About interconnections of chemostats

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Team MODEMIC

UMR MISTEA - Montpellier

An initial framework

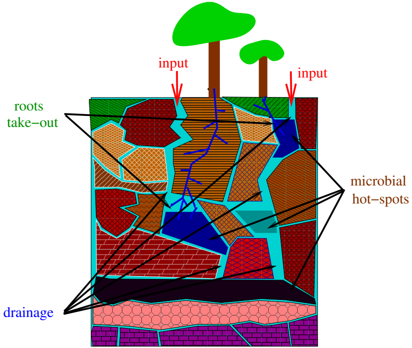
The ARC INRIA / AIP INRA VITELBIO 2009-10
(VIrtual TELluric BIOreactors)

Objective : **study simple spatial representations of soil as a structured fermentor**.

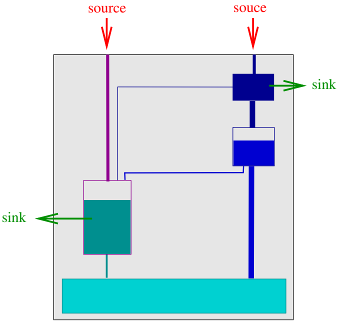
Main participants : UMR EcoSols (Montpellier), UMR Géosciences (Univ. Rennes 1), UREP (INRA Theix), ITK.

Web site : `https://sites.google.com/site/vitelbio/`

The VITELBIO project

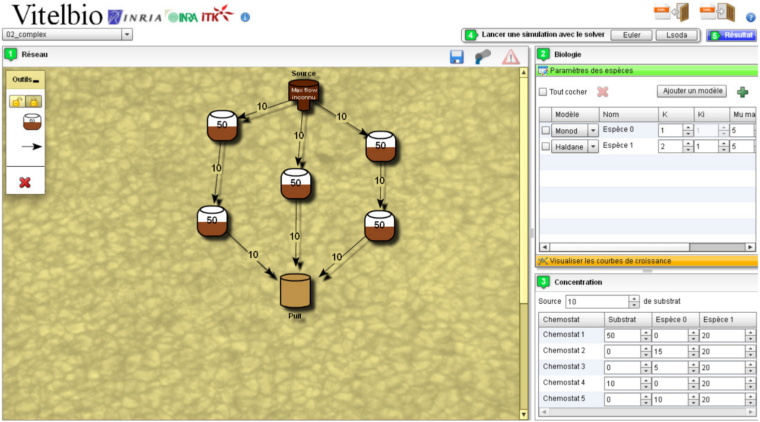


cross section of soil



structured bioreactor

The VITELBIO project



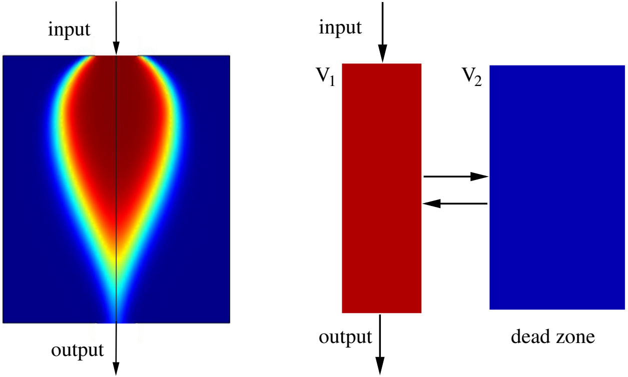
Main studies

- Effects of spatial structure and diffusion on the performances of the chemostat
  - co-supervision of a PhD student with UMR EcoSols
- About the benefit of the buffered chemostat
  - properties discovered thanks to simulations
- About niches and overyielding
  - primary work on the two species case
  - a lot remain to be done and understood...

Present and future directions

- Waste water treatment in natural environments
  within associated team with Chile
  collaboration with MOISE team
- Input-output equivalence of hydric systems
  automatic control viewpoint
  collaboration with GéoSciences Rennes

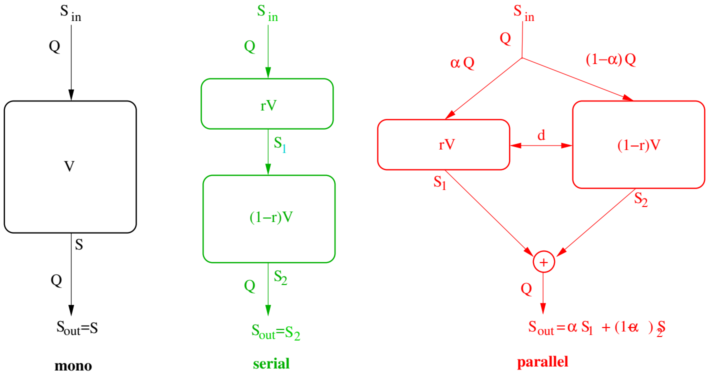
The spirit



Effects of spatial structure and diffusion on the performances of the chemostat

Participants : F. Gérard, I. Haidar, A. Rapaport.

