HW2: Molecular Biophysics

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October 15, 2019

1 Q1

For this problem first I will use the relationship defined in Eq 1 which relates flux ϕ to the diffusion constant D, change in concentration ΔC, and change in distance Δx. I searched and found a literature value for $D = 5.5 * 10^{-6} \frac{cm^2}{s}$. Based ont eh problem setup we go from a concentration of $4mM$ to $0mM$, thus $\Delta c = c2 - c1 = -4.4mM$. The length of the axon is $1m = \Delta x$. Now for some unit conversion. $-4.4mM = -0.004M = 0.004 * 6.023 * 10^{23} \frac{molecules}{L} = \frac{-0.004*6.023*10^{23}}{1000} \frac{molecules}{cm^3} = -2.409 * 10^{18} \frac{molecules}{cm^3}$, $\Delta x = 1m = 100cm$. Now that everything is in terms of cm, s, and molecules we can evaluate Eq 1, which results in a vlaue of $1.32 * 10^{11} \frac{molecules}{cm^2 s}$. By multiplying this flux per area by the crossectional area of the axon we get the quantity of molecules per second out the end of the axon by diffusion. The axon has a diameter of $10\mu m = 1 * 10^{-3} cm$. Thus the area is $\pi r^2 = \pi(d/2)^2 = \pi(5 * 10^{-4)cm})^2 = 7.8 * 10^{-7} cm^2$. Multiplying this area by the flux we get a total of $1.04 * 10^5 \frac{molecules}{second}$. For a signal the described delivery amounts to 3 million molecules per impulse. Using the diffusion rate we just solved for this would take 3million/104000 = 28.8 seconds. This rate of fire is way too slow, as a neuron is typically able to fire many many times a second.

$$\phi = -D \frac{\Delta c}{\Delta x} \tag{1}$$

2 Q2

For this section I used the convection equation as described by Eq 2, where t is time (80 seconds), u is position, m is number of particles (10^9), v is drift velocity ($1 \frac{\mu m}{s}$), and G is the diffusion constant ($10^{-6} \frac{cm^2}{s}$). If we consider that diffusion happens in all directions, and that it follows a normal or gaussian distribution, then it makes sense that even if a force is pushing objects in a certain direction, this only acts to move the center of the distribution, and it is still possible to find particles on both sides of the distribution (both with and against the applied force). By plugging in u = 0 to Eq 2 we get the molecules/cm = $2.58 * 10^{10}$.

$$convection = \frac{e^{-\frac{(u-tv)^2}{4Gt}} m}{2\sqrt{\pi}\sqrt{Gt}} \tag{2}$$

3 Q3

Using the relationship established in Eq 3 we can determine the radius of the nano particles by using the effective mass (m) which is equal to $v(D_{gold} - D_{water})$ where v is the volume of the particle $= \frac{4}{3}\pi r^3$. A simple substitution and rearrangement to solve for r yields Eq 4 where k is the Boltzmann's constant, T is the temperature (assumed to be room temperature of 293 K), g is acceleration due to gravity (9.8 m/s^2) and λ is the distance at which the density decreases by e-fold, 9 mm. The density of water is $1000 kg/m^3$ thus the difference between gold and water is $19.3 * D_{water} - D_{water} = 19.3 * 1000 - 1000 = 18300 kg/m^3$. Using this equation and the known values from the problem we get $r = 8.43^10{-}9m = 8.43nm$ thus the diameter $d \approx 17nm$.

$$\lambda = \frac{kT}{mg} \tag{3}$$

$$r = (\frac{3kT}{4\pi(D_{gold} - D_{water})g\lambda})^{\frac{1}{3}} \tag{4}$$

4 Q4

Assuming a room temperature of 273 K. When there is no force the diffusion is equal to $D = \frac{x_0^2}{2D} = 13\mu s$. When there is a force the relationship shown in Eq 5 was provided. When the particle is moving with the force then the force is positive, and when the particle is moving against the force the force is negative. (the same could be done by negating the position instead of the force) Plugging in the known values the time to diffuse going with the force is $2.4\mu s$, whereas the time to diffuse against the force is $5.5ms$.

$$t = 2(\frac{x_0^2}{2D})(\frac{kT}{FX_0})^2(e^{-\frac{Fx_0}{kT}} - 1 + \frac{Fx_0}{kT}) \tag{5}$$

5 Q5

Attached page has the visual and written equations for problem 5. The first section (A) shows all of the different binding options. Next to each configuration is the number of possible arrangements for that configuration. In B I write out the full expansion of this polynomial, adding the f term to each binding interaction based on the number of cooperative (adjacent) bindings of the ligand on the 6 sites. In C I simplify this expansion by combining like terms and remove the protein term to get the polynomial Q. In D I show the average number bound as a function of ligand concentration.

6 Appendix

Below is the matlab code I used for the calculations in each of the problems.

```
%Q1

dC = -(0.004 * 6.023e23)/1000;
dX = 100;%cm
D = 5.5e-6;%cm^2/s
phi = -D*(dC/dX);
d = 1e-3;%cm
r = d/2;
area = pi * r^2;%cm^2
flow = phi*area;
timeToDiffuse = 3000000/flow;
%Q2
u = 0;
m = 10^9;
v = 1e-4;
G = 10^-6;
t = 80;
convection = (exp(-(u-t*v)^2/(4*G*t))*m)/...
(2*sqrt(pi)*sqrt(G*t));

%Q3
k = 1.38e-23;%m^2 kg/K s
T = 293;%K
g = 9.8;%m/s^2
Ddiff = 19.3*1000 - 1000;%
lambda = 0.009;%m
r = ((3*k*T)/(4*g*pi*Ddiff*lambda))^(1/3);
d = 2*r;

%Q4
k = 1.38e-23;%m^2 kg/K s
T = 292;%k
f = 1e-12;%kg m/s^2
x0 = 4e-8;%m
D = 6e-11;%m/s

tnoforce = x0^2/(2*D);

%Now with force
%With the force
t1 = 2*(x0^2/(2*D))*...
((k*T)/(f*x0))^2*(exp(-(f*x0)/(k*T))...
- 1 + (f*x0)/(k*T));
%f = -f;%either works
x0 = -x0;
```

```
%Against the force
t2 = 2*(x0^2/(2*D))*...
((k*T)/(f*x0))^2*(exp(-(f*x0)/(k*T))...
- 1 + (f*x0)/(k*T));
```