Spherical diffusion equation

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1 The problem

Develop a steady-state solution for a spherical cell excreting a metabolic product. This product diffusing from the cell is governed by the following equation for pure diffusion

Where the diffusivity constant is D everywhere inside and outside of the cell. The concentration of some substance inside the cell is C(r) is independent of time t spherical coordinates and . The product is produced at a rate proportional to its distance from the origin, being a maximum $Q(particles/m3s)$ at $r = -$ and going to 0 at the radius R, also Q stas 0 for $r > R$.

a set up the equation for P(r) and plot it

b making the simplifying assumptions and setting up the remining differential equation in r using spherical coordinates. Remember there is no angular dependence in the Laplacian since we are assuming no angular dependence.

c Solve the differential equation obtained in (b) for inside and outside the cell. To find the particular solution use the variation of parameters

d finish the solution by applying the following boundary conditions

1 The concentration is finite at the origin r=0

2 The concentration goes to zero at infinity

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3 . The solution at the boundary of the cell (that is at the radius R) must match up.

Hint: use Ficks second law modified to include the production term Q and with the concentration not changing with time

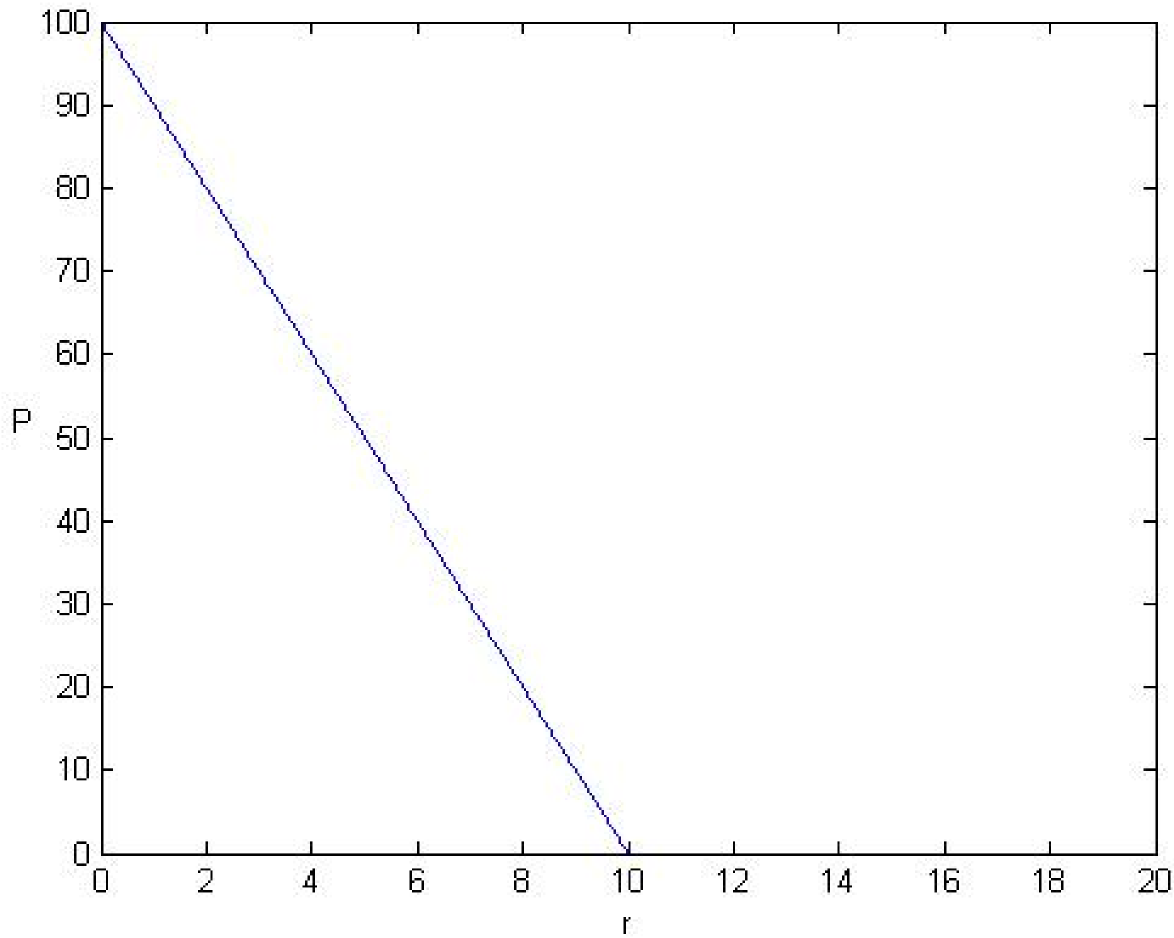

Figure 1: The function $P(r)$, the radius of the sphere is $R = 10$.

