Appendix A

This appendix provides further details of the derivation of the analytical solution for the diffusion equation in the inner domain Ω_1, that is given in equation (16).

It is convenient to first introduce the nondimensionalization,

$$\hat{u} = 1 - \frac{c}{c_s} \qquad \hat{r} = r\frac{h}{D} \qquad \hat{s} = s\frac{D}{R_1^2} \qquad \hat{\beta} = h\frac{R_1}{D}. \tag{A-1}$$

Using the definitions in (A-1), the equation for radial diffusion (11), the boundary condition on Γ_1 (14), and the initial condition (13) can be written as,

$$\begin{cases} \dfrac{\partial \hat{u}}{\partial \hat{s}} = \hat{\beta}^2 \dfrac{1}{\hat{r}} \dfrac{\partial}{\partial \hat{r}} \left(\hat{r} \dfrac{\partial \hat{u}}{\partial \hat{r}} \right) & \hat{r} \in [0, \hat{\beta}] \text{ and } \hat{s} > 0, \\ \dfrac{\partial \hat{u}}{\partial \hat{r}} = -\hat{u} & \text{at } \hat{r} = \hat{\beta}, \qquad \hat{s} > 0, \\ \hat{u}(\hat{r}, 0) = 1, & \hat{r} \in [0, \hat{\beta}], \qquad \hat{s} = 0, \end{cases} \tag{A-2}$$

Using standard methods of separation of variables (see, for example, Carlslaw and Jaeger [46]), we look for a factorized solution $\hat{u} = \hat{T}(\hat{s})\hat{R}(\hat{r})$ for (A-2), from which it follows, that $\hat{T}(\hat{s})$ and $\hat{R}(\hat{r})$ must satisfy

$$\hat{T}' + \alpha^2 \hat{\beta}^2 \hat{T} = 0, \qquad \hat{R}'' + \frac{1}{\hat{r}}\hat{R}' + \alpha^2 \hat{R} = 0, \tag{A-3}$$

for $\hat{s} > 0$ and $\hat{r} \in [0, \hat{\beta}]$, where α^2 is a positive, real constant and we have used the "$'$" notation to denote differentiation with respect to the independent variable. The well known solutions to (A-3) are

$$\hat{T} = Ae^{-\alpha^2 \hat{\beta}^2 \hat{s}}, \qquad \hat{R} = BJ_0(\alpha \hat{r}) \tag{A-4}$$

where we have imposed the boundedness of the solution at $\hat{r} = 0$. The equation for $\hat{R}(\hat{r})$ in (A-3) is a (singular), Sturm-Liouville problem, where

$$L[\hat{R}] \equiv (\hat{r}\hat{R}')' \tag{A-5}$$

with corresponding differential equation and boundary conditions,

$$\begin{array}{ll} L[\hat{R}] = -\alpha^2 \hat{r}\hat{R} & \hat{r} \in [0, \hat{\beta}] \\ \hat{R}' + \hat{R} = 0 & \text{at}\, \hat{r} = \hat{\beta}. \end{array} \tag{A-6}$$

The Lagrange identity holds for this singular problem (A-6) (e.g. page 659 Boyce and DiPrima) [47], and we therefore have the completeness of the set of eigenfunctions $\hat{R}(\hat{r})$ in the appropriate function space, so the solution $\hat{u}$ can be represented as the following series

$$\hat{u} = \sum_{n=1}^{\infty} A_n e^{-\alpha_n^2 \hat{\beta}^2 \hat{s}} J_0(\alpha_n \hat{r}). \tag{A-7}$$

Applying the boundary condition given in (A-2) on surface Γ_1 ($\hat{r} = \hat{\beta}$), we obtain,

$$\sum_{n=1}^{\infty} A_n e^{-\alpha_n^2 \hat{\beta}^2 \hat{s}} [J_0(\alpha_n \hat{\beta}) - \alpha_n J_1(\alpha_n \hat{\beta})] = 0 \tag{A-8}$$

and therefore, α_n are the the roots of

$$J_0(\alpha_n \hat{\beta}) - \alpha_n J_1(\alpha_n \hat{\beta}) = 0 \qquad n = 1, 2, 3 \cdots \tag{A-9}$$

