx 7$. Using the same sort of set up as for (a) we find:

$$N_{H+}^{Peri} = 10^{-7}(\text{N}_A)(0.4\text{x}V_{Ecoli}) = 16.13\frac{\text{ions}}{\text{perispace}}. \tag{4}$$

2

(a) Given $R = 18\text{Å}$, $T = 298K$, Q=-10e, and [NaCl]=0.05$\frac{\text{mol}}{\text{L}}$. For NaCl $\approx 0.05M$, $\kappa^{-1} = 13.6\text{Å}$.

$$\overline{V} = \frac{eV}{k_BT} = \frac{Cqe}{Dk_BTa(1+\kappa a)} \tag{5}$$

Using equation 5, and the values provided we obtain $\overline{V} = -1.075$.

(b) $[\text{Na}^+] = 0.05e^{1.705} = 275$ mM
$[\text{Cl}^-] = 0.05e^{-1.705} = 9.1$ mM

(c) We can rewrite the first part of equation 5 to obtain 6.

$$\frac{eV}{k_BT} = \frac{eV}{k_BT}\frac{a}{r}e^{-\kappa(r-a)} \tag{6}$$

From this we can find $\frac{eV}{k_BT} = -1.172$, which allows us to then arrive at $[\text{Na}^+] = 0.05e^{1.172} = 161$ mM and $[\text{Cl}^-] = 0.05e^{-1.172} = 15.5$ mM.

3

(a) The energy of interest can be written according to 7 where V(R) is given by equation 8.

$$U = \int_0^Q V(R)dq \tag{7}$$

$$V(R) = k_BT\frac{Q\,l_B\lambda_D}{e^2\;R(R+\lambda_D)} \tag{8}$$

Using this as well as substituting in Q=Ne, and substituting further that N = $\frac{4\pi R^2}{\pi r^2}$, we can pass through the following steps.

$$U = \frac{1}{2}Q^2\frac{k_BT}{e^2}\frac{l_B\lambda_D}{R\,(R+\lambda_D)} = \frac{N^2k_BT}{2}\frac{l_B\lambda_D}{R(R+\lambda_D)} \tag{9}$$

Which can then be rewritten and simplified to give:

$$U = \frac{8k_BTR^3}{r^4}\left(\frac{l_B\lambda_D}{(R+\lambda_D)}\right) \tag{10}$$

(b) Here we use that $\lambda_D = \frac{1}{\sqrt{c}}$, and $l_B = \frac{e^2}{4\pi\epsilon k_BT}$, and make the approximation from class for $R >> \lambda_D$. This gives

$$U \approx \frac{8k_BTR^3}{r^4}(\frac{l_B\lambda_D}{R}) = \frac{8k_BTR^2l_B\lambda_D}{r^4} \tag{11}$$

The plot generated from this equation is shown in figure 1 where r = 5Å, R is 1,...,9 nm and $c_\infty = 1, 10,$ and 100 mM. From the figure it can be seen that at higher salt concentrations, larger radii will result at lower energies. This suggests the salt will change the charge state of the protein such that it denatures out of it's folded conformation.

