Biofilm kinetics III

Today's lecture

- Biofilm analysis: pseudo-analytical solution
  - Concept and master equations
  - Non-dimensionalization of variables
  - Calculation procedure
  - Example question

Biofilm analysis

- Key points from last two lectures
  - Idealized biofilm: uniform X_f and L_f, external mass transport by film theory, internal mass transport by Fick's 2nd law of diffusion
  - Deep biofilm vs. Shallow biofilm
  - Governing eq. & BCs

$$0 = D_f \frac{d^2 S_f}{dz^2} - \frac{\hat{q} X_f S_f}{K + S_f} \qquad 0 = \left.\frac{dS_f}{dz}\right|_{z=L_f} \qquad \frac{D}{L}(S - S_s) = D_f \left.\frac{dS_f}{dz}\right|_{z=0}$$

$$0 = YJ - b' X_f L_f$$

Biofilm analysis

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$$0 = YJ - b' X_f L_f$$

For numerical analysis, we are happy with these equations; but people want to have analytical solutions as well!

Pseudo-analytical solution

By Sáez and Rittmann (1992)

$$J = f \cdot J_{deep}$$

J = the steady-state substrate flux of the actual biofilm [M/L^2/T]

J*deep* = the substrate flux into a deep biofilm having the S_s (substrate concentration at the biofilm surface) value same as the actual biofilm

recall that $J_{deep} = \left[2\hat{q}X_f D_f\left(S_s + K\ ln\left(\frac{K}{K+S_s}\right)\right)\right]^{1/2}$ [Eq. 4.10]

f = the ratio expressing how much the actual flux is reduced because the steady-state biofilm is not deep

$0 \leq f \leq 1$, f approaches 1 for deep biofilm

Pseudo-analytical solution

$$J = f \cdot J_{deep}$$

Our goal is to calculate *J*.

We don't know *f* yet and we need S_s to calculate J_{deep}.

Note that we have eight variables:

$$\hat{q}, K, Y, b', D_f, D, L, and\ S$$

First, let's non-dimensionalize the variables.

Pseudo-analytical solution

- Non-dimensionalized variables
  - S^*_{min}: represents growth potential

$$S^*_{min} = \frac{b'}{Y\hat{q} - b'} = \frac{S_{min}}{K}$$

$S^*_{min} \ll 1$: very high growth potential
$S^*_{min} > 1$: very low grow potential
(hard to maintain steady-state biomass)

  - K^*: compares external and internal mass transport

$$K^* = \frac{D}{L}\left[\frac{K}{\hat{q}X_f D_f}\right]^{1/2}$$

$K^* < 1$: external mass transport controls the substrate flux into the biofilm

$K^* \gg 1$: external mass transport resistance does not affect the substrate flux

Pseudo-analytical solution

- Non-dimensionalized variables
  - S^*: dimensionless substrate concentration

$$S^* = \frac{S}{K}$$

$S^* < 1$: the substrate utilization rate is less than the maximum value throughout the biofilm

$S^* \gg 1$: the substrate utilization rate is at its maximum at least in the outer portion of the biofilm

Pseudo-analytical solution

- The non-dimensional flux

$$J^* = J/\left(K\hat{q}X_f D_f\right)^{1/2}$$

$$= J^*_{deep} \cdot f \qquad \text{(from J} = J_{deep} \cdot f\text{)}$$

$$= K^*(S^* - S_s^*) \qquad \text{(from J} = \frac{D}{L}(S - S_s)\text{)}$$

J^*_{deep} = the non-dimensional substrate flux into a deep biofilm having the S_s^* (dimensionless substrate concentration at the biofilm surface) value same as the actual biofilm

J^*_{deep} is calculated as:

$$J^*_{deep} = (2[S_s^* - ln(1 + S_s^*)])^{1/2} \qquad \text{(from eq. [4.10])}$$

Pseudo-analytical solution

- Calculating *f*

  by numerical analysis, Sáez and Rittmann (1992) found following relationship (this is why the solution is pseudo-analytical):

$$f = tanh\left[\alpha\left(\frac{S_S^*}{S_{min}^*} - 1\right)^{\beta}\right]$$

  where

$$\alpha = 1.5557 - 0.4117\, tanh[log_{10} S_{min}^*]$$

$$\beta = 0.5035 - 0.0257 tanh[log_{10} S_{min}^*]$$

Pseudo-analytical solution

Now, the following equations including differentials

$$0 = D_f \frac{d^2 S_f}{dz^2} - \frac{\hat{q} X_f S_f}{K + S_f} \qquad 0 = \left.\frac{dS_f}{dz}\right|_{z=L_f} \qquad \frac{D}{L}(S - S_s) = D_f \left.\frac{dS_f}{dz}\right|_{z=0}$$

$$0 = YJ - b' X_f L_f$$

are made into algebraic equations

$$J^* = J^*_{deep} \cdot f = K^*(S^* - S^*_s)$$

with J^*_{deep} a function of S^*_s and f as a function of S^*_s and S^*_{min}.

(Two unknowns, two equations, three input parameters)

Using the pseudo-analytical solution

The procedures to compute the substrate flux, J, and the biomass accumulation per unit area, XfLf from the pseudo analytical solution is as follows:

1. *Compute the non-dimensional parameters,* $S^*,\ K^*,\ S^*_{min}$
2. *Compute* α *and* β
3. *Compute* S^*_s *by:* $S^*_s = S^* - J^*_{deep} \cdot f / K^*$
4. *Compute* J^* *by:* $J^* = J^*_{deep} \cdot f = K^*(S^* - S^*_s)$
5. *Convert* J^* *into J*
6. *Compute* $X_f L_f$ *by:* $X_f L_f = YJ/b'$

Pseudo-analytical solution

Q: Following parameters are given for a steady-state biofilm:

$$L = 0.01\ cm \qquad b' = 0.1\ d^{-1}$$
$$K = 0.01\ mg/cm^3 \qquad D = 0.8\ cm^2/d$$
$$X_f = 40\ mg/cm^3 \qquad D_f = 0.64\ cm^2/d$$
$$\hat{q} = 8\ d^{-1} \qquad Y = 0.5$$

Compute the steady-state substrate flux (J) and the biofilm accumulation ($X_f L_f$) when the bulk liquid substrate concentration is 0.5 mg/L.