A biofilm mathematical model

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What is a biofilm?

- **Solids in suspension**
- **Liquid**
- **Solids in biofilm**
- **Biofilm**
- **Substratum**
- **Solid deposits**
- **Solid precipitates**
- **EPS**
- **Cells**
Biofilm models are based upon three principles elements:

1. Transport mechanisms (advection, diffusion): for bringing nutrients into the biofilm.
2. Consumption and growing mechanisms.
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Modelling

Let $\Omega \subset \mathbb{R}^2$ be the rectangle $\Omega = (0, 1) \times (0, 1.5)$, divided into two subregions: the biofilm region $z < h(x, t)$ and aqueous region $z > h(x, t)$, with curve interface $z = h(x, t)$ (the interface need not to be expressible as a function of $x$).
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The biofilm is modelled as a homogeneous viscous fluid, which satisfies Darcy law

\[ \bar{u} = -\lambda \nabla p \]

\( \lambda \) constant, \( \bar{u}, p \) velocity and pressure resp. The biofilm may be growing or decaying, so that

\[ \nabla \cdot \bar{u} = g \]

for some \( g \) prescribed growing function.
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$$\nabla \cdot \bar{u} = g$$

for some $g$ prescribed growing function.
Thus, we have that
\[ -\lambda \nabla^2 p = g, \]
with the following boundary and transmissions conditions:

\[
\begin{align*}
\left. p \right|_{z=h} &= 0, \\
\left. \frac{\partial p}{\partial z} \right|_{z=0} &= 0, \\
\text{p periodic in } x \text{ direction.}
\end{align*}
\]
The growing function \( g \) depends on the concentration of a single substrate \( S(x, z, t) \) (e.g. oxygen, or glucose) through usage function or substrate uptake rate \( U \), i.e., \( g = g(U(S)) \). A typical choice for \( U \) is the Monod function

\[
U(S) = U_{\text{max}} \frac{S}{S + K_S}
\]

where \( U_{\text{max}} \) and \( K_S \) are the maximum usage and half-saturation, resp. This form is also often used for the growing function \( g \). In particular, \( g(S) \propto U(S) \).
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Substrate diffuses through the aqueous region into the biofilm, where it also diffuses and is consumed. We assume that there is a function $H(x, t)$, with $H \geq h$, s.t. for $z \geq H$ the concentration of substrate is at its maximum, i.e.

$$S(x, y, z, t) = S_{\text{max}}, \quad \text{for } z > H.$$ 

This models a bulk flow region away from the biofilm, where the substrate is constantly replenished ($\{z > H\}$: zone of saturation).
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Biofilm modelling
Discretization of the model
Perspectives

The biofilm model
Substrate equations
The full biofilm model

\[ z > H \text{ (zona de saturacion)} \]
\[ h < z < H \]
\[ z < h \text{ (biofilm)} \]

\[ z = h \]
\[ z = H \]

\[ \Omega \]
Thus, we obtain:

\begin{align*}
S_t - D_1 \nabla^2 S &= 0, \quad h < z < H, \\
S_t - D_2 \nabla^2 S &= -U(S), \quad z < h,
\end{align*}

with the following boundary and transmissions conditions:

\begin{align*}
S \bigg|_{z=H} &= S_{max}, \\
\frac{\partial S}{\partial z} \bigg|_{z=0} &= 0, \\
S \bigg|_{z=h^+} &= S \bigg|_{z=h^-}, \\
D_1 \nabla S \bigg|_{z=h^+} &= D_2 \nabla S \bigg|_{z=h^-}, \\
S \text{ periodic in } x \text{ direction,}
\end{align*}

\[ S(x, z, 0) = S_0(x, z) \text{ (prescribed)}. \]
Substrate equations

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D_1 \nabla S|_{z=h^+} &= D_2 \nabla S|_{z=h^-}, \\
S &\text{ periodic in } x \text{ direction,} \\
S(x, z, 0) &= S_0(x, z) \text{ (prescribed).}
\end{aligned}
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Key issue: evolution of the biofilm front is a *unknown* of the model ⇒ problem highly *non linear*.

