1.1 Derivation of Concentration Profile within a Porous Catalyst with a 1st Order Reaction

The concentration through a porous catalyst for a first order reaction can be described by the differential equation,

$$\frac{\mathrm{d}^2 C_A}{\mathrm{d}\, r^2} + \frac{2}{r}\frac{\mathrm{d}\, C_A}{\mathrm{d}\, r} - \frac{k_1'' S_a \rho_c}{D_e} C_A = 0 \tag{1.1.1}$$

This equation can be turned into a dimensionless version by defining 2 dimensionless variables,

$$\varphi = \frac{C_A}{C_{As}} \tag{1.1.2}$$

$$\lambda = \frac{r}{R} \tag{1.1.3}$$

This means that we can write,

$$r = \lambda R \tag{1.1.4}$$

$$\mathrm{d}\, r = R \mathrm{d}\, \lambda \tag{1.1.5}$$

and,

$$C_A = C_{As}\varphi \tag{1.1.6}$$

$$\frac{\mathrm{d}\, C_A}{\mathrm{d}\, r} = C_{As}\frac{\mathrm{d}\, \varphi}{\mathrm{d}\, r} \tag{1.1.7}$$

$$\frac{\mathrm{d}^2 C_A}{\mathrm{d}\, r^2} = C_{As}\frac{\mathrm{d}^2 \varphi}{\mathrm{d}\, r^2} \tag{1.1.8}$$

Combining with our definition of $\mathrm{d}\, r$ we then produce,

$$\frac{\mathrm{d}\, C_A}{\mathrm{d}\, r} = \frac{C_{As}}{R}\frac{\mathrm{d}\, \varphi}{\mathrm{d}\, \lambda} \tag{1.1.9}$$

$$\frac{\mathrm{d}^2 C_A}{\mathrm{d}\, r^2} = \frac{C_{As}}{R^2}\frac{\mathrm{d}^2 \varphi}{\mathrm{d}\, \lambda^2} \tag{1.1.10}$$

Substituting this into equation 1.1.1 produces,

$$\frac{C_{As}}{R^2}\frac{\mathrm{d}^2 \varphi}{\mathrm{d}\, \lambda^2} + \frac{2C_{As}}{\lambda R^2}\frac{\mathrm{d}\, \varphi}{\mathrm{d}\, \lambda} - \frac{k_1'' S_a \rho_c}{D_e} C_{As}\varphi = 0$$

$$\frac{\mathrm{d}^2 \varphi}{\mathrm{d}\, \lambda^2} + \frac{2}{\lambda}\frac{\mathrm{d}\, \varphi}{\mathrm{d}\, \lambda} - \frac{k_1'' S_a \rho_c R^2}{D_e}\varphi = 0 \tag{1.1.11}$$

We can now define a final dimensionless parameter,

$$\phi^2 = \frac{k_1'' S_a \rho_c R^2}{D_e} \tag{1.1.12}$$

Thus producing a dimensionless form of the differential equation for the concentration through a porous catalyst,

$$\frac{\mathrm{d}^2 \varphi}{\mathrm{d}\, \lambda^2} + \frac{2}{\lambda}\frac{\mathrm{d}\, \varphi}{\mathrm{d}\, \lambda} - \phi^2\varphi = 0 \tag{1.1.13}$$

The boundary conditions can also be defined in terms of the dimensionless parameters,

$$\begin{aligned} C_A &= C_{As} \text{ at } r = R \Rightarrow \varphi = 1 \text{ at } \lambda = 1 \\ \frac{\mathrm{d}\, C_A}{\mathrm{d}\, r} &= 0 \text{ at } r = 0 \Rightarrow \frac{\mathrm{d}\,\varphi}{\mathrm{d}\,\lambda} = 0 \text{ at } \lambda = 0 \end{aligned} \tag{1.1.14}$$

