INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

# *Team MERE*

# *Modelling and Water Ressources*

*Sophia Antipolis*

THEME BIO

Activity Report

2004

# Table of contents

# 1. Team

*MERE is a joint research team INRIA and INRA (UMR Analyse des Systèmes et Biométrie, Montpellier, France).*

**Head of project-team**

Claude Lobry [Université de Nice, INRIA Sophia Antipolis]

**Administrative assistant**

Catherine Martin [AI, part time]

**Staff member INRIA**

Frédéric Mazenc [CR1, INRIA Sophia-Antipolis]

**Staff member INRA**

Jérôme Harmand [CR1, half time, Laboratoire de Biotechnolgie de l'Environnement, Narbonne]
Patrice Loisel [CR1, half time, Laboratoire d'Analyse des Systèmes et Biométrie, Montpellier]
Alain Rapaport [CR1, half time, Laboratoire d'Analyse des Systèmes et Biométrie, Montpellier]

**Ph. D. student**

Abdou Khadry Dramé [allocataire AUF]
Djalel Mazouni [boursier projet EOLI]

# 2. Overall Objectives

Biological WasteWater Treatment Plants (WWTP) are used to transform organic compounds present in wastewaters in soluble form (also called substrates) into solids (micro-organisms or biomass also called sludge). In more general terms, such a system where a micro-organism is used to transform substrates into others is called a bioreactor. In the context of wastewater treatment, substrates are consumed by the biomasses under adequate environmental conditions. Once the substrate concentrations have reached normative constraints, the solids (the biomass) and the clean water are separated: the liquid is rejected to the natural environment while the sludge is either incinerated, used in agriculture or, until recently, stored in wetlands. The treatment industry can be considered as the first industry in terms of matter to be processed. Therefore, the design, the control and in more general terms, the optimization of treatment processes are real challenges. Our objective is to better understand these processes in order to optimize their functioning in the presence of uncertainty and of unknown and unmeasured external disturbances. To do so,

1. we approach the problems at two levels: the microscopical scale (the micro-organism) and the macroscopical one (the plant),
2. we use macroscopical modeling and control system science tools to develop new design rules, estimation techniques and control systems that we calibrate on real biological pilot plants.

Our methodology consists in the development of mathematical models of the biological reactions and transports in the reactor. At this stage, we have very strong interactions with micro-biologists. After that we analyze the model with the available mathematical tools or/and through computer simulations. Our main emphasis is put on the effects of the spatial distribution of the biomass. This questioning can be understood at various scales.

- At the macroscopic level we compare the performances of various designs, from infinitely stirred reactors to purely non mixed reactors through cascade of reactors.
- At the microscopic level we are interested in the growth process of the biomass, limitations caused by the diffusion of the substrate, the role of the biofilms.

We are interested in fundamental questions of microbial ecology, like biodiversity of biomasses, competition and predation since they are at the roots of the understanding of biological wastewater treatment and, at the same time we address very practical questions like the minimization of the size of the bioreactors.

# 3. Scientific Foundations

**Keywords:** *control systems*, *ecology*, *environment*, *mathematical modeling*, *observers*, *process engineering*.

The chemostat is a laboratory device which goes back to the second world war, with the work of Monod and Szilard. It is used to study the growth of micro-organisms. The principle is simple: a continuous flow rate through a constant volume reactor provides nutrients to a population or a community of micro-organisms. At equilibrium the growth-rate must equal the artificial mortality induced by the outflow of the reactor. A simple model, for the case where the reactor is perfectly stirred, is given by a set of two differential equations, one for the variations of the nutrient concentration, the other one for the biomass concentration. This model is based on the classical law of mass action used in the modeling of chemical kinetics: the rate of a reaction is proportional to the product of the concentrations of the two reactants. In the case of population growth this means that the growth-rate of a population depends of the nutrient concentration. This system of two equations has been perfectly well understood for more than half a century.

The chemostat model is a good first approximation of the running of a wastewater treatment plant. From this simple model one can rdevelop models which incorporate more realistic assumptions like:

- Existence of a complicated trophic chain in the digestion process.
- Consideration of non perfect mixing inducing diffusion processes,
- Consideration of mass transport in plug-flow reactors,
- Parallel or cascade connections of reactors,
- Re-circulation of the biomass,

which lead to complicated systems of coupled partial differential equations of transport-diffusion type. Due to the presence of non monotonic kinetics the theory of equations of this type is not yet perfectly understood. Determination of stable stationary solutions is often a question of current research and numerical simulations are used. Moreover the control of industrial plants addresses new questions in the domain of robust control and observers.

