Mathematical Optimization in Industrial Processes

Application to the design of bioreactors for water treatment.

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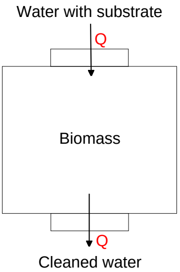
- Postulate: We consider water resources polluted with biochemical substances (glucose,sulfate,etc), called substrates.
- Objective: Clean this water by using biological microorganisms (bacteria,enzymes,etc), called biomasses, which develop by substrate consumption.
- How?: Connecting the water resource in a closed circuit with a bioreactor.

Contents

Bioreactors

The bioreactors operating continuously are also called *chemostats*. The chemostat was studied by Jacques Monod, Aaron Novick and Leo Szilard in 1950.



The bioreactor is fed from the resource with a flow rate Q, and its output returns the cleaned water with the same flow rate Q.

Mathematical Model for a bioreactor: An ODE Approach

Homogeneous distribution of the contaminant in the bioreactor:

$$\begin{cases} \frac{\mathrm{d}S_{\mathrm{r}}}{\mathrm{d}t}(t) = -\mu(S_{\mathrm{r}}(t))B_{\mathrm{r}}(t) + \frac{Q(t)}{V_{\mathrm{r}}}(S_{\mathrm{e}}(t) - S_{\mathrm{r}}(t)) & t > 0, \\ \frac{\mathrm{d}B_{\mathrm{r}}}{\mathrm{d}t}(t) = \mu(S_{\mathrm{r}}(t))B_{\mathrm{r}}(t) - \frac{Q(t)}{V_{\mathrm{r}}}B_{\mathrm{r}}(t) & t > 0, \\ S_{\mathrm{r}}(0) = S_{\mathrm{e}}(0), \qquad B_{\mathrm{r}}(0) = B_{\mathrm{r},0}, & \end{cases} \tag{1}$$

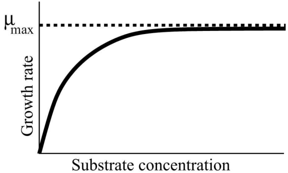
-Q: flow rate (m^3/s).
-S_{r}: substrate concentration inside the reactor (mol/m^3).
-B_{r}: biomass concentration inside the reactor (mol/m^3).
-S_{e}: substrate concentration that enters the bioreactor (mol/m^3).
-V_{r}: reactor volume(m^3).
-μ: growth rate function (s^{-1}).

Assumption:

1. Function $\mu(\cdot)$ is increasing and $\mu(0) = 0$.
2. Function $\mu(\cdot)$ es concave.

An example of growth rate function is given by the Monod Equation:

$$\mu(S) = \mu_{\max} \frac{S}{K+S}$$



P. Gajardo, J. Harmand, H. Ramírez C., and A. Rapaport. Minimal time bioremediation of natural water resources. *Automatica*, 47(8), 2011.

Particular case: $S_{\rm e}$ and Q are constant.

System (1) has two fixed points:

- $E_1 = (S_{\rm e}, 0) \Rightarrow$ No decontamination (leaching)
- $E_2 = (S_{\rm r}^{\rm Q}, S_{\rm e} - S_{\rm r}^{\rm Q})$, where $S_{\rm r}^{\rm Q}$ fulfills $Q = V_{\rm r}\mu(S_{\rm r}^{\rm Q})$.

Theorem (Stability analysis)

1. *If* $Q < V_{\rm r}\mu(S_{\rm e}) \Rightarrow E_1$ *unstable,* E_2 *is asymptotically stable.*
2. *If* $Q > V_{\rm r}\mu(S_{\rm e}) \Rightarrow E_1$ *asymptotically stable,* E_2 *is unstable.*
3. *If* $Q = V_{\rm r}\mu(S_{\rm e}) \Rightarrow E_1 = E_2$ *asymptotically stable.*

Proof.

