

Problem Set 3: Diffusion

1 Diffusion scales

The diffusion constant, D , of a suspended spherical particle of radius R in a fluid with viscosity μ is given by the Stokes-Einstein relation

$$D = \frac{k_B T}{6\pi R \mu},$$

where k_B is the Boltzmann's constant and T is the temperature.

(a) Approximate the diffusion constants in water for the following organisms:

- i. a cell of E.coli
- ii. an amoeba
- iii. a frog
- iv. a hippopotamus
- v. a blue whale

Use rough orders of magnitude, but state any assumptions that you make.

(b) What is the typical time scale it would take each one of these organisms to diffuse their own body length? The mean-squared displacement of a diffusing particle in 1D is $\langle x^2 \rangle = 2Dt$ for a time period t .

2 Pain killer

A sphere of radius R_1 is immersed in water. A chemical reaction on the surface of the sphere produces particles that diffuse into the water with a diffusion constant D . The particles are produced at a rate of \dot{N} particles per second. The concentration of particles in the bath far away from the sphere is maintained at C_0 .

(a) What are the boundary conditions of the problem?

(b) Calculate and sketch the steady state concentration profile of particles between the two boundaries. (Hint: Write the diffusion equation in suitable coordinates.)

3 Krogh-Erlang model

Oxygen diffusion and consumption can be modeled in a one-dimensional, linear tissue. The original version of this model, called the Krogh-Erlang model, was formulated in cylindrical coordinates. In this model, blood flows along the z direction in a capillary of radius R_1 surrounded by a tissue of radius R_2 , as shown in Figure 1 below.

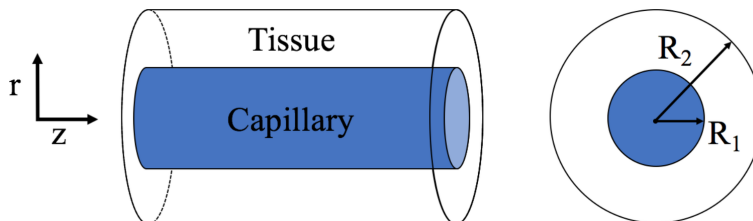


Figure 1: Diffusion of oxygen from a blood vessel into the surrounding tissue. See problem 3.

Oxygen from the blood enters the tissue, diffuses in the radial direction, and is consumed at a constant rate M . The consumption of oxygen enters the diffusion equation as a sink term:

$$\frac{\partial C(r)}{\partial t} = D\nabla^2 C(r) - M.$$

The oxygen concentration at the capillary wall is $C(r = R_1) = C_0$. It is also assumed that no oxygen leaves the tissue at the outermost region, so the flux of oxygen is zero at $r = R_2$.

- (a) Calculate the concentration profile of oxygen in the tissue at steady state, $C(r)$.
- (b) Plot (e.g. with MATLAB) the concentration profile $C(r)$. Check that it satisfies the boundary conditions.

4 Unsteady diffusion: the modal approach

Consider the diffusion equation for the concentration $C(x, t)$,

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

in a finite domain $x \in [0, L]$ with the boundary conditions

$$C(0, t) = 0,$$

$$C(L, t) = 0,$$

and the initial condition

$$C(x, 0) = C_0 \frac{x}{L} \left(1 - \frac{x}{L}\right).$$

(a) Solve the PDE with the boundary conditions and the initial condition by the method of separation of variables.

Hint: You may need the following indefinite integrals:

$$\begin{aligned} \int x \sin(ax) dx &= \frac{1}{a^2} [\sin(ax) - ax \cos(ax)], \\ \int x^2 \sin(ax) dx &= \frac{1}{a^3} [(2 - a^2 x^2) \cos(ax) + 2ax \sin(ax)]. \end{aligned}$$

(b) Use the result you found in part (a) and plot it for $L = 1 \text{ m}$, $D = 0.5 \text{ m}^2/\text{s}$ and $C_0 = 1 \text{ m}^{-1}$ at times $t = 0 \text{ s}$, 0.1 s , 0.2 s , 0.5 s , 1 s and with $N = 1, 2, 3$ modes. For every N plot the results at the different times in a single plot and label your plots clearly. Plot also the 3 differences between the 3 solution approximations. By how much do additional higher modes improve the solution?

5 Unsteady diffusion: finite differences approach

Consider the diffusion equation with the following boundary and initial conditions (same as problem 2):

$$\begin{aligned}\frac{\partial C(x, t)}{\partial t} &= D \frac{\partial^2 C(x, t)}{\partial x^2}, \\ C(0, t) &= 0, \\ C(L, t) &= 0, \\ C(x, 0) &= C_0 \frac{x}{L} \left(1 - \frac{x}{L}\right).\end{aligned}$$

Calculate the concentration at N equally spaced points in the domain. For equally spaced points, the second derivative of C for the i -th point can be approximated by

$$\frac{\partial^2 C_i}{\partial x^2} = \frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2},$$

where Δx is the distance between two successive points.

(a) Apply the approximation of the second derivative to the diffusion equation to obtain a system of ordinary differential equations (ODE) for the time variation $dC_i(t)/dt$ of concentration C_i at each point i .

(b) How many equations can you set up in this way? How many equations are required to solve this system uniquely (What is the number of unknowns)?

(c) How can you represent the boundary conditions in the discretized system? Use these to complete the system of equations.

(d) Solve the system of ODEs numerically with MATLAB. (*Hint:* The function `ode45` is well suited for this integration.)

(e) Plot the result for $L = 1\text{ m}$, $D = 0.5\text{ m}^2/\text{s}$ and $C_0 = 1\text{ m}^{-1}$ at times $t = 0\text{ s}, 0.1\text{ s}, 0.2\text{ s}, 0.5\text{ s}, 1\text{ s}$ and with $N = 3, 5, 11$ grid points. For each N plot the results at different times in a single plot and label your plots clearly. Plot also the 3 differences between the 3 solution approximations. By how much do additional grid points improve the solution?

(f) Compare your results with the results of problem 2.