Since a Waste Water plant is a microbial ecosystem, microbial ecology is fundamental for the understanding of our processes. An ecosystem is a system in which various populations of different species are interacting between them and reacting to the environmental abiotic parameters. Concepts of competition, predation, symbiosis are used to describe these interactions and try to understand important questions like the biodiversity and the productivity of the ecosystem. The biodiversity is the number of species which is supported by the ecosystem and the productivity measures the rate at which abiotic resources are transformed into biomass. An old prediction of theoretical population models says that, in a constant environment, an ecosystem with $n$ different kinds of resources can support at most $n$ different species (different means that the ways two species use resources are different). This prediction is not realized in wastewater treatment plants where it was demonstrated, using tools of molecular biology (SSCP), that a small number of resources (maintened at a constant level) are able to maintain a huge number of species. This shows that the classical model of the perfectly stirred reactor is no longer valid if one wants to model the biodiversity in the reactor. We explore alternative models based on the consideration of growth-rates which are not solely nutrient-dependent, but are also density-dependent, which means that the growth-rate decreases with the density of the biomass. A special case of density-dependence is the ratio dependence which was much discussed recently.

Since a density-dependent model is a macroscopic model, it is important to understand how the density-dependence is a consequence of the microscopic behaviors of individuals. Since direct observation of the behavior of bacteria is difficult, mathematical modeling is of great help. The hypotheses, at the microscopic level, are expressed in terms of partial differential equations or in terms of individually based models so that macroscopic consequences are derived, either by using mathematical reasonings or computer simulations. Mathematical modeling also helps designing experiments which could validate hypotheses.

# 4. Application Domains

### *4.1.1. Design of Wastewater treatment plants*

The question of the optimal design of chemical or biochemical systems has been assessed by several authors during the last thirty years. An important effort has been made by the chemical engineering community to synthesize plants with the smallest possible volume in order to minimize the investment cost. This task turns out to be much more complex in the case of biological systems. One reason for that is the difficulty of finding simple and yet accurate models to represent all the important dynamics of living organisms interacting in a bio-system.

A plant that is made of a cascade of homogeneous Continuous Stirred Tank Reactors (CSTR or chemostats) has a particular practical interest: in most cases, it allows to approximate the behavior of diffusive systems (also called Plug Flow Reactors or PFR) which usually exhibit better performances than a single CSTR. In other terms, a given conversion rate can be obtained with a PFR of smaller volume than with a CSTR of identical volume. However, a PFR is very difficult to operate in practice while CSTR operability and reliability are better.

Biological processes can usually be classified into two classes of systems: micro-biological and enzymatic reactions. In simple terms, micro-biological-based reactions define (bio)reactions where a substrate degradation is associated with the growth of certain organisms while the second, the enzymatic reaction, may be viewed as a chemical reaction with specific kinetic functions.

Given a model of a series of CSTRs, representing either enzyme or micro-biological reactions, and a flow rate to be treated, the problem of determining optimal conditions for steady-state operation has been studied. In particular, conditions have been proposed to minimize the Total Retention Time (TRT) required to attain a given conversion rate $1 - S_N/S_0$ (here $S_0$ and $S_N$ denote respectively the input and output substrate concentrations), or equivalently to minimize the total volume of the plant given that the flow rate to be treated is constant.

### *4.1.2. Observation and control of wastewater treatment plants*

Control problems frequently arise in the context of the study of biological systems such as wastewater treatment plants. In general, in order to cope with disturbances, modeling errors or uncertainty of parameters, one has to take advantage of robust nonlinear control design results. These results are based on central theories of modern non-linear control analysis, like for instance those based on the input-to-state stable (ISS) notion and the backstepping and the forwarding techniques. Observe that most of these results are based on the construction of families of Control Lyapunov Functions.

Waste water treatments plants are often unstable as soon as bacteria growths exhibit some inhibition. Typically, under a constant feed rate, the wash-out of the reactor (i.e. when biomass is no longer present) becomes an attracting but undesirable equilibrium point. Choosing the dilution rate as the manipulated input is usually a mean for the stabilization about a desired a set point, but the most efficient control laws often require a perfect knowledge of the state variables of the system, namely the online measurement of all the concentrations, which are generally not accessible (for technical or economical reasons). Most often, only a few sensors are available.

A popular way to achieve stabilization of a control dynamical system under partial knowledge of the state is to first design an “observer” or “software sensor” for the reconstruction of the unobserved variables, and then to couple this estimate with a stabilizing feedback control law, if some “separation principle” is satisfied. Unfortunately, in industrial operating conditions, one cannot thoroughly trust the models that were developed and identified in well controlled environments such as in laboratory experiments. Engineers have to deal with several uncertainties on parts of the model, as well as on the output delivered by the sensors. During the initialization stage or hitches on the process, the system can be far away from the nominal state, where few empirical data are available. Generally, probabilistic hypotheses cannot be justified regarding the nature of the uncertainty for stochastic models to be considered. On the opposite, reasonable bounds on the unknown parts of the models are available, so that uncertainties can be considered as unknown deterministic inputs.