Equation 1.1.13 can be solved by defining a new variable $y = \varphi\lambda$, which means that,

$$\varphi = \frac{y}{\lambda} \tag{1.1.15}$$

$$\frac{\mathrm{d}\,\varphi}{\mathrm{d}\,\lambda} = \frac{1}{\lambda}\frac{\mathrm{d}\,y}{\mathrm{d}\,\lambda} - y\frac{1}{\lambda^2} \tag{1.1.16}$$

$$\begin{aligned} \frac{\mathrm{d}^2\,\varphi}{\mathrm{d}\,\lambda^2} &= \frac{1}{\lambda}\frac{\mathrm{d}^2\,y}{\mathrm{d}\,\lambda^2} - \frac{1}{\lambda^2}\frac{\mathrm{d}\,y}{\mathrm{d}\,\lambda} - \frac{1}{\lambda^2}\frac{\mathrm{d}\,y}{\mathrm{d}\,\lambda} + y\frac{2}{\lambda^3} \\ &= \frac{1}{\lambda}\frac{\mathrm{d}^2\,y}{\mathrm{d}\,\lambda^2} - \frac{2}{\lambda^2}\frac{\mathrm{d}\,y}{\mathrm{d}\,\lambda} + \frac{2}{\lambda^3}y \end{aligned} \tag{1.1.17}$$

Substituting these into equation 1.1.13 produces,

$$\begin{aligned} \frac{1}{\lambda}\frac{\mathrm{d}^2\,y}{\mathrm{d}\,\lambda^2} - \frac{2}{\lambda^2}\frac{\mathrm{d}\,y}{\mathrm{d}\,\lambda} + \frac{2}{\lambda^3}y + \frac{2}{\lambda^2}\frac{\mathrm{d}\,y}{\mathrm{d}\,\lambda} - \frac{2}{\lambda^3}y - \phi^2\frac{1}{\lambda}y &= 0 \\ \frac{1}{\lambda}\frac{\mathrm{d}^2\,y}{\mathrm{d}\,\lambda^2} - \phi^2\frac{1}{\lambda}y &= 0 \\ \frac{\mathrm{d}^2\,y}{\mathrm{d}\,\lambda^2} - \phi^2 y &= 0 \end{aligned} \tag{1.1.18}$$

This differential equation can now be solved by substituting an exponential form for y as,

$$y = e^{\beta\lambda} \tag{1.1.19}$$

where β is a value to find. Substituting this expression into equation 1.1.18 allows β to be calculated as,

$$\begin{aligned} \beta^2 e^{\beta\lambda} - \phi^2 e^{\beta\lambda} &= 0 \\ \beta^2 - \phi^2 &= 0 \\ (\beta - \phi)(\beta + \phi) &= 0 \\ \beta &= \pm\,\phi \end{aligned} \tag{1.1.20}$$

This means that from the linear combination of all solutions, then the full integrated expression can be given as,

$$y = Ae^{\phi\lambda} + Be^{-\phi\lambda} \tag{1.1.21}$$

or using the definition of y, equation 1.1.15,

$$\varphi = \frac{A}{\lambda}e^{\phi\lambda} + \frac{B}{\lambda}e^{-\phi\lambda} \tag{1.1.22}$$

We can now use the boundary conditions, equation 1.1.14, to find the constants A and B. The differential of equation 1.1.22 is,

$$\frac{\mathrm{d}\,\varphi}{\mathrm{d}\,\lambda} = \frac{A}{\lambda^2}e^{\phi\lambda}(\phi\lambda - 1) - \frac{B}{\lambda^2}e^{-\phi\lambda}(\phi\lambda + 1) \tag{1.1.23}$$

Thus with our boundary condition at the centre of the particle we get,

$$\begin{aligned} 0 &= A(1)(-1) - B(1)(1) \\ A &= -B \end{aligned} \tag{1.1.24}$$

With this and our boundary condition at the surface of the particle we get,

$$\begin{aligned} 1 &= Ae^{\phi} + Be^{-\phi} \\ 1 &= A\left(e^{\phi} - e^{-\phi}\right) \\ 1 &= 2A\sinh\phi \\ A &= \frac{1}{2\sinh\phi} = -B \end{aligned} \tag{1.1.25}$$

where we have used the mathematical definition of $\sinh ax = \dfrac{e^{ax} - e^{-ax}}{2}$. Substituting these constant values into equation 1.1.22 gives,

$$\begin{aligned} \varphi &= \frac{1}{\lambda\sinh\phi}\left(\frac{e^{\phi\lambda} - e^{-\phi\lambda}}{2}\right) \\ \varphi &= \frac{1}{\lambda}\frac{\sinh\phi\lambda}{\sinh\phi} \end{aligned} \tag{1.1.26}$$