For (1) and (2) we use *Hartman-Grobman Theorem*.
For (3) we use *Poincare-Bendixson Theorem* and *Dulac's Criterion*. □

Nonlinear system: $\begin{cases} x\acute{=}F(x) \\ x(0) = x_0 \end{cases} \qquad (*)$

Let x^* a critical point of $(*)$, i.e, $F(x^*) = 0$.

Linearization: $z' = DF(x^*)z$, where $z = x - x^*$.

Theorem (Hartman-Grobman)

Suppose x^* is a hyperbolic critical point (i,.e the real part of the eigenvalues of DF are not zero). Then the phase portrait of the linearization and the nonlinear equations are locally homeomorphic.

Theorem

- *Real part of the eigenvalues of DF are negative $\Rightarrow x^*$ is asymptotically stable.*
- *At least one eigenvalue of DF is positive $\Rightarrow x^*$ is unstable.*

Theorem (Generalized Poincare Bendixson)

If the positive orbit $\gamma^+(x)$ in $(*)$ is contained in a compact set K, where K only contains a finite number of critical points, then:

- *$\omega(x)$ critical point, or*
- *$\omega(x)$ periodic orbit, or*
- *$\omega(x)$ connected set composed of finite number of fixed points.*

Theorem (Dulac Criterion - Only for $F = (F_1, F_2)$)

Let D be a simply connected region in the phase plane. If there exists $\mathcal{C}^1$ function $\psi(x, y)$ such that

$$\frac{\mathrm{d}}{\mathrm{d}x}(\psi(x, y)F_1(x, y)) + \frac{\mathrm{d}}{\mathrm{d}y}(\psi(x, y)F_2(x, y))$$

has constant sign in D, then (2) has no closed orbits lying in D.

Nondimensionalization of the system

Definition

Partial or full removal of units from an equation involving physical quantities by a suitable substitution of variables

1. List all of the variables, parameters, and their dimensions:

Variable	Dimension	Parameter	Dimension
B_r	mol/m^3	V_r	m^3
S_r	mol/m^3	$S_e(0)$	mol/m^3
t	s	$B_{r,0}$	mol/m^3
Q	m^3/s		
S_e	mol/m^3		
μ	s^{-1}		

2. Take each variable and create a new variable dividing by a combination of parameters that has the same dimension:

$$s_{\mathrm{e}} = \frac{S_{\mathrm{e}}}{S_{\mathrm{e}}(0)}, \quad s_{\mathrm{r}} = \frac{S_{\mathrm{r}}}{S_{e}(0)}, \quad b_{\mathrm{r}} = \frac{B_{\mathrm{r}}}{S_{e}(0)}, \quad \tilde{\mu}(s_{\mathrm{r}}) = \frac{\mu(S_{\mathrm{r}})}{\mu(S_{\mathrm{e}}(0))}$$

$$q = \frac{Q}{V_{\mathrm{r}}\mu(S_{\mathrm{e}}(0))}, \qquad \boxed{t_{\mathrm{r}} = \frac{t}{\frac{1}{\mu(S_{\mathrm{e}}(0))}}}$$

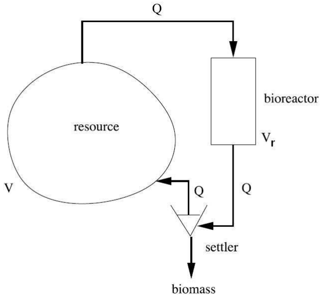
3. Rewrite the differential equation in terms of the new variables:

$$\begin{cases} \frac{\mathrm{d}s_{\mathrm{r}}}{\mathrm{d}t_{\mathrm{r}}}(t_{\mathrm{r}}) = -\tilde{\mu}(s_{\mathrm{r}}(t_{\mathrm{r}}))b_{\mathrm{r}}(t_{\mathrm{r}}) + q(t_{\mathrm{r}})(s_{\mathrm{e}}(t_{\mathrm{r}}) - s_{\mathrm{r}}(t_{\mathrm{r}})), & t_{\mathrm{r}} > 0, \\ \frac{\mathrm{d}b_{\mathrm{r}}}{\mathrm{d}t_{\mathrm{r}}}(t_{\mathrm{r}}) = \tilde{\mu}(s_{\mathrm{r}}(t_{\mathrm{r}}))b_{\mathrm{r}}(t_{\mathrm{r}}) - q(t_{\mathrm{r}})b_{\mathrm{r}}(t_{\mathrm{r}}), & t_{\mathrm{r}} > 0, \\ s_{\mathrm{r}}(0) = 1, \qquad b_{\mathrm{r}}(0) = \alpha, \end{cases}$$

where $\alpha = \frac{B_{\mathrm{r},0}}{S_{\mathrm{e}}(0)}$.

