Diffusion: Particles and Heat.

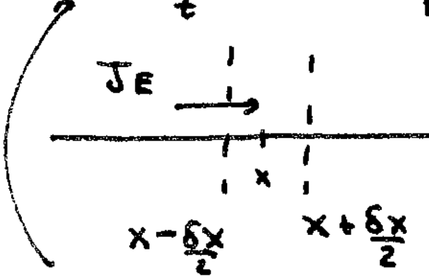
Fourier's law of heat flow $J_E = -K\,\partial_x T$

Thermal conductivity.

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

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

$$u = cT$$



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

energy content of "slice" at x

Expanding to 1^{st} order in δx:

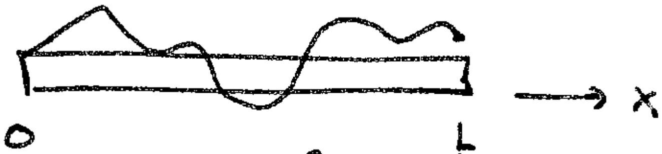
$$c\,\partial_t T = -K\left[\partial_x T - \tfrac{1}{2}\delta x\, \partial_x^2 T - \partial_x T - \tfrac{1}{2}\delta x\, \partial_x^2 T\right]$$

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

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: $\left.\begin{array}{l} T(0,t) = T_0 \\ T(L,t) = T_L. \end{array}\right\}$ Boundary Conditions.

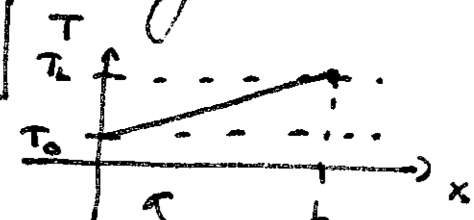
Can we find a steady-state solution?
i.e., one with $\partial_t T = 0$

$\Rightarrow \quad \partial_x^2 T = 0 \Rightarrow T_{ss}(x) = A + Bx$; two constants to be set by the boundary conditions.

"steady-state"

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

Steady State solution



constant energy current from hot to cold.

Can we find more interesting solutions?

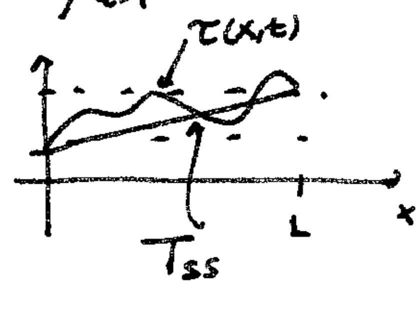
Before we look at time-dependent solutions, note that, since the diffusion equation is linear a sum of solutions is also a solution

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

constants.

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

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



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 $T(t)\sin(qx)$

$\partial_t T = D\,\partial_x^2 T \Longrightarrow \sin(qx)\,T'(t) = -Dq^2 \sin(qx)\,T(t)$

so $\dfrac{d}{dt}\log T(t) = -Dq^2$ or $T(t) = T(0)\,e^{-Dq^2 t}$

related to the initial condition

So we should have a sol'n with: $A\,e^{-Dq^2 t}\sin(qx) = \tau(x,t)$.

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

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

In general we have a solution of the form:

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

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

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

or $T_{decay}^{(n)} = \dfrac{1}{n^2}\,T_{decay}^{(1)}$.

Time scales grow as L^2: $T^{(1)}_{decay} \cong \frac{L^2}{D}$ "diffusive scaling"

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

Recall the initial conditions

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

$$\uparrow$$

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

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

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

$\uparrow$

known from initial condition

Fourier Series!

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:

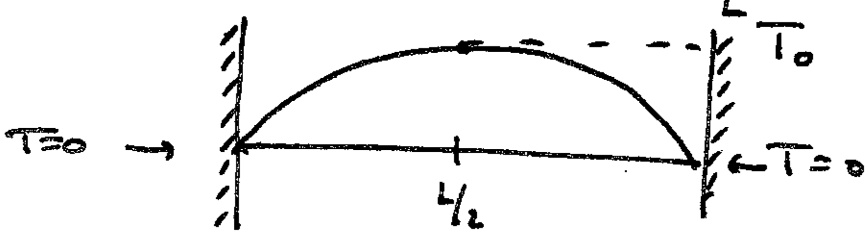
$$\int_0^L f(x)\sin\left(\frac{m\pi x}{L}\right)dx = \sum_{n=1}^{\infty}\Big\{\underbrace{\int_0^L dx\,\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)dx}_{=\ \delta_{n,m}\,L/2}\Big\}A_n$$

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

$$\Rightarrow \boxed{A_m = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{mx\pi}{L}\right)dx.}$$ This completes the solution.