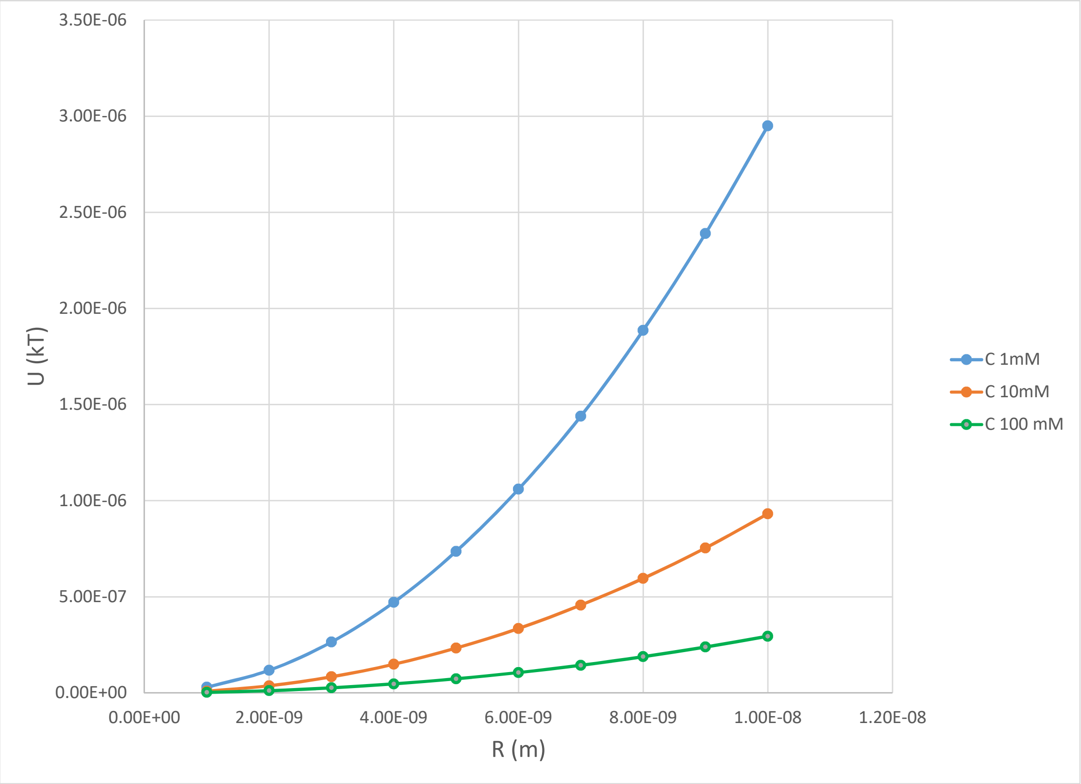

Figure 1: Electrical energy as a function of radius for three concentrations c_∞=1mM, 10mM and 100mM.

4

We are given the reaction $ATP \rightleftharpoons ADP + P_i$, where the reaction is catalyzed by the presence of kinesin. If we label ATP as the substrate, S, kinesin as the enzyme, E, and call ADP and P_i collectively as the products, P, we can re-write this as:

$$E + S \rightleftharpoons ES \longrightarrow E + P \tag{12}$$

This follows Michealis-Menton kinetics such that [ATP] $= K_m$ at $1/2 v_{max}$, and we can model v such that,

$$v = \frac{v_{max}[S]}{K_m + [S]} = \frac{[ATP]v_{max}}{[ATP] + K_m} \tag{13}$$

Using this model we create the plot in figure 2, which plots the values of v as a function of the substrate concentration in µM. From the plot it can be seen that the relationship obeys the kinetics expected of Michaelis-Menton kinetics were there is an initial rise in speed with increased substrate that eventually reaches a plateau.