Dynamics in the water resource and coupled system

Natural water resource polluted with a substrate concentration S_1.
$\Longrightarrow$ Objective: Reduce the concentration of the pollutant to a prescribed value S_{lim}.



Settler: Collect the biomass $\Rightarrow$ avoids new contamination.

The dynamics in the water resource can be described

$$\begin{cases} \frac{\mathrm{d}S_1}{\mathrm{d}t}(t) = \frac{Q(t)}{V}(S_\mathrm{r}(t) - S_1(t)), \quad t > 0, \\ S_1(0) = S_{1,0} \end{cases} \tag{2}$$

- **Dimensional Analysis**

Variable	Dimension	Parameter	Dimension
S_1	$\mathrm{mol/m}^3$	V	m^3
t	s	$S_{1,0}$	$\mathrm{mol/m}^3$
S_r	$\mathrm{mol/m}^3$		
Q	m^3/s		

$s_1 = \frac{S_1}{S_1(0)}$, $\quad s_\mathrm{r} = \frac{S_\mathrm{r}}{S_1(0)}$, $\quad q = \frac{Q}{V_\mathrm{r}\mu(S_1(0))}$, $\quad t_1 = \frac{t}{\frac{V}{V_\mathrm{r}\mu(S_1(0))}}$

$$\begin{cases} \frac{\mathrm{d}s_1}{\mathrm{d}t_1}(t_1) = -q(t_1)(s_1(t_1) - s_\mathrm{r}(t_1)), \\ s_1(0) = 1. \end{cases}$$

Quasi-Steady State Approximation

Hypothesis: $V >> V_\mathrm{r} \Rightarrow \boxed{\tau_1 \sim \frac{V}{V_\mathrm{r}} \frac{1}{\mu(S_1(0))} >> \tau_\mathrm{r} \sim \frac{1}{\mu(S_1(0))}}$

Reasonable time scale for the bioreactor $\Rightarrow S_1$, Q negligibly changes.

Remember: When $Q < V_\mathrm{r}\mu(S_1)$, the equilibrium point $(S_\mathrm{r}^\mathrm{Q}, S_1 - S_\mathrm{r}^\mathrm{Q})$ is asymptotically stable.

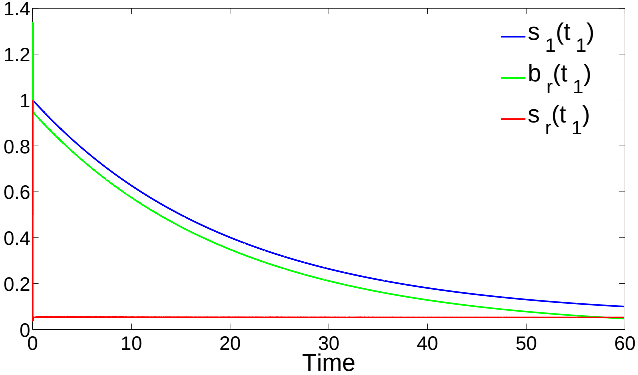
Reasonable time scale for the water resource $\Rightarrow$ the bioreactor attains its equilibrium point.

Thus, System (2) can be approximated as:

$$\begin{cases} \frac{\mathrm{d}S_1}{\mathrm{d}t}(t) = \frac{Q(t)}{V}(S_\mathrm{r}^\mathrm{Q}(t) - S_1(t)), & t > 0, \\ S_1(0) = S_{1,0}. \end{cases} \tag{3}$$

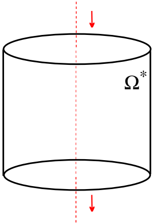
where $S_\mathrm{r}^\mathrm{Q}(t) \in [0, S_1(t))$.