Using the initial condition $\hat{u} = 1$ at $\hat{s} = 0$ in (A-7), it follows that,

$$\sum_{n=1}^{\infty} A_n J_0(\alpha_n \hat{r}) = 1 \tag{A-10}$$

and therefore,

$$\sum_{n=1}^{\infty} \int_0^{\hat{\beta}} A_n J_0(\alpha_n \hat{r}) J_0(\alpha_m \hat{r}) \hat{r} d\hat{r} = \int_0^{\hat{\beta}} J_0(\alpha_m \hat{r}) \hat{r} d\hat{r}, \qquad m = 1, 2, 3, \cdots \tag{A-11}$$

Using well known orthogonality properties of the solution with (A-9),

$$\int_0^{\hat{\beta}} J_0(\alpha_n \hat{r}) J_0(\alpha_m \hat{r}) \hat{r} d\hat{r} = \begin{cases} 0 & m \neq n \\ \frac{\hat{\beta}^2 (1+\alpha_n^2)}{2\alpha_n^2} J_0^2(\alpha_m \hat{\beta}) & m = n \end{cases} \tag{A-12}$$

and hence,

$$A_n = \int_0^{\hat{\beta}} J_0(\alpha_n \hat{r}) \hat{r} d\hat{r} \Bigg/ \int_0^{\hat{\beta}} J_0^2(\alpha_n \hat{r}) \hat{r} d\hat{r} \tag{A-13}$$

It follows from standard integral results for Bessels functions and (A-9) that

$$\int_0^{\hat{\beta}} J_0(\alpha_n \hat{r}) \hat{r} d\hat{r} = \frac{\hat{\beta}}{\alpha_n} J_1(\alpha_n \hat{\beta}) = \frac{\hat{\beta}}{\alpha_n^2} J_0(\alpha_n \hat{\beta}) \tag{A-14}$$

Using this last result with (A-12) in (A-13), we obtain the solution for $\hat{u}$ in Ω_1 (see, e.g. page 201 of Carslaw and Jaeger) [46],

$$\hat{u} = \sum_{n=1}^{\infty} \frac{2\, J_0(\alpha_n \hat{r})}{\hat{\beta}\, (1 + \alpha_n^2)\, J_0(\alpha_n \hat{\beta})}\ e^{-\alpha_n^2 \hat{\beta}^2 \hat{s}} \qquad \hat{r} \in [0, \hat{\beta}] \text{ and } \hat{s} > 0 \tag{A-15}$$

Using the definitions in (A-1), the solution for the concentration given in equation (16) is obtained.

Appendix B

This appendix provides further details of the derivation of the analytical solution given in equation (25) for radial diffusion in the outer domain Ω_2. It is useful to first write the equations in dimensionless form. Using the following non-dimensionalization

$$\hat{u} = 1 - \frac{c}{c_s} \qquad \hat{r} = r\frac{h}{D} \qquad \hat{s} = s\frac{D}{R_2^2} \qquad \hat{\beta} = h\frac{R_2}{D} \qquad \gamma = \frac{R_2}{R_3} \tag{B-16}$$

the system of equations for the outer domain can be written as,

$$\begin{cases} \dfrac{\partial \hat{u}}{\partial \hat{s}} = \hat{\beta}^2 \dfrac{1}{\hat{r}} \dfrac{\partial}{\partial \hat{r}} \left(\hat{r} \dfrac{\partial \hat{u}}{\partial \hat{r}} \right) & \hat{r} \in [\hat{\beta}, \hat{\beta}/\gamma] \qquad \hat{s} > 0, \\ \dfrac{\partial \hat{u}}{\partial \hat{r}} = \hat{u} & \text{at } \hat{r} = \hat{\beta}, \qquad \hat{s} > 0, \\ \dfrac{\partial \hat{u}}{\partial \hat{r}} = 0 & \text{at } \hat{r} = \hat{\beta}/\gamma, \qquad \hat{s} > 0, \\ \hat{u}(\hat{r}, 0) = 1, & \hat{r} \in [0, \hat{\beta}]. \end{cases} \tag{B-17}$$

