**ME-280: Fluid Mechanics**
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# Problem Set 3: Solutions

## 1 Diffusion scales

**Problem:** The diffusion constant, $D$, of a suspended spherical particle of radius $R$ in a fluid with viscosity $\mu$ 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 $t$.

**Solution:** **(a)** In this problem we will be using rough orders of magnitude only.

$$k_B \approx 10^{-23}\,\frac{J}{K},$$
$$T \approx 300\,K,$$
$$\mu_{water} = 10^{-3}\,\frac{kg}{m\,s},$$
$$D = \frac{k_B T}{6\pi R\mu} \approx \frac{\left(10^{-23}\,\frac{J}{K}\right)(300\,K)}{(6\pi R)\left(10^{-3}\,\frac{kg}{m\,s}\right)} \approx \frac{10^{-19}\,\frac{m^3}{s}}{R}.$$

*E.coli:* Approximating a sphere of diameter $d \approx 1.25\,\mu m \to R_{E.coli} \approx 10^{-6}\,m$

$$D = \frac{10^{-19}\,\frac{m^3}{s}}{10^{-6}\,m} = 10^{-13}\,\frac{m^2}{s}.$$

*Amoeba:* Approximating a sphere of diameter $d \approx 500\,\mu m \to R_{Amoeba} \approx 10^{-4}\,m$

$$D = \frac{10^{-19}\,\frac{m^3}{s}}{10^{-4}\,m} = 10^{-15}\,\frac{m^2}{s}.$$

*Frog:* Approximating a sphere of diameter $d \approx 5\,cm \to R_{Frog} \approx 10^{-2}\,m$

$$D = \frac{10^{-19}\,\frac{m^3}{s}}{10^{-2}\,m} = 10^{-17}\,\frac{m^2}{s}.$$

*Hippo:* Approximating a sphere of diameter $d \approx 2\,m \rightarrow R_{Hippo} \approx 1\,m$

$$D = \frac{10^{-19}\,\frac{m^3}{s}}{1\,m} = 10^{-19}\,\frac{m^2}{s}.$$

*Blue whale:* Approximating a sphere of diameter $d \approx 20\,m \rightarrow R_{Blue\,whale} \approx 10\,m$

$$D = \frac{10^{-19}\,\frac{m^3}{s}}{10\,m} = 10^{-20}\,\frac{m^2}{s}.$$

**(b)** The time period relates to diffusion length scale by

$$t = \frac{x^2}{2D}.$$

$$E.coli \qquad t = \frac{\left(10^{-6}\,m\right)^2}{2\left(10^{-13}\,\frac{m^2}{s}\right)} \approx 5\,s$$

$$Amoeba \qquad t = \frac{\left(10^{-4}\,m\right)^2}{2\left(10^{-15}\,\frac{m^2}{s}\right)} \approx 5\cdot 10^{6}\,s \approx 8\,weeks$$

$$Frog \qquad t = \frac{\left(10^{-2}\,m\right)^2}{2\left(10^{-17}\,\frac{m^2}{s}\right)} \approx 5\cdot 10^{12}\,s \approx 100\,millenia$$

$$Hippo \qquad t = \frac{\left(1\,m\right)^2}{2\left(10^{-19}\,\frac{m^2}{s}\right)} \approx 5\cdot 10^{18}\,s \approx 10^{8}\,millenia$$

$$Blue\ whale \qquad t = \frac{\left(10\,m\right)^2}{2\left(10^{-20}\,\frac{m^2}{s}\right)} \approx 5\cdot 10^{21}\,s \approx 10^{11}\,millenia$$

## 2 Pain killer

**Problem:** 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.)

**Solution:** To take advantage of the rotational symmetry that exists in this problem, it is reasonable to employ spherical coordinates so that the concentration depends only on the radial distance from the center of the sphere and derivatives with respect to rotational axes are canceled, and solving the problem is much easier.