Study of interconnected chemostats



The role of spatial structure

Proposition. For any monotonic increasing $\mu(\cdot)$, there exists a thershold $\bar{s}_{in}$ such that

- $s_{in} > \bar{s}_{in}$, the exists a serial configuration s.t.
  $$s^{\star}_{out}(\text{serial}) < s^{\star}_{out}(\text{mono}) < s^{\star}_{out}(\text{parallel})$$
  for any parallel configuration,

- $s_{in} < \bar{s}_{in}$, there exists a parallel configuration s.t.
  $$s^{\star}_{out}(\text{parallel}) < s^{\star}_{out}(\text{mono}) < s^{\star}_{out}(\text{serial})$$
  for any serial configuration.

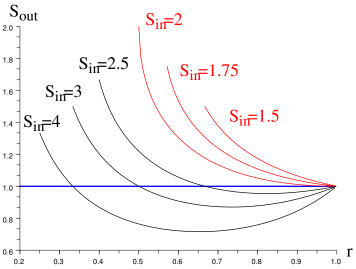
The role of diffusion

Proposition. For any monotonic increasing $\mu(\cdot)$, the parallel configuration satisfies the properties

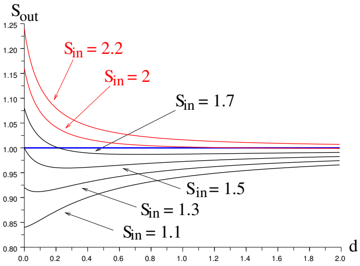
- $s_{in} > \bar{s}_{in}$, the map $d \mapsto s_{out}^{\star}(d)$ is **decreasing**,
- $s_{in} < \bar{s}_{in}$, the map $d \mapsto s_{out}^{\star}(d)$ admits an **unique minimum** for $d^{\star} < +\infty$.

  Furtermore, there exists another threshold $\underline{s}_{in} < \bar{s}_{in}$ s.t. $d^{\star} = 0$ for $s_{in} < \underline{s}_{in}$.

Comparaison of performances



serial



parallel

About the benefit of the buffered chemostat

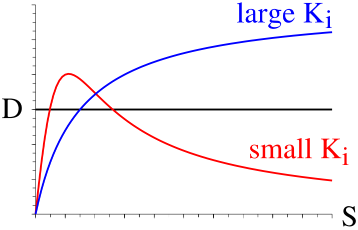
Participants : I. Haidar, J. Harmand, A. Rapaport.

The chemostat with inhibited growth

$$\begin{array}{rcll} \dot{s} & = & -\mu(s)x + D(s_{in} - s) & \text{(substrate concentration)} \\ \dot{x} & = & \mu(s)x - Dx & \text{(biomass concentration)} \end{array}$$

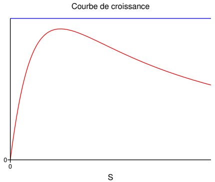
where $\mu(\cdot)$ is an **Haldane** function.

$$\boxed{\mu(s) = \frac{\bar{\mu}s}{K + s + s^2/K_i}}$$



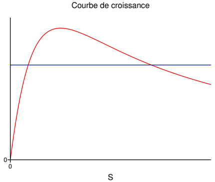
Example : J. F. Andrews, *A mathematical model for the continuous culture of microorganisms utilizing inhibitory substrates*, Biotech. Bioengrg., 10 (1968), pp. 707-723.

Stability analysis for non-monotonic growth



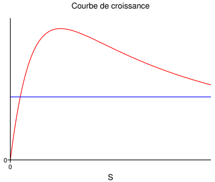
$$D > \max_{s \in [0, S_{in}]} \mu(s)$$

1 equilibrium : wash-out



$$\mu(s_{in}) < D < \max_{s \in [0, S_{in}]} \mu(s)$$

3 equilibria : bi-stability

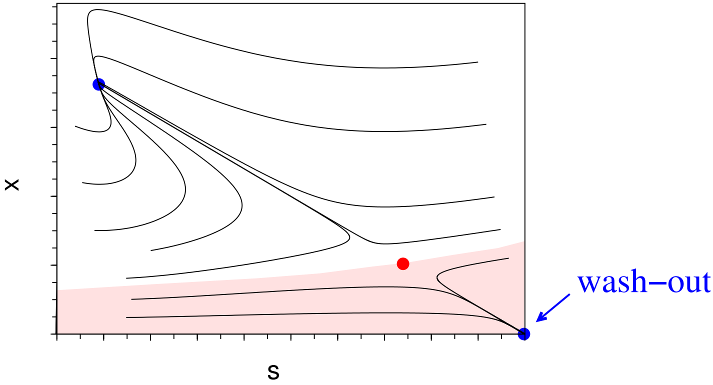


$$D < \mu(s_{in})$$

2 equilibria : stability

The bi-stability case

Under the condition $\mu(s_{in}) < D < \max_{s \in [0, S_{in}]} \mu(s)$



We are looking to ways to eliminate or reduce the attraction basin of the wash-out equilibrium

Solution A : feedback control

Example 1 : linearizing feedback control

$$D(s,x) = \frac{\mu(s)x - \lambda(s - s^\star)}{s_{in} - s}$$

see Bastin Dochain 1986

Example 2 : P.I. controller

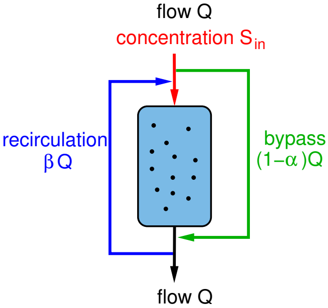
$$D(s) = G_1(s - s^\star) + G_2 \int_0^t (s(\tau) - s^\star) d\tau$$

see Shaum Alvarez Lopez-Arenas 2012

and many other contributors...