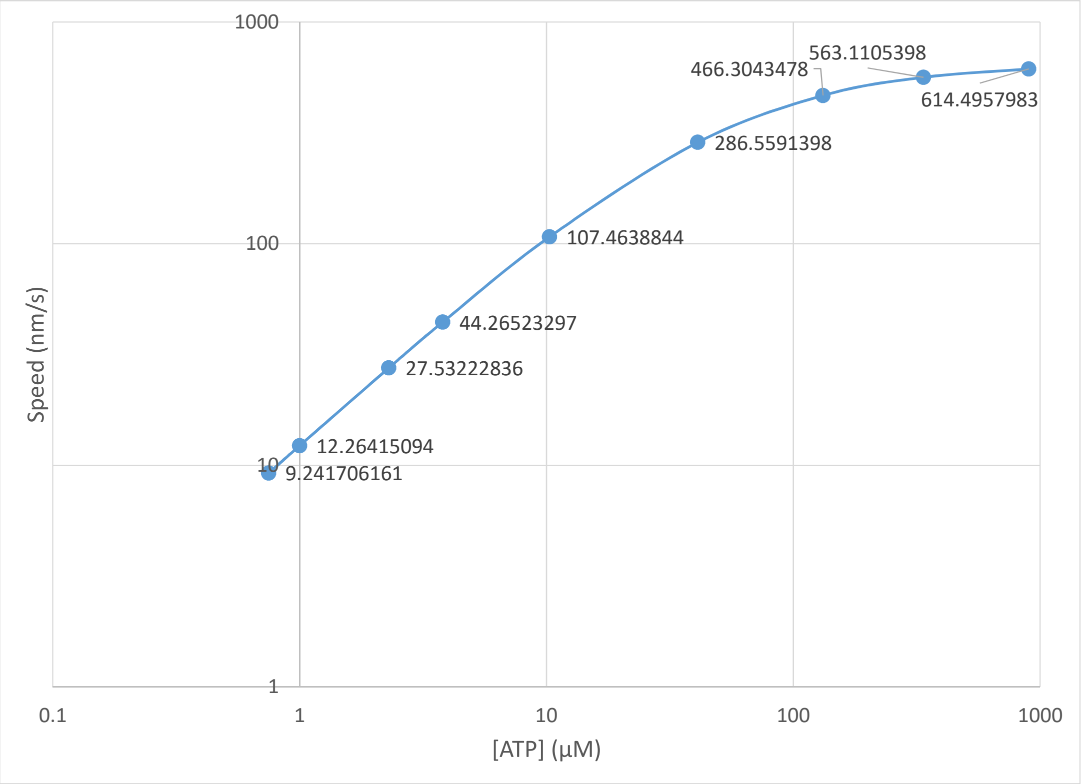

Figure 2: Relationship between speed and substrate concentration.

In the cases given we have v = $0.1v_{max}$ and v = $0.9v_{max}$. This gives:

$$0.1v_{max}([ATP] + K_m) = [ATP]v_{max} \Rightarrow 0.1([ATP] + K_m) = [ATP] \tag{14}$$

This ultimately gives [ATP]=$\frac{K_m}{9}$. Performing a similar calculation for the v=$0.9v_{max}$ case gives [ATP]$'$ = $9K_m$. The difference is then Δ[ATP] = $9K_m - \frac{K_m}{9}$ = $8.89K_m$, where $K_m \approx 52\mu M$, giving Δ[ATP] $\approx$ $462.3\mu M$.

5

(a) Want capacitance for membrane; given $k = 2$ and d = 2nm for only lipid tail portion of bilayer. Using $C = \frac{k\epsilon_o A}{d}$, and further $C_m = \frac{C}{A}$ we obtain:

$$C_m = \frac{2(8.85 \text{ x } 10^{-12}\frac{F}{m})}{2 \text{ x } 10^{-9}m} = 0.00885\frac{F}{m^2} \tag{15}$$

(b) $\epsilon_{H_2O} = 80$ and $d_{H_2O} = 0.7$ nm.
Applying the same formulae as before we get $C_m^{H_2O} = 1.011\frac{F}{m^2}$. Using then that:

$$C_T = \frac{1}{\frac{1}{c_1} + \frac{1}{c_2}} \tag{16}$$

We find $C_T = 0.877\frac{\mu F}{cm^2}$.

6

(a) C = 1µF/cm^{-2}, ΔV = 60mV.
Q = CV = (0.01F/m^2)(0.06V) = 6 x 10^{-4}C/m^2.

(b) ΔV = Q/C; C=cA where c = 1µF/cm^2; and r = 0.5mm.

ΔV = $\frac{ne}{cA} = \frac{ne}{C}$ where n is the number of protons (Q = ne).

$\frac{Q}{L} = 2\pi r\sigma = \frac{C\Delta V}{L}$.