**(a)** On the surface of the sphere particles are produced at a constant rate and go into the surrounding water, so there is a constant flux of particles at the surface into water of $j = \dot{N}/4\pi R_1^2$ in the normal direction. Due to the rotational symmetry, the flux must be constant everywhere on the surface. Thus, *Fick's first law* defines one boundary condition

$$j = -D\frac{\partial C}{\partial r}\bigg|_{r=R_1} = \frac{\dot{N}}{4\pi R_1^2} \rightarrow \frac{\partial C}{\partial r}\bigg|_{r=R_1} = -\frac{\dot{N}}{4\pi R_1^2 D}.$$

Also concentration is kept constant far away from the sphere:

$$C(r \rightarrow \infty) = C_0.$$

**(b)** The steady state concentration profile is given by the equation

$$D\nabla^2 C = 0.$$

Knowing that the concentration depends only on $r$, the Laplacian in spherical coordinates becomes

$$D\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C}{\partial r}\right)\right] = 0,$$

and because $D$ is non-zero we can divide:

$$\frac{\partial}{\partial r}\left(r^2\frac{\partial C}{\partial r}\right) = 0.$$

Integrating this equation once with respect to $r$, we obtain

$$r^2\frac{\partial C}{\partial r} = \alpha_1,$$

where $\alpha_1$ is a constant. By rearranging this equation and integrating again, we find that

$$C(r) = -\frac{\alpha_1}{r} + \alpha_2,$$

where $\alpha_2$ is also a constant. By applying the boundary conditions to the general solution, we can solve for $\alpha_1$ and $\alpha_2$ as follows:

$$C(r \rightarrow \infty) = \alpha_2 = C_0 \ \rightarrow \ \alpha_2 = C_0,$$

$$\frac{\partial C}{\partial r}\bigg|_{r=R_1} = \frac{\alpha_1}{R_1^2} = -\frac{\dot{N}}{4\pi R_1^2 D} \ \rightarrow \ \alpha_1 = -\frac{\dot{N}}{4\pi D}.$$

Thus, the solution to the steady state concentration profile is

$$C(r) = \frac{\dot{N}}{4\pi D}\frac{1}{r} + C_0.$$

The concentration profile is plotted in the figure below:

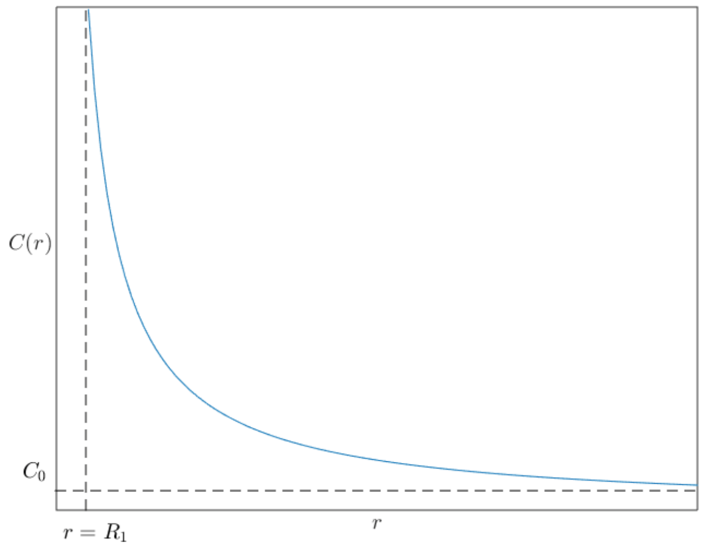


Figure 1: see problem 2

## 3 Krogh-Erlang model

**Problem:** 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 2 below.

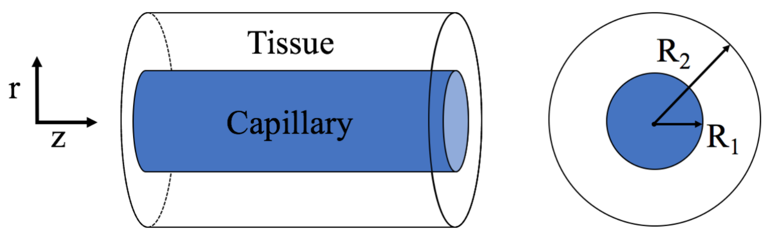


Figure 2: Diffusion of oxygen from a blood vessel into the surrounding tissue. See problem 3.