Drawback : requires an upstream tank while D is above its nominal value $D^\star$, whose volume can be very large depending on the initial condition...

Solution B : re-circulation loops



D is fixed.

Let $u = \dfrac{\alpha + \beta}{1 + \beta} \in [0, 1]$

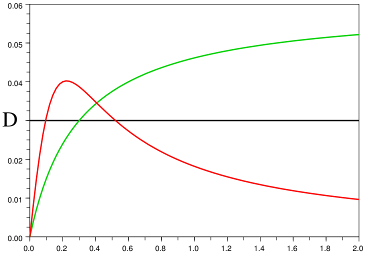
Proposition. See Harmand Mazenc R. 2004

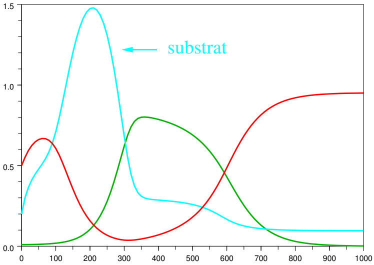
$$u(s) = \left| \begin{array}{l} \min\left(1, \dfrac{\mu(s) - \mu(s^\star) + D}{D}\right) \text{ if } s > s^\star \\ \dfrac{s_{in} - s^\star}{s_{in} - s} \text{ if } s \leq s^\star \end{array} \right.$$

G.A.S. the chemostat about $(s^\star, s_{in} - s^\star)$.

Drawback : In the transient, output s can be above $s^\star$ for a long time...

Solution C : the "bio-control"





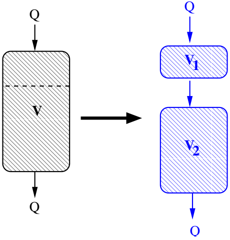
The presence of the "green" species at initial time allows a G.A.S. equilibrium with the "red" species (alone). See Harmand R. 2008.

Drawback : Requires to find and add the "good" species...

The role of spatialisation

Consider V and Q such that $\mu(s_{in}) < \dfrac{Q}{V} < \max\limits_{s \in [0, S_{in}]} \mu(s)$.

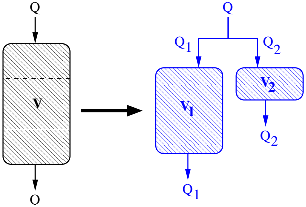
Serial structure with $V = V_1 + V_2$:



$$V_i < V \Rightarrow \frac{Q}{V_i} > \mu(s_{in}) \quad (i = 1, 2)$$

$\Rightarrow$ both wash-out are attractive !

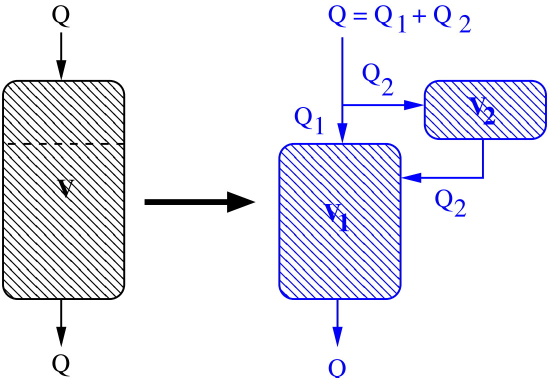
Parallel structure with $V = V_1 + V_2$ and $Q = Q_1 + Q_2$:



$$\frac{Q_i}{V_i} < \frac{Q}{V} \Rightarrow \frac{Q_j}{V_j} > \frac{Q}{V} \quad (i \neq j)$$

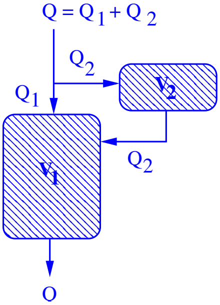
$\Rightarrow$ at least one wash-out is attractive !