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

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



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

We get $A_m = \frac{48LT_0}{m^3\pi^3}\frac{2}{L}\left(2-2\cos(m\pi)\right)$

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

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

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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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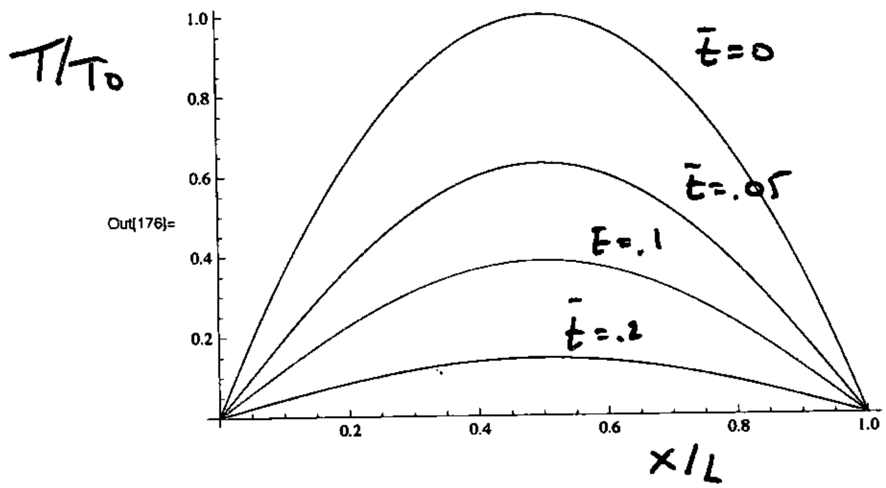
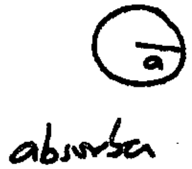


What does the solution Look like? Ans.

"Feeding" at the microscale: Diffusion to capture.

A. Steady-state Solutions: Isotropic absorber w/ fixed concentration at ∞.



c_∞.

$$\frac{\partial c}{\partial t} = D\nabla^2 c \qquad \text{Time-independent}$$

$\Rightarrow \nabla^2 c = 0$ Recall $\vec{\nabla}\cdot\vec{E} = 0$ $\quad \vec{E} = -\vec{\nabla}\Phi$

Look for isotropic solution: $\Rightarrow \nabla^2\Phi = 0$ 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 boundy conditions?

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

$r=\infty$ $\quad C=C_\infty$

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

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

current $\quad \vec{J} = -D\dfrac{\partial c}{\partial r}\hat{r} \Rightarrow J_r = -D C_\infty \dfrac{a}{r^2}$ $\quad$ Current ↔ "Electric field"

particles per time per unit area.

What is the rate of particle accumulation at the absorber?

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

had to be true → linearity!

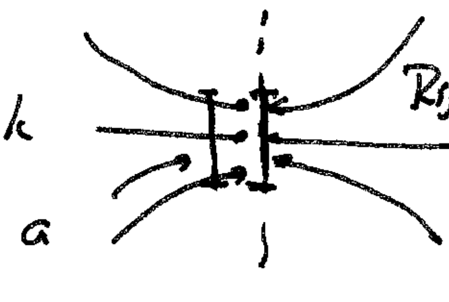
$\boxed{I = 4\pi D C_\infty a}$ Oddly, we get $I \propto a$ not proportional to the surface area! $I \not\propto a^2$. Why?

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

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

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

B. Diffusion to a disk



C_∞

Right 1/2: $\boxed{I = 4 D a C_\infty}$

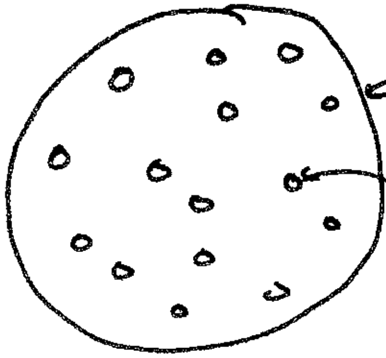
C. Diffusion to an ellipsoidal absorber

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

$$I \cong \frac{4\pi D a C_\infty}{\log(2a/b)}$$

← like a sphere.
← But a bit less efficient!

