

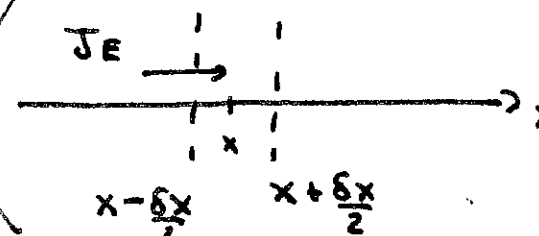
Diffusion: Particles and Heat.

Fourier's law of heat flow $J_E = -K \partial_x T$
Thermal conductivity.

Conservation of energy: $u \propto T$ and $u = \text{energy density}$

$$\delta x \partial_t u = J_E(x - \delta x/2) - J_E(x + \delta x/2)$$

$u = cT$



$$c \delta x \partial_t T = -K \left[\partial_x T(x - \frac{\delta x}{2}, t) + \partial_x T(x + \frac{\delta x}{2}, t) \right]$$

energy content of "slice" at x

Expanding to 1st order in δx :

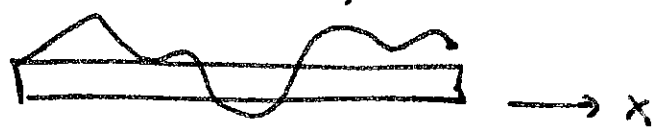
$$c \partial_t T = -K \left[\partial_x T - \frac{1}{2} \delta x \partial_x^2 T - \partial_x T - \frac{1}{2} \delta x \partial_x^2 T \right]$$

$$\Rightarrow \boxed{\partial_t T = D \partial_x^2 T} \quad D = K/c$$

Diffusion Eqn for heat. Required 1) currents \propto gradient
2) local conservation.

\Rightarrow Should be generally true. We will come back to this.

How can we solve this? Example: heat diffusion on a finite bar.



$T(x, 0)$ specified Initial condition.

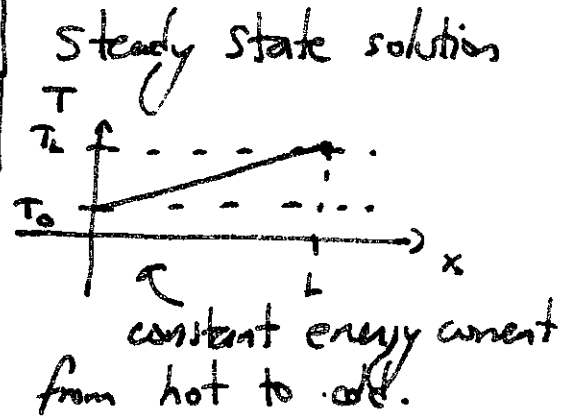
What about the boundaries? We can specify the temperature or the energy flux at each end.

A. Specify temperature: $T(0, t) = T_0$ } Boundary
 $T(L, t) = T_L$ } Conditions.

Can we find a steady-state solution?
i.e., one with $\partial_t T = 0$

$\Rightarrow \partial_x^2 T = 0 \Rightarrow T(x) = A + Bx$; two constants to be set by the boundary conditions.
↑
"steady-state"

$T_{ss}(x) = T_0 + (T_L - T_0) \frac{x}{L}$



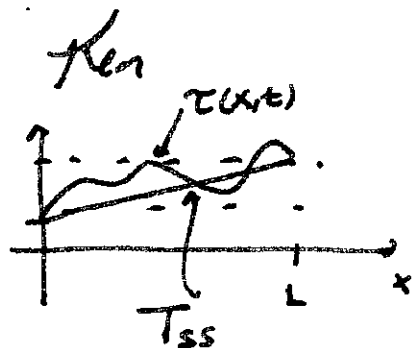
Can we find more interesting solutions?

Before we look at time-dependent solutions, note that since the diffusion equation is linear a sum of solutions is also a solution

If T_1, T_2 solve the equation $c_1 T_1 + c_2 T_2$ is one too.

