A biofilm extension of Freter’s model of a bioreactor with wall attachment and a failed attempt to optimize it

Hermann J. Eberl\textsuperscript{1} and Alma Mašić\textsuperscript{2}

\textsuperscript{1} Dept. Mathematics and Statistics, University of Guelph
\textsuperscript{2} Center for Mathematics, Lund University

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• Freter’s model of a CSTR with wall attachment (since 1983)

\[ \dot{S} = D(S_0 - S) - \gamma^{-1}(u\mu_u(S) + \delta w\mu_w(S)) \]

\[ \dot{u} = u(\mu_u(S) - D - k_u) + \beta\delta w + \delta w\mu_w(S)(1 - G(W)) - \alpha u(1 - W) \]

\[ \dot{w} = w(\mu_w(S)G(W) - \beta - k_w) + \alpha u (1 - W) \delta^{-1} \]

with

\[ \mu_u(S) = \frac{m_u S}{a_u + S}, \quad \mu_w(S) = \frac{m_w S}{a_w + S}, \quad W = \frac{w}{w_{max}}, \quad G(W) = \frac{1 - W}{1.1 - W} \]

\( S \): substrate concentration
\( u \): unattached bacteria
\( w \): wall attached bacteria

- major assumptions:
  ◦ growth, lysis, attachment, detachment, washout of unattached cells
  ◦ available wall space for attachment is limited
  ◦ same substrate conditions for attached and unattached bacteria

- studied in 1990s and 2000s by Smith, Ballyk, Jones, Kojouharov,... in this and extended versions (plug flow, etc): principle of competitive exclusion does not hold
Extension of Freter’s model for a biofilm reactor: setup

- wastewater treatment processes: activated sludge vs. biofilm processes
- biofilm reactors are designed to provide ample surface for colonization (retention of biomass): Trickling Filters, Membrane Aerated Biofilm Reactors, Moving Bed Biofilm Reactors (MBBR), etc
- MBBR is an attempt to provide CSTR conditions for biofilms
- due to biomass detachment suspended bacteria cannot be avoided; typically not accounted for in design of biofilm processes
- similar hybrids: IFAS (Integrated Fixed Film Activated Sludge)
- **limitation of the Freter model**: in biofilm reactors wall attached bacteria develop in thick biofilms with substrate gradients \(\Rightarrow\) heterogeneous, spatially structured populations \(\Rightarrow\) **need to include a biofilm model for wall attached bacteria**
Extension of Freter’s model for a biofilm reactor: model

\[
\dot{S} = D(S^0 - S) - \frac{u \mu_u(S)}{\gamma V} - \frac{J(S, \lambda)}{V} \\
\dot{u} = u (\mu_u(S) - D - k_u) + A \rho E \lambda^2 - \alpha u \\
\dot{\lambda} = v(\lambda, t) + \frac{\alpha u}{A \rho} - E \lambda^2
\]

where \( \lambda \): biofilm thickness: biofilm expansion due to microbial growth

\( J(S, \lambda) \): substrate flux into biofilm (substrate consumption by biofilm)

\[
J(S, \lambda) = Ad_c C''(\lambda)
\]

\( v(\lambda, t) \): ”expansion velocity” of biofilm (biofilm growth)

\[
v(z, t) = \int_0^z \left( \frac{m_\lambda C}{K_\lambda + C} - k_\lambda \right) d\zeta
\]  

\( C(z) \): substrate concentration in biofilm

\[
C''' = \frac{\rho m_\lambda}{dC \gamma K_\lambda + C}, \quad C''(0) = 0, \quad C'(\lambda) = S
\]

- observe: \( v \) and \( J \) can be ”obtained” by integrating (\( * \)) once
• Extension of Freter’s model for a biofilm reactor: analysis

- formally re-write model as an ODE system

\[
\dot{S} = D(S^0 - S) - \frac{1}{V} \left( \frac{u\mu_u(S)}{\gamma} + AD_C j(S, \lambda) \right)
\]

\[
\dot{u} = u(\mu_u(S) - D - k_u) + A\rho E\lambda^2 - \alpha u
\]

\[
\dot{\lambda} = \frac{\gamma d_C}{\rho} j(\lambda, S) - k_\lambda \lambda + \frac{\alpha u}{A\rho} - E\lambda^2
\]

where after integrating substrate BVP once

\[
j(\lambda, S) := \frac{\rho}{\gamma d_C} \int_0^\lambda \mu_\lambda(C(z))dz
\]

- ODE can be studied with elementary techniques
- NOTE: evaluating R.H.S still requires to solve BVP!!

