Theoretical Notes for Model

CHAN Man Yau, WONG Chi Yan
iGEM2016 NUS_Singapore Team
National University of Singapore

July 29, 2016

Contents

1 Diffusion in a cylindrical vessel

1.1 General solution

The general solution for diffusion of the concentration, c, in a cylinder with impermeable walls, in the absence of force/potential fields and source/sink processes is:

$$\begin{aligned} c\left(r,\phi,z,t\right) = &\sum_{i,j,k}^{\infty} K_{ijk}^{(1)} \exp\left(-D\lambda_{ijk}^2 t\right) J_0\left(\frac{\zeta_i r}{L_R}\right) \cos\left(j\phi\right) \cos\left[\frac{2\pi k}{L_z}\left(z-z_0\right)\right] \\ &+ \sum_{i,j,k}^{\infty} K_{ijk}^{(2)} \exp\left(-D\lambda_{ijk}^2 t\right) J_0\left(\frac{\zeta_i r}{L_R}\right) \sin\left(j\phi\right) \cos\left[\frac{2\pi k}{L_z}\left(z-z_0\right)\right] \end{aligned} \tag{1}$$

where L_R and L_Z are the radius and vertical length of the cylinder. Also, z_0 λ_{ijk} and ζ_i are such that:

$$z_0 = \frac{z_a + z_b}{2}, \tag{2}$$

$$\lambda_{ijk}^2 = \zeta_i^2/L_R^2 + j^2/r^2 + 4\pi^2 k^2/L_Z^2, \tag{3}$$

$$\left.\frac{\partial J_0\left(\zeta\right)}{\partial \zeta}\right|_{\zeta=\zeta_i} = J_1\left(\zeta_i\right) = 0. \tag{4}$$

where z_a and z_b are the z-coordinates of the top and bottom of the cylinder respectively.

For a given $c_0\left(r,\phi,z\right)$ as initial conditions, the spectral coefficients, $K_{ijk}^{(1)}$ and $K_{ijk}^{(2)}$ can be determined by:

$$\begin{cases} K_{ijk}^{(1)} = \dfrac{\int_0^{L_R}\int_{-\pi}^{\pi}\int_{-L_Z/2}^{L_Z/2} c_0\ J_0\left(\dfrac{\zeta_i r}{L_R}\right)\sin\left(j\phi\right)\cos\left(\dfrac{2\pi k z'}{L_z}\right) r\ dr\ d\phi\ dz'}{\dfrac{\pi L_Z}{2}\int_0^{L_R} J_0\left(\dfrac{\zeta_i r}{L_R}\right)^2 rdr}, \\ \\ K_{ijk}^{(2)} = \dfrac{\int_0^{L_R}\int_{-\pi}^{\pi}\int_{-L_Z/2}^{L_Z/2} c_0\ J_0\left(\dfrac{\zeta_i r}{L_R}\right)\cos\left(j\phi\right)\cos\left(\dfrac{2\pi k z'}{L_z}\right) r\ dr\ d\phi\ dz'}{\dfrac{\pi L_Z}{2}\int_0^{L_R} J_0\left(\dfrac{\zeta_i r}{L_R}\right)^2 rdr}. \end{cases} \tag{5}$$

1.2 Derivation of general solution

1.2.1 Diffusion equation

The general diffusion equation for the concentration of a chemical species,c, in the absence of any force/potential field and source/sinks is:

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

In cylindrical coordinates, the equation can be expanded as:

$$\frac{\partial c}{\partial t} = D\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 c}{\partial \phi^2} + \frac{\partial^2 c}{\partial z^2}\right] \tag{6}$$

where r, ϕ and z are radius, polar angle and z coordinates of the cylindrical coordinate system [1].

