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Antoine Rousseau, Alain Rapaport

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Reduced Models (and control) of in-situ decontamination of large water resources

Antoine ROUSSEAU,
Inria, Team LEMON (Montpellier)

In honor of my "brother in sciences" Claudius

June 9th, 2017, SFC2MAC, Xiamen

Joint work with Alain Rapaport (INRA)
Outline

1. Introduction: the Taihu problem
2. A simple ODE model
3. A PDE-based model for the lake
4. Back to ODEs
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**Applicative Framework**

Polluted Taihu (algae), Yangtze Delta plain, Wuxi, China.

**Objectives:**
- use a bioreactor to remove pollution from the lake
- do it as efficiently as possible
Bioremediation problem

Parameters and unknowns

- $V_L$ and $V_R$ the volumes of the resource and bioreactor,
- $X_R$ the biomass concentration in the bioreactor,
- $S_L$ and $S_R$ the pollutant concentrations,
- $\mu(\cdot)$ the biomass growth law,
- $Q = Q(t)$ the pump discharge, controlled by the user.
1. Introduction: the Taihu problem
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ODE-based model: the homogeneous case \( S_L = S_L(t) \)

\[
\begin{aligned}
\dot{X}_R &= \mu(S_R) X_R - \frac{Q}{V_R} X_R, \\
\dot{S}_R &= -\mu(S_R) X_R + \frac{Q}{V_R} (S_L - S_R), \\
\dot{S}_L &= \frac{Q}{V_L} (S_R - S_L),
\end{aligned}
\]
ODE-based model: the homogeneous case $S_L = S_L(t)$

\[
\begin{align*}
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\end{align*}
\]

Chemostat equations: J. Monod (1910-1976)
ODE-based model: the homogeneous case $S_L = S_L(t)$

\[
\begin{align*}
\dot{X}_R & = \mu(S_R) X_R - \frac{Q}{V_R} X_R, \\
\dot{S}_R & = -\mu(S_R) X_R + \frac{Q}{V_R} (S_L - S_R), \\
\dot{S}_L & = \frac{Q}{V_L} (S_R^\infty - S_L),
\end{align*}
\]

Slow-fast approximation:

\[\varepsilon = \frac{V_R}{V_L} \ll 1\]

ODE-based model: the homogeneous case $S_L = S_L(t)$

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\end{align*}
\]

Slow-fast approximation:
\[
\varepsilon = \frac{V_R}{V_L} \ll 1
\]


Theorem (case $\mu(X) = \mu X$)

For any $X_R(0) > 0$ and $S_R(0) = S_L > 0$, our system has a unique global solution. In addition, there exists a critical flow rate $Q_c > 0$, depending on $S_L$, such that asymptotically:

- if $Q > Q_c$, then $(S_R(s), X_R(s))$ converges towards $(S_L, 0)$,
- if $0 < Q < Q_c$, then $(S_R(s), X_R(s))$ converges towards $(S_R^\infty, X_R^\infty)$ with $S_R^\infty = \frac{Q}{\mu V_R} < S_L$. 

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Decontamination of large water resources
SFC2MAC, Xiamen
Optimal flow rate for the bioremediation (linear $\mu$)

Back to the lake equations...

$$\dot{S}_L = \frac{Q}{V_L} \left( \frac{Q}{\mu V_R} - S_L \right),$$

What is the best flow rate $Q$?
Optimal flow rate for the bioremediation (linear $\mu$)

Back to the lake equations...

$$\dot{S}_L = \frac{Q}{V_L} \left( \frac{Q}{\mu V_R} - S_L \right),$$

What is the best flow rate $Q$?

$$Q(t) = \frac{\mu V_R}{2} S_L(t)$$
Optimal flow rate for the bioremediation (linear $\mu$)

Back to the lake equations...

$$\dot{S}_L = \frac{Q}{V_L} \left( \frac{Q}{\mu V_R} - S_L \right),$$

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The non-homogeneous case: 

\[ S_L = S_L(t, x, y) \]

Navier Stokes & transport equations in the resource

\[
\begin{align*}
\frac{\partial u}{\partial t} + u \cdot \nabla u - \nu_u \Delta u + \nabla p &= 0, \\
\nabla \cdot u &= 0,
\end{align*}
\]

Boundary conditions

\[
\begin{align*}
\frac{\partial S_L}{\partial t} + u \cdot \nabla S_L - \nu_S \Delta S_L &= 0.
\end{align*}
\]

\[
\begin{align*}
u_{in}(t) &= A \times Q(t), \\
u_{out}(t) &= A \times Q(t), \\
B.C \text{ on } S_L
\end{align*}
\]
Simulations

Circular lake : 1 pump
Comparing models

Pollution concentration in the lake with ODE (black) and PDE (red)
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Active and dead zones model

New ODE model

\[
\begin{align*}
\dot{X} &= \mu(S_R)X - \frac{Q}{V_R}X, \\
\dot{S}_R &= -\mu(S_R)X + \frac{Q}{V_R}(S_1 - S_R), \\
\dot{S}_1 &= \frac{Q}{V_1}(S_R - S_1) + \frac{d}{V_1}(S_2 - S_1), \\
\dot{S}_2 &= \frac{d}{V_2}(S_1 - S_2).
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\end{align*}
\]

Existence, uniqueness, optimal control for two zones


Two parameters we can play with: \( \frac{V_1}{V_1 + V_2} \) and \( d \).
Comparing models (with A. Rapaport and S. Barbier)

Optimization on the parameters \( \frac{V_1}{V_1 + V_2} \) and \( d \)

Pollution concentration in the lake
1 ODE (black)
2 ODEs (blue)
PDE (red)

Best parameter \( d \) vs viscosity \( \nu_S \) (dashed blue)
Best meansquare fit (plain red)
In summary...

\[ d = 0, \ r = 1 \]

\[ V \gg V_R \]

H1

H2, H3
Conclusion

The “take home” message is...

- we have designed a first model and questioned it,
- we proposed a more complicated (too much ?) one,
- we took an intermediary model, which seems satisfactory, on which optimal control can be done.

BUT: is the reference (PDE) model a realistic model? Certainly not...
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*Sino-French project ANSWER:*

Analysis and Numerical Simulation of Water Ecosystems in Response to anthropogenic environmental changes
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*The more we fail, the more chances we have to succeed*
Thank you for your attention

A few references...

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