As for the solution in the inner domain (Appendix A), the classical method of separation of variables is used and we look for a solution of the form $\hat{u} = \hat{T}(\hat{s})\hat{R}(\hat{r})$. It follows from (B-17) that

$$\hat{T}(\hat{t}) = Ae^{-\alpha^2\hat{\beta}^2\hat{s}}, \qquad \hat{R}(\hat{r}) = AJ_0(\alpha\hat{r}) + BY_0(\alpha\hat{r}) \tag{B-18}$$

where α is once again a real, positive constant. Hence, the solution for $\hat{u}$ in the outer domain Ω_2 is

$$\hat{u} = \sum_{n=1}^{\infty} [A_n J_0(\alpha_n \hat{r}) + B_n Y_0(\alpha \hat{r})] e^{-\alpha_n^2 \hat{\beta}^2 \hat{s}} \tag{B-19}$$

Applying the boundary condition at the outer boundary, Γ_3 ($\hat{r} = \hat{\beta}/\gamma$) given in (B-17), it follows that,

$$A_n \alpha_n J_1(\alpha_n \frac{\hat{\beta}}{\gamma}) + B_n \alpha_n Y_1(\alpha_n \frac{\hat{\beta}}{\gamma}) = 0, \qquad n = 1, 2, 3, \cdots \tag{B-20}$$

It is useful to define the function, $\phi_0(\alpha_n\hat{r})$, as a linear combination of $J_0(\alpha_n\hat{r})$ and $Y_0(\alpha_n\hat{r})$

$$\phi_0(\alpha_n\hat{r}) \doteq J_0(\alpha_n\hat{r})Y_1(\alpha_n\frac{\hat{\beta}}{\gamma}) - Y_0(\alpha_n\hat{r})J_1(\alpha_n\frac{\hat{\beta}}{\gamma}) \tag{B-21}$$

Using (B-20) to eliminate B_n in (B-19) and using the notation in (B-21), we have

$$\hat{u} = \sum_{n=1}^{\infty} C_n \, \phi_0(\alpha_n \hat{r}) \, e^{-\alpha_n^2 \hat{\beta}^2 \hat{s}} \tag{B-22}$$

It follows from (B-22) and (B-17) that $\phi_0(\alpha_n \hat{r})$ are eigenfunctions that satisfy

$$\begin{aligned} &(\hat{r}\phi_0')' = -\alpha^2 \, \hat{r}\phi_0 && \hat{r} \in [\hat{\beta}, \hat{\beta}/\gamma] \\ &\phi_0' - \phi_0 = 0 && \text{at } \hat{r} = \hat{\beta} \\ &\phi_0' = 0 && \text{at } \hat{r} = \hat{\beta}/\gamma. \end{aligned} \tag{B-23}$$

Applying the boundary condition at Γ_2 ($\hat{r} = \hat{\beta}$) given in $(\text{B-23})_2$ with (B-21), we obtain an equation for the eigenvalues α_n as the roots of,

$$\begin{aligned} \alpha_n \, J_1(\alpha_n \hat{\beta}) Y_1(\alpha_n \tfrac{\hat{\beta}}{\gamma}) - \alpha_n \, Y_1(\alpha_n \hat{\beta}) J_1(\alpha_n \tfrac{\hat{\beta}}{\gamma}) \\ = J_0(\alpha_n \hat{\beta}) Y_1(\alpha_n \tfrac{\hat{\beta}}{\gamma}) - Y_0(\alpha_n \hat{\beta}) J_1(\alpha_n \tfrac{\hat{\beta}}{\gamma}). \end{aligned} \tag{B-24}$$

