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

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- **Freter's model of a CSTR with wall attachment (since 1983)**

$$\dot{S} = D\big(S^0 - S\big) - \gamma^{-1}\big(u\mu_u(S) + \delta w \mu_w(S)\big)$$
$$\dot{u} = u\big(\mu_u(S) - D - k_u\big) + \beta\delta w + \delta w \mu_w(S)\big(1 - G(W)\big) - \alpha u(1 - W)$$
$$\dot{w} = w\big(\mu_w(S)G(W) - \beta - k_w\big) + \alpha u\,(1 - W)\,\delta^{-1}$$

with

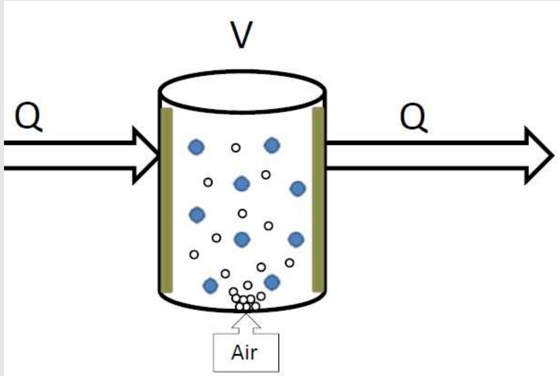
$$\mu_u(S) = \frac{m_u S}{a_u + S}, \quad \mu_w(S) = \frac{m_w S}{a_w + S}, \quad W = \frac{w}{w_{max}}, \quad G(W) = \frac{1 - W}{1.1 - W}$$

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 $\Longrightarrow$ heterogeneous, spatially structured populations $\Longrightarrow$ **need to include a biofilm model for wall attached bacteria**

- **Extension of Freter's model for a biofilm reactor: model**

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

where λ: 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)

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

$C(z)$: substrate concentration in biofilm

$$C'' = \frac{\rho m_\lambda}{d_C \gamma}\frac{C}{K_\lambda + C}, \quad C'(0) = 0, \quad C(\lambda) = S$$

– **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

$$\dot{S} = D(S^0 - S) - \frac{1}{V}\left(\frac{u\mu_u(S)}{\gamma} + AD_C j(S,\lambda)\right)$$
$$\dot{u} = u\left(\mu_u(S) - D - k_u\right) + A\rho E\lambda^2 - \alpha u$$
$$\dot{\lambda} = \frac{\gamma d_c}{\rho} j(\lambda, S) - k_\lambda \lambda + \frac{\alpha u}{A\rho} - E\lambda^2$$

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:

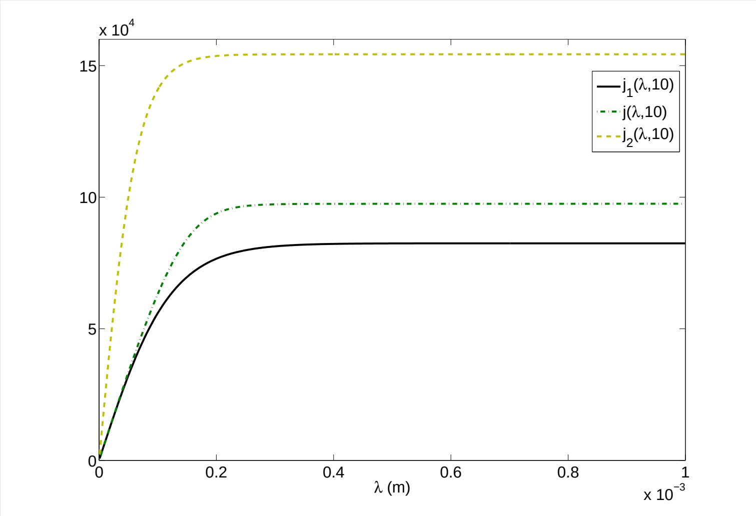
  (a) $j(\cdot, 0) = j(0, \cdot) = 0$

  (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

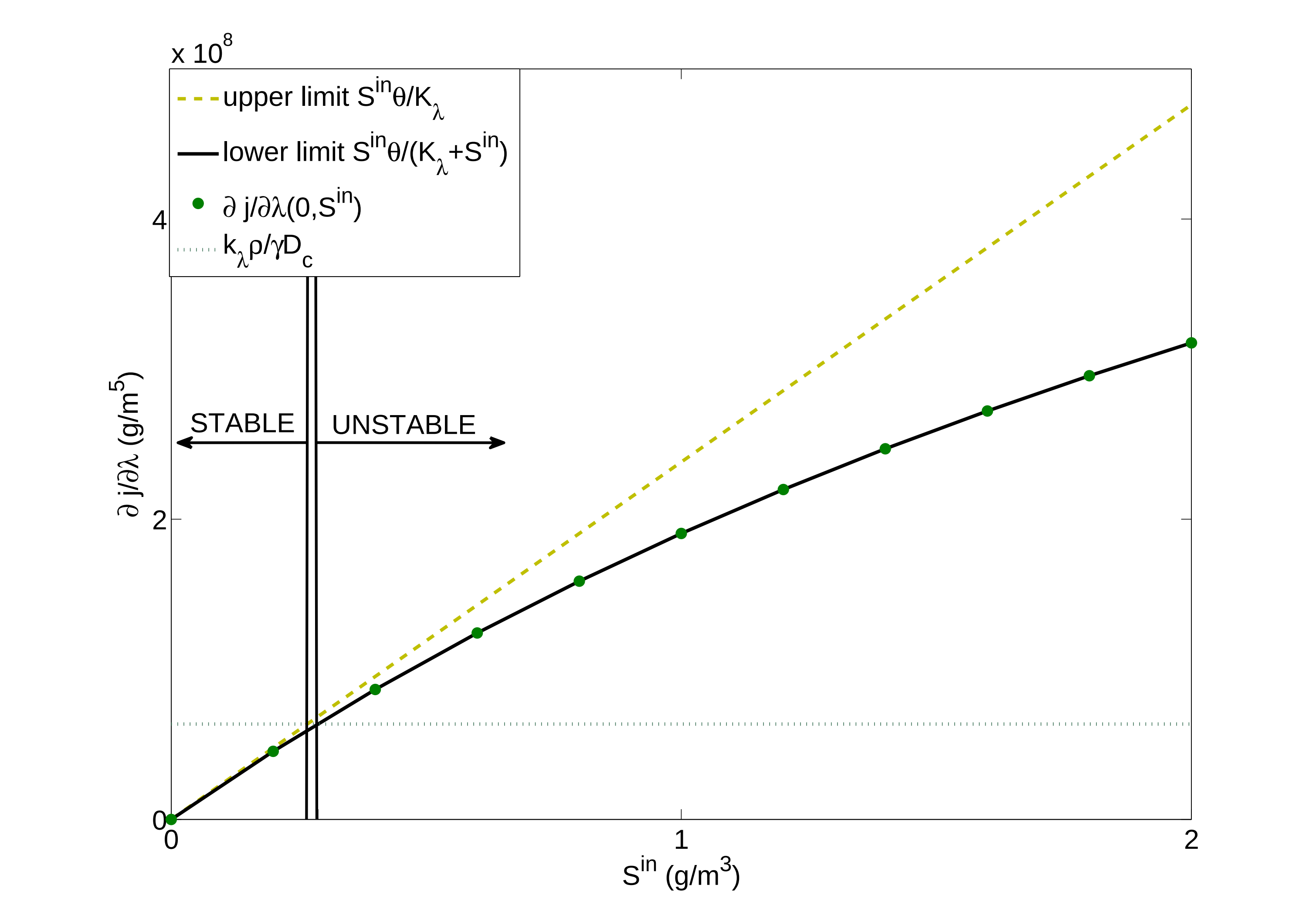
$$\mu_u(S^0) < D + k_u + \alpha \quad \text{and} \quad \frac{S^0}{K_\lambda} < \frac{k_\lambda}{m_\lambda}.$$