Consequently, robust observers and control laws need to be developed to cope with the particularities of the uncertainty on the models.

#### *4.1.3. Interpretation of SSCP profiles*

The SSCP (Single Strand Conformation Polymorphism) is a molecular analysis technique which allows us to estimate the relative abundance of a given species in a complex ecosystem at a given time $t$. The result of this analysis is delivered under the form of a graphic in which the x-axis is related to the species while the y-axis gives the relative abundance of the corresponding species. Ideally, under the assumption that two different species do not respond on the same abscissa, a SSCP spectrum would be a succession of rays, the heights of which would correspond to the abundances of these species. From a technical point of view, the method is based on the fact that regions of the DNA remain unchanged during the cellular division, or at least that the variation rate of these regions is very low. Thus, these regions (called 16S) are assumed to be constant and have been designated as being a real signature for a given species. Being able to detect, to mark and to specifically amplify these regions using the PCR (Polymerase Chain Reaction) technique, it has become possible - for about ten years now - to specify "who is there?" in a complex microbial ecosystem. After the PCR, in adequate conditions, the RNA strands are separated on a gel by electrophoresis. The size of the strands and their spatial conformations allow them to be discriminated with respect to the time it takes for each of them to reach a laser detector, the intensity of which depends on the actual quantity of strands (it gives the relative abundance of the corresponding species). Because the detector is not perfect and because the strands of a given species do not move exactly together, the result is not a succession of rays but rather the sum of individual Gaussian-like curves. Furthermore, a real microbial ecosystem may comprise hundreds of species and it is expected that a number of DNA16S strands almost respond at the same time (and thus are very close in the x-axis of the SSCP spectrum). These facts introduce an important uncertainty about the analysis of such signals.

Until now, the micro-biologists analyze their SSCP profile in the following way. Usually, they empirically identify the visible peaks as being the responses of species which are major quantities in the ecosystem. The height of the peak is used as a measure of its relative abundance into the ecosystem. However, with respect to the uncertainty sources described above, it is straightforward to see that the picture cannot be considered as so simple. For instance, imagine that two species respond on the same x-axis: only one peak (the sum of all DNA16S detected at a given instant by the detector) will be visible on the spectrum and it will be concluded that one species is present at an abundance that is directly related to the magnitude of the peak while, in reality, this peak is due to two (or why not even to a greater number) species. And indeed, our preliminary works show that the results given by these molecular techniques under the form of spectra must be carefully analyzed in order not to establish bad conclusions. Our objective is to better understand what exactly happens during the analysis in order to identify, characterize and extract the correct information given by this technique.

#### *4.1.4. Experimentation in ecology*

Mathematics and simulations show that substrate dependent models of competition and density-dependent models have radically different predictions in terms of extinction of species. A substrate dependent model is likely to be a reasonably good model for the case of low densities of biomass, the density-dependent model being a good one for high densities. The mathematical treatment on realistic parameters predicts outcomes which are to be tested. In connection with biologists (J.-J. Godon from LBE and R. Arditi from INAPG) we are currently working on this subject.

# 5. Software

We produce our own softwares for the simulations we are currently doing. These softwares are, most of the time, uniquely designed for research purposes. However it might sometimes happen that some software has some wider interest. In that case we try to design it in such a way that it is useful for a larger community.

# 6. New Results

## 6.1.1. Theoretical results

### 6.1.1.1. Asymptotic behavior of reaction diffusion-transport equation

**Participants:** Abdou Khadry Dramé, Claude Lobry, Frédéric Mazenc, Alain Rapaport.

We consider the system of two partial differential equations with boundary conditions of Robin type

$$
\begin{aligned}
&\frac{\partial S}{\partial t} = -\frac{q}{\sigma(z)}\frac{\partial S}{\partial z} + d\frac{\partial^2 S}{\partial z^2} - \mu(S)X \\
&\frac{\partial X}{\partial t} = -\frac{q}{\sigma(z)}\frac{\partial X}{\partial z} + d\frac{\partial^2 X}{\partial z^2} + \mu(S)X \\
&d\frac{\partial S}{\partial z}(t,0) = \frac{q}{\sigma(0)}(S(t,0) - S_{in}), \quad d\frac{\partial S}{\partial z}(t,l) = 0 \\
&d\frac{\partial X}{\partial z}(t,0) = \frac{q}{\sigma(0)}(X(t,0) - X_{in}), \quad d\frac{\partial X}{\partial z}(t,l) = 0
\end{aligned}
$$