Let $T(x, t) = T_{ss}(x) + \tau(x, t)$

$\tau(0, t) = \tau(L, t) = 0$.



What kind of solution can we find?

Recall $\partial_x^2 \begin{cases} \sin qx \\ \cos qx \end{cases} = -q^2 \begin{cases} \sin qx \\ \cos qx \end{cases}$

Look for a solution of the form $T(t) \sin(qx)$

$$\partial_t T = D \partial_x^2 T \Rightarrow \sin(qx) T'(t) = -D q^2 \sin(qx) T(t)$$

so $\frac{d}{dt} \log T(t) = -D q^2$ or $T(t) = T(0) e^{-D q^2 t}$

So we should have a sol'n

related to the initial condition

with: $A e^{-D q^2 t} \sin(qx) = \tau(x, t).$

But we need $\sin(qL) = 0 \Rightarrow qL = n\pi$ $n=1, 2, 3, \dots$

$$q_n = \frac{n\pi}{L}$$

In general we have a solution of the form:

$$\tau(x, t) = \sum_{n=1}^{\infty} A_n e^{-D q_n^2 t} \sin\left(\frac{n\pi}{L} x\right);$$

Note: Information at short length scales get erased faster than at long length scales.

decay time of n th mode: $T_{\text{decay}}^{(n)} = \frac{1}{D q_n^2} = \frac{L^2}{D \pi^2 n^2}$

or $T_{\text{decay}}^{(n)} = \frac{1}{n^2} T_{\text{decay}}^{(1)}$

Time scales grow as L^2 : $T_{\text{decay}}^{(1)} \approx \frac{L^2}{D}$ "diffusive scaling"

Back to our problem. How do we get the set of A_n 's?

Recall the initial conditions

$$T(x,0) = f(x) = \sum_{n=1}^{\infty} A_n e^{-Dq_n^2 t} \sin(q_n x)$$

$$T(x,0) - T_{SS}(x)$$

We need to determine the set $\{A_n \mid n=1, \dots\}$ to get

$$f(x) = \sum_{n=1}^{\infty} A_n \sin(q_n x) ; \quad q_n = n\pi/L$$

known

Fourier Series!

from initial condition

A refresher on Fourier series.

The sine functions are orthogonal:

$$\int_0^L \sin\left(m\pi\frac{x}{L}\right) \sin\left(n\pi\frac{x}{L}\right) dx = 0 \text{ unless } m=n.$$

If $m=n$, then we have:

$$\int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2}.$$

Using the orthogonality of the sines:

$$\int_0^L f(x) \sin\left(\frac{m\pi x}{L}\right) dx = \sum_{n=1}^{\infty} \left\{ \int_0^L dx \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx \right\} A_n$$

$\delta_{n,m} \frac{L}{2}$

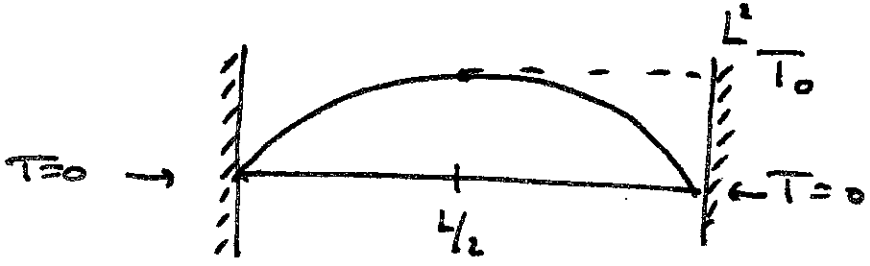
$$= \frac{L}{2} A_m$$

$$\Rightarrow A_m = \frac{2}{L} \int_0^L f(x) \sin\left(\frac{m\pi x}{L}\right) dx.$$

This completes the solution.

