

Biofilm Model Theory

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Abstract

Summary of theory used in biofilm model.

1 Nomenclature

Variable	Description	Units
μ_{\max}	Maximum specific growth rate	1/days
K_m	Monod half saturation coefficient	g/m ³
Y_{xs}	Biomass yield coefficient on substrate	g·g/s
V	Volume	m ³
Q	Flowrate	m ³ /day
S_A	Wetted surface area	m ²
S_{in}	Influent substrate concentration	g/m ³
S_o	Initial bulk fluid substrate concentration in tank	g/m ³
X_o	Initial biomass concentration in tank	g/m ³
D_{aq}	Diffusion coefficient of substrate in water	m ² /day
D_e	Effective diffusion coefficient of substrate in biofilm	m ² /day
X_b	Biomass density in biofilm	g/m ³
L_f	Biofilm thickness	m
L_L	Concentration boundary layer thickness	m
k_{det}	Detachment rate coefficient	1/(m·days)

2 Tank Environment

The environment is modeled in this function as a continuous stirred tank reactor (CSTR), with the existence of an inflow and outflow which carries biomass and substrate into the bulk liquid. The concentration rates of the biomass and substrate are modeled by the following ordinary differential equations

$$\frac{dx}{dt} = \left(\mu(S) - \frac{Q}{V} \right) x + \frac{V_{det} S_A X_b}{V}, \quad (2.1)$$

$$\frac{dS}{dt} = -\frac{\mu(S)x}{Y_{xs}} + \frac{QS_{in}}{V} - \frac{QS}{V} - \frac{S_A B_{flux}}{V}. \quad (2.2)$$

with initial condition $x(t=0) = x_o$ and $S(t=0) = S_o$.

These two ordinary differential equations are packaged into a function f

$$f(t, y) = \left[\frac{dx}{dt}(y(1), t, y(2), V_{det}), \frac{dS}{dt}(y(1), t, y(2)) \right] \quad (2.3)$$

A 4th Order Runge-Kutta Method is used to discretize and solve the packed differential equations in this function. The Runge-Kutta Numerical Method calculates the slope of function at four points between each step of the iteration process in order to boost the accuracy of the next-point estimation. The first of these four slope calculations is the most simple, and occurs at the beginning of the interval,

$$S_1 = f(t_n, y_n). \quad (2.4)$$

The next slope estimation occurs at the midpoint of the iterative step, using the slope calculated at the beginning of the interval to increase its accuracy,

$$S_2 = f\left(t + \frac{1}{2}dt, y + \frac{1}{2}dtS_1\right) \quad (2.5)$$

The third calculation occurs at the 3/4 point of the step,

$$S_3 = f\left(t + \frac{3}{4}dt, y + \frac{3}{4}dtS_2\right) \quad (2.6)$$

The final calculation of the slope at the next step uses the previous three calculations to produce the most accurate estimation of the slope possible.

$$t_{new} = t + dt \quad (2.7)$$

$$y_{new} = y + \frac{1}{9}dt(2S_1 + 3S_2 + 4S_3) \quad (2.8)$$

$$S_4 = f(t_{new}, y_{new}) \quad (2.9)$$

The final portion of each iterative step is to calculate the error of the step by comparing it to the Butcher Tableau coefficients produced by an Adaptive Runge-Kutta Method,

$$\text{error} = \frac{1}{72}dt(-5S_1 + 6S_2 + 8S_3 - 9S_4). \quad (2.10)$$

This error term allows for each variable time step to be analyzed and adjusted according to its deviation from the standard timestep. This occurs by establishing thresholds for error which keep it from getting too big or too small as given for an arbitrary tolerance 'tol'.

For instance, when the timestep becomes too small, if $\text{abs}(\text{error}) \leq \text{tol}/100$

$$dt = 2dt. \quad (2.11)$$

When the timestep becomes too big, if $\text{abs}(\text{error}) \geq \text{tol}$

$$dt = \frac{1}{2}dt. \quad (2.12)$$

This error term maintains the variable timestep within a reasonable range during the iteration process.