which models a single biomass growing in a bioreactor which is not well stirred. The growth-rate $\mu(S)$ is supposed to be positive, non monotonic (increasing, having a maximum, decreasing). Our purpose is to first determine equilibria and next to analyze their stability properties. Since the T.P.B.V.P. is in four dimensions and its study is not an easy task, we reduce the problem by the following trick. Consider the quantity $U(t,z) = X(t,z) + S(t,z)$. It is trivial to show that it tends to $M = X_{in} + S_{in}$. Replacing $X$ by $U$-$S$ we get:

$$
\begin{aligned}
&\frac{\partial S}{\partial t} = -\frac{q}{\sigma(z)}\frac{\partial S}{\partial z} + d\frac{\partial^2 S}{\partial z^2} - \mu(S)(U(t) - S) \\
&d\frac{\partial S}{\partial z}(t,0) = \frac{q}{\sigma(0)}(S(t,0) - S_{in}), \quad d\frac{\partial S}{\partial z}(t,l) = 0
\end{aligned}
$$

which is an asymptotically autonomous equation. We prove [14] that its asymptotic behavior is the same as the one of the limiting system. This last one is a one dimensional equation for which the T.P.B.V.P. is solved using asymptotic methods and computer simulations, for small and large values of $d$ (that correspond to the models, respectively, of flow plug and perfectly stirred reactors).

$$
\begin{aligned}
&\frac{\partial S}{\partial t} = -\frac{q}{\sigma(z)}\frac{\partial S}{\partial z} + d\frac{\partial^2 S}{\partial z^2} - \mu(S)(M - S) \\
&d\frac{\partial S}{\partial z}(t,0) = \frac{q}{\sigma(0)}(S(t,0) - S_{in}), \quad d\frac{\partial S}{\partial z}(t,l) = 0
\end{aligned}
$$

In a work in progress we prove that, under a mild condition on the growth-rate, there exist at most two stable and one unstable solutions.

### 6.1.1.2. Multiple steady state solutions for a cascade of well stirred reactors with non monotonic growth-rate

**Participants:** Abdou Khadry Dramé, Claude Lobry, Frédéric Mazenc, Alain Rapaport.

We prove [15] that a cascade of well stirred reactors with non monotonic growth-rate may present a complex set of stable equilibria which join together in a unique equilibrium when the number of reactors tends to the infinity. The proof is very simple but uses a graphical representation which is not usual. The result is qualitative in the sense that it does not only apply in the case when the growth-rate admits a specific form but also for general non monotonic growth-rates.

### 6.1.1.3. Interconnection of bioreactors

**Participants:** Abdou Khadry Dramé, Claude Lobry, Jérôme Harmand, Alain Rapaport.

Whatever the reason for which it is desirable to optimize a biological process, very few studies related to the design and the control of interconnected biosystems can be found in the literature. Yet, it is particularly important to deal with this problem in the field of WWTP since any treatment process is precisely composed of a number of different tanks connected together by the way of pipes, valves and pumps.

As already mentioned, a cascade of chemostats presents a number of practical interests:

- Non homogeneous systems (also called tubular or plug flow reactors) may exhibit better performances than homogeneous ones. However, operating a real plug flow system is almost impossible in practice. In such a case, the use of a cascade of homogeneous reactors allows us, in adequate conditions, to approximate the behavior of the plug flow system.
- The presence of a gaseous phase usually increases the homogeneity of the mixed liquid. Again, separating the reaction scheme between several reactors can be useful to overcome this problem.
- When operating a tubular reactor, a continuous biomass sow is necessary in order to initiate the biological reaction at the entrance of the process. In others terms, it is necessary to have some biomass in the input flow rate. The use of a recirculation can be appropriate. However, again, very few studies have studied the influence of a recirculation loop on a biological system.

As a consequence, the study of interconnected biological systems is of particular theoretical as well as of practical importance.

In the project, we have more particularly studied mono-fed and multi-fed cascades of homogeneous bioreactors for which we have analyzed the role of the recirculation on the performances of the system. These studies have led to the proposition of an equivalence principle: conditions have been derived under which there exists an infinity of equivalent systems (of identical volumes) and that only differ from the way they are fed and by the way they are connected together via a recirculation loop.

Finally, let us mention that the stability of interconnected nonlinear systems can be guaranteed with the help of small-gain theorems, for which an extension has been proposed [27].

#### 6.1.1.4. Robust observers and control

**Participants:** Frédéric Mazenc, Alain Rapaport.

Even in the case of perfectly known observable models, the theory of observation of nonlinear systems and synthesis of nonlinear observers presents some technicalities for its application to biological systems (see for instance the contribution [31]).