  On the other hand,

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

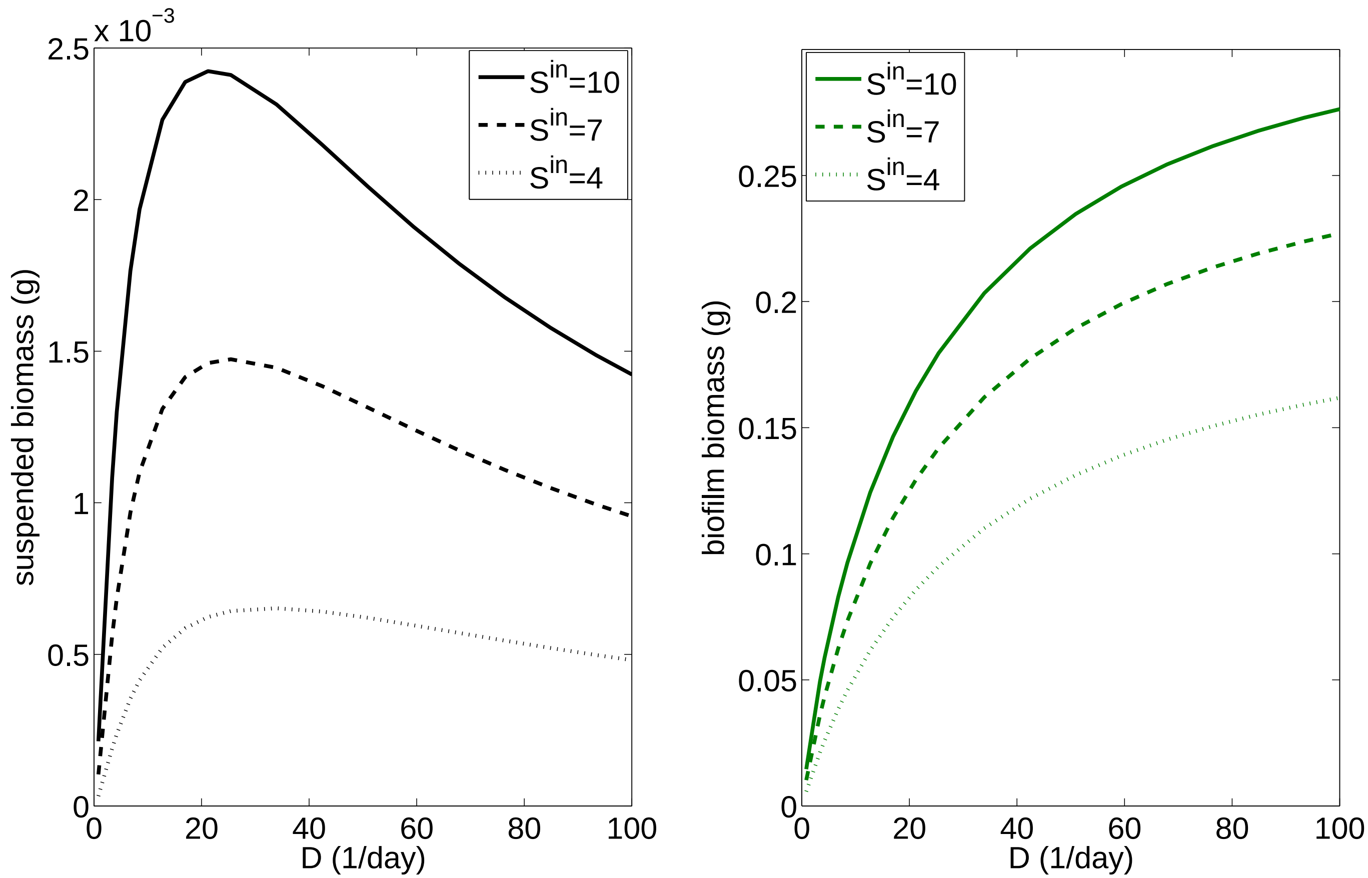
  is sufficient for instability.