1.1 Answer

1.1.1 Part a

The production $P(r)$ is given by

$$P(r) = \begin{cases} 0 & r > R\,, \\ Q(R-r) & r \leq R\,. \end{cases} \tag{1}$$

Figure 1 shows a plot of the production as a function of r, for the case $R = 10$.

1.1.2 Part b

Let us reconsider the diffusion equation,

$$\frac{\partial C}{\partial t} = \frac{D}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial C}{\partial r}) + \frac{1}{r^2\sin\theta}(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial C}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 C}{\partial\phi^2} + P(r) \tag{2}$$

with

$$\frac{\partial C}{\partial t} = \frac{\partial C}{\partial\theta} = \frac{\partial C}{\partial\phi} = 0$$

the diffusion equation simplifies to

$$0 = \frac{D}{r^2}\frac{d}{dr}(r^2\frac{dC}{dr}) + P(r) \tag{3}$$

The equation for the concentration $C(r)$ is

$$\frac{d}{dr}(r^2\frac{dC}{dr}) = \begin{cases} 0 & r > R\,, \\ -\frac{r^2}{D}Q(R-r) & r \leq R\,. \end{cases} \tag{4}$$

1.1.3 Part c

Outer solution. Let us consider the external region $r > R$, the equation for the concentration is

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dC_e}{dr}) = 0 \tag{5}$$

from the above equation we get

$$(r^2\frac{dC_e}{dr}) = a, \qquad \frac{dC_e}{dr} = \frac{a}{r^2} \tag{6}$$

integrating the above equation give us

$$C_e(r) = -\frac{a}{r} + b \tag{7}$$

Inner solution. Let us consider the internal region $r \leq R$, the equation for the concentration is

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dC_i}{dr}) = -\frac{1}{D}P(r) \tag{8}$$

$$\frac{d}{dr}(r^2\frac{dC_i}{dr}) = -\frac{r^2}{D}P(r) = -\frac{r^2}{D}Q(R-r) \tag{9}$$

integrating once, we get

$$r^2 \frac{dC_i}{dr} = -\frac{QR}{3D}\, r^3 + \frac{Q}{4D}\, r^4 \,+\, A \tag{10}$$

the above equation can be written as

$$\frac{dC_i}{dr} = -\frac{QR}{3D}\, r + \frac{Q}{4D}\, r^2 \,+\, \frac{A}{r^2} \tag{11}$$

integrating the above equation we get

$$C_i(r) = -\frac{QR}{6D}\, r^2 + \frac{Q}{12D}\, r^3 \,-\, \frac{A}{r} + \, B \tag{12}$$

1.1.4 Variation of parameters

We know that the complementary solution of Eq.(8) is

$$C_c(r) \;=\; \frac{A}{r} + \, B \tag{13}$$

the above expression is the general solution of the homogeneous equation

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

The variation of parameters states that we may construct a particular solution to Equation (8) by

$$C_p(r) \;=\; u_1(r)\,\frac{A}{r} + \, u_2(r)\, B \tag{14}$$

where $u_1(r)$ and $u_2(r)$ are functions to be determined. The proposed solution must satisfy the differential equation, so we will get the first equation by substituting the proposed solution into Equation (8), which can be re-written as

$$\frac{d^2C_p}{dr^2} + \frac{2}{r}\,\frac{dC_p}{dr} = -\frac{1}{D}P(r) \tag{15}$$

using Eq.(14), we obtain

$$\frac{dC_p}{dr} = -\, u_1(r)\,\frac{A}{r^2} + \frac{A}{r}\,\frac{du_1}{dr} + B\,\frac{du_2}{dr} \tag{16}$$