**Proposition.** Initial value problem possess a unique, non-negative and bounded solution for all \(t > 0\). We have either \(u(t) = \lambda(t) = 0\) or \(u(t) > 0, \lambda(t) > 0\) for all \(t > 0\).
• Extension of Freter’s model for a biofilm reactor: analysis

Lemma (Properties of $j(\lambda, S)$). For $\lambda \geq 0, S \geq 0$ the function $j(\lambda, S)$ is well-defined and differentiable. It has the following properties:

(a) $j(\cdot, 0) = j(0, \cdot) = 0$
(b) $\frac{\partial j}{\partial S}(0, S) = 0$
(c) $\sqrt{\frac{\theta}{K_\lambda}} \tanh \sqrt{\frac{\lambda^2 \theta}{K_\lambda}} \leq j(\lambda, S) \leq \sqrt{\frac{\theta}{K_\lambda + S}} \tanh \sqrt{\frac{\lambda^2 \theta}{K_\lambda + S}}$
(d) with $\theta := \rho m_\lambda / \gamma d_c$ we have

$$\frac{S \theta}{K_\lambda + S} \leq \frac{\partial j}{\partial \lambda}(0, S) \leq \frac{S \theta}{K_\lambda}$$
• Extension of Freter’s model for a biofilm reactor: analysis

**Proposition (stability of washout equilibrium).** Washout equilibrium \((S^0, 0, 0)\) exists for all parameters. It is asymptotically stable

\[
\mu_u(S^0) < D + k_u + \alpha \quad \text{and} \quad \frac{\partial j}{\partial \lambda}(0, S^0) < \frac{k_{\lambda \rho}}{\gamma d_C}
\]

and unstable if either

\[
\mu_u(S^0) > D + k_u + \alpha \quad \text{or} \quad \frac{\partial j}{\partial \lambda}(0, S^0) > \frac{k_{\lambda \rho}}{\gamma d_C}.
\]

**Corollary.** A sufficient condition for asymptotic stability of the trivial equilibrium is

\[
\mu_u(S^0) < D + k_u + \alpha \quad \text{and} \quad \frac{S^0}{K_\lambda} < \frac{k_{\lambda}}{m_\lambda}.
\]

On the other hand,

\[
\mu_u(S^0) > D + k_u + \alpha \quad \text{or} \quad \frac{S^0}{K_\lambda + S^0} > \frac{k_{\lambda}}{m_\lambda}
\]

is sufficient for instability.
Extension of Freter’s model for a biofilm reactor: analysis
• Extension of Freter’s model for a biofilm reactor: Simulations

Steady state values of $u$, $\lambda$ in dependence of dilution rate
Extension of Freter’s model for a biofilm reactor: Simulations

Contribution of suspended biomass to substrate removal

Summary: for small colonization area and flow rate, suspendeds can contribute substantially to substrate removal
- previous analysis is concerned with long term behaviour of the reactor in the case of continuous inflow of substrate
- now: treat finite amount of substrate in finite time
- can the process be optimized by controlling flow rate $Q$?
  - *treat as much substrate as possible*
  - *in as short a time as possible*
- vector optimization problem

$$\min_{Q \in \Omega} \left( \int_0^T Q S dt \right)$$

where $Q : [0, T_{max}] \rightarrow \mathbb{R}_0^+$ reactor flow rate, $\Omega$ specified later
Vector optimization