Q is constant in time , $\mu(\cdot)$ Monod Equation.
$(S_{\rm r}^*, B_{\rm r}^*) = (S_{\rm r}^{\rm Q}, S_1(t) - S_{\rm r}^{\rm Q})$ where $S_{\rm r}^{\rm Q}$ fulfills $Q = V_{\rm r}\mu(S_{\rm r}^{\rm Q})$.



Mathematical Model for the Bioreactor: A PDE Approach

Spatial disparity of the contaminant in the bioreactor.



- Substrate and Biomass concentrations ⇒ Convection-Diffusion-Reaction equation.
- Fluid Flow ⇒ Vertical inflow: $\mathbf{u} = (0, 0, -\bar{Q}(t))$ where $\bar{Q}$ (m/s) is the flow rate per unit of area.

$$\begin{cases} \frac{\mathrm{d}S_\mathrm{r}}{\mathrm{d}t} = \nabla \cdot (D_\mathrm{S} \nabla S_\mathrm{r}) - \mathbf{u} \nabla S_\mathrm{r} - \mu(S_\mathrm{r}) B_\mathrm{r} & \text{in } \Omega^*, \ t > 0, \\ \frac{\mathrm{d}B_\mathrm{r}}{\mathrm{d}t} = \nabla \cdot (D_\mathrm{B} \nabla B_\mathrm{r}) - \mathbf{u} \nabla B_\mathrm{r} + \mu(S_\mathrm{r}) B_\mathrm{r} & \text{in } \Omega^*, \ t > 0. \end{cases} \quad (4)$$

$D_\mathrm{S}, D_\mathrm{B}$ substrate and biomass diffusion coefficients $(\mathrm{m}^2/\mathrm{s})$.

We consider suitable initial conditions:

- $S_{\mathrm{r}}(0,x) = S_1(0), \qquad B_{\mathrm{r}}(0,x) = B_{\mathrm{init}} \qquad \forall x \in \Omega^*,$

and boundary conditions:

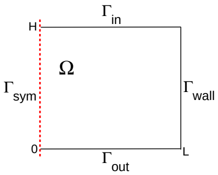
Flux of the system: $\boxed{J = -D\nabla c + \mathbf{u}c}$

D is the diffusion, $\mathbf{u}$ is the fluid flow and c is the concentration.

- $$\begin{cases} \mathbf{n}\cdot(-D_{\mathrm{S}}\nabla S_{\mathrm{r}} + \mathbf{u}S_{\mathrm{r}}) = -\bar{Q}(t)S_{\mathrm{e}}(t) \\ \mathbf{n}\cdot(-D_{\mathrm{B}}\nabla B_{\mathrm{r}} + \mathbf{u}B_{\mathrm{r}}) = 0 \end{cases} \qquad \forall x \in \Gamma^*_{\mathrm{in}},\ \ t > 0,$$

- $$\begin{cases} \mathbf{n}\cdot(-D_{\mathrm{S}}\nabla S_{\mathrm{r}}) = 0 \\ \mathbf{n}\cdot(-D_{\mathrm{B}}\nabla B_{\mathrm{r}}) = 0 \end{cases} \qquad \forall x \in \Gamma^*_{\mathrm{wall}} \cup \Gamma^*_{\mathrm{out}},\ \ t > 0.$$

Simplification:



⇒ Change to cylindrical coordinates (r, z) where r is the distance to the cylinder axis.