Now, an example: Take $T_{ss}(x) = 0$ and

$$T(x,0) = T(x,\infty) = x(L-x) \frac{4T_0}{L^2}$$



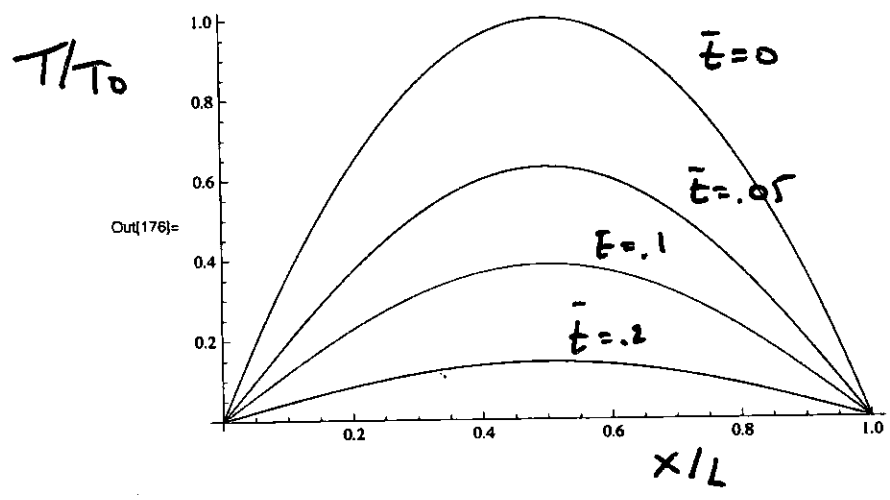
A parabolic temperature profile of $T=0$ at the boundaries.

We get $A_m = \frac{4 \cdot L T_0}{m^3 \pi^3} \frac{2}{L} (2 - 2 \cos(m\pi))$

$$= \frac{16 T_0}{m^3 \pi^3} [1 - (-1)^m] = \begin{cases} \frac{32 T_0}{\pi^3 m^3} & , m \text{ odd} \\ 0 & , m \text{ even.} \end{cases}$$

$$\bar{t} = \frac{t}{\tau} \left(\frac{D}{L^2} \right)$$

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In[176]= Plot[{f[x, 0.], f[x, 0.05],  
f[x, 0.1], f[x, 0.2], 4 x (1 - x)}, {x, 0, 1}]
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What does the solution look like? An.
 "Feeding" at the microscale: Diffusion to capture.
 A. Steady-state solutions: Isotropic absorber w/
 fixed concentration at ∞ .



absorber

$$\frac{\partial C}{\partial t} = D \nabla^2 C$$

C_{∞} .
Time-independent

$\Rightarrow \nabla^2 C = 0$ Recall $\nabla \cdot \vec{E} = 0$ $\vec{E} = -\nabla \Phi$
 look for isotropic solutions: $\Rightarrow \nabla^2 \Phi = 0$ Laplace's Eq.

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dC}{dr} \right) = 0$$

Of course we know the answer! $C = A + B/r$

What are the boundary conditions?

$r = a$ Perfect absorber $C = 0$

$r = \infty$ $C = C_{\infty}$

$$\Rightarrow C(r) = C_{\infty} - \frac{C_{\infty} a}{r} = C_{\infty} \left(1 - \frac{a}{r}\right)$$

What is the ("Fickian") flux of particles?

current $\vec{J} = -D \frac{\partial C}{\partial r} \hat{r} \Rightarrow J_r = -D C_{\infty} \frac{a}{r^2}$ Currents "Electric field"

particles per time per unit area.

What is the rate of particle accumulation at the absorber?

$$I = - \oint_{r=a} r^2 d\Omega \hat{r} \cdot \vec{J} = \frac{D C_{\infty} a^2}{a^2} 4\pi$$

$r=a$ had to be true \rightarrow linearity!