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.

**Solution:** Given the axial symmetry of the problem, we should employ cylindrical coordinates, where the concentration only varies in the radial direction.

**(a)** The steady state concentration profile in the tissue, $C(r)$, is defined in the interval $R_1 \le r \le R_2$, with the boundary conditions:

$$C(r = R_1) = C_0,$$
$$\frac{\partial C}{\partial r}(r = R_2) = 0.$$

The governing equation for the diffusion of oxygen in the tissue is:

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

Because we are interested in the steady state solution, the $\partial C(r)/\partial t$ term is zero. Also, since concentration depend only on radial direction, derivatives with respect to axial and rotational axes in the Laplacian are zero. Therefore, the governing differential equation is:

$$\nabla^2 C(r) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) = \frac{M}{D}.$$

This equation is solved as follows:

$$\begin{aligned}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right) &= \frac{M}{D}r \\ \Rightarrow r\frac{\partial C}{\partial r} &= \frac{M}{2D}r^2 + \alpha_1 \\ \Rightarrow \frac{\partial C}{\partial r} &= \frac{M}{2D}r + \frac{\alpha_1}{r},\end{aligned}$$

and the general solution is

$$C(r) = \frac{M}{4D}r^2 + \alpha_1 \ln(r) + \alpha_2,$$

where $\alpha_1$ and $\alpha_2$ are integration constants. By applying the boundary conditions:

$$\frac{\partial C}{\partial r}(r = R_2) = 0 \rightarrow \frac{M}{2D}R_2 + \frac{\alpha_1}{R_2} = 0 \rightarrow \alpha_1 = -\frac{M}{2D}R_2^2,$$
$$C(r = R_1) = C_0 \rightarrow \frac{M}{4D}R_1^2 + \alpha_1 \ln(R_1) + \alpha_2 = C_0$$
$$\rightarrow \alpha_2 = C_0 - \frac{M}{4D}R_1^2 - \alpha_1 \ln(R_1) = C_0 - \frac{M}{4D}R_1^2 + \left(\frac{M}{2D}R_2^2\right)\ln(R_1),$$

so the solution becomes

$$\begin{aligned}C(r) &= \frac{M}{4D}r^2 - \frac{M}{2D}R_2^2\ln(r) + C_0 - \frac{M}{4D}R_1^2 + \frac{M}{2D}R_2^2\ln(R_1) \\ &= \frac{M}{4D}\left[r^2 - R_1^2 + 2R_2^2\ln\left(\frac{R_1}{r}\right)\right] + C_0.\end{aligned}$$

**(b)** The concentration is plotted in the figure below. The concentration at $r = R_1$ should be $C_0$ and the slope of the curve should be zero at $r = R_2$.