Solution D : the "buffered" chemostat



with $\mathbf{V = V_1 + V_2}$

Solution D : the “buffered” chemostat



Two degrees of freedom : (α, r) with

$$\frac{Q_2}{V_2} = \alpha D \text{ and } V_1 = rV$$

- *buffer tank :* the classical chemostat model

$$\Rightarrow \text{unique positive eq. } s_2^\star(\alpha) \text{ if } \alpha D < \mu(s_{in})$$

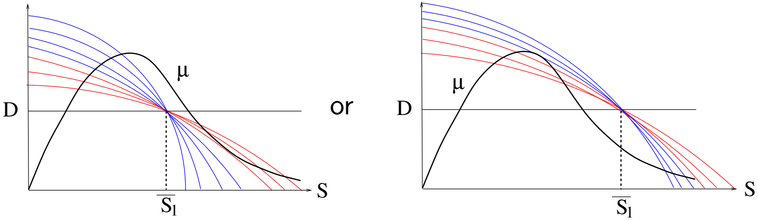
- *main tank :* chemostat with two inputs :

$$\boxed{\mu(s_1^\star) = \frac{D}{r} - \alpha D \left(1 - \frac{1}{r}\right) \frac{s_{in} - s_2^\star(\alpha)}{s_{in} - s_1^\star} = \phi_{\alpha,r}(s_1^\star)}$$

Solution D : the "buffered" chemostat

Proposition. See Haidar R. Harmand 2013
For any $\alpha \in (0, \mu(s_{in})$, there exists $\bar{r}(\alpha) \in (0, 1)$ such that

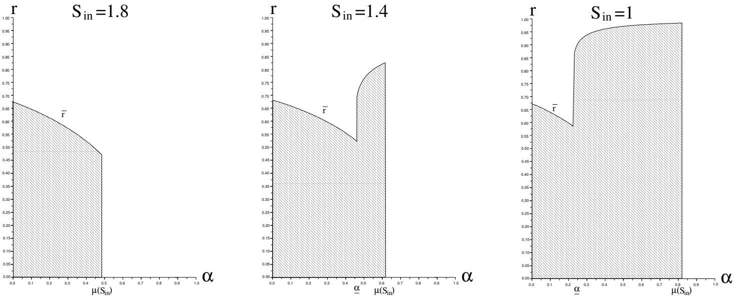
- for any $r < \bar{r}(\alpha)$, the dynamics admits an unique positive equilibrium,
- for any $r > \bar{r}(\alpha)$, the dynamics admits at least three positive equilibrium.



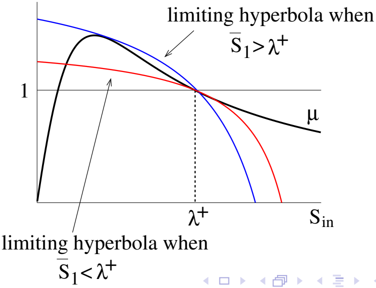
where $\bar{s}_1 = \alpha s_2^\star(\alpha) + (1-\alpha)s_{in}$ fulfills $\boxed{\phi_{\alpha,r}(\bar{s}_1) = 1, \ \forall r}$

The set of G.A.S. configurations

Examples with the Haldane law and $D = 1$:



Limiting cases : $\bar{s}_1 = \lambda^+$



Performances of the "buffered" chemostat

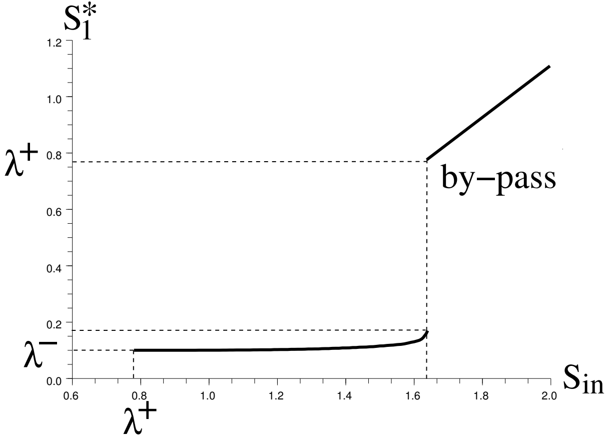
Consider $\boxed{\psi(s) = \mu(s)(S_{in} - s)}$

Let $\psi^\star = \max_{s\in[0,\bar{s}]} \psi(s)$ where $\mu(\bar{s}) = \mu(s_{in})$.
Let $s^\star \in \arg\max \psi^\star$ and define $\alpha^\star = \mu(s^\star)$.

Proposition. See Haidar R. Harmand 2013
The best stable configuration consists in having $\alpha = \alpha^\star$ and

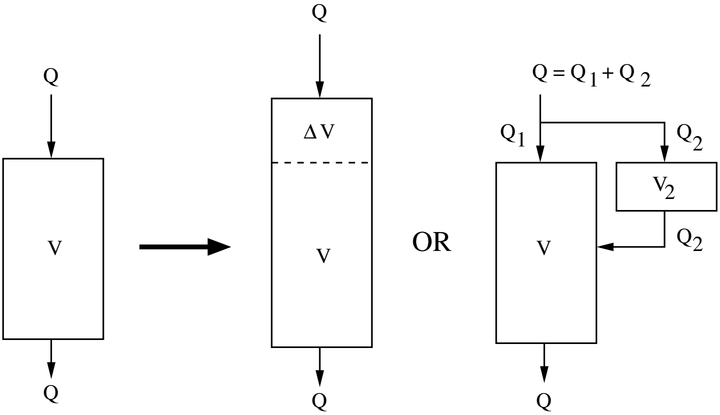
- making a **by-pass** of the volume V with a flow rate equal to $(1 - \alpha^\star)Q$, when $\psi^\star < S_{in} - \lambda_+$.
- choosing any value of $r \in (0, \bar{r}(\alpha^\star))$, when $\psi^\star = S_{in} - \lambda_+$.
- taking r smaller and arbitrarily close to $\bar{r}(\alpha^\star)$, when $\psi^\star > S_{in} - \lambda_+$.