System (4) can be rewritten as:

$$\begin{cases} \frac{\mathrm{d}S_{\mathrm{r}}}{\mathrm{d}t} = \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(rD_{\mathrm{S}}\frac{\mathrm{d}S_{\mathrm{r}}}{\mathrm{d}r}\right) + \frac{\mathrm{d}}{\mathrm{d}z}\left(D_{\mathrm{S}}\frac{\mathrm{d}S_{\mathrm{r}}}{\mathrm{d}z}\right) + \bar{Q}(t)\frac{\mathrm{d}S_{\mathrm{r}}}{\mathrm{d}z} - \mu(S_{\mathrm{r}})B_{\mathrm{r}} & \text{in } \Omega, t > 0, \\ \frac{\mathrm{d}B_{\mathrm{r}}}{\mathrm{d}t} = \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(rD_{\mathrm{B}}\frac{\mathrm{d}B_{\mathrm{r}}}{\mathrm{d}r}\right) + \frac{\mathrm{d}}{\mathrm{d}z}\left(D_{\mathrm{B}}\frac{\mathrm{d}B_{\mathrm{r}}}{\mathrm{d}z}\right) + \bar{Q}(t)\frac{\mathrm{d}B_{\mathrm{r}}}{\mathrm{d}z} + \mu(S_{\mathrm{r}})B_{\mathrm{r}} & \text{in } \Omega, t > 0, \end{cases} \quad (5)$$

We consider suitable initial conditions:

- $S_{\mathrm{r}}(0,r,z) = S_1(0), \qquad B_{\mathrm{r}}(0,r,z) = B_{\mathrm{init}} \qquad \forall (r,z) \in \Omega,$

and boundary conditions:

- $$\left\{ \begin{array}{l} D_{\mathrm{S}} \frac{\mathrm{d}S_{\mathrm{r}}}{\mathrm{d}z} + \bar{Q}(t) S_{\mathrm{r}} = \bar{Q}(t) S_{\mathrm{e}}(t) \\ D_{\mathrm{B}} \frac{\mathrm{d}B_{\mathrm{r}}}{\mathrm{d}z} + \bar{Q}(t) B_{\mathrm{r}} = 0 \end{array} \right. \qquad \forall (r,z) \in \Gamma_{\mathrm{in}}, \ \ t > 0,$$

- $$\left\{ \begin{array}{l} \frac{\mathrm{d}S_{\mathrm{r}}}{\mathrm{d}r} = 0 \\ \frac{\mathrm{d}B_{\mathrm{r}}}{\mathrm{d}r} = 0 \end{array} \right. \qquad \forall (r,z) \in \Gamma_{\mathrm{wall}} \cup \Gamma_{\mathrm{sym}} \cup \Gamma_{\mathrm{out}}, \ \ t > 0.$$

The dynamics of the water resource can be described as follows:

$$\begin{cases} \frac{\mathrm{d}S_1}{\mathrm{d}t}(t) = \frac{Q(t)}{V}(S_{\mathrm{out}}(t) - S_1(t)), \quad t > 0, \\ S_1(0) = S_{1,0}. \end{cases} \tag{6}$$

where $S_{\mathrm{out}}(t) = \frac{\int_{\Gamma_{out}} S_{\mathrm{r}}(t,r,z)\mathrm{d}\mathrm{r}}{L}$ and Γ_{out} is the outlet through which treated water leaves the reactor.

Optimization problem: Bioreactor with ODE model

$$\left\{ \begin{array}{l} \text{Find } Q^{\text{opt}} \in X, \text{ such that} \\ T(Q^{\text{opt}}) = \min_{Q \in X} T(Q), \end{array} \right. \tag{7}$$

where $T(Q)$ is the time required for achieving $S_1(T(Q)) = S_{\text{lim}}$, with S_1 being the solution of (2) (or 6).
$X = \{Q \text{ piecewise } C^1([0,+\infty)) : 0 \leq Q(t) < V_r \mu(S_1(t)) \ \forall t \geq 0\}$.

- **Flux is constant in time**

Theorem

If Q is constant, then the time required for the solution of (3) to attain the value S_{lim} is:

$$T(S_r^Q) = \frac{1}{\frac{V_r}{V} \mu(S_r^Q)} \ln \left(\frac{S_{1,0} - S_r^Q}{S_{\text{lim}} - S_r^Q} \right)$$

- **Q is a time variable**

Definition

If a functional relation of the form

$$S_{\mathrm{r}}^{\mathrm{Q}}(t) = \omega(S_1(t)) \qquad \forall t \in [0, +\infty)$$

can be found for the optimal control at time t for problem (7), then ω is called optimal feedback.