To obtain $c(r,\phi,z,t)$, it is convenient to assume that the $c(r,\phi,z,t)$ is variable separable. *I.e.*, it can be written in the following form:

$$c(r,\phi,z,t) = T(t)\,R(r)\,\Phi(\phi)\,Z(z)\,. \tag{7}$$

Substituting Eqn (7) into Eqn (6) and dividing the resulting equation by $TR\Phi Z$ yields:

$$\frac{1}{T}\frac{\partial T}{\partial t} = D\left[\frac{1}{rR}\frac{\partial}{\partial r}\left(r\frac{\partial R}{\partial r}\right) + \frac{1}{r^2\Phi}\frac{\partial^2 \Phi}{\partial \phi^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right]$$

Since the left hand side is completely independent of r, ϕ and z and the right hand side is completely independent of t, the only way for both sides to be equivalent is that both are equal to a a constant. For convenience, let us have $-D\lambda^2$ as our constant.

$$\frac{1}{T}\frac{\partial T}{\partial t} = -D\lambda^2 = D\left[\frac{1}{rR}\frac{\partial}{\partial r}\left(r\frac{\partial R}{\partial r}\right) + \frac{1}{r^2\Phi}\frac{\partial^2 \Phi}{\partial \phi^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right] \tag{8}$$

Since each of the terms on the right hand side are independent of each other, let us consider allowing:

$$\frac{1}{rR}\frac{\partial}{\partial r}\left(r\frac{\partial R}{\partial r}\right) = -\alpha^2 \quad , \quad \frac{1}{r^2\Phi}\frac{\partial^2 \Phi}{\partial \phi^2} = -\frac{\beta^2}{r^2} \quad , \quad \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = -\gamma^2$$

which then yields the indentity:

$$\lambda = \alpha^2 + \frac{\beta^2}{r^2} + \gamma^2$$

This identity will be evoked later when we have obtained the general solution.

1.2.2 Time component, $T(t)$

$$\frac{1}{T}\frac{\partial T}{\partial t} = -D\lambda^2 \implies T = Ae^{-D\lambda^2 t}$$

where A is a constant that depends on the initial conditions of the concentration field. This will be dealt with after we have completed our derivation of the general solution.

[1] See `http://mathinsight.org/cylindrical_coordinates` if you are unfamiliar with cylindrical coordinates.

1.2.3 Nature of λ, $\lambda \in \mathbb{R}$

Before proceeding any further, we must first discern the nature of λ. λ can be either a complex number with a non-zero imaginary component or purely a real number. $\mathrm{Im}\,(\lambda) \neq 0$ clearly implies that $\lambda^2 < 0$ or $\mathrm{Im}\,(\lambda^2) \neq 0$. We will now show that λ must be a real number.

We can rule out $\lambda^2 < 0$ easily. Suppose we have the concentration field $c = \delta\,(r, \phi, z)$ at $t = 0$, where δ is the 3D Dirac delta function, then the substance should spread out with time from $r = 0, \phi = 0, z = 0$. The concentration of the substance at the origin cannot increase! Hence, λ^2 cannot be smaller than zero.

$\mathrm{Im}\,(\lambda^2) \neq 0$ can also be ruled out. If $\mathrm{Im}\,(\lambda^2) \neq 0$, then T is a periodic function in time[2]. In the absence of source/sinks, this is completely unphysical.

Hence, we can safely say that:

$$\lambda \in \mathbb{R}$$

1.2.4 Radial component, $R\,(r)$

Let us consider that $\dfrac{1}{rR}\dfrac{\partial}{\partial r}\left(r\dfrac{\partial R}{\partial r}\right) = -\alpha^2$. This is a Bessel differential equation, which can be solved by Bessel functions. Since our concentration fields are real and finite everywhere in the region of consideration, then the solution are Bessel functions of the first kind[3]:

$$J_n\,(\alpha r) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!\Gamma\,(m+n+1)} \left(\frac{\alpha r}{2}\right)^{2m+n}$$

where Γ refers to the gamma function and $n \in \mathbb{Z}$. It is known that for $n \in \mathbb{Z}$ and $n \neq 0$, for $r = 0$, $J_n\,(\alpha r) = 0$. This is clearly not always the case! Hence, we can safely say that only $n = 0$ yields a physical Bessel function in our case.