Nevertheless, our main interest is the study of un-observable models in presence of unknown inputs, that is to say when the collected information facing the uncertainty is not rich enough for an univalued state reconstruction. We have developed a method for set membership reconstructions, with the help of "intervals observers" [13][30]. The spirit of our approach can be summarized as follows.

| guaranteed intervals |
| --- |
| for the unknown inputs |
| and measures |

$$\Longrightarrow$$

| guaranteed intervals |
| --- |
| for the state variables |

More precisely, for models of the form

$$\dot{x} = f(t, x, u, w(t)), \qquad x(0) = x_0 \tag{1}$$

(where $u$ is the input and $w(t)$ the unknown input) along with observation vectors $y^-(\dot{})$, $y^+(\dot{})$ such that

$$h(t, x(t), u(t), w(t)) \in [y^-(t), y^+(t)], \qquad \forall t \geq t_0,$$

for a given observation model $h(\dot{})$, we design two coupled estimators (instead of one for the usual observable cases) of the form

$$\left\{ \begin{array}{l} \dot{x}^- = f^-(t, x^-, x^+, y^-(t), y^+(t)) \\ \dot{x}^+ = f^+(t, x^-, x^+, y^-(t), y^+(t)) \end{array} \right. \tag{2}$$

such that for any given bounds on unknown $w(.)$ and initial condition $x_0$, it is possible to initialize system (2) so that the following property is fulfilled

$$x^-(t) \leq x(t) \leq x^+(t), \qquad \forall t \geq t_0,$$

without having to require the convergence of vector $x^-(\dot{})$, $x^+(\dot{})$.
Then, robust control problems for uncertain models (1) can be reformulated into control problems of models (2) with perfect knowledge. Notice that when the realization of the disturbance vector $w(\cdot)$ in (1) is known or observed online, one deals with differential games: the "player" $u(\cdot)$ is playing against the "player" $w(\cdot)$. Recent contributions in this field have been obtained and will be published.

*6.1.1.5. Time optimal control of a sequencing batch reactor*

**Participants:** Jérôme Harmand, Claude Lobry, Djalel Mazouni, Alain Rapaport.

From an engineering point of view, biological reactors are classified according to the way they are fed. When treating industrial as well as urban waste-waters, batch processes present a number of advantages with respect to continuous ones. In particular, the reaction rates are usually faster and the separation step, during which the biomass is removed from the effluent to be finally rejected into the environment, is much easier to control than during continuous operation. A batch process operates in a sequential mode (this is why they are called Sequencing Batch Reactors or SBR): the water to be treated is first introduced into a closed tank. Then, the reaction takes place (the biomass degrades the substrates), the biomass settles and the supernatant (clean water) is finally discharged from the process before another cycle begins.

In order to improve the functioning of these processes, we have studied a minimal time optimal problem for a SBR treating both the organic carbon and nitrogen. To do so, two different operating conditions are needed: one aerated period (also called the "aerobic phase") and one without aeration (also called the "anoxic phase"). Depending on the initial concentrations of the different components (biomasses and substrates), the objective is to find the switching instants (from the aerobic phase to the anoxic one or conversely from the anoxic phase to the aerobic one) such that the total reaction time is minimized. Because several components and biological reactions are simultaneously present in the different reaction phases, the problem is far from being solved and a rigorous study has been realized within the framework of the European project EOLI.

In a first step, a reachability study has been realized [34]: the set of all initial conditions for which there exists a control sequence allowing for the state to reach a final target has been determined. In particular, it has been established that any initial state in this reachability set can reach the target with a control sequence involving at most two switches (aerobic/anoxic/aerobic). For practical reasons (minimize the number of switches), a suboptimal time control problem has been defined (determine the switching instants $t_1$ and $t_2$ such that any initial state in the reachability set attains the target set in a minimal time using a control sequence (aerobic/anoxic/aerobic)) and solved using the Pontryagin Maximum Principle. This new control algorithm is now to be implemented on a real 200 liters pilot plant available at the INRA-LBE, Narbonne.

Singular arcs in time optimal control problems present some similitude with the so-called "turnpike" optimality in calculus of variation. Extensions of a recent result obtained with P. Cartigny (Univ. Mediterranée) in this last framework [28][29] will be investigated.

*6.1.1.6. Analysis of an SSCP profile*

**Participants:** Jérôme Harmand, Patrice Loisel.

Because of the complexity and the reduction of information due to the analysis, we can at most hope to identify the majority species (species representing a significant percentage). By construction, a majority species generates a peak, but to any peak we cannot systematically associate a majority species. Indeed, a preliminary simulated study showed that for a mixture made up of a very high number of minority species (as it is the case in nature, typically 5000 species with $0.01\%$) and without any majority species, the SSCP analysis provides a curve with peaks of significant amplitude.