Performances of the “buffered” chemostat



smallest output concentration at steady state
as function of s_{in}

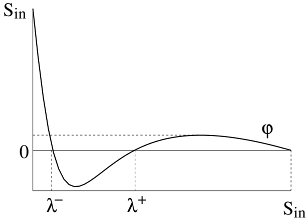
Adding a "buffer"



What is the smallest volume to add to obtain global stability ?

The “buffered” interconnection

Let $\boxed{\varphi(s) = (s_{in} - s)(D - \mu(s))}$

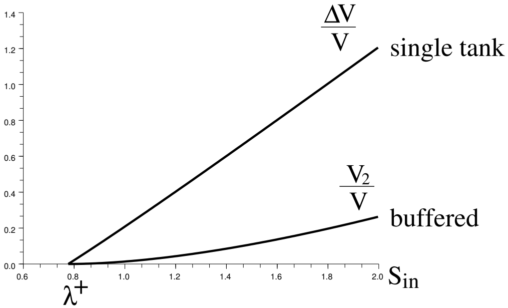


Proposition. See Haidar R. Harmand 2013.
The G.A.S. property is fulfilled for an additional volume such that

$$V_2 > \frac{V}{\psi^\star} \max_{s \in (\lambda^+, S_{in})} \varphi(s)$$

Comparison with a single tank

For a single tank, one should have $\Delta V > V\left(\frac{1}{\mu(s_{in})} - 1\right)$.



Main messages

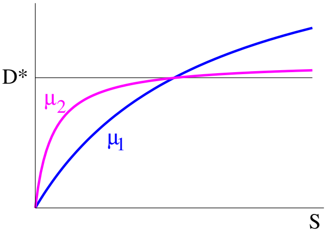
- A buffered interconnection of two volumes can globally stabilize the chemostat, preserving the total volume and input rate (while this is not possible with serial or parallel interconnections).
- We have characterized the set $\mathcal{C}$ of such configurations and among them the one that presents the best conversion.
- The input concentration impacts the shape of $\mathcal{C}$. There exits a threshold above it a by-pass is more efficient.
- The minimum volume to add to a given single tank for obtaining the global stability van be significantly reduced using a “buffered” interconnection.

About niches and overyielding

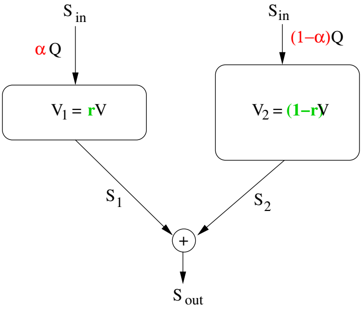
Participants : D. Dochain, P. de Leenheer, A. Rapaport.

Two species two habitats

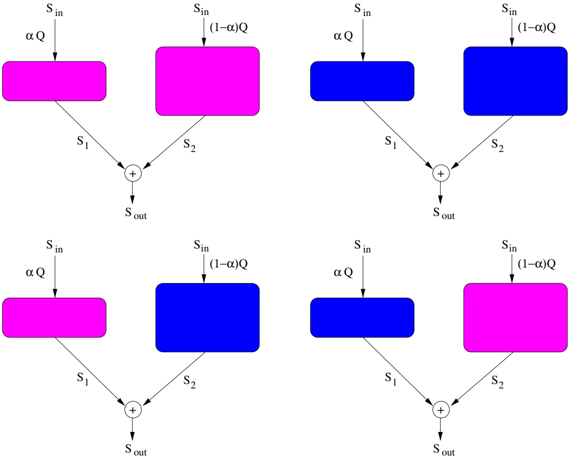
Consider two species



and a spatial structure



Bioconversion overyielding



Which is the best configuration ?

Steady state overyielding

Assumption : $\mu(\cdot)$ is increasing.

$$\text{Let } \lambda(D) = \left| \begin{array}{ll} \mu^{-1}(D) & \text{if } D \leq \mu(s_{in}) \\ s_{in} & \text{if } D > \mu(s_{in}) \end{array} \right.$$

$$\text{Define } \boxed{F(\alpha, r) := \alpha\lambda\left(\frac{\alpha}{r}D\right) + (1-\alpha)\lambda\left(\frac{1-\alpha}{1-r}D\right)}$$

Definition : There is **overyielding** exactly when

$$G(\alpha, r) := \alpha\lambda_1\left(\frac{\alpha}{r}D\right) + (1-\alpha)\lambda_2\left(\frac{1-\alpha}{1-r}D\right) < \min(F_1(\alpha, r), F_2(\alpha, r))$$

Steady state overyielding

$$C = \{(\alpha, r) \in [0,1]^2 \mid (\alpha/r)D \le \mu(s_{in}) \text{ and } ((1-\alpha)/(1-r))\, D \le \mu(s_{in})\}$$

$$T_1 = \{(\alpha, r) \in [0,1]^2 \mid (\alpha/r)D > \mu(s_{in})\}$$

$$T_2 = \{(\alpha, r) \in [0,1]^2 \mid ((1-\alpha)/(1-r))\, D > \mu(s_{in}))\}$$

Proposition. If $\mu(\cdot)$ is concave then the restriction of F on C is convex.