3 Tank Environment - v2

Assuming steady-state with full penetration of substrate into biofilm, i.e., substrate concentration is a constant within the tank and biofilm.

3.1 Biofilm Thickness

The thickness of the biofilm is described by

$$\frac{dL_f}{dt} = \bar{\mu}L_f - k_{\text{det}}L_f^2, \quad (3.1)$$

which at steady state leads to

$$\bar{\mu}L_f = k_{\text{det}}L_f^2. \quad (3.2)$$

3.2 Biomass Concentration in Tank

Biomass in the tank is described by

$$\frac{dxV}{dt} = \mu xV - Qx + V_{\text{det}}S_A x_b \quad (3.3)$$

At steady state, this equation simplifies to

$$Qx = \mu xV + V_{\text{det}}S_A x_b \quad (3.4)$$

$$Qx = \mu xV + \mu L_f S_A x_b \quad (3.5)$$

where we used $V_{\text{det}} = K_{\text{det}}L_f^2 = \mu L_f$ from Eq. 3.2.

3.3 Substrate Concentration

The substrate concentration in the tank is described by

$$\frac{dSV}{dt} = -\frac{\mu x V}{Y_{xs}} + QS_{\text{in}} - QS - S_A B_{\text{flux}}. \quad (3.6)$$

The flux term B_{flux} can be computed using the growth of biomass in the biofilm, i.e.,

$$B_{\text{flux}} = \int_0^{L_f} \frac{\mu(S)x_b}{Y_{xs}} dz = \frac{x_b}{Y_{xs}} \int_0^{L_f} \mu(S) dz = \frac{x_b}{Y_{xs}} L_f \bar{\mu}. \quad (3.7)$$

Using this definition of the flux, Eq. 3.6 can be written as

$$\frac{dSV}{dt} = -\frac{\mu x V}{Y_{xs}} + QS_{\text{in}} - QS - \frac{\bar{\mu} x_b V_b}{Y_{xs}} \quad (3.8)$$

where $V_b = S_A L_f$ is the volume of the biofilm. At steady-state this simplifies to

$$x = \frac{Y_{xs}}{\mu V} (QS_{\text{in}} - QS) - \frac{\bar{\mu} V_b}{\mu V} x_b \quad (3.9)$$

4 Growth-rate μ

μ represents the variable growth rate of the species within the biofilm. These equations model the consumption of substrate within the biofilm and are used in a variety of different equations, including the bulk liquid concentration rates, the biofilm thickness, and the diffusion within the biofilm.

Different equations are required to represent different growth profiles. The standard growth equation is the Monod Growth Rate

$$\mu = \mu_{\text{max}} \frac{S}{K_m + S}. \quad (4.1)$$

There is also the Double Monod Growth Rate to model multiple substrates ‘a’ and ‘b’

$$\mu = \mu_{\text{max}} \frac{S_a}{K_{ma} + S_a} \frac{S_b}{K_{mb} + S_b}. \quad (4.2)$$

The final equation that may be used is an Inhibition Model

$$\mu = \mu_{\text{max}} \frac{S_a}{K_{ma} + S_a} \frac{1}{1 + \frac{S_b}{K_{mb}}}. \quad (4.3)$$

The μ function ‘mu’ defines all these equations and allows for the desired growth rate to be called throughout the rest of the code when needed.

