7. Diffusion with Chemical Reaction in a One Dimensional Slab

7.1 Numerical Methods

Solution of second order ordinary differential equations with two point boundary conditions.

7.2 Concepts Utilized

Methods for solving second order ordinary differential equations with two point boundary values typically used in transport phenomena and reaction kinetics.

7.3 Course Useage

Transport Phenomena and Reaction Engineering.

7.4 Problem Statement

The diffusion and simultaneous first order irreversible chemical reaction in a single phase containing only reactant A and product B results in a second order ordinary differential equation given by

$$\frac{d^2 C_A}{dz^2} = \frac{k}{D_{AB}} C_A \qquad \textbf{(23)}$$

where C_A is the concentration of reactant A (kg mol/m^3), z is the distance variable (m), k is the homogeneous reaction rate constant (s^{-1}) and D_{AB} is the binary diffusion coefficient (m^2/s). A typical geometry for Equation (23) is that of a one dimension layer which has its surface exposed to a known concentration and allows no diffusion across its bottom surface. Thus the initial and boundary conditions are

$$C_A = C_{A0} \qquad \text{for } z = 0 \qquad \textbf{(24)}$$

$$\frac{dC_A}{dz} = 0 \qquad \text{for } z = L \qquad \textbf{(25)}$$

where C_{A0} is the constant concentration at the surface (z = 0) and there is no transport across the bottom surface (z = L) so the derivative is zero.

This differential equation has an analytical solution given by

$$C_A = C_{A0} \frac{\cosh[L(\sqrt{k/D_{AB}})(1 - z/L)]}{\cosh(L\sqrt{k/D_{AB}})} \qquad \textbf{(26)}$$

(a) Numerically solve Equation (23) with the boundary conditions of (24) and (25) for the case where C_{A0} = 0.2 kg mol/m^3, $k = 10^{-3}$ s^{-1}, D_{AB} = 1.2 10^{-9} m^2/s, and $L = 10^{-3}$ m. This solution should utilized an ODE solver with a shooting technique and employ Newton's method or some other technique for converging on the boundary condition given by Equation (25).

(b) Compare the concentration profiles over the thickness as predicted by the numerical solution of (a) with the analytical solution of Equation (26).