Theorem

An optimal feedback $S_{\mathrm{r}}^{\mathrm{opt}}$ must fulfill

$$S_{\mathrm{r}}^{\mathrm{opt}}(t) = \arg \min_{S_{\mathrm{r}}^{\mathrm{Q}}(t) \in (0, S_1(t))} \mu(S_{\mathrm{r}}^{\mathrm{Q}}(t))(S_{\mathrm{r}}^{\mathrm{Q}}(t) - S_1(t)).$$

Moreover $t \to Q(t)$ is decreasing along any optimal trajectory.

Q is constant in time $\Rightarrow \Theta = [0, V_{\mathrm{r}}\mu(S_{\mathrm{lim}}))$.

Q is a time variable: $Q(t)$ is $\mathcal{C}^1$ and should be decreasing on time!
We work with 5 optimization parameters:

$$(Q_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4) \in \Theta = [0, V_{\mathrm{r}}\mu(S_1(0))) \times [0, 1]^4$$

such that

$$Q(t) = \begin{cases} Q_0 & t = 0 \\ Q_0 \cdot \alpha_1 & t = t_1 \\ Q_0 \cdot \alpha_1 \cdot \alpha_2 & t = t_2 \\ Q_0 \cdot \alpha_1 \cdot \alpha_2 \cdot \alpha_3 & t = t_3 \\ Q_0 \cdot \alpha_1 \cdot \alpha_2 \cdot \alpha_3 \cdot \alpha_4 & t = t_4 \end{cases}$$

for 4 different fixed times t_1, t_2. t_3 and t_4
In the time intervals (t_i, t_{i+1}) $(i = 0, \ldots, 3)$, $Q(t)$ is calculated with Cubic Hermite Spline

It is reasonable to think that in practice it is easier to use Piecewise Constant $Q(t)$.

$$Q(t) = \begin{cases} Q_0 & t \in [0, t_1) \\ Q_0 \cdot \alpha_1 & t \in [t_1, t_2) \\ Q_0 \cdot \alpha_1 \cdot \alpha_2 & t \in [t_2, t_3) \\ Q_0 \cdot \alpha_1 \cdot \alpha_2 \cdot \alpha_3 & t \in [t_3, t_4) \\ Q_0 \cdot \alpha_1 \cdot \alpha_2 \cdot \alpha_3 \cdot \alpha_4 & t \in [t_4, t_5) \end{cases}$$

Genetic Algorithms

Global optimization method based on a natural selection process that mimics biological evolution.

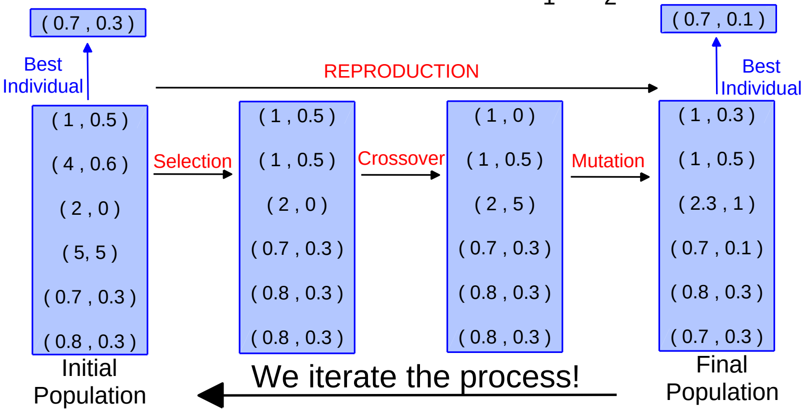
$$\min_{x \in \Theta} f(x)$$

$\Theta \subset R^{\mathrm{N}}$ is the search space.

- Creation a random initial population in the search space.
- Successive reproduction of the population by the stochastic steps Selection, Crossover, Mutation and Elitism.