In our system, the bacteria's walls are impermeable. For there to be no flux out of the bacteria, with a cylindrical shell wall at $r = L_R$, the radial gradient must be zero at the wall. Considering that[4]:

$$\frac{\partial J_0\,(\zeta)}{\partial \zeta} = -J_1\,(\zeta)$$

Then:

$$\left.\frac{\partial J_0\,(\alpha r)}{\partial r}\right|_{r=L_R} = -\alpha J_1\,(\alpha L_R) = 0 \implies J_1\,(\alpha L_R) = 0$$

If the solutions to $J_1\,(\zeta) = 0$ is $z = \zeta_i$ for $i \in \mathbb{Z}^+$ and $i \geq 0$, then α can possess multiple values, all of which fulfill the original Bessel differential equation. Thus, by the principle of

[2]See Euler's identity for complex numbers

[3]For more information, see `https://en.wikipedia.org/wiki/Bessel_function`.

[4]See `http://people.math.sfu.ca/~cbm/aands/toc.htm`.

superposition:

$$R(r)=\sum_{i=1}^{\infty} B_i J_0(\alpha_i r) \quad , \quad \alpha_i=\zeta_i/L_R \tag{9}$$

Also, $\alpha_i \in \mathbb{R}$ for all $i \in \mathbb{Z}^+$ to ensure that the concentration field is always real.

1.2.5 Azimuthal component, $\Phi(\phi)$

It is very easy to determine Φ. Considering that:

$$\frac{1}{r^2\Phi}\frac{\partial^2\Phi}{\partial\phi^2}=-\frac{\beta^2}{r^2} \implies \frac{\partial^2\Phi}{\partial\phi^2}=-\beta^2\Phi$$

and that $\Phi(\phi')=\Phi(\phi'+2\pi)$ for all $\phi \in \mathbb{R}$, then the solution is:

$$\Phi(\phi)=\sum_{j=1}^{\infty}\left[C_j\cos(\beta_j\phi)+D_j\sin(\beta_j\phi)\right]$$

where to satisfy periodic boundaries, $\beta_j \in \mathbb{Z}$. For simplicity, we can remove β completely:

$$\Phi(\phi)=\sum_{j=1}^{\infty}\left[C_j\cos(j\phi)+D_j\sin(j\phi)\right] \tag{10}$$

1.2.6 Z component, $Z(z)$

Let us consider that:

$$\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}=-\gamma^2.$$

If we consider that the lower and upper walls of the cylinder occur at $z=z_a$ and $z=z_b$, respectively, and that these walls are impermeable, then:

$$\left.\frac{\partial Z}{\partial z}\right|_{z=z_a}=\left.\frac{\partial Z}{\partial z}\right|_{z=z_b}=0.$$

It is also obvious that the center of the bacteria occurs at $z_0=(z_a+z_b)/2$. To make our lives easier, consider a new coordinate $z'=z-z_0$. It should thus be obvious that:

$$\frac{1}{Z}\frac{\partial^2 Z}{\partial z'^2}=-\gamma^2,$$

$$\left.\frac{\partial Z}{\partial z'}\right|_{z'=z'_a}=\left.\frac{\partial Z}{\partial z'}\right|_{z'=z'_b}=0 \quad \text{for} \quad z'_a=z_a-z_0 \ , \ z'_b=z_b-z_0$$

Since $\|z'_a\|=\|z'_b\|$, Z can thus be written as:

$$Z(z')=\sum_{k=1}^{\infty}\left[E_k\cos(\gamma_k z')+F_k\sin(\gamma_k z')\right]$$