(c) [Na]$_{\text{i}}$ = 50mM and r$_{\text{axon}}$= 0.5x10^{-3}m ⇒ v$_{\text{axon}}$ = πr^{2}l.
Thus we obtain $\frac{n}{l}$ = [Na]$_iA$ = 50mM($\pi(0.5$ x $10^{-3})^2$) x N$_A$, which leads to an end value of 2.36 x 10^{10}ions/nm inside.

Using then [Na]$_o$ = 440mM, and the same equation leads to a value of 2.08 x 10^{11}ion/nm. The difference between these is then given as $\Delta n/l$ = 1.84 x 10$^{11}\,\frac{\text{ion}}{\text{mm}}$.

(d) Even after the pumps have shut down there remains a high number of Na+ ions for transmission to continue.

7

(a) $A \approx 1nm^2$ and $j = \frac{D\Delta c}{L}$ where L = 5nm, Δc = 100mM and D$_{Na}$ ≈ 1 µm^2/ms. Plugging this in we obtain:

$$j = \frac{(10^{-9}m^2/s)(100mol/m^3)}{5 \text{ x } 10^{-9}m} = 20\ s^{-1}m^{-2}mol \tag{17}$$

And so jA = 20 $s^{-1}m^{-2}mol(1$ x $10^{-18}m^2)$ = 2 x 10^{-17} mol/s x N$_A$ = 12.04 x 10^6 ion/s.

(b) j = I/A ⇒ $JA \approx I$, where I = 5 x 10^{-12} A = 5 x 10^{-12} C/s. We thus perform the following:

$$\Rightarrow 5 \text{ x } 10^{-12}\ C/s \text{ x } \left(\frac{1 \text{ ion charge}}{1.6 \text{ x } 10^{-19}}\right) \tag{18}$$

This gives the end result of ≈ 31.25 x 10^6 ion/s. The results differ by seemingly a lot, however, they are the same order of magnitude, so given that the quantity of interest is for number of ions the relative difference isn't so bad.

(c) let O = the total time channel is open (i.e. open = $O_1 + O_2 + ... + O_n$) and let C = the total time the channel is closed (i.e. closed = $C_1 + C_2 + ... + C_n$).
The probability is then:

$$P_O = \frac{O}{O + C} = \frac{4 \text{ ms}}{(4 + 27) \text{ ms}} = 0.129 \approx 13\%. \tag{19}$$

If the probability is then 0.5, this becomes:

$$0.5 = \frac{O}{O + C} \Rightarrow O = 0.5O + 0.5C \Rightarrow 0.5C = 0.5C \tag{20}$$

A sketch of what this current might look like is shown in figure 3 below.

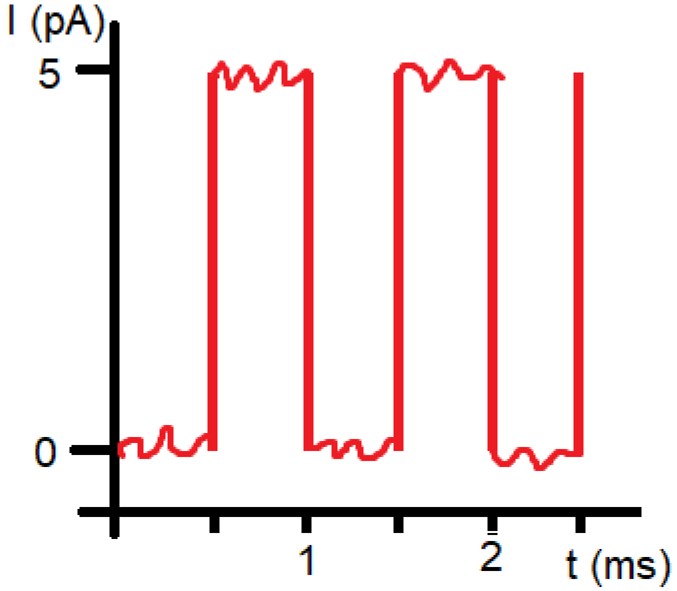

Figure 3: Sketch of possible current recording for a P_o=0.5.