Proposition. Define $T^{in}(D) = \lambda(D) + D\lambda'(D)$. One has

$$\min_{[0,1]^2} F = \left| \begin{array}{l} \lambda(D) = F(\alpha, \alpha),\ \forall \alpha \in [0,1],\ \text{for } s_{in} \ge T^{in}(D) \\ \min_{\alpha} F(\alpha, 0) < \lambda(D),\ \text{for } s_{in} < T^{in}(D) \end{array} \right.$$

Steady state overyielding

Assume that there exists $D^\star$ such that $\lambda_1(D^\star) = \lambda_2(D^\star)$.

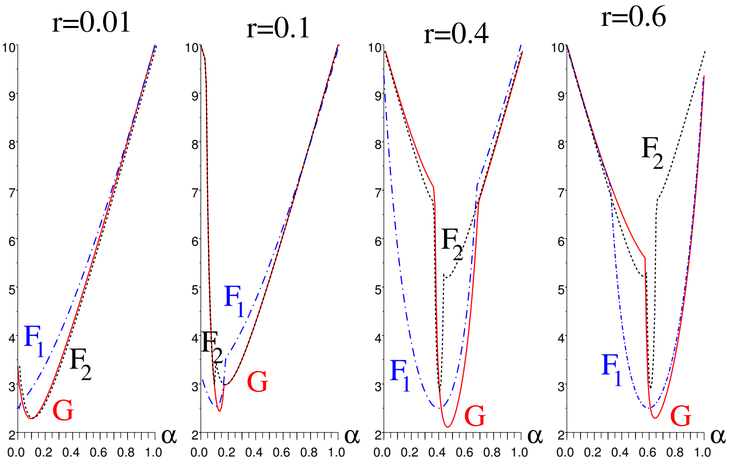
Proposition. When $D = D^\star$ and $\alpha \in (0,1)$, there exist configurations close to (α, α) that present overyielding.

Proposition. When $D \neq D^\star$, there exists (α, r) with

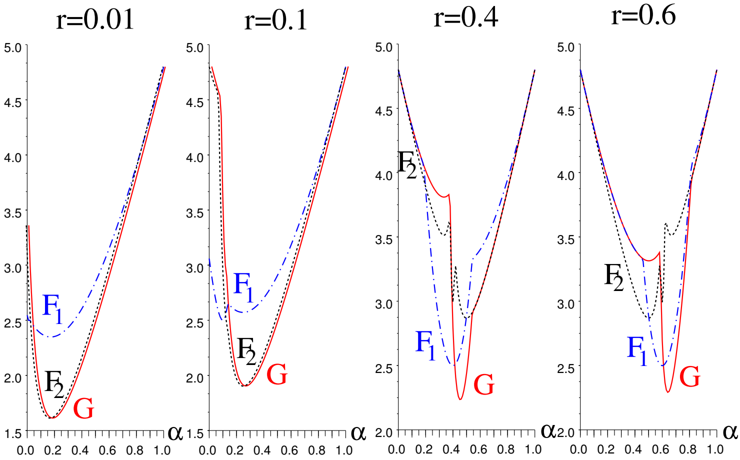
$$\frac{\alpha}{r} D < D^\star < \frac{1-\alpha}{1-r} D < \min(\mu_1(s_{in}), \mu_2(s_{in}))$$

that corresponds to overyelding.

Example (large s_{in})



Example (small s_{in})



Waste water treatment in natural environments

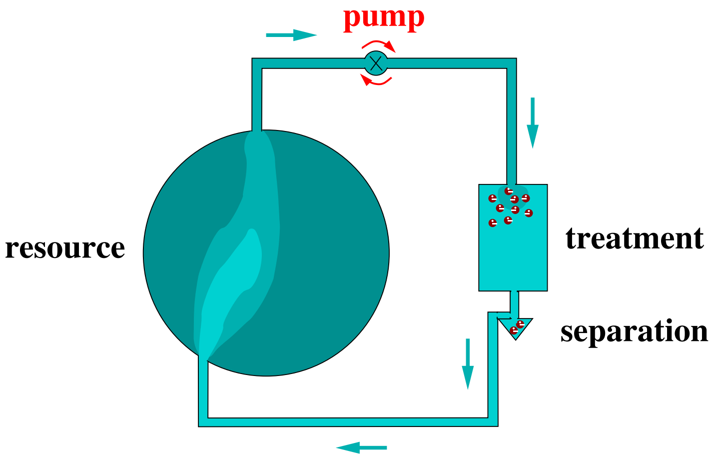
Participants : P. Gajardo, J. Harmand, A. Rapaport, H. Ramirez, V. Riquelme, A. Rousseau.