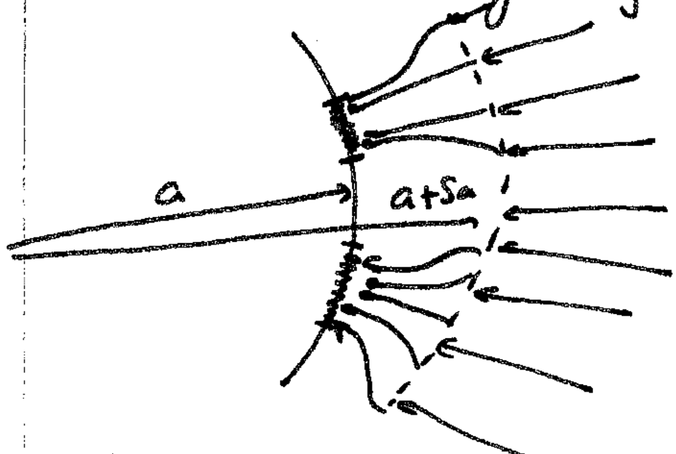
Note that cells are not perfect absorbers. More like:



cell of radius $a \approx 3\,\mu m$ ← for a bacterium.

chemoreceptor $s \approx 1\,nm$

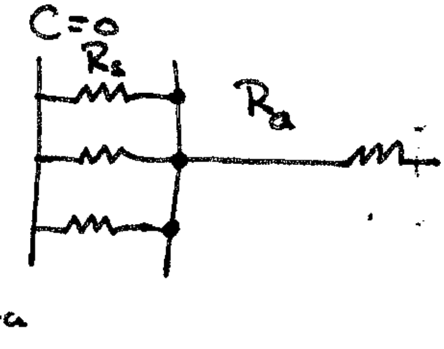
How efficient is this system? Or, how many receptors do we need to do a good job?



Far enough away the absorber looks perfect.

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

Effective Circuit:

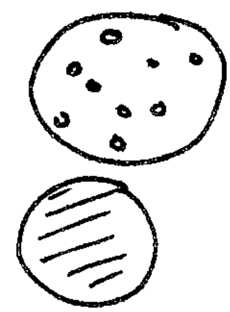


$$R = R_a + R_s/N = \frac{1}{4\pi D a} + \frac{1}{4DNs}$$

R_a: Roughly $\frac{1}{4\pi D a}$ R_s: $1/4Ds$.

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

$\Rightarrow$ particles per time absorbed by



I

compared to

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

Now what fraction of the surface need be covered.

$s \sim 1nm$ $a \sim 10^3 nm$ want $\frac{\pi a}{Ns} \sim \mathcal{O}(1)$

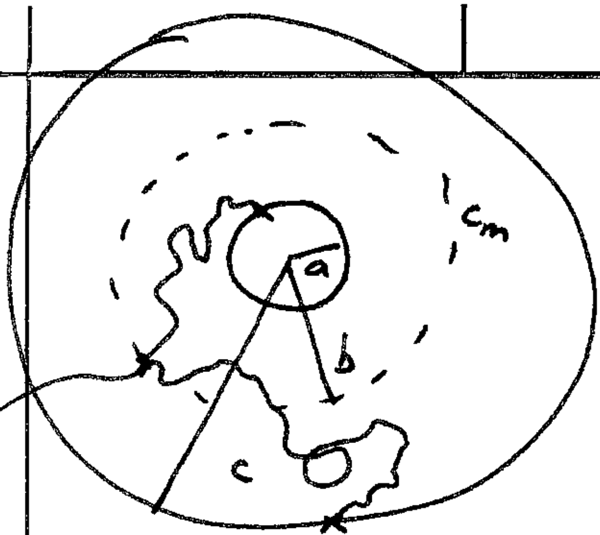
$\Rightarrow$ $N \sim \frac{\pi a}{s} \sim 10^3$ receptors on one bacterium.

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

of the surface area of the cell.

Saves receptors and allow for multiplexing!

C. Probability of Capture.



release here — where do they go?

Solution

$$C(r) = \begin{cases} \dfrac{c_m}{1-a/b}\left(1-\dfrac{a}{r}\right), & a \le r \le b \\[2ex] \dfrac{c_m}{\frac{c}{b}-1}\left(\dfrac{c}{r}-1\right) & b \le r \le c \end{cases}$$

What is the radial flux?

$$J_r(r) = \begin{cases} \dfrac{-Dc_m}{1-a/b}\,\dfrac{a}{r^2}, & a \le r \le b \\[2ex] \dfrac{Dc_m}{c/b-1}\,\dfrac{c}{r^2}, & b \le r \le c \end{cases}$$

Inner shell collects particles at a rate of:

$$I_{in} = \frac{Dc_m}{(1-a/b)}\,\frac{a}{a^2}\,4\pi a^2 = \frac{4\pi D c_m a}{1-a/b}$$

$$I_{out} = \frac{4\pi D c_m \; c}{c/b - 1}$$

Ratio: $\dfrac{I_{in}}{I_{in}+I_{out}} = \dfrac{a(c-b)}{b(c-a)}$ Prob that particle released at $r=b$ get absorbed at $r=a$ <u>before</u> wandering off to c.