To ensure that $\left.\frac{\partial Z}{\partial z'}\right|_{z'=z'_a} = \left.\frac{\partial Z}{\partial z'}\right|_{z'=z'_b} = 0$, $F_k = 0$ for all $k \in \mathbb{Z}$ and that:

$$\gamma_k = \frac{2\pi k}{L_Z} \ , \ L_Z \equiv z'_b - z'_a$$

I.e., L_Z is the vertical length of the cylinder. Thus:

$$Z\left(z'\right) = \sum_{k=1}^{\infty} E_k \cos\left(\frac{2\pi k}{L_z} z'\right)$$

$$Z\left(z\right) = \sum_{k=1}^{\infty} E_k \cos\left[\frac{2\pi k}{L_z}\left(z - z_0\right)\right] \quad , \quad z_0 \equiv \frac{z_a + z_b}{2} \tag{11}$$

1.2.7 Putting all the components together

Since the basis of this whole derivation is that $c\left(r, \phi, z, t\right) = T\left(t\right) R\left(r\right) \Phi\left(\phi\right) Z\left(z\right)$, then if we put all the components together, we obtain:

$$\begin{aligned} c\left(r, \phi, z, t\right) = &\sum_{i,j,k}^{\infty} K_{ijk}^{(1)} \exp\left(-D\lambda_{ijk}^2 t\right) J_0\left(\frac{\zeta_i r}{L_R}\right) \cos\left(j\phi\right) \cos\left[\frac{2\pi k}{L_z}\left(z - z_0\right)\right] \\ &+ \sum_{i,j,k}^{\infty} K_{ijk}^{(2)} \exp\left(-D\lambda_{ijk}^2 t\right) J_0\left(\frac{\zeta_i r}{L_R}\right) \sin\left(j\phi\right) \cos\left[\frac{2\pi k}{L_z}\left(z - z_0\right)\right] \end{aligned}$$

where ζ_i are the roots of $J_1\left(\zeta\right)$, the Bessel function of the first kind of order 1. Note also that $K_{ijk}^{(1)} \equiv AB_iC_jE_k$, $K_{ijk}^{(2)} \equiv AB_iD_jE_k$ and that:

$$\left\{\begin{array}{c} \lambda_{ijk}^2 = \alpha_i^2 + \beta_j^2/r^2 + \gamma_k^2 \\ \alpha_i = \zeta_i/L_R \\ \beta_j = j \\ \gamma_k = 2\pi k/L_Z \end{array}\right\} \implies \lambda_{ijk}^2 = \zeta_i^2/L_R^2 + j^2/r^2 + 4\pi^2 k^2/L_Z^2 \tag{12}$$

1.2.8 Determining spectral coefficients

Clearly, if we know what $K_{ijk}^{(1)}$ and $K_{ijk}^{(2)}$ are for each set of i, j, k, we know the behavior of the system at all positions and times. To determine $K_{ijk}^{(1)}$ and $K_{ijk}^{(2)}$, we will utilize the initial conditions of the system ($t = 0$). Suppose the initial concentration field is $c_0\left(r, \phi, z\right)$, then clearly:

$$\begin{aligned} c_0\left(r, \phi, z\right) &= c\left(r, \phi, z, t = 0\right) \\ \Leftrightarrow c_0\left(r, \phi, z\right) &= \sum_{i,j,k}^{\infty} K_{ijk}^{(1)} J_0\left(\frac{\zeta_i r}{L_R}\right) \cos\left(j\phi\right) \cos\left[\frac{2\pi k}{L_z}\left(z - z_0\right)\right] \\ &\quad + \sum_{i,j,k}^{\infty} K_{ijk}^{(2)} J_0\left(\frac{\zeta_i r}{L_R}\right) \sin\left(j\phi\right) \cos\left[\frac{2\pi k}{L_z}\left(z - z_0\right)\right] \end{aligned}$$