The required goal being to determine the majority species, it is necessary to find a criterion to trust the information given by a peak. A first criterion is the width of the peak (standard deviation for Gaussians). This idea comes from the following observations:

- the variance of the peak of an isolated species does not depend on the species but on specific materials used to make analysis SSCP.
- if, in a mixture of $n$ minority species (with $n$ large), one adds some majority species, one notes that the variance of the peak corresponding to the majority species is of the same order as the variance of an isolated species. On the other hand, for the peaks resulting from contributions of the minority ones, the variance is doubled (or more) with respect to the variance of an isolated species.

*6.1.1.7. Competition in the chemostat for density-dependent growth-rates*

**Participants:** Claude Lobry, Frédéric Mazenc, Alain Rapaport.

We prove the following result. Consider the system:

$$\begin{aligned}\dot{S} &= D(S_{in} - S) - \sum_{i=1}^{n} g_i(X_1, \cdots, X_n)\mu_i(S)X_i \\ \dot{X}_i &= (g_i(X_1, \cdots, X_n)\mu_i(S) - D)\, X_i \qquad (i = 1, \cdots, n)\end{aligned}$$

where $g_i$ are positive coupling functions. It has a unique strictly positive (each $X_i$ is strictly positive) globally asymptotically stable equilibrium, provided that:

- $D$ is small enough,
- $S_{in}$ is large enough,
- $\frac{\partial g_i}{\partial X_j} \leq 0$ for all $i, j$ and $|\frac{\partial g_i}{\partial X_j}| << |\frac{\partial g_i}{\partial X_i}|$ for all $i \neq j$.

The ecological interpretation of this result is the following. If the intra-specific competition is much larger than the inter-specific one, then, $n$ species competing for a single resource can survive. This result is accepted for anouncement in C. R. Acad. Sci. Mathématiques and an extended version in currently in preparation.

### 6.1.2. Applications

*6.1.2.1. Optimal design of a series of biorectors*

**Participants:** Abdou Khadry Dramé, Jérôme Harmand, Claude Lobry, Alain Rapaport.

When the objective is to optimize a series of bioreactors, existing results in the literature can be classified into two distinct classes: those dealing with mono-fed systems composed of $N$ bioreactors with different volumes and those dealing with multi-fed systems composed of $N$ equal size reactors. From the authors knowledge, the determination of the optimal volumes of the tanks (not necessarily equal) in the case where the input flow is distributed among the units of the series and where a recirculation loop is present has never been investigated.

Considering this new class of systems, we have shown - for both enzyme or microbial reacting systems - that the optimal solution of the problem of minimizing the TRV depends on the ratio $S_1'/\overline{S}_2$ where $S_1'$ is one of the two roots of a particular second order equation whose coefficients are determined from the system data and $\overline{S}_2$ is the output substrate concentration to be obtained (cf.[16] for the optimal design of catalytic systems). More specifically, if $S_1' > \overline{S}_2$, the optimal design is obtained by considering the feeding only into the first reactor while no recirculation is needed. At one end, one has $S_1' = \overline{S}_2$ corresponding to the case when only one tank is needed. For the case in which $S_1' < \overline{S}_2$, it was shown that the TRV can be significantly decreased (when compared to the existing design procedures found in the literature) by distributing the input flow rate and introducing a recirculation loop with a certain flow rate. In such a case, the optimal solution is not unique and the concept of "Steady State Equivalent Biological Systems" was introduced to help the designer to choose one among all the possible equivalent TRV-optimal solutions. In particular, we have pointed out the existence of an infinity of processes which have the same total volume, the same input-output behavior and which only differ by the way the input is distributed among the tanks and by the magnitude of the recirculation loop.

This new concept is particularly interesting because it allows the designer to take additional properties of each one of the TRV-optimal solution into account such as observability or controllability, and then to decide which one is the "best" with respect to these additional criteria.

*6.1.2.2. Monitoring and estimation techniques for the SBRs*

**Participants:** Jérôme Harmand, Djalel Mazouni, Alain Rapaport.

One of the most important problems when dealing with biological processes is the quasi-systematic lack of sensors able - at a reasonable cost - to deliver on-line information about the composition of the matter to be processed. This is why the development of "software sensors" (observation techniques) are of particular interest in this field of research. When dealing with the optimal time control of SBRs, it was assumed that the entire state of the system was measured on-line. In reality, only parts of the state can be measured and an important experimental work has been realized

1. to generate data that are rich enough to be used for the modeling of a 200 liters SBR pilot plant,
2. to design estimators that use the available on-line information to reconstruct unmeasured state variables,
3. to validate these sensors that will be used for the time-optimal control of the SBR.

*6.1.2.3. Physical bases of density-dependence in the chemostat*

**Participants:** Jérôme Harmand, Claude Lobry.

In cooperation with three biologists (R. Arditi (INAPG), J.-J. Godon (LBE), A. Sciandra (Observatoire Océanographique Villefranche sur Mer)), we establish that the density-dependence used in Section 6.1.7. can be explained by purely abiotic causes. Namely we are able to show that the diffusion of the substrate, associated to the fact that populations are increasing through the division of cells, is a possible explanation of a more intense intra-specific competition that the inter-specific one.