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

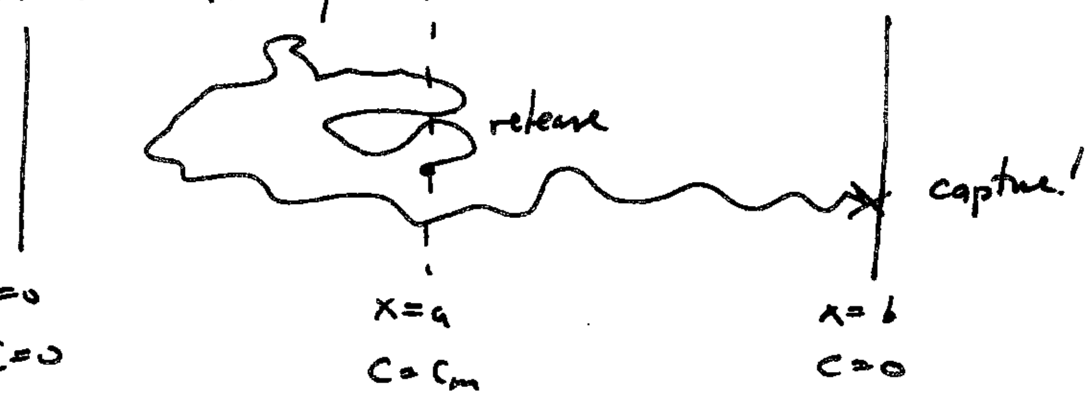
Prob that particle visits the sphere once before wandering away for good. $p = a/b$.

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

mean # trips $\langle n \rangle = \sum_{n=0}^{\infty} n p^n (1-p) = \dfrac{p}{1-p}$

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

Mean time to capture.



$W(a)$ = mean time to capture when released at a.

$W(x) = ?$

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

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

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

$$\boxed{\frac{d^2W}{dx^2} + \frac{1}{D} = 0}$$ Differential equation for $W(x)$.

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

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

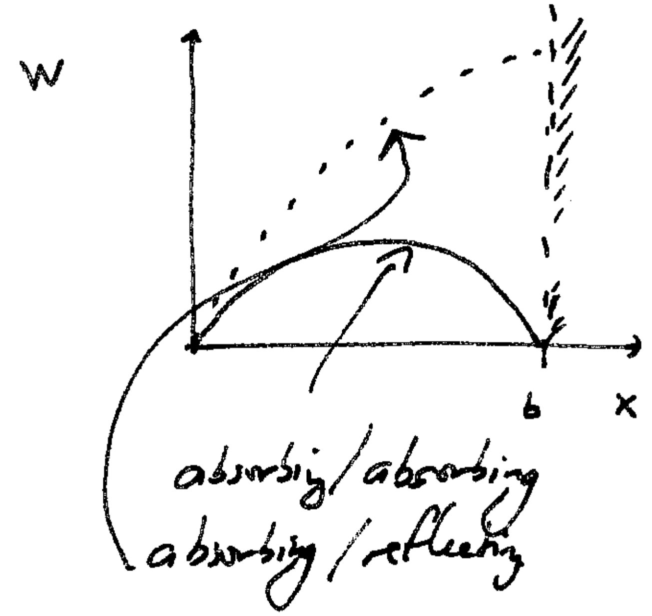
$W(b/2) = b^2/8D$ longest time.

Averaged time over release pts:

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

What is we make the right wall reflecting? $W(0)=0$, $\frac{d}{dx}W(b) = 0.$

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



Note: what are diffusion constants in cells? in water?

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

Diffusion w/ drift.

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

Fick's Eqn $\quad J = -D\frac{\partial c}{\partial x} + v\,C$

$\Rightarrow$ Advection / Diffusion Eqn

$$\frac{\partial c}{\partial t} = D\,\partial_x^2 c - v\frac{\partial c}{\partial x}$$

Diffusion $\qquad$ Drift.

Consider approach to equilibrium.

Extra stuff in case of additional time...