applying the condition for the variation of parameters

$$\frac{A}{r}\,\frac{du_1}{dr} + B\,\frac{du_2}{dr} = 0 \tag{17}$$

we obtain,

$$\frac{dC_p}{dr} = -\,u_1(r)\,\frac{A}{r^2} \tag{18}$$

taking the derivative of the above equation we get

$$\frac{d^2C_p}{dr^2} = \;u_1(r)\,\frac{2\,A}{r^3} - \frac{A}{r^2}\,\frac{du_1}{dr} \tag{19}$$

substituting Eqs.(18)-(19) into Eq.(15) give us

$$\big(\,u_1(r)\,\frac{2\,A}{r^3} - \frac{A}{r^2}\,\frac{du_1}{dr}\big) + \frac{2}{r}\,\big(-\;u_1(r)\,\frac{A}{r^2}\big) = -\frac{1}{D}P(r) \tag{20}$$

The above equation simplifies to

$$\frac{A}{r^2}\,\frac{du_1}{dr} = \frac{1}{D}P(r), \qquad \frac{du_1}{dr} \;=\; \frac{r^2}{A\,D}P(r), \tag{21}$$

and integratig the above equation we get

$$u_1(r) \;=\; \int \frac{(r')^2}{A\,D}Q(R-r')\,dr' = \frac{Q}{A\,D}\big(\frac{Rr^3}{3} - \frac{r^4}{4}\big) + B' \tag{22}$$

and using Eq.(21) and the condition Eq.(17) we get,

$$\frac{du_2}{dr} = -\frac{A}{B\,r}\,\frac{du_1}{dr} \;=\; -\,\frac{r}{B\,D}P(r), \tag{23}$$

integrating the above equation we get,

$$u_2(r) \;=\; \int -\,\frac{r'}{B\,D}Q(R-r')\,dr' = -\,\frac{Q}{B\,D}\big(\frac{Rr^2}{2} - \frac{r^3}{3}\big) + E \tag{24}$$

Now, putting together all the above results we get the inner solution

$$C_i(r) = C_c(r) + C_p(r) = \;\frac{A}{r} + \;B + \;\frac{A}{r}\,\Big(\frac{Q}{A\,D}\big(\frac{Rr^3}{3} - \frac{r^4}{4}\big) + B'\Big) + B\Big(-\;\frac{Q}{B\,D}\big(\frac{Rr^2}{2} - \frac{r^3}{3}\big) + E\Big) \tag{25}$$

It is important to point out that the above equation can be rewritten as Equation (12),

$$C_i(r) = \;d'\,r^2 \;+\; e'\,r^3 \;+\; \frac{a'}{r} + b' \tag{26}$$

where the coefficients a', b', d', e', are given in terms of Q, A, B, D.

1.1.5 Part d

The constant b must be zero because the concentration must be zero far from the cell, on the other hand since the concentration must be finite at $r = 0$, the constant $A = 0$ or $a' = 0$ (which appears at the concentration $C_i(r)$), finally at the boundary $r = R$ we have to satisfy the matching boundary conditions,

$$C_i(r = R) = C_e(r = R), \quad \frac{dC_i(r = R)}{dr} = \frac{dC_e(r = R)}{dr} \tag{27}$$

$$-\frac{Q}{6D} R^3 + \frac{Q}{12D} R^3 + B = -\frac{a}{R} \tag{28}$$

$$-\frac{Q}{3D} R^2 + \frac{Q}{4D} R^2 = \frac{a}{R^2} \tag{29}$$

solving the above system of equations we get

$$a = -\frac{Q}{3D} R^4 + \frac{Q}{4D} R^4 = -\frac{Q}{12D} R^4 \tag{30}$$

$$B = (\frac{Q}{3D} R^3 - \frac{Q}{4D} R^3) + \frac{Q}{6D} R^3 - \frac{Q}{12D} R^3 = \frac{Q}{6D} R^3 \tag{31}$$

putting together all the above results we get

$$C_e(r) = (\frac{Q\,R^4}{12D})\frac{1}{r} \quad r > R \tag{32}$$

$$C_i(r) = -\frac{QR}{6D} r^2 + \frac{Q}{12D} r^3 + \frac{Q}{6D} R^3 \quad r \leq R \tag{33}$$