Thankfully, the Bessel and trigonometric functions shown above possess orthogonal relations. For the sake of brevity, we will employ the following orthogonal relations without derivation:

$$\int_0^{L_R} J_0\left(\frac{\zeta_i r}{L_R}\right) J_0\left(\frac{\zeta_{i'} r}{L_R}\right) r dr = \delta_{ii'} \int_0^{L_R} J_0\left(\frac{\zeta_i r}{L_R}\right)^2 r dr \tag{13}$$

$$\int_{-L_Z/2}^{L_Z/2} \cos\left(\frac{2\pi k z'}{L_z}\right) \cos\left(\frac{2\pi k' z'}{L_z}\right) dz' = \frac{L_Z}{2}\delta_{kk'} \tag{14}$$

$$\int_{-\pi}^{\pi} \sin(j\phi)\sin(j'\phi)\, d\phi = \pi\delta_{jj'} \tag{15}$$

$$\int_{-\pi}^{\pi} \cos(j\phi)\cos(j'\phi)\, d\phi = \pi\delta_{jj'} \tag{16}$$

where $\delta_{ii'}$ is the Kronecker delta, which is defined as: $\delta_{ii'} = \begin{cases} 1, i = i' \\ 0, i \neq i' \end{cases}$.

It is also very useful to consider that[5]:

$$\int_{-\pi}^{\pi} \sin(j\phi)\cos(j'\phi)\, d\phi = 0 \tag{17}$$

It can thus be shown that,

$$\int_0^{L_R}\int_{-\pi}^{\pi}\int_{-L_Z/2}^{L_Z/2} c_0\ J_0\left(\frac{\zeta_{i'} r}{L_R}\right)\sin(j'\phi)\cos\left(\frac{2\pi k' z'}{L_z}\right) r\ dr\ d\phi\ dz'$$
$$= \delta_{ii'}\delta_{jj'}\delta_{kk'}K^{(1)}_{ijk}\frac{\pi L_Z}{2}\int_0^{L_R} J_0\left(\frac{\zeta_i r}{L_R}\right)^2 r dr$$

Since $\int x^n J_{n-1}(x)\, dx = J_n(x) + C$, then:

$$\int_0^{L_R}\int_{-\pi}^{\pi}\int_{-L_Z/2}^{L_Z/2} c_0\ J_0\left(\frac{\zeta_{i'} r}{L_R}\right)\sin(j'\phi)\cos\left(\frac{2\pi k' z'}{L_z}\right) r\ dr\ d\phi\ dz'$$
$$= \delta_{ii'}\delta_{jj'}\delta_{kk'}K^{(1)}_{ijk}\frac{\pi L_Z}{2}\int_0^{L_R} J_0\left(\frac{\zeta_i r}{L_R}\right)^2 r dr$$

Hence,

$$K^{(1)}_{ijk} = \frac{\int_0^{L_R}\int_{-\pi}^{\pi}\int_{-L_Z/2}^{L_Z/2} c_0\ J_0\left(\frac{\zeta_i r}{L_R}\right)\sin(j\phi)\cos\left(\frac{2\pi k z'}{L_z}\right) r\ dr\ d\phi\ dz'}{\frac{\pi L_Z}{2}\int_0^{L_R} J_0\left(\frac{\zeta_i r}{L_R}\right)^2 r dr} \tag{18}$$

Likewise:

$$K^{(2)}_{ijk} = \frac{\int_0^{L_R}\int_{-\pi}^{\pi}\int_{-L_Z/2}^{L_Z/2} c_0\ J_0\left(\frac{\zeta_i r}{L_R}\right)\cos(j\phi)\cos\left(\frac{2\pi k z'}{L_z}\right) r\ dr\ d\phi\ dz'}{\frac{\pi L_Z}{2}\int_0^{L_R} J_0\left(\frac{\zeta_i r}{L_R}\right)^2 r dr} \tag{19}$$

Thus, we have obtained the general solution to the diffusion equation.

[5] See `http://tutorial.math.lamar.edu/Classes/DE/PeriodicOrthogonal.aspx`.