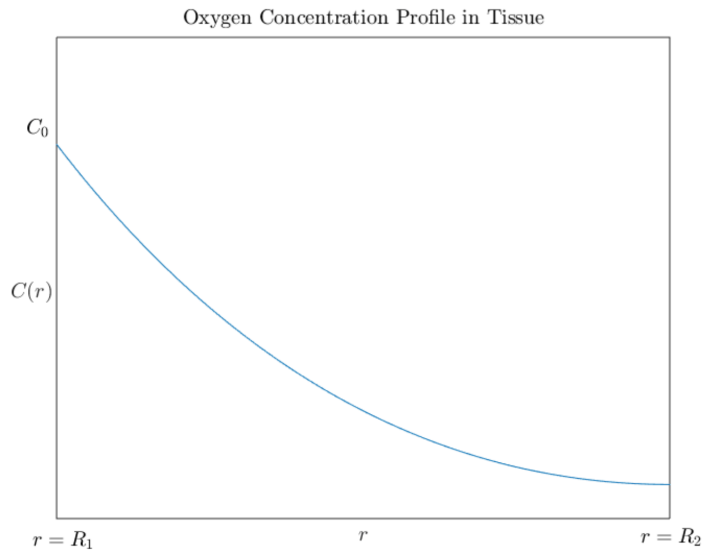


Figure 3: see problem 3

# 4 Unsteady diffusion: the modal approach

**Problem:** 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:

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

**(b)** Use the result you found in part (a) and plot it for $L = 1\,m$, $D = 0.5\,m^2/s$ and $C_0 = 1\,m^{-1}$ at times $t = 0\,s$, $0.1\,s$, $0.2\,s$, $0.5\,s$, $1\,s$ 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?

**Solution:** **(a)** We construct the solution following the steps outlined in class (see *recipe*). The PDE is linear and homogeneous. The boundary conditions (BC) are homogeneous. Thus, the general solution can be expressed as

$$C(x,t) = \sum_{n=1}^{\infty} A_n \varphi_n(x,t)$$

with

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

subject to boundary conditions

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

**Step 1**: Base solution by "separation of variables" ansatz: $\varphi_n(x,t) = X_n(x)T_n(t)$:

$$\frac{1}{D\,T_n(t)}\frac{dT_n(t)}{dt} = \frac{1}{X_n(x)}\frac{d^2X_n(x)}{dx^2} = -\lambda_n = \text{const.}$$

Time ODE:

$$\frac{dT_n(t)}{dt} = -\lambda_n D T_n(t) \Rightarrow \int \frac{dT_n(t)}{T_n(t)} = -\lambda_n D \int dt \Rightarrow T_n(t) = T_{0,n}\, e^{-\lambda_n D t}.$$

Space ODE:

$$\frac{d^2X_n(x)}{dx^2} = -\lambda_n X_n(x).$$

The solution of this ODE depends on the sign of $\lambda_n$:
Case $\lambda_n < 0$:

$$X_n(x) = \alpha_1\, e^{+\sqrt{-\lambda}\,x} + \alpha_2\, e^{-\sqrt{-\lambda}\,x}.$$

BCs give $\alpha_1 = \alpha_2 = 0$, which is the trivial solution.
Case $\lambda_n = 0$:

$$X_n(x) = \alpha_1\, x + \alpha_2.$$

BCs give $\alpha_1 = \alpha_2 = 0$, which is the trivial solution.
Case $\lambda_n > 0$:

$$X_n(x) = \alpha_1\, \cos(\sqrt{\lambda_n} x) + \alpha_2\, \sin(\sqrt{\lambda_n} x).$$

$$\begin{aligned} \text{BC}\,1: \quad 0 =& \alpha_1\, \cos(\sqrt{\lambda_n}\cdot 0) + \alpha_2\, \sin(\sqrt{\lambda_n}\cdot 0) \Rightarrow \alpha_1 = 0, \\ \text{BC}\,2: \quad 0 =& \alpha_2\, \sin(\sqrt{\lambda_n}\,L). \end{aligned}$$

The solution is only non-trivial ($\alpha_2 \neq 0$) for $\sqrt{\lambda_n}\,L = n\pi$. Therefore,

$$\lambda_n = \left(\frac{n\,\pi}{L}\right)^2,$$
$$X_n(x) = \alpha_n\, \sin\left(\frac{n\,\pi}{L} x\right).$$

Integration constants $T_{0,n}$ and $\alpha_n$ are absorbed in coefficients $A_n$ for the general solution expansion

$$C(x,t) = \sum_{n=1}^{\infty} A_n\, \sin\left(\sqrt{\lambda_n}\, x\right)\, e^{-D\lambda_n t},$$

with $\lambda_n = (n\pi/L)^2$. The general solution satisfies the BCs.