Industrial or municipal waste treatment

waste

discharge

Closed circuit treatment

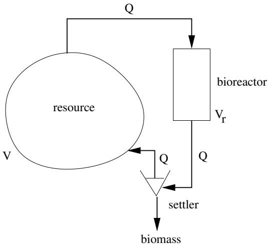


The control problem

Objective : clean up in minimal time .

- which information on the parameters of the model are useful for reaching the target in minimal time ?
- could it be better operating a non-constant flow Q ?
- which variable(s) have to be measured on-line ?
- what is the influence of an **inhomogeneity** of the substrate concentration of the resource ?

The homogeneous case



$$
\begin{aligned}
\dot{S} &= \frac{Q}{V}(S_r - S) \\
\dot{S}_r &= -\mu(S_r)X_r + \frac{Q}{V_r}(S - S_r) \\
\dot{X}_r &= \mu(S_r)X_r - \frac{Q}{V_r}X_r
\end{aligned}
$$

Target : $S \leq \underline{S}$

Hypotheses : $V >> V_r$, $\mu(\cdot)$ increasing concave.

Slow-fast approximation :

$$\boxed{\mu(S_r(Q)) = \frac{Q}{V_r}} \quad \Rightarrow \quad \boxed{\dot{S} = \frac{Q}{V}(S_r(Q) - S)}$$

Optimization among feedbacks

Proposition. $Q^{opt}(S) = V_r \mu(S_r^{opt}(S))$ is an optimal feedback with

$$S_r^{opt}(S) \in \arg \max_{S_r \in (0,S)} \mu(S_r)(S - S_r)$$

- $\mu(\cdot)$ linear,

$$\boxed{S_r^{opt}(S) = \frac{S}{2}}$$

- $\mu(\cdot)$ Monod : $\mu(s) = \mu_{\max} \dfrac{s}{K + s}$

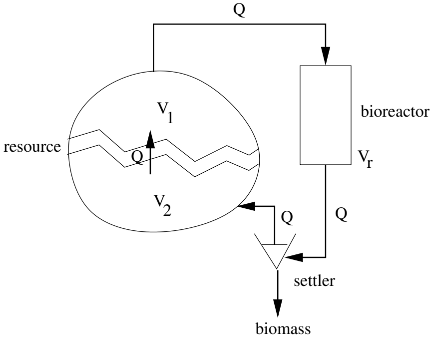
$$\boxed{S_r^{opt}(S) = \sqrt{K^2 + KS} - K} \, .$$

Numerical simulations

$\mu_{\max}$	K	V	V_r	$S(0)$
1.0	1.0	1000	1	1

$\underline{S}$	$T_f^\star$	T_{opt}	gain
0.5	5420	5293	1.9%
0.4	8064	7719	3.7%
0.3	12499	11606	7.2%
0.2	21663	19062	12%
0.1	51626	40425	22%

Modelling the inhomogeneity



with $V = V_1 + V_2$
$p = V_1 / V_l$

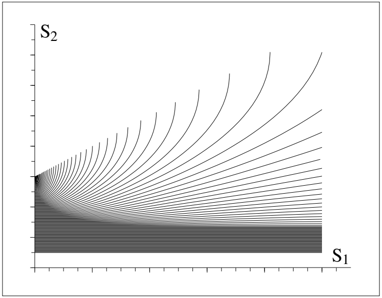
$$\begin{cases} \dot{S}_1 & = & \dfrac{Q}{V_1}(S_2 - S_1) = \mu(S_r)\dfrac{V_r}{V_1}(S_2 - S_1) \\ \dot{S}_2 & = & \dfrac{Q}{V_2}(S_r(Q) - S_2) = \mu(S_r)\dfrac{V_r}{V_2}(S_r - S_2) \end{cases}$$

$\mathcal{D} = \{(S_1, S_2) \in \mathbb{R}_+^2 \mid S_1 \geq S_2\}$ is invariant.

Optimization among feedbacks

Proposition. For any initial condition in $\mathcal{D}$, the optimal policy Q^{opt} consists in two steps :

1. (possibly void) a non constant feedback until S_2 reaches a value $\underline{S}_2 < \underline{S}_l$,
2. a constant control $Q^{opt} = V_r\mu(\underline{S}_2)$ until S_1 reaches $\underline{S}$.