This addresses the question whether, in the real world, chemical communications between individuals, the so called “quorum sensing”, occurs in this context or not. We are trying to start experimental works on this subject.

*6.1.2.4. Software design*

**Participants:** Jérôme Harmand, Patrice Loisel.

A software for the analysis of SSCP profiles is currently designed (see above).

# 7. Contracts and Grants with Industry

**Participants:** Jérôme Harmand, Alain Rapaport.

Biological processes are not only used to treat liquid wastes but are also useful to treat organic solid wastes, for instance urban organic wastes (green wastes, activated sludges, molasses,...) We have been contacted by the industrial leader of this treatment domain (the Suez-Lyonnaise des eaux group by the way of the SITA company) to develop a software that is able to simulate the aerobic process that can stabilize the organic waste in order to get a high quality compost that can be used in agriculture (transforming it into gas, inert matter in order to avoid odors and minimizing the pathogens rate, aerobic fermentation being processed at high temperature, around 60 to 70°C for several days).

# 8. Other Grants and Activities

### *8.1.1. International*

The MERE project-team is very actively involved in cooperation with Africa in two different but related ways.

- C. Lobry, as a former director of CIMPA, has been involved for a long time in cooperation with African mathematical teams. He visits Africa very often and delivers lectures in summer schools or universities.([18][19][20]).
- The team has a close relationship with the LANI (Laboratoire d'Ananlyse Numérique et Informatique de l'Université Gaston Berger de Saint-Louis du Sénégal). The LANI is a team of about ten permanent researchers working on partial differential equations applied to problems of development in Sahel and mainly to questions related to water. The LANI is involved in a regional network devoted to the same problems and located in Ouagadougou.

### *8.1.2. European initiatives*

The EOLI project, European contract number ICA4-CT-2002-10012.
EOLI (an acronym for "Efficient Operation of [Low Investment] cost wastewater treatments plants") is an INCO (for International Cooperation) European project (2003-2005) involving eight European/Latin-American partners, the LBE being the INRA partner. It is dedicated to the optimization of a class of WasteWater Treatment Processes (WWTP) through the use of control engineering science tools. The objective of the EOLI project is to design a low-cost, modular and reliable monitoring and control system for wastewater treatment processes dedicated to the treatment of wastewater from urban settlements, especially from those urbanized areas where industries heavily contribute to water pollution. The aerobic treatment of domestic and industrial wastewaters by activated sludge is a common process, but the characteristics of many industrial discharges often cause operational problems in continuous flow systems. Therefore, discontinuous processes, as sequencing batch reactors (SBRs), are considered in this project because, in terms of investment and operation costs, process stability, and operation reliability, they are better than the conventional continuous activated sludge process. The monitoring and control system, relying upon information technologies and automatic control, is designed to provide a tool for reliable and efficient operation of SBRs. It is expected to provide a framework for the ISO14001 certification and allows small and medium units (mainly SMEs, not only in Latin America but also in Europe, that cannot afford high investment processes for wastewater treatment) to meet the pollution constraints (like the European Directives 91/271/EEC and 98/15/EEC). The EOLI project is aiming at developing a general, yet adaptable, supervision and monitoring system for the types of wastewater described above. The framework of the EOLI project will integrate the data collected by the sensors, detect fault or abnormal working conditions, and activate model based controllers to optimize the technology and operation of SBRs. The efficient, low-cost and safe operation of the SBRs is expected to be achieved by the integration of high performance controllers, affordable hardware and software sensors and a supervision system to guarantee the reliability of the process operation. In practice, Djalel Mazouni (a PhD student of the LBE granted by EOLI) has taken benefit from the MERE expertise for the development of a time optimal control law of a 200 liters SBR pilot plant available at the LBE.

For further information, see http://www.auto.ucl.ac.be/EOLI/index.html.

# 9. Dissemination

### *9.1.1. Teaching*

J. Harmand teaches a module "Automatic control" (25 h/year) at the UPS, Toulouse, for the "Préparation à l'Agrégation de Sciences Physiques Appliquées, Option Procédés Physico-Chimiques".

A. Rapaport regularly gives lectures on calculus of variation for Master degree, and on control theory for pre-PhD degree at the University of Montpellier.
A. Rapaport is responsible of a two-weeks lectures “Mathématiques pour la gestion de ressources renouvelables” at Ecole Nationale Supérieure d’Agronomie de Montpellier (optional second year module, see the web page http://www.montpellier.inra.fr/DRN/COURS/). J. Harmand and A. Rapaport deliver each year several lectures and training periods.
C. Lobry, J. Harmand and A. Rapaport have participated with P. Cartigny (Univ. Mediterranée) to a one week lectures series at CMM (Centro de Modelamiento Matematico), Santiago, Chili on the modelisation of natural resources.
Web site: http://www.cmm.uchile.cl/renewres/workshop04/lectures/lectures.htm.
C. Lobry gives 15h/year course at the Institut National D’Agronomie Paris-Grignon (INAPG). He also delivers lectures at the University of Saint-Louis du Sénégal.