$I = 4\pi D C_{\infty} a$

Oddly, we get $I \propto a$ not

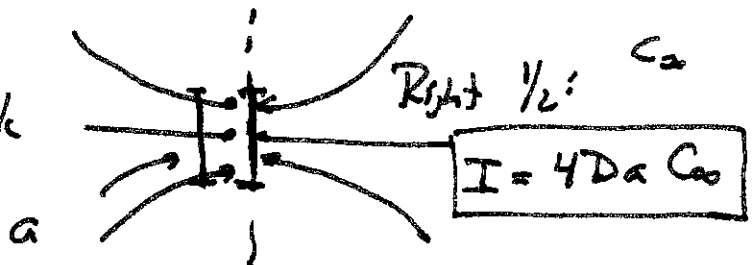
proportional to the surface area! $I \propto a^2$ why?

$I = (\text{surface area}) \times (\text{current})$ and current $\propto \nabla C$

$$I \sim a^2 \times \frac{1}{a} = a.$$

Small absorbers do "better" than you might have guessed!

B. Diffusion to a disk



c. Diffusion to an elliptical absorber

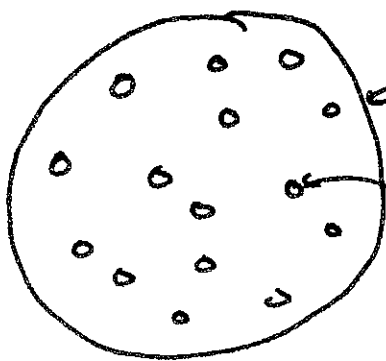


if $a^2 \gg b^2$ then

$$I \cong \frac{4\pi D a C_\infty}{\log(2a/b)} \quad \leftarrow \text{like a sphere.}$$

$\log(2a/b)$ \leftarrow But a bit less efficient!

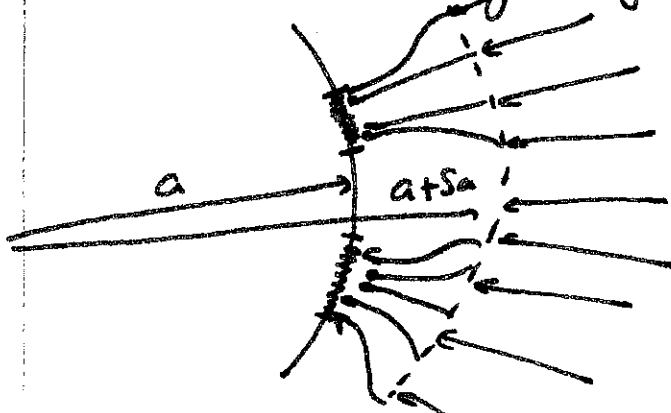
Note that cells are not perfect absorbers. more like:



all of radius $a \approx 3 \mu m$

chemoreceptor $s \approx 1 \mu m$ for a bacterium.

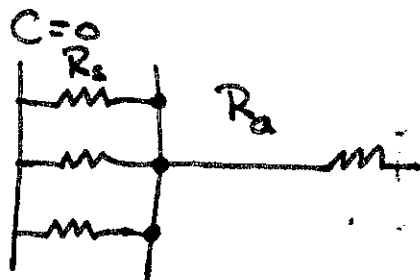
How efficient is this system? Or, how many receptors do we need to do a good job?



Far enough away the absorber looks perfect.

Note in steady-state $I = C_\infty / R$ \leftarrow "diffusion resistance"

Effective Circuit:



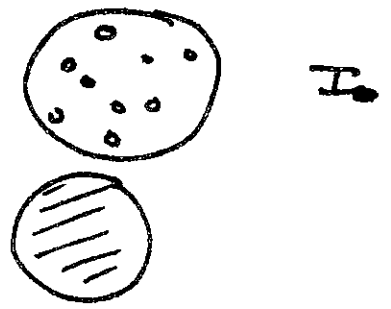
$r = a$

$$R = R_a + R_s/N = \frac{1}{4\pi Da} + \frac{1}{4DN_s}$$

Roughly $\frac{1}{4\pi Da}$ \swarrow $\frac{1}{4Da}$.

$$R = \frac{1}{4\pi Da} \left[1 + \frac{\pi a}{N_s} \right]$$

\Rightarrow particles per time absorbed by
compared to



$$\Rightarrow \frac{I}{I_0} = \frac{1}{1 + \pi a/N_s}$$

Now what fraction of the surface need be covered.