- **Extension of Freter's model for a biofilm reactor: analysis**



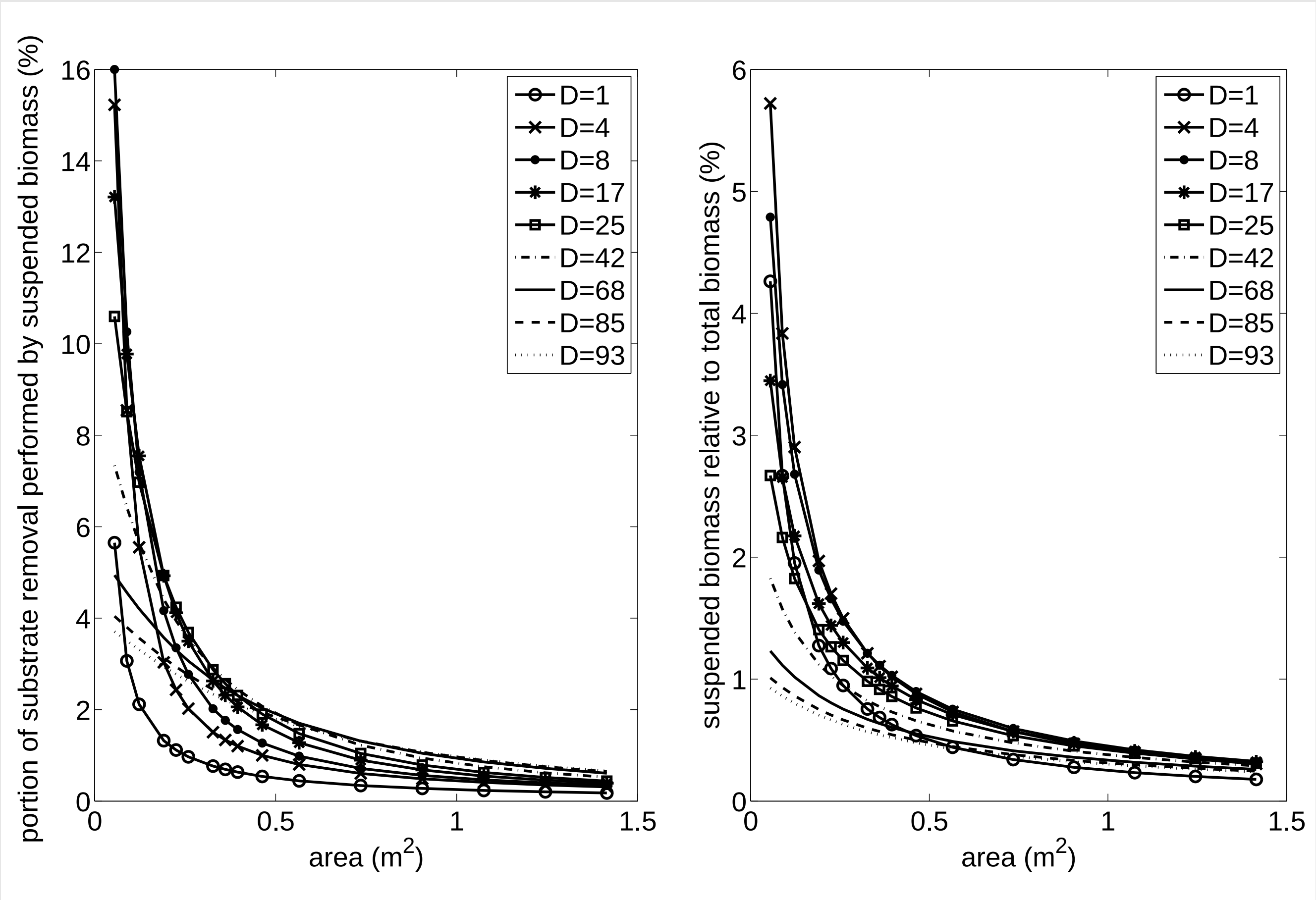
- **Extension of Freter's model for a biofilm reactor: Simulations**

  Steady state values of u, λ in dependence of dilution rate



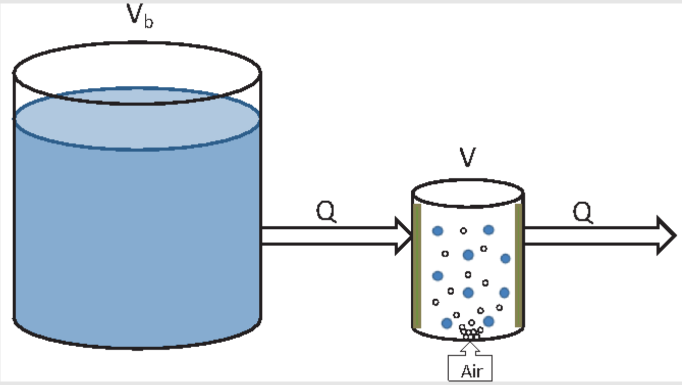
- **Extension of Freter's model for a biofilm reactor: Simulations**