5 Biofilm Diffusion

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

$$\frac{d^2 S_b}{dz^2} = \frac{\mu(S_b) X_b}{Y_{xs} D_e}. \quad (5.1)$$

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

5.1 Discretization and Linearization

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

$$\frac{S_{b,i-1} - 2S_{b,i} + S_{b,i+1}}{dz^2} = \frac{\mu(S_{b,i}) X_b}{Y_{xs} D_e}, \quad (5.2)$$

which is valid at all the interior grid points, i.e., for $i = 2, 3, \dots, N_z - 1$. 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. 5.2 becomes

$$\frac{S_{b,i-1}^{(k)} - 2S_{b,i}^{(k)} + S_{b,i+1}^{(k)}}{\Delta z^2} = \frac{\mu \left(S_{b,i}^{(k)} \right) X_b}{Y_{xs} D_e} = g \left(S_{b,i}^{(k)} \right). \quad (5.3)$$

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

$$g \left(S_{b,i}^{(k)} \right) = g \left(S_{b,i}^{(k-1)} \right) + \left(S_{b,i}^{(k)} - S_{b,i}^{(k-1)} \right) \frac{dg}{dS_b} \Big|_{S_{b,i}^{(k-1)}} + \dots \quad (5.4)$$

Combining Eqs. 5.3 and 5.4 and keeping only the linear terms in the Taylor series leads to

$$\frac{S_{b,i-1}^{(k)} - 2S_{b,i}^{(k)} + S_{b,i+1}^{(k)}}{\Delta z^2} = g \left(S_{b,i}^{(k-1)} \right) + \left(S_{b,i}^{(k)} - S_{b,i}^{(k-1)} \right) \frac{dg}{dS_b} \Big|_{S_{b,i}^{(k-1)}} \quad (5.5)$$

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

$$-S_{b,i-1}^{(k)} + \left(2 + \Delta z^2 \frac{dg}{dS_b} \Big|_{S_{b,i}^{(k-1)}} \right) S_{b,i}^{(k)} - S_{b,i+1}^{(k)} = \Delta z^2 \left(S_{b,i}^{(k-1)} \frac{dg}{dS_b} \Big|_{S_{b,i}^{(k-1)}} - g \left(S_{b,i}^{(k-1)} \right) \right) \quad (5.6)$$

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

$$\frac{dg}{dS_b} \Big|_{S_{b,i}^{(k-1)}} = \frac{g \left(S_{b,i}^{+} \right) - g \left(S_{b,i}^{-} \right)}{\Delta S} \quad (5.7)$$

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.

5.2 Boundary Conditions

Eq. 5.6 for $i = 2, 3, \dots, N_z - 1$ 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.,

$$\frac{dS_b}{dz} \Big|_{z=0} = \frac{S_2 - S_1}{\Delta z} = 0. \quad (5.8)$$

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

$$D_e \frac{dS_b}{dz} \Big|_{z=L_f} = D_{aq} \frac{S - S_b(L_f)}{L_L}. \quad (5.9)$$

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

$$D_e \frac{S_{b,N_z} - S_{b,N_z-1}}{\Delta z} = D_{aq} \frac{S - S_{b,N_z}}{L_L}. \quad (5.10)$$

Rearranging leads to

$$(D_e L_l + D_{aq} \Delta z) S_{b,N_z} - D_e L_l S_{b,N_z-1} = D_{aq} \Delta z S \quad (5.11)$$

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

5.3 Solution of System of Equations

The previous two section describe the equations used to solve the diffusion problem through the biofilm and apply appropriate boundary conditions. In summary, Eq. 5.5 for $i = 2, 3, \dots, N_z - 1$ provides $N_z - 2$ equations with Eq. 5.8 and Eq. 5.11 providing the two other equations for a total of N_z equations for the N_z unknowns $S_{b,i}$ for $i = 1, \dots, N_z$.

The N_z equations are solved by iteratively solving for S_b using the matrices

$$\begin{bmatrix} 1 & -1 & & & \\ L & D & U & & \\ & L & D & U & \\ & & \ddots & \ddots & \ddots \\ & & & L & D & U \\ & & & & C_1 & C_2 \end{bmatrix} \begin{bmatrix} S_{b,1}^{(k)} \\ S_{b,2}^{(k)} \\ S_{b,3}^{(k)} \\ \vdots \\ S_{b,N_z-1}^{(k)} \\ S_{b,N_z}^{(k)} \end{bmatrix} = \begin{bmatrix} 0 \\ R_2 \\ R_3 \\ \vdots \\ R_{N_z-1} \\ C_3 \end{bmatrix} \quad (5.12)$$