$a \sim 1 \mu m$ $a \sim 10^3 nm$ want $\frac{\pi a}{N_s} \sim O(1)$

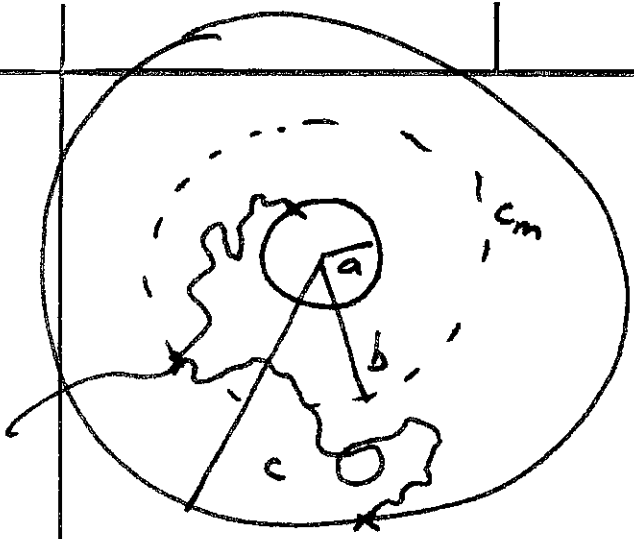
$\Rightarrow NN \frac{\pi a}{s} \sim 10^3$ receptors on one bacterium.

But they take up only $\frac{N\pi a^2}{\pi a^2} \sim 10^3 \times \left(\frac{1}{10^3}\right)^2 \sim 10^{-3}$

of the surface area of the cell.

Save receptors and allow for multiplexing!

C. Probability of Capture.



Solution

$$C(r) = \begin{cases} \frac{C_m}{1-a/b} \left(1 - \frac{a}{r}\right), & a \leq r \leq b \\ \frac{C_m}{\frac{c}{b}-1} \left(\frac{r}{c} - 1\right) & b \leq r \leq c \end{cases}$$

release here - where do they go?

What is the radial flux?

$$J_r(r) = \begin{cases} \frac{-DC_m}{1-a/b} \frac{a}{r^2}, & a \leq r \leq b \\ \frac{DC_m}{c/b-1} \frac{c}{r^2}, & b \leq r \leq c \end{cases}$$

Inner shell collect particles at a rate of:

$$I_{in} = \frac{DC_m}{(1-a/b)} \frac{a}{a^2} 4\pi a^2 = \frac{4\pi DC_m a}{1-a/b}$$

$$I_{out} = \frac{4\pi DC_m c}{c/b-1}$$

Ratio: $\frac{I_{in}}{I_{in} + I_{out}} = \frac{a(c-b)}{b(c-a)}$ Prob that particles released at $r=b$ get absorbed at $r=a$ before wandering off to c .

Take $c \rightarrow \infty$ Prob $\sim a/b \leftarrow$ decreases as $1/b$ not $1/b^2$! ? like the solid angle.