- Edgeworth-Pareto optimality: a solution is optimal is further improvement of one objective is only possible at the expense of making the other one worse
- enforces a trade-off between objectives
- solution is not unique, typically infinitely many optima exist
- solution can be represented graphically as **Pareto front**
- convert vector optimization problem into a family of scalar problems:
  - scalarization by *monotonic (linear) functionals* $F : \mathbb{R}^2 \rightarrow \mathbb{R}$
    \[
    \min_{Q \in \Omega} F(Z(Q)) = \min_{Q \in \Omega} \omega \beta \int_0^T QSdt + (1 - \omega)T, \quad 0 < \omega < 1
    \]
  - modified Pollack algorithm: For every $T \in (T_{\min}, T_{\max})$ solve
    \[
    \min_{Q \in \Omega} \int_0^T QSdt
    \]
Optimization: Optimal control problem in Bolza form

\[
\min_{Q \in \Omega} \int_0^T Q S dt + (1 - w) T
\]

with \( \Omega = \{ Q \text{ measureable}, 0 \leq Q \leq Q_{max} \} \)

subject to

\[
\begin{align*}
\dot{S} &= \frac{Q}{V}(S^0 - S) - \frac{1}{V} \left( \frac{u \mu_u(S)}{\gamma} + AD_C j(S, \lambda) \right) \\
\dot{u} &= u \left( \mu_u(S) - \frac{Q}{V} - k_u \right) + A \rho E \lambda^2 - \alpha u \\
\dot{\lambda} &= \frac{\gamma d_c}{\rho} j(\lambda, S) - k_\lambda \lambda + \frac{\alpha u}{A \rho} - E \lambda^2 \\
\dot{V}_b &= -Q \\
S(0) &= 0, \quad u(0) \geq u_0, \quad \lambda(0) \geq 0, \quad V_b(0) = V_{b, max}
\end{align*}
\]

-- linear in control variable \( Q \implies \) optimal control chatters
Optimization: Off-on functions

- look for optimal flow rate $Q$ in the class of functions

$$Q(t) = \begin{cases} 0, & \text{for } t < T_{\text{switch}} \\ \frac{V_{b,\text{max}}}{T - T_{\text{switch}}}, & \text{for } T_{\text{switch}} \leq t \leq T \end{cases}$$

and solve (using Pollack’s method)

$$\min_{T_{\text{switch}}, T} \left( \int_0^T QSdt \right), \quad \text{s.t. } 0 < T_{\text{min}} \leq T_{\text{switch}} \leq T \leq T_{\text{max}}$$
- Optimization: Off-on functions continued

- strong dependence on initial data:

- initial data typically not known \(\Rightarrow\) optimum difficult to find
- the less biomass initially in reactor the higher potential for control
- overall very moderate compared to \(Q = V_{b,max}/T = \text{const}\)
\(\Rightarrow\) for all practical purposes, no control benefits
- **Optimization: Other approaches that we tried**

- zero-max functions: divide $[0, T_{max}]$ into $n$ subintervals of length $\Delta t = T/n$ and search for optimal $Q : t \mapsto \{0, Q_{max}\}$

- an industry standard software package

- a free academic software package that did not converge

- all these approaches are computationally much more expensive than simple off-on functions

- none performs better than simple off-on functions

$\Rightarrow$ increased complexity does not give better solutions
• **Take home**

- extended the Freter model for a bioreactor with wall attachment by combining it with a Wanner-Gujer style biofilm model (single species, single substrate) to assess contribution of suspended bacteria to substrate degradation in a biofilm reactor

- model can formally be written as ODE, and qualitatively studied with elementary techniques

- in biofilm reactors, at lower flow rates suspended bacteria can make a major contribution to substrate removal

- at higher flow rates suspended are washed out

- qualitative behaviour of model similar than simple Freter model, quantitative big differences (did not have time to emphasize this)

- multi-species setup will be essentially more complex: free boundary value problem for a coupled nonlocal parabolic-hyperbolic system (did not have time to cover this)

- finite time treatment: optimization not worth the effort