Biofilm Model Theory

Austen, Tukumi, Mark, Phil

Abstract

Summary of theory used in biofilm model.

1 Overview

2 Tank Environment

3 Growth-rate μ

4 Biofilm Diffusion

Substrates that exist within the tank will diffuse into the biofilm. The diffusion process is described by

$$\frac{d^2 S_b}{dz^2} = \frac{\mu(S_b) X_b}{Y_{xs} D_e}. \tag{1}$$

This differential equation is, typically, non-linear due the growth-rate μ.

4.1 Discretization and Linearization

To solve it we use the direct, finite-difference method, which leads to the following discretized equation

$$\frac{S_{b,i-1} - 2S_{b,i} + S_{b,i+1}}{dz^2} = \frac{\mu(S_{b,i}) X_b}{Y_{xs} D_e}, \tag{2}$$

which is valid at all the interior grid points, i.e., for $i = 2, 3, \ldots, N_z - 1$. This non-linear equation is solved by linearizing and then iterating the solution from an initial guess until converged. The iterations are denoted by a superscript, i.e., $S_b^{(k)}$. With this notation Eq. 2 becomes

$$\frac{S_{b,i-1}^{(k)} - 2S_{b,i}^{(k)} + S_{b,i+1}^{(k)}}{\Delta z^2} = \frac{\mu\left(S_{b,i}^{(k)}\right) X_b}{Y_{xs} D_e} = g\left(S_{b,i}^{(k)}\right). \tag{3}$$

where we have introduced g as the right-hand-side of the equation.

To linearize this equation, we employ the Taylor series of g about the previous iteration $S_{b,i}^{(k-1)}$ which is

$$g\left(S_{b,i}^{(k)}\right) = g\left(S_{b,i}^{(k-1)}\right) + \left(S_{b,i}^{(k)} - S_{b,i}^{(k-1)}\right) \left.\frac{dg}{dS_b}\right|_{S_{b,i}^{(k-1)}} + \ldots \tag{4}$$

Combining Eqs. 3 and 4 and keeping only the linear terms in the Taylor series leads to

$$\frac{S_{b,i-1}^{(k)} - 2S_{b,i}^{(k)} + S_{b,i+1}^{(k)}}{\Delta z^2} = g\left(S_{b,i}^{(k-1)}\right) + \left(S_{b,i}^{(k)} - S_{b,i}^{(k-1)}\right) \left.\frac{dg}{dS_b}\right|_{S_{b,i}^{(k-1)}} \tag{5}$$

which is linear with-respect-to $S_{b,i}^{(k)}$ and can be rearranged to

$$-S_{b,i-1}^{(k)} + \left(2 + \Delta z^2 \left.\frac{dg}{dS_b}\right|_{S_{b,i}^{(k-1)}}\right) S_{b,i}^{(k)} - S_{b,i+1}^{(k)} = \Delta z^2 \left(S_{b,i}^{(k-1)} \left.\frac{dg}{dS_b}\right|_{S_{b,i}^{(k-1)}} - g\left(S_{b,i}^{(k-1)}\right)\right) \tag{6}$$

The derivative $\left.\frac{dg}{dS_b}\right|_{S_{b,i}^{(k-1)}}$ needs to be approximated and we use

$$\left.\frac{dg}{dS_b}\right|_{S_{b,i}^{(k-1)}} = \frac{g\left(S_{b,i}^{+}\right) - g\left(S_{b,i}^{-}\right)}{\Delta S} \tag{7}$$

where

$$S_{b,i}^{+} = S_{b,i}^{(k-1)} + \delta \quad \text{and}$$
$$S_{b,i}^{-} = \max\left[S_{b,i}^{(k-1)} + \delta, 0\right]$$

and $\Delta S = S_{b,i}^{+} - S_{b,i}^{-}$ and $\delta = 1 \times 10^{-3}$ is an specified constant. The maximum on $S_{b,i}^{-}$ ensures the concentration remains non-negative.

4.2 Solution of System of Equations

Eq. 6 for $i = 2, 3, \ldots, N_z - 1$ provides $N_z - 2$ equations for $S_b^{(k)}$. The remaining equations come from the boundary conditions. At the bottom of the biofilm ($z = 0$) there is a wall and a no-flux boundary condition is appropriate, i.e.,

$$\left.\frac{dS_b}{dz}\right|_{z=0} = \frac{S_2 - S_1}{\Delta z} = 0. \tag{8}$$

At the top of the biofilm the substrate is diffusing from the tank into the biofilm. Depending on the conditions in the tank, e.g., how well it is mixed, the flux of substrate into the biofilm may be controlled by the diffusion through the liquid in the tank. This leads to a flux-matching condition that can be written as

$$D_e \left.\frac{dS_b}{dz}\right|_{z=L_f} = D_{\text{aq}} \frac{S - S_b(L_f)}{L_L}. \tag{9}$$

where a simple diffusion model through the liquid has been used. Discretizing the derivative using a finite-difference operator leads to

$$D_e \frac{S_{b,N_z} - S_{b,N_z-1}}{\Delta z} = D_{\text{aq}} \frac{S - S_{b,N_z}}{L_L}. \tag{10}$$

Rearranging leads to

$$\left(D_e L_l - D_{\text{aq}} \Delta z\right) S_{b,N_z} - D_e L_l S_{b,N_z-1} = D_{\text{aq}} \Delta z S \tag{11}$$

which is a useful form because if $L_l = 0$ it simplifies to $S_{b,N_z} = S$ as expected without dividing by zero.

In summary, Eq. 5 for $i = 2, 3, \ldots, N_z - 1$ provides $N_z - 2$ equations with Eq. 8 and Eq. 11 providing the two other equations for a total of N_z equations for the N_z unknowns $S_{b,i}$ for $i = 1, \ldots, N_z$.