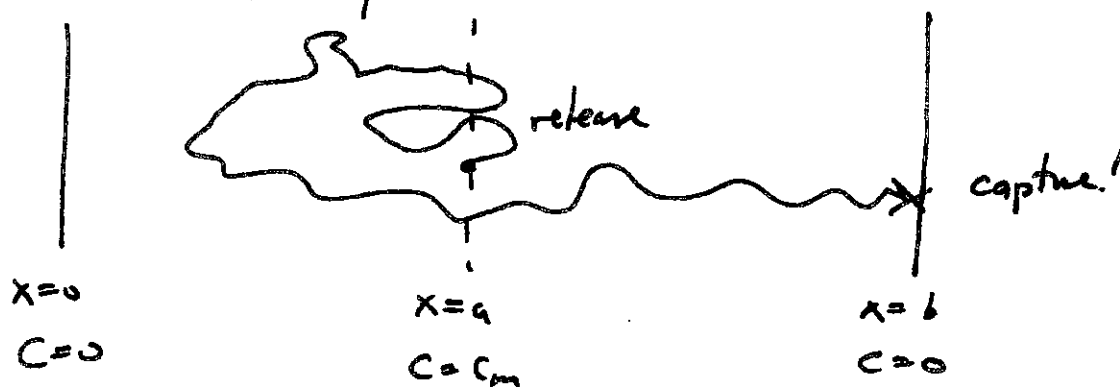
Prob that particle visits the sphere once before wandj⁽⁷²⁾
away for good. $p = a/b$.

Prob that the particle makes n trips to the sphere
before wandj away: $p^n (1-p)$

$$\text{mean \# trip } \langle n \rangle = \sum_{n=0}^{\infty} n p^n (1-p) = \frac{p}{1-p}$$

$$= \frac{a}{b-a}$$

Mean time to capture.



$W(a) = \text{mean time to capture when released at } a$.

$W(x) = ?$

Take steps of size δ every τ $D = \delta^2 / 2\tau$

$$W(x) = \tau + \frac{1}{2} [W(x+\delta) + W(x-\delta)]$$

$$\Rightarrow \frac{dW}{dx} \Big|_x - \frac{dW}{dx} \Big|_{x-\delta} + \frac{2\tau}{\delta} = 0 ;$$

$$\boxed{\frac{d^2 W}{dx^2} + \frac{1}{D} = 0}$$

Differential equation for $W(x)$.

Boundary Conditions $W(0) = W(b) = 0$

$$\Rightarrow W(x) = \frac{1}{2D} (bx - x^2)$$

$$W(b/2) = b^2/8D \text{ longest time.}$$

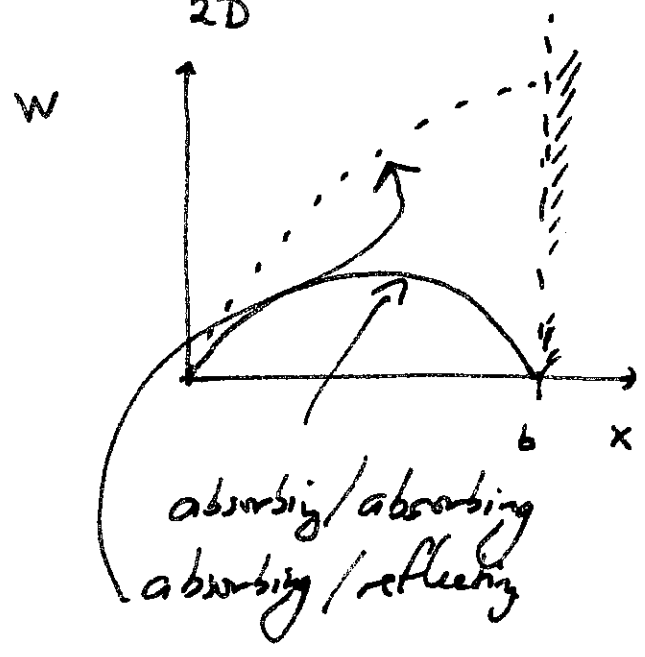
Averaged time over release pt:

$$\frac{1}{b} \int_0^b W(x) dx = b^2/12D$$

What if we make the right wall reflecting? $W(0) = 0$

$$W(x) = \frac{1}{2D} (2bx - x^2)$$

$$\frac{dW(b)}{dx} = 0.$$



Note: what are diffusion constants in water?

In higher dimension: $\nabla^2 W + \frac{1}{D} = 0.$

Diffusion w/ drift.

$$v_d = \frac{\mu}{\zeta} F / \zeta \leftarrow \text{friction constant.}$$