The first row comes from Eq. 5.8. The second through $N_z - 1$ rows are Eq. 5.6 written with $i = 2, \dots, N_z - 1$ and the constants are $L = U = -1$,

$$D = \left(2 + \Delta z^2 \frac{dg}{dS_b} \Big|_{S_{b,i}^{(k-1)}} \right) \quad \text{and} \\ R_i = \Delta z^2 \left(S_{b,i}^{(k-1)} \frac{dg}{dS_b} \Big|_{S_{b,i}^{(k-1)}} - g \left(S_{b,i}^{(k-1)} \right) \right)$$

The last row is Eq. 5.11 with $C_1 = D_e L_l$, $C_2 = (D_e L_l + D_{aq} \Delta z)$, and $C_3 = D_{aq} \Delta z S$.

The right-hand-side depends $S_{b,i}^{(k-1)}$, which is the concentration at the previous iteration. The solution process is started with a guess, e.g., $S_b = 0$. Iteration continues until

$$\max |S_{b,i}^{(k)} - S_{b,i}^{(k-1)}| < \text{tol},$$

for a specified tolerance tol.

6 Biofilm Thickness

With the current time-step's substrate concentrations throughout the thickness of the biofilm computed, the new thickness of the biofilm may now be computed by solving the first order differential equation

$$\frac{dL_f}{dt} = \bar{\mu} L_f - k_{\text{det}} L_f^2, \quad (6.1)$$

in which the first term of the right hand side is equal to the growth velocity and the second term is equal to the detachment velocity of the biofilm's biomass.

$$v_g = \bar{\mu} L_f \quad (6.2)$$

$$v_{\text{det}} = k_{\text{det}} L_f^2 \quad (6.3)$$

Eq. 6.1 is discretized and a future time step's solution is obtained using Euler's method and the information known at the current time step. The resulting expression is as follows, where the superscript *i.e.* L_f^t denotes the biofilms state at the respective time-step.

$$L_f^{t+1} = L_f^t + \Delta t (v_g^t + v_{\text{det}}^t) \quad (6.4)$$

6.1 Growth Velocity

Since the growth rate μ is specified as an average value within the biofilm in Eq. 6.2, and the specifics of the growth rate at each point within the biofilm depends on μ and S_b a result for the growth velocity within the biofilm is obtained by numerically evaluating the integral

$$v_g^t = \int_0^{L_f^t} \mu(S_b(z)^t) dz. \quad (6.5)$$

Using trapezoidal integration, Eq. 6.5 becomes

$$v_g^t = \sum_{i=1}^{N_z-1} \frac{\Delta z^t}{2} (\mu(S_{b,i}^t) + \mu(S_{b,i+1}^t)). \quad (6.6)$$

6.2 Detachment Velocity

The detachment velocity of biomass from the biofilm is computed as follows

$$v_{det}^t = k_{det} L_f^{t^2}. \quad (6.7)$$

7 Test Cases for Validity

In order to determine the accuracy of the methods and equations used in this model, test cases were created to verify results produced by this model. This almost always involved solving a portion of the problem with a certain set of parameters so that an analytical solution could be obtained for the same problem. The following is a collection of the tests created.

7.1 Test for when LL=0

In the implementation of flux matching boundary conditions within the biofilm diffusion function as well as in the setup of the substrate concentration within the tank environment function there were issues with LL in the denominator. This lead to errors in further computations as substrate concentration values became NaN within the program and subsequent operations could not be completed.

The purpose of this test is to show that no error occurs in the code as the boundary layer thickness goes to zero, as well as to ensure that the physics of the problem act as expected. When the boundary layer thickness goes to zero the substrate concentration at the top of the biofilm should match the substrate concentration in the tank at the given time-step.