Applyting the initial condition $\hat{u} = 1$ at $t = 0$ to the solution (B-22)

$$\sum_{n=1}^{\infty} C_n \; \phi_0(\alpha_n \hat{r}) = 1. \tag{B-25}$$

Therefore from (B-25)

$$\sum_{n=1}^{\infty} \int_{\hat{\beta}}^{\frac{\hat{\beta}}{\gamma}} C_n \, \phi_0(\alpha_n \hat{r}) \phi_0(\alpha_m \hat{r}) \, \hat{r} \, d\hat{r} = \int_{\hat{\beta}}^{\frac{\hat{\beta}}{\gamma}} \phi_0(\alpha_m \hat{r}) \hat{r} d\hat{r}. \tag{B-26}$$

The eigenfunctions $\phi_0(\alpha_n \hat{r})$ are linear combinations of bessel functions $J_0(\alpha_n \hat{r})$ and $Y_0(\alpha_n \hat{r})$ and are orthogonal, so that from (B-26),

$$C_n \; = \int_{\hat{\beta}}^{\frac{\hat{\beta}}{\gamma}} \phi_0(\alpha_n \hat{r}) \hat{r} d\hat{r} \Bigg/ \int_{\hat{\beta}}^{\frac{\hat{\beta}}{\gamma}} \phi_0^2(\alpha_n \hat{r}) \, \hat{r} \, d\hat{r}. \tag{B-27}$$

Making use of (B-23), the following simplifications follow for the integral in (B-27)

$$\begin{aligned} \int_{\hat{\beta}}^{\frac{\hat{\beta}}{\gamma}} \phi_0(\alpha_n \hat{r}) \hat{r} d\hat{r} \; &= -\tfrac{1}{\alpha_n^2} \int_{\hat{\beta}}^{\frac{\hat{\beta}}{\gamma}} (\hat{r}\phi_0')' d\hat{r} = -\tfrac{1}{\alpha_n^2} \left[\tfrac{\hat{\beta}}{\gamma} \phi_0'(\alpha_n \tfrac{\hat{\beta}}{\gamma}) - \hat{\beta}\phi_0'(\alpha_n \hat{\beta}) \right] \\ &= \tfrac{\hat{\beta}}{\alpha_n^2} \, \phi_0(\alpha_n \hat{\beta}) \end{aligned} \tag{B-28}$$

and, after multiplying $(\text{B-23})_1$ by the quantity $(2r\phi')$, rearranging terms and integrating over the domain, we obtain,

$$\int_{\hat{\beta}}^{\frac{\hat{\beta}}{\gamma}} \phi_0^2(\alpha_n \hat{r})\hat{r}d\hat{r} = \left[\frac{\hat{r}^2}{2\alpha_n^2}\left((\phi_0'(\alpha_n\hat{r}))^2 + \alpha_n^2\,\phi_0^2(\alpha_n\hat{r})\right)\right]_{\hat{\beta}}^{\frac{\hat{\beta}}{\gamma}} \tag{B-29}$$

$$= \frac{\hat{\beta}^2}{2}\left[\frac{1}{\gamma^2}\phi_0^2(\alpha_n\frac{\hat{\beta}}{\gamma}) - \phi_0^2(\alpha_n\hat{\beta})(1+\frac{1}{\alpha_n^2})\right] \tag{B-30}$$

Using these last two results with (B-27), it follows that the solution for $\hat{u}$ in the outer domain Ω_2 is

$$\hat{u} = \sum_{n=1}^{\infty} C_n\,\phi_0(\alpha_n\hat{r})e^{-\alpha_n^2\hat{\beta}^2\hat{s}} \tag{B-31}$$

with

$$C_n = \frac{2\phi_0(\alpha_n\hat{\beta})}{\hat{\beta}\left[\alpha_n^2\phi_0^2(\alpha_n\frac{\hat{\beta}}{\gamma})/\gamma^2 - (1+\alpha_n^2)\phi_0^2(\alpha_n\hat{\beta})\right]} \tag{B-32}$$

where it should be recalled that α_n can be determined through (B-24) and $\phi_n(\alpha_n\hat{r})$ is defined in (B-21).