Contribution of suspended biomass to substrate removal



Summary: for small colonization area and flow rate, suspendeds can contribute substantially to substrate removal

- **Optimization: setup**



  - 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

$$\min_{Q\in\Omega} \begin{pmatrix} \int_0^T QS dt \\ T \end{pmatrix}$$

where $Q : [0, T_{max}] \to \mathbb{R}_0^+$ reactor flow rate, Ω 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* $\mathcal{F} : \mathbb{R}^2 \to \mathbb{R}$

$$\min_{Q \in \Omega} \mathcal{F}(Z(Q)) = \min_{Q \in \Omega} \omega\beta \int_0^T QS dt + (1-\omega)T, \quad 0 < \omega < 1$$

    - ◇ *modified Pollack algorithm*: For every $T \in (T_{min}, T_{max})$ solve

$$\min_{Q \in \Omega} \int_0^T QS dt$$

- **Optimization: Optimal control problem in Bolza form**

$$\min_{Q\in\Omega} w\beta \int_0^T QS dt + (1-w)T$$

with $\Omega = \{Q \text{ measureable}, 0 \leq Q \leq Q_{max}\}$
subject to

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

$$\dot{u} = u\left(\mu_u(S) - \frac{Q}{V} - k_u\right) + A\rho E\lambda^2 - \alpha u$$

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

$$\dot{V}_b = -Q$$

$$S(0) = 0, \quad u(0) \geq u_0, \quad \lambda(0) \geq 0, V_b(0) = V_{b,max}$$

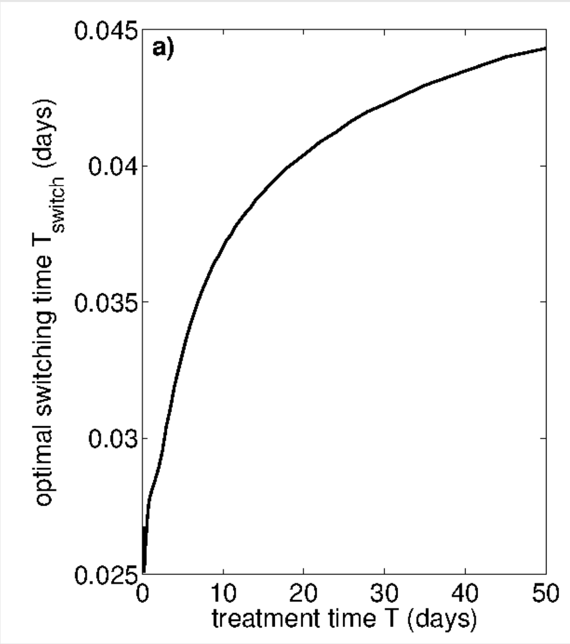
-- **linear in control variable $Q \Longrightarrow$ optimal control chatters**