Genetic Algorithm: Sketch

We want to minimize: $J(x)=x_1^2 + x_2^2$

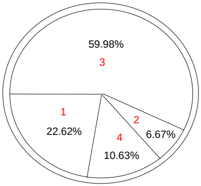


- **Selection:** Individuals are selected according to their fitness value.

Roulette Wheel Selection:

Individual number	Individual	Fitness value	% of Total
1	$(0,1)$	169	22.72
2	$(1,0)$	576	6.67
3	$(0,0)$	64	59.99
4	$(1,1)$	361	10.63
Total		1170	100.0

Table: Roulette Wheel Selection.



- **Crossover:** Create a new solution candidate by combining the characteristics of two existing individuals
  Arithmetic Crossover

$$\text{Chil1} = a \cdot \text{Parent1} + (1-a) \cdot \text{Parent2}$$

$$a \in [0,1]$$

$$\text{Chil2} = (1-a) \cdot \text{Parent1} + a \cdot \text{Parent2}$$

- **Mutation:** Randomly modifies the value of one or more genes of an individual.
  Non-Uniform mutation: To mutate an individual x, we compute

$$x' = \begin{cases} x + \Delta(g, b-x) & \text{if } \tau = 0 \\ x - \Delta(g, b-x) & \text{if } \tau = 1 \end{cases}$$

where $\Delta(g,y) = (1 - r^{(1-\frac{g}{g_{\max}})^b})$.

- **Elitism:** Ensures that at least one copy of the best individual(s) of the current generation is directly copied to the next generation.

  Matrix formulation

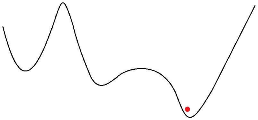
  $$\boxed{X^{i+1} = (I_N - \mathcal{E}^i)(\mathcal{C}^i \mathcal{S}^i X^i + \mathcal{M}^i) + \mathcal{E}^i X^i}$$

  -X^i: Current generation
  -$\mathcal{E}^i$: Elitism operator
  -$\mathcal{C}^i$: Crossover operator
  -$\mathcal{S}^i$: Selection operator
  -$\mathcal{M}^i$: Mutation operator
  -I_N: Identity matrix

- **Stopping criteria:**
  Generation number
  No Improvement generation number

Hybrid Genetic Algorithm

1. Coarse search of global minimum with GA

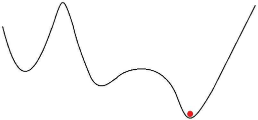


2. Refine the local search by using a Gradient Descent method.

$$x_{k+1} = x_k - \nabla f(x_k)\alpha_k,$$

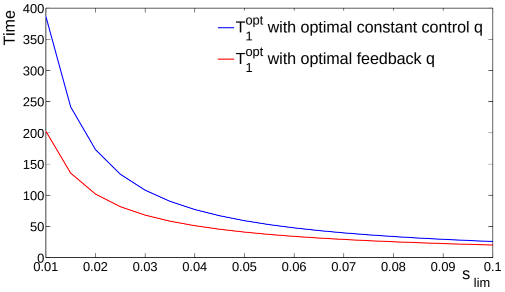
where α_k is the step length which must fulfill

$$f(x_k - \nabla f(x_k)\alpha_k) \leq f(x_k - \nabla f(x_k)\alpha) \quad \text{for all } \alpha \geq 0.$$



Numerical Optimization Results: ODE Approach

$\mu(\cdot)$ Monod Function



Optimal feedback can reduce the decontamination time by half!

Numerical Optimization Results: PDE Approach

$\mu(\cdot)$ Monod, $S_{\mathrm{lim}} = 0.1$, $Q(t)$ continuously differentiable.

$S_1(0)$ (mol/m^3)	Time $Q^{\mathrm{opt}}_{\mathrm{HGA}}$(const) (s)	Time $Q^{\mathrm{opt}}_{\mathrm{HGA}}$(Tdep) (s)
$D_{\mathrm{S}} = D_{\mathrm{B}} = 100$ (m^2/s)		
5	72750	46650
10	81840	48090
20	90760	49360
$D_{\mathrm{S}} = D_{\mathrm{B}} = 0.01$ (m^2/s)		
5	87710	55120
10	100360	57870
20	58870	26460

Time dependent Q can reduce the decontamination time in 55%!

