Supporting Information:

A Steady-State Biofilm Model for Simultaneous Reduction of Nitrate and Perchlorate -- Part 1: Model Development and Numerical Solution

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A steady-state mass balance for solid-component i can be written for a differential volume element $A'dz$ of the biofilm,

$$A'dz\mu_{oi(z)}X_f f_{i(z)} = A'J_{Xi(z+dz)} - A'J_{Xi(z)} \qquad (i = 1,2,3,4,5) \qquad \textbf{[S1]}$$

In Equation S1, A' is the biofilm volume element's lateral area for mass transport (L^2), and $J_{x(z)}$ and $J_{x(z+dz)}$ are the flux of solid-component i through area A' at the points z and (z + dz) in the biofilm. The sum of the volume fraction of every solid-component must equal 1.

$$\sum_{i=1}^{i=5} f_i = 1 \qquad \textbf{[S2]}$$

Equation S1 divided by $A'dzX_f$ yields

$$\mu_{oi(z)} f_{i(z)} = \frac{1}{X_f}\frac{J_{Xi(z+dz)} - J_{X\,i(z)}}{dz} \qquad (i = 1,2,3,4,5) \qquad \textbf{[S3]}$$

which for dz approaching 0 leads to

$$\mu_{oi(z)} f_{i(z)} = \frac{1}{X_f}\frac{\partial J_{X\,i(z)}}{\partial z} \qquad (i = 1,2,3,4,5) \qquad \textbf{[S4]}$$

The biomass flux can be expressed by the velocity u at which the biomass moves with respect to the support medium multiplied by the concentration $X_f f_i$ of the solid component.

$$J_{X\,i(z)} = u_{(z)} X_f f_{i(z)} \qquad (i = 1,2,3,4,5) \qquad \textbf{[S5]}$$

Using Equation S5, Equation S4 can be rewritten as:

$$\begin{aligned} \mu_{oi(z)} f_{i(z)} &= \frac{1}{X_f}\frac{\partial(u_{(z)} X_f f_{i(z)})}{\partial z} = \frac{\partial(u_{(z)} f_{i(z)})}{\partial z} \\ &\overset{\text{chain rule}}{=} f_{i(z)}\frac{\partial u_{(z)}}{\partial z} + u_{(z)}\frac{\partial f_{i(z)}}{\partial z} \qquad (i = 1,2,3,4,5) \end{aligned} \qquad \textbf{[S6]}$$

The average observed specific growth rate of all solid components at a location z in the biofilm is defined as

$$\overline{\mu_{o(z)}} = \sum_{i=1}^{i=5} (\mu_{oi(z)} f_{i(z)}) \quad \textbf{[S7]}$$

which can be converted to

$$\begin{aligned}
\overline{\mu_{o(z)}} &= \sum_{i=1}^{i=5} (\mu_{oi(z)} f_{i(z)}) \\
&= \sum_{i=1}^{i=5} \left(\frac{1}{X_f} \frac{\partial J_{X\,i(z)}}{\partial z}\right) \ (\textit{obtained from equation } \text{S4}) \\
&= \frac{1}{X_f} \frac{\partial \sum_{i=1}^{i=5} (J_{X\,i(z)})}{\partial z} \\
&= \frac{1}{X_f} \frac{\partial \sum_{i=1}^{i=5} (u_{(z)} X_f f_{i(z)})}{\partial z} \ (\textit{obtained from equation } \text{S5}) \\
&= \frac{\partial \sum_{i=1}^{i=5} (u_{(z)} f_{i(z)})}{\partial z} = \frac{\partial (u_{(z)} \times \sum_{i=1}^{i=5} f_{i(z)})}{\partial z} \\
&= \frac{\partial u_{(z)}}{\partial z} \ (\textit{obtained from equation } 10) \qquad (i = 1, 2, 3, 4, 5)
\end{aligned} \quad \textbf{[S8]}$$

Substituting Equation S8 into Equation S6 gives

$$\begin{aligned}
&\mu_{oi(z)} f_{i(z)} = f_{i(z)} \frac{\partial u_{(z)}}{\partial z} + u_{(z)} \frac{\partial f_{i(z)}}{\partial z} = f_{i(z)} \overline{\mu_{o(z)}} + u_{(z)} \frac{\partial f_{i(z)}}{\partial z} \\
&\textit{or} \\
&(\mu_{oi(z)} - \overline{\mu_{o(z)}}) f_{i(z)} - u_{(z)} \frac{\partial f_{i(z)}}{\partial z} = 0 \\
&\textit{or} \\
&\frac{\partial f_{i(z)}}{\partial z} = \frac{(\mu_{oi(z)} - \overline{\mu_{o(z)}}) f_{i(z)}}{u_{(z)}} \qquad (i = 1,2,3,4,5)
\end{aligned} \quad \textbf{[S9]}$$

The physical meaning of Equation S9 is that the fraction variation of a solid component at the position z ($\frac{\partial f_{i(z)}}{\partial z}$) is in direct proportion to the difference between the specific growth rate of this solid component and the average specific growth rate of all solid components at the position z ($(\mu_{oi(z)} - \overline{\mu_{o(z)}})$) and the fraction of this solid component at the position z ($f_{i(z)}$), but it is in inverse proportion to the velocity at which the biomass moves in respect to the support media ($u_{(z)}$).

The $u_{(z)}$ term in Equation S9 can be calculated using Equation S5

$$\begin{aligned} u_{(z)} &= \frac{J_{X\,i(z)}}{X_f f_{i(z)}} = \frac{f_{i(z)} \int_{L_f}^{z} (net\ growth\ rate\ of\ all\ species) dz}{X_f f_{i(z)}} \\ &= \frac{\int_{L_f}^{z} (net\ growth\ rate\ of\ all\ species) dz}{X_f} \\ &= \frac{\int_{L_f}^{z} (\sum_{i=1}^{i=5} \mu_{oi} f_i X_f) dz}{X_f} = \int_{L_f}^{z} (\sum_{i=1}^{i=5} \mu_{oi} f_i) dz \end{aligned} \qquad \textbf{[S10]}$$

Substitution of Equations S7 and S10 into Equation S9 provides the final form of the mass balance for solid component i,

$$(\int_{L_f}^{z} (\sum_{i=1}^{i=5} \mu_{oi} f_i) dz) \frac{\partial f_{i(z)}}{\partial z} = (\mu_{oi(z)} - \sum_{i=1}^{i=5} (\mu_{oi(z)} f_{i(z)})) f_{i(z)} \qquad (i = 1, 2, 3, 4, 5) \qquad \textbf{[S11]}$$