Field of extremals

Numerical simulations

	$p=0$	$p=0.2$			$p=0.5$		
$\underline{S}$	$T_f^\star$	$T_f^\star$	T_{opt}	%	$T_f^\star$	T_{opt}	%
0.7	2387	2708	2661	1.7	2931	2881	1.7
0.6	3660	3816	3756	1.6	3993	3951	1.1
0.5	5420	5325	5194	2.5	5385	5317	1.2
0.4	8064	7567	7329	3.2	7395	7250	2.0
0.3	12499	11338	10754	5.4	10696	10320	3.6
0.2	21663	19137	17297	11	17389	16 180	7.4

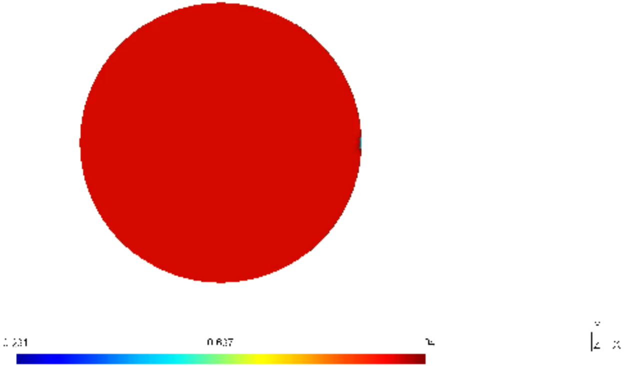
Facing realistic simulations

$$\boxed{\begin{array}{l} u_t + u.\nabla u - \nu_u \Delta u + \nabla p = 0 \\ \nabla . u = 0 \\ S_t + u \nabla S - \nu_S \Delta S = 0 \end{array}}$$

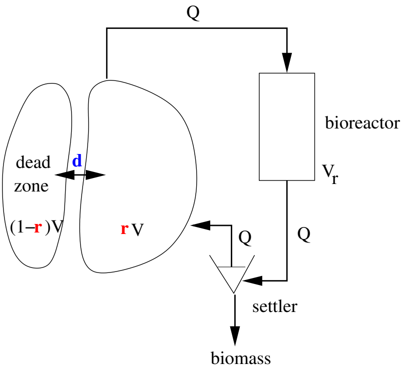
Boundary of the domain : $\Gamma = \Gamma_0 \cup \Gamma_{in} \cup \Gamma_{out}$

$$\begin{array}{lll} u = 0, & & x \in \Gamma_0 \\ u.n = Qf(x), & u.\tau = 0, & x \in \Gamma_{in} \cup \Gamma_{out} \\ \frac{\partial S}{\partial n} = 0, & & x \in \Gamma_0 \cup \Gamma_{out} \\ S = S_r(Q), & & x \in \Gamma_{in} \end{array}$$

Numerical simulation

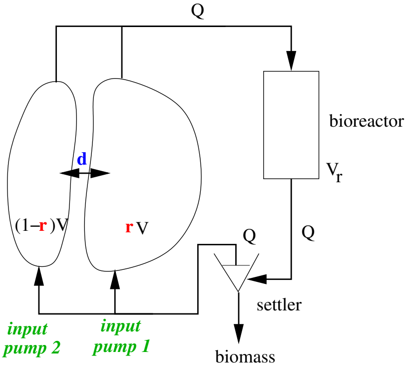


Consideration of a dead zone



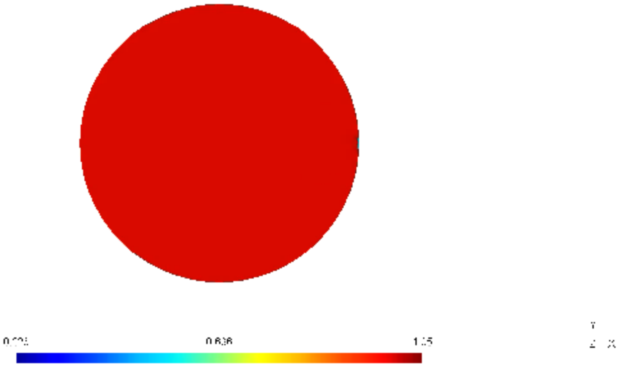
Proposition The same feedback as without dead zone is optimal, whatever are parameters r and d.

Multi-input pumps consideration

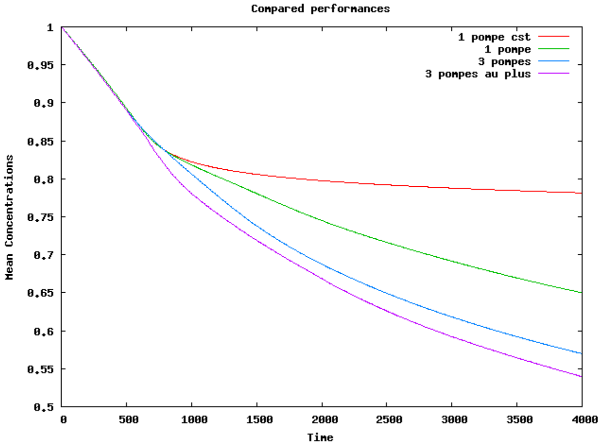


Proposition The optimal strategy consists in reaching $S_1 = S_2$ with only one input pump, and then to stay on the *singular arc* $S_1 = S_2$ using the two input pumps.

Multi-ouput pumps simulation



Numerical comparison



Main messages

- A feedback strategy can significantly improve the total duration of treatment,
- A resource with an inhomogeneous concentration reduces the treatment duration under large concentrations,
- One needs to know the shape of the growth function to choose optimally the feedback.