7.2 Test for Tank Biomass Concentration when no Inflow Q

This is the first of three tests created to establish the validity of the 4th Order Runge-Kutta Method used to solve for the tank biomass and substrate concentrations. This test focuses on the biomass concentration. It takes the equation,

$$\frac{dxV}{dt} = \mu xV - Qx + V_{det} S_A x_b \quad (7.1)$$

and sets Q=0, establishing no inflow of biomass or substrate and eliminating said term from the differential equation. This test also sets bflux=0 in order to eliminate the diffusion of biomass into the biofilm. When there is no inflow and no diffusion into the biofilm, the biomass within the tank is expected to remain at its initial state, xo. This was verified by the following lines of code,

```
[ , , x , , ] = tankenvironment(t, x, S, Vdet, dt, bflux, param)
actSolution = x
expSolution = xo
tol = 1e - 1
verifyLessThan(testCase, abs(actSolution - expSolution), tol)
```

These lines of code verify that the result which the code produces matches the expected analytic result to a specified tolerance.

7.3 Test for Tank Substrate Concentration when no Inflow Q

This test aims to replicate the previous test for the substrate concentration within the tank. When there is no inflow Q of substrate, nor any substrate diffusing into the biofilm, it is expected to remain at its initial value, So. This test is verified by the following lines of code, which look very similar to the previous test.

```
[ , , , S, ] = tankenvironment(t,x,S,Vdet,dt,bflux,param)
actSolution = S
expSolution = So
tol = 1e - 1
verifyLessThan(testCase,abs(actSolution - expSolution),tol)
```

Again, when the code is producing results which match the expected analytic solution to a tolerance, it can be verified that the 4th Order Runge-Kutta Method is implemented correctly.

7.4 Test Diffusion

A test was setup in which the analytical solution for substrate concentrations throughout the biofilm would be compared to those computed numerically in the biofilm diffusion function. An analytical solution was able to be created for the substrate concentrations within the biofilm by enlarging parameters mu and Km so that external mass transfer can be eliminated and therefore the tank concentration S remains at a fixed value. From here the analytical solution for substrate concentrations within the biofilm was computed at each location z within the biofilm.

$$Sb_{ana} = \frac{S * \cosh(\frac{\phi z}{L_f})}{\cosh(\phi)} \quad (7.2)$$

$$\text{where } \phi = \frac{\mu_{max} X_b L_f^2}{D_e K_m Y_{xs}} \quad (7.3)$$

This test was completed for 5 different grid sizes of biofilm. Convergence of the substrate concentrations for the analytical and numerical methods can be seen as the grid size grows. The results are displayed in the figure below

7.5 Test Steady-State with Large Diffusivities such that Substrate Concentration is Relatively Constant

7.6 Test Variable Time Dynamic of Tank Environment Calculations

The 4th Order Runge-Kutta Method used in the 'tankenvironment' function utilizes an additional 'error' step which compares the coefficients calculated to the coefficients of the Butcher Tableau. This is done to ensure that the numerical method never varies from the analytic solution beyond a certain tolerance. This error term is coupled to the step size term dt so that maximum accuracy is obtained.

This coupling establishes the boundaries of the allowable step size, so that that when the error is too large, the step size can shrink and reduce the inaccuracy. When the error is small, the step size can be increased to expedite the solving and improve efficiency.

This test analyzes this operation by comparing a simplified model of the substrate environment to its corresponding analytic solution. This simulated model eliminates the biomass within the tank as well as

any initial substrate concentration and profiles the development of the substrate until it reaches steady state. The analytic solution used is,

$$S_{anal} = Sin1(-e^{-\frac{Q}{V}t}) \quad (7.4)$$

If the simulated and analytic methods converge, it can be determined that the time step is properly adjusting to the magnitude of the error calculated at each point. This convergence is determined by the following lines.

$$\begin{aligned} maxError &= max(abs(S - S_{anal})) \\ expTol &= param.ttol \\ verifyLessThan(testCase, maxError, expTol) \end{aligned}$$

If the simulated and analytic methods produce results which match according to an established tolerance, the test will pass.