Numerical Optimization Results: PDE Approach

$\mu(\cdot)$ Monod, $S_{\mathrm{lim}} = 0.1$, $Q(t)$ Piecewise constant.

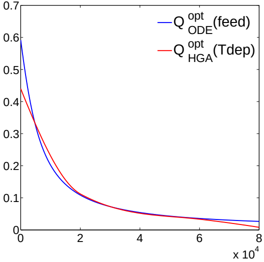
$S_1(0)$ (mol/m^3)	Time $Q^{\mathrm{opt}}_{\mathrm{HGA}}$(const) (s)	Time $Q^{\mathrm{opt}}_{\mathrm{HGA}}$(Tdep) (s)
$D_S = D_B = 100$ (m^2/s)		
5	72750	49390
10	81840	51560
20	90760	55010
$D_S = D_B = 0.01$ (m^2/s)		
5	87710	60120
10	100360	62990
20	58870	23340

Time dependent Q can reduce the decontamination time in 60%!

Comparison between ODE and PDE Approaches: $Q(t)$ continuously differentiable

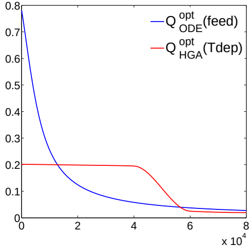
$$D_S = D_B = 100 \ (m^2/s)$$

- Both fluxes are suitable.
- Decontamination times are comparable.



$$D_S = D_B = 0.01 \ (m^2/s)$$

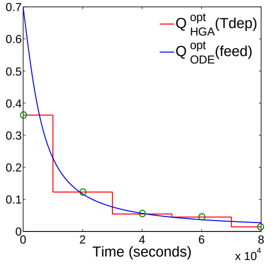
- Optimal fluxes obtained with the ODE approach are not suitable $\Rightarrow$ we are not able to achieve the target.



Comparison between ODE and PDE Approaches: $Q(t)$ piecewise constant

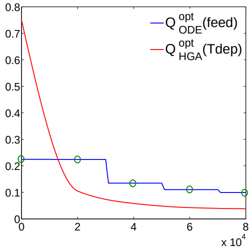
$$D_S = D_B = 100 \ (\mathrm{m}^2/\mathrm{s})$$

- Both fluxes are suitable.
- Decontamination times are comparable.



$$D_S = D_B = 0.01 \ (\mathrm{m}^2/\mathrm{s})$$

- Optimal fluxes obtained with the ODE approach are not suitable $\Rightarrow$ we are not able to achieve the target.



Numerical Optimization Results: Comparison between $Q(t)$ continuously differentiable and piecewise constant

$\mu(\cdot)$ Monod, $S_{\rm lim} = 0.1$

$S_1(0)$ (mol/m^3)	Time $Q^{\rm opt}_{\rm HGA}$(CD) (s)	Time $Q^{\rm opt}_{\rm HGA}$(PC) (s)
$D_S = D_B = 100$ (m^2/s)		
5	46650	49390
10	48090	51560
20	49360	55010
$D_S = D_B = 0.01$ (m^2/s)		
5	55120	60120
10	57870	62990
20	26460	23340

$Q(t)$ continuously differentiable can reduce the decontamination time in 10%!

Conclusions

- ODE approach for the bioreactor: We obtain the optimal flux with theoretical results.
- PDE approach for the bioreactor: We obtain the optimal flux using an Hybrid Genetic Algorithm.
- The decontamination time can be reduced by half if the optimal flux is chosen as a time variable rather than constant in time.
- For small diffusivities D_{S} and D_{B} the theoretical results obtained for the ODE approach are not suitable. We are not able to achieve the target.

Future work

- Give an existence and uniqueness result for the system presented in the PDE approach for the bioreactor.
- Give a suitable nondimensionalization for the system presented in the PDE approach.
- More intensive study of HGA.
- Consider inhomogeneity in the water resource.

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