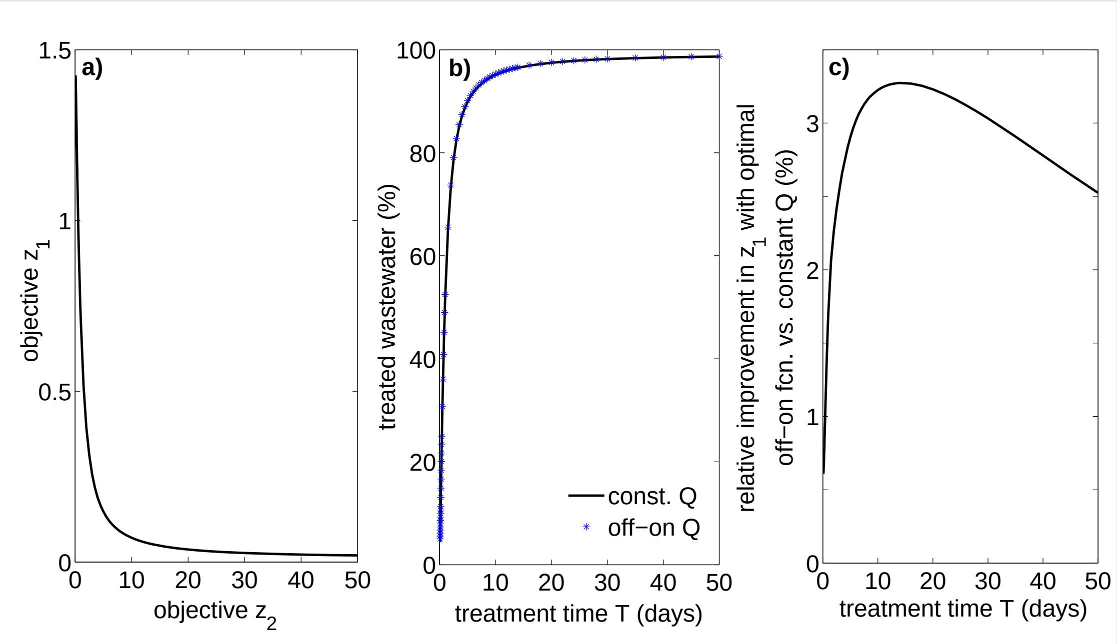
- **Optimization: Off-on functions**
  - look for optimal flow rate Q in the class of functions

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

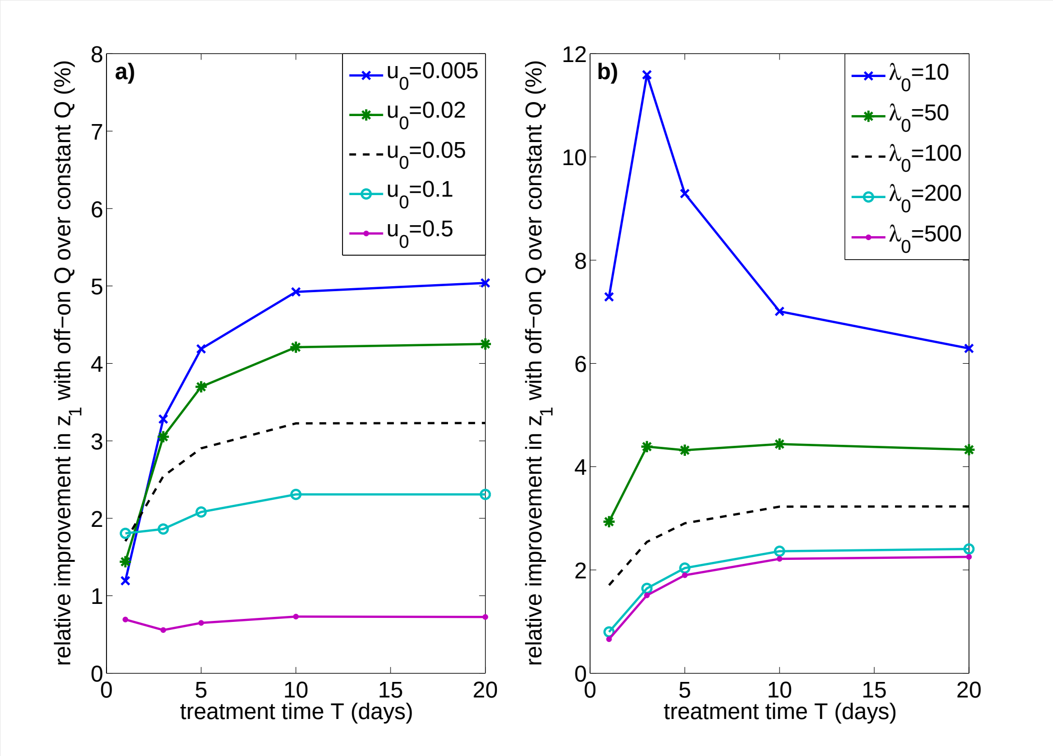
and solve (using Pollack's method)

$$\min_{T_{switch}, T} \left(\frac{\int_0^T QS dt}{T} \right), \quad s.t. \quad 0 < T_{min} \le T_{switch} \le T \le T_{max}$$