**Step 2:** Calculating the coefficients $A_n$ from the initial condition (IC):

$$C(x,t=0) = \sum_{n=1}^{\infty} A_n\, \sin\left(\frac{n\pi}{L} x\right)\, e^{-D(\frac{n\pi}{L})^2\cdot 0} = C_0\left(\frac{x}{L} - \left(\frac{x}{L}\right)^2\right).$$

The exponential term is unity. Multiplication with $\sin(m\pi x/L)$ and integration from 0 to $L$ ("Fourier-Trick"):

$$\int_0^L \sin\left(\frac{m\pi}{L}\, x\right) \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi}{L}\, x\right)\, dx = C_0 \int_0^L \left(\frac{x}{L} - \left(\frac{x}{L}\right)^2\right) \sin\left(\frac{m\pi}{L}\, x\right)\, dx$$

Sum and integral commute:

$$\sum_{n=1}^{\infty} A_n \int_0^L \underbrace{\sin\left(\frac{m\pi}{L}x\right)\sin\left(\frac{n\pi}{L}x\right)}_{\frac{1}{2}\left[\cos\left((m-n)\frac{x\pi}{L}\right)-\cos\left((m+n)\frac{x\pi}{L}\right)\right]} dx = C_0 \int_0^L \left(\frac{x}{L} - \left(\frac{x}{L}\right)^2\right) \sin\left(\frac{m\pi}{L}x\right) dx.$$

Integral is only non-zero for $m = n$, thus only one term in the sum is left:

$$A_n \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx \;=\; \frac{C_0}{L}\int_0^L x\sin\left(\frac{n\pi}{L}x\right) dx \;-\; \frac{C_0}{L^2}\int_0^L x^2 \sin\left(\frac{n\pi}{L}x\right) dx.$$

Evaluation of the three integrals

$$\begin{aligned}
\int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx &= \int_0^L \frac{1}{2}\left(1-\cos\left(2\frac{n\pi}{L}x\right)\right) dx = \frac{1}{2}\left[x - \frac{L}{2n\pi}\sin\left(2\frac{n\pi}{L}x\right)\right]_0^L = \frac{L}{2},\\
\int_0^L x\,\sin\left(\frac{n\pi}{L}x\right) dx &= \left(\frac{L}{n\pi}\right)^2 \left[\sin\left(\frac{n\pi}{L}x\right) - \frac{n\pi}{L}x\,\cos\left(\frac{n\pi}{L}x\right)\right]_0^L\\
&= \left(\frac{L}{n\pi}\right)^2 (0 - 0 - n\pi\,\cos(n\pi) + 0) = -\frac{(-1)^n L^2}{n\pi},\\
\int_0^L x^2\,\sin\left(\frac{n\pi}{L}x\right) dx &= \left(\frac{L}{n\pi}\right)^3 \left[\left(2-\left(\frac{n\pi}{L}\right)^2 x^2\right)\cos\left(\frac{n\pi}{L}x\right) + 2\frac{n\pi}{L}x\,\sin\left(\frac{n\pi}{L}x\right)\right]_0^L\\
&= \left(\frac{L}{n\pi}\right)^3 \left((2-(n\pi)^2)(-1)^n - 2 + 0 - 0\right)\\
&= -\frac{L^3}{n\pi}(-1)^n + \frac{2L^3}{(n\pi)^3}((-1)^n - 1)\\
\Rightarrow A_n &= \frac{4C_0}{(n\pi)^3}(1-(-1)^n).
\end{aligned}$$

The coefficients $A_n$ are only non-zero if $n$ is odd: $A_n = (2/n\pi)^3\,C_0$. If we substitute $n = 2n' - 1$, only odd multiples of $\pi$ form the series. The final solution reads

$$C(x,t) = \sum_{n=1}^{\infty} \frac{8\,C_0}{((2n-1)\pi)^3} \sin\left(\frac{(2n-1)\pi}{L}x\right) \exp\left(-D\left(\frac{(2n-1)\pi}{L}\right)^2 t\right).$$

**(b)** The solution of (a) is plotted in Figure 4. The single mode solution is already a good approximation and improvements become only apparent for differences. Each additional mode improves the solution by approximately one order of magnitude.