We so deal with a *free boundary value problem*. It is then necessary a law for the evolution of the biofilm front. For instance:

\[ [\bar{u}]_{\gamma(t)}(P) = C \kappa(P) \bar{n}(P), \quad P \in \gamma(t) \]

where \( C \) is a parameter depending on *local composition of the biofilm, EPS concentration*, ....
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Level set formulation of the biofilm model

Let $\phi(x, z, t)$ be s.t. $\phi(x, z, t) > 0$ for $(x, z)$ in the aqueous region and $\phi(x, z, t) < 0$ for $(x, z)$ in the biofilm region. Then, by continuity $\phi(x, z, t)$ satisfies

$$(x, z) \in \text{Biofilm front} \iff \phi(x, z, t) = 0.$$ 

Thus, the biofilm front motion is modelled by:

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = 0, \quad \text{for } (x, z) \in \Omega, \ t > 0,$$

$$\phi(x, z, 0) = \phi_0(x, z), \quad \text{for } (x, z) \in \Omega,$$

where $\phi_0(x, z)$ implicitly defines the initial biofilm front.
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Some previous simplifications

For small values of $S$, we can assume that $U(S) \approx S$. Moreover, the evolution time of the biofilm is large compared with the diffusion time of the substrate, and thus we can assume that the diffusion of the substrate is time-independent. Then, it is easily shown that the boundary value problem for the substrate becomes:

$$
\left\{ \begin{array}{l}
\nabla \cdot (D \nabla S) = \chi_{\{z<h\}} S, \quad (x, z) \in \Omega, \ z < H \\
S|_{z=H} = 1, \quad \frac{\partial S}{\partial z}\bigg|_{z=0} = 0,
\end{array} \right.
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where $\chi_{\{z<h\}}$ denotes the characteristic function of the biofilm region and $D = D(x, z)$ denotes the piecewise constant diffusion coefficient.
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Algorithm

Step 1. \( n \leftarrow 0 \). Initialize \( \phi_0(x, z) \) such that it implicitly defines the initial biofilm front.

Step 2. Solve the boundary value problem for the substrate, with the piecewise constant diffusion coefficient smoothed near the interface.

Step 3. Solve the boundary value problem for the pressure in the biofilm region. Extend \( p \) across (above and near) the interface.

Step 4. Solve the level set equation with the velocity field \( \vec{u} = -\nabla p \).

Step 5. Reinitialize the above computed level set function \( \phi \) in such a way of keeping it as the signed distance function from the interface. \( n \leftarrow n + 1 \) and repeat Steps 2-5.
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We approximate the convective terms by using a second-order ENO upwind scheme. For doing so, define

\[
\text{minmod} (a, b) = \begin{cases} 
\text{sgn} (a) \min (|a|, |b|) & \text{if } a \cdot b > 0, \\
0 & \text{if } a \cdot b \leq 0.
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Then, the second-order ENO scheme reads as follow:

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\begin{cases}
\quad u_{ij} \left( D_x^- \phi_{ij} + \frac{1}{2} \text{minmod} \left( D_x^2 \phi_{ij}, D_x^2 \phi_{i-1,j} \right) \right), & \text{if } u_{ij} > 0, \\
\quad u_{ij} \left( D_x^+ \phi_{ij} - \frac{1}{2} \text{minmod} \left( D_x^2 \phi_{ij}, D_x^2 \phi_{i+1,j} \right) \right), & \text{if } u_{ij} < 0.
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For the reinitialization of the level set function, we solve the equation:

$$\frac{\partial \phi}{\partial t} + S(\phi_0)(|\nabla \phi| - 1) = 0,$$

to the steady state, using as initial condition $\phi_0$, the advected function with the velocity field $\vec{u}$. Here above, $S(\phi_0)$ is the signum function. The previous equation can be handled as a motion in normal direction equation, with source term $S(\phi_0)$. Numerically, it is convenient to smooth the signum function near the interface.
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Research perspectives

- Computational implementation of numerical methods. The delicate part is to extend the pressure across the interface (in progress).
- Calibration of constitutive law for the biofilm front.
- Application to bioleaching process in mining industry.
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