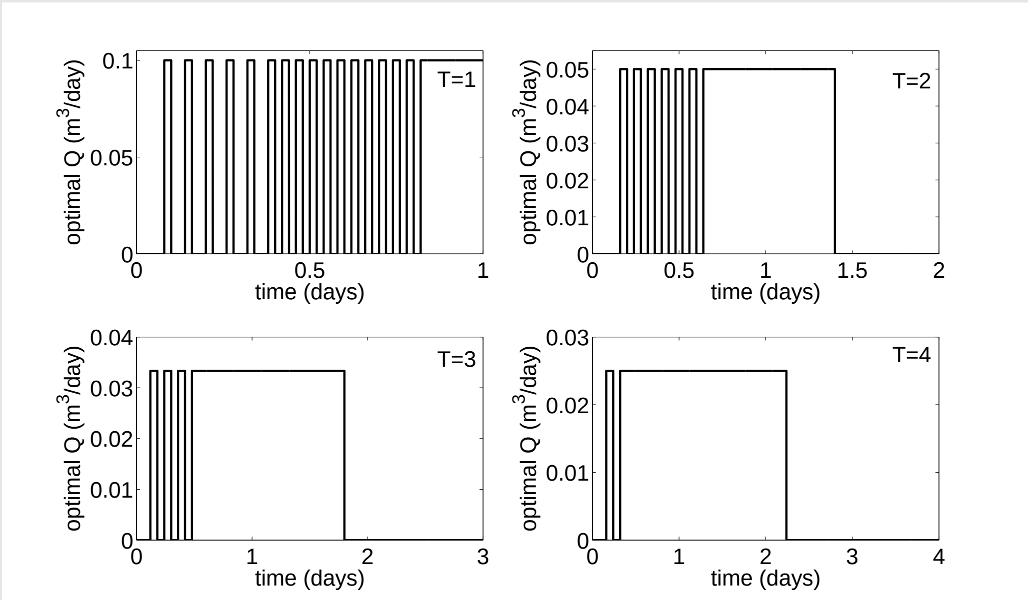
- **Optimization: Off-on functions continued**
  - strong dependence on initial data:

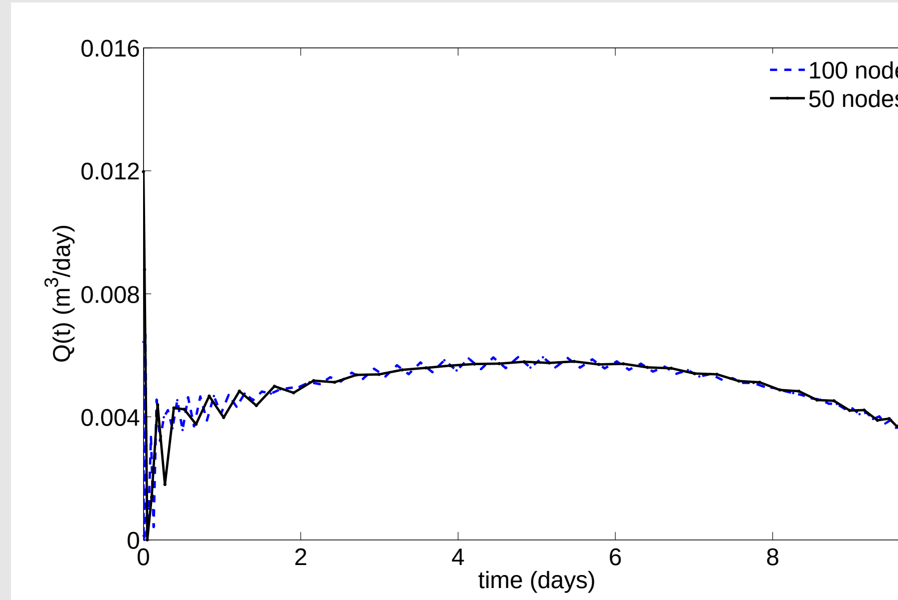


  - initial data typically not known $\Longrightarrow$ optimum difficult to find
  - the less biomass initially in reactor the higher potential for control
  - overall very moderate compared to $Q = V_{b,max}/T = const$

$\Longrightarrow$ 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

$\Longrightarrow$ 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