# 5 Unsteady diffusion: finite differences approach

**Problem:** 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

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

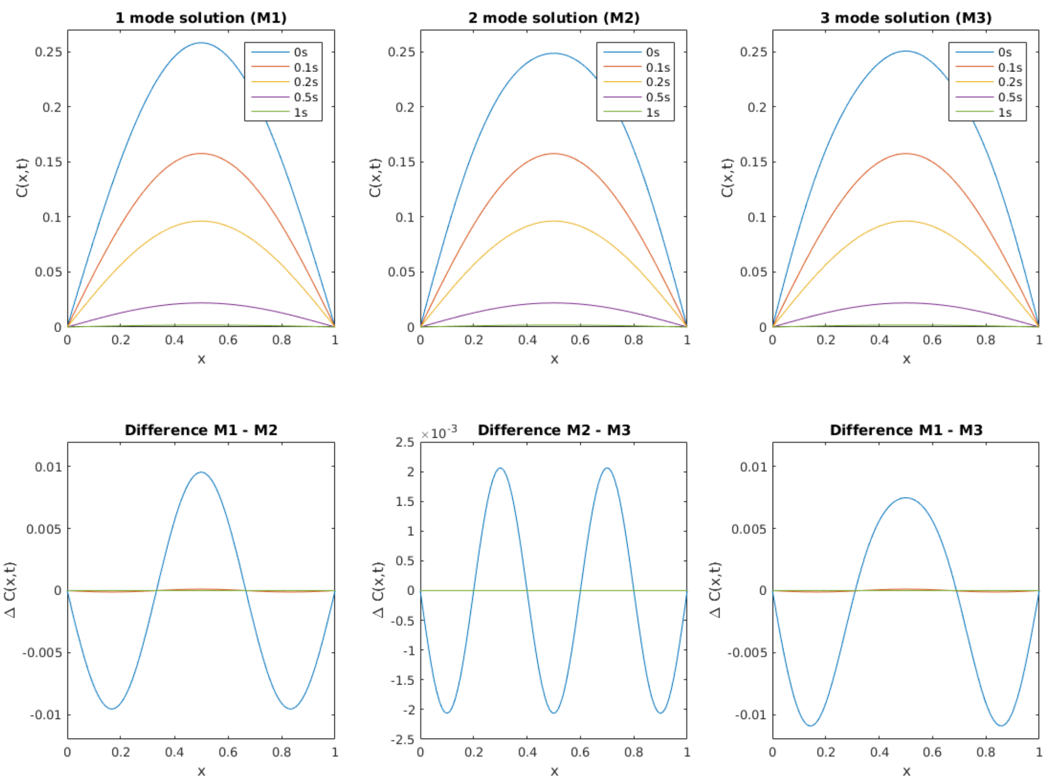


Figure 4: Concentration profiles and differences from the solution of problem 4a at given times.

where $\Delta x$ 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 $\mathrm{d}C_i(t)/\mathrm{d}t$ 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 $L = 1\,m$, $D = 0.5\,m^2/s$ and $C_0 = 1\,m^{-1}$ at times $t = 0\,s$, $0.1\,s$, $0.2\,s$, $0.5\,s$, $1\,s$ 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.

**Solution:** **(a)** Inserting the given finite difference approximation of the Laplacian into the diffusion equations gives a system of coupled ODE:

$$\frac{d}{dt}C_i(t) = \frac{D}{\Delta x^2}\left(C_{i+1}(t) - 2C_i(t) + C_{i-1}(t)\right).$$

**(b)** There are $(N-2)$ ODEs of this form for $2 \leq i \leq N-1$. Still we have discretized space with $N$ points which creates $N$ unknowns $C_i$ for which we need $N$ equations.

**(c)** The two missing equations are given by the boundary conditions:

$$C_1 = 0,$$
$$C_N = 0.$$

**(d)** There are different implementations in MATLAB possible. One is to define a right hand side (RHS) as an anonymous function

```
rhs = @(t,C) D*( [0;C(1:end-1)] - 2.0*C + [C(2:end);0] )./dx^2;
```

and pass it to

```
[t3,C3] = ode45(rhs,times,initC);
```

with the given times and initial condition

```
times=[0 0.1 0.2 0.5 1];
```

```
initC = C0*(x11/L - x11.^2/L^2);
```

**(e)** The solutions are plotted in Figure 5. The solutions for $N = 3$ and $N = 5$ are very coarse. $N = 11$ captures the curved profile better. The corrections are at about 10% of the solution values.

**(f)** The relative errors are higher in the finite difference approach than in the modal approach. This is the case although the number of modes $N$ in problem 2 is smaller than the number of points in problem 3. The ansatz functions in problem 3 are straight lines between the points while in problem 2 the calculated modes are global.

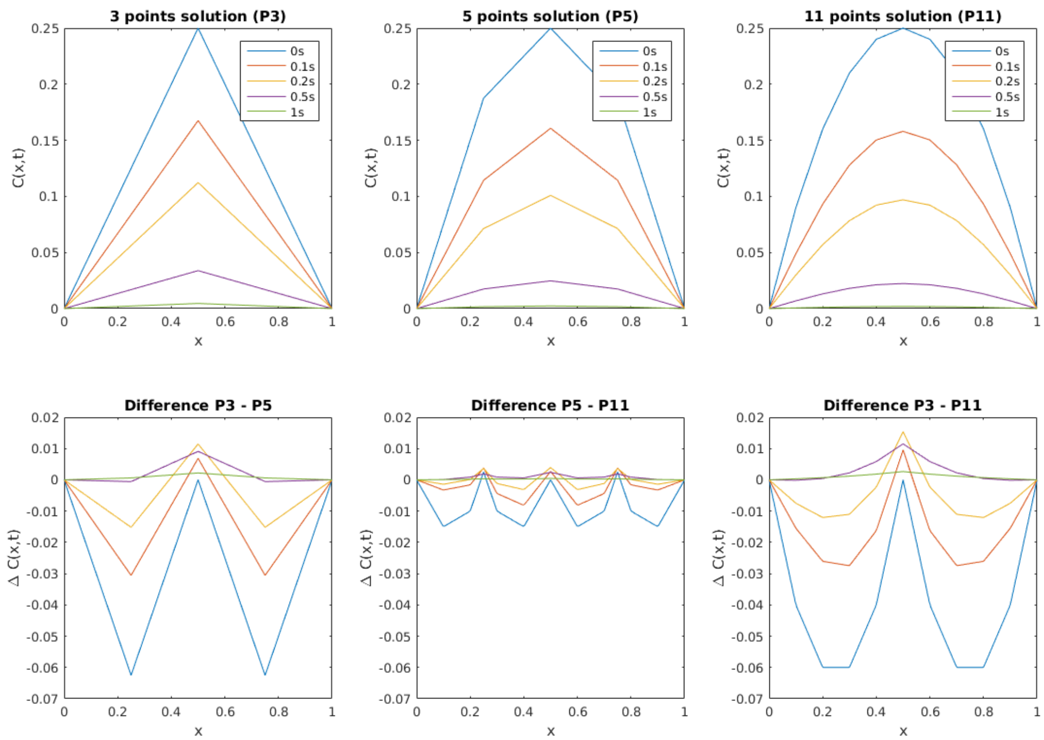


Figure 5: Concentration profiles and differences from finite difference method (Problem 5).