### *9.1.2. Ongoing thesis*

- Dramé PhD’s is supported by a grant from AUF. He is part time in the MERE project at Montpellier, part time at the University of Saint Louis du Sénégal. The thesis is devoted to the study of the question of existence of multi equilibria in a non perfectly stirred reactor when the kinetic is non monotonous. He has published three papers in journals, two in 2004 [14], [16].
- Djalel Mazouni is preparing his PhD at the LBE. He is granted by the LBE within the framework of the European EOLI project dedicated to the modeling and the optimization, through the development of control and supervision algorithms, of aerobic SBRs able to treat a large class of wastewaters. His work is more particularly devoted to the generation of experimental data (he has started up and has been operating a 200 liters SBR pilot plant since the beginning of the project in 2002), the design of estimation techniques and the development and the validation of a time-optimal control law able to minimize the reaction period lengths. He is the author of two international conference papers ([35] and [34]), he has submitted two others at the world IFAC 2005 and one paper in an international journal ).

### *9.1.3. Conferences, Invited conferences*

*9.1.3.1. Saint-Louis du Sénégal*

A. Dramé and C. Lobry where invited lecturers at the international conference: “Mathématiques et Applications Aux Problèmes de Développement du Sahel”, Saint-Louis du Sénégal, 15–20 décembre 2003.

*9.1.3.2. Santiago de Chile*

In connection with the lectures series given at the CMM, Santiago, Chili (see Section 9.1), C. Lobry, J. Harmand and A. Rapaport have participated to a one day workshop on modeling and control of renewable resources.
Web site: http://www.cmm.uchile.cl/renewres/workshop04.

# 10. Bibliography

## Major publications by the team in recent years

[1] J. Harmand, A. Rapaport, A. Trofino. *Optimal design of interconnected bioreactors : new results*, in "AIChE", vol. 49, n° 6, 2003, p. 1433–1450.

[2] J. Lobry, C. Lobry. *Evolution of DNA base composition under the no-strand bias conditions when the substitution rates are not constant*, in "Journal of Mol. Biol Evol.", vol. 16, n° 6, 1999, p. 719–723.

[3] C. LOBRY, T. SARI, S. TOUHAMI. *Slow and fast feed-back in control systems*, in "Journal of Biological Systems", vol. 7, n$^o$ 3, 1999.

[4] C. LOBRY, A. SCIANDRA, P. NIVAL. *Effets paradoxaux des fluctuations de l'environnement sur la croissance des populations et la compétition entre espèces*, in "C.R. Acad. Sci. Sciences de la Vie", vol. 317, 1994, p. 102–107.

[5] S. D. MARCO, A. RAPAPORT. *Characterization and Approximation of Value Functions of Differential Games with Maximum cost in Infinite Horizon*, in "International Game Theory Review", 2005, to appear.

[6] F. MAZENC, S. BOWONG. *Backstepping with bounded feedbacks for time-varying systems*, in "SIAM Journal on Control and Optimization", vol. 43, n$^o$ 3, 2004, p. 856–871.

[7] F. MAZENC, D. NESIC. *Strong Lyapunov functions for systems satisfying the conditions of La Salle*, in "IEEE Trans. Aut. Contr.", vol. 49, n$^o$ 6, 2004, p. 1026–1030.

[8] A. RAPAPORT, P. CARTIGNY. *Turnpike Theorems in Infinite Horizon by a Value Function Approach*, in "ESAIM Control, Optimization and Calculus of Variations", vol. 10, 2004, p. 123–141.

[9] A. RAPAPORT, J.-L. GOUZÉ. *Parallelotopic and practical observers for nonlinear uncertain systems*, in "International Journal of Control", vol. 76, n$^o$ 3, 2003, p. 237–251.

[10] A. RAPAPORT, M. MALOUM. *Design of exponential observers for nonlinear systems by embedding*, in "International Journal of Robust and Nonlinear Control", vol. 14, 2004, p. 273–288.

## Doctoral dissertations and Habilitation theses

[11] J. HARMAND. *Contribution à l'analyse et au contrôle des systèmes biologiques : application aux bioprocdédés de dépollution*, Habilitation à diriger des recherches (en Automatique), Univ. Lyon I, Juin 2004.

[12] A. RAPAPORT. *Contribution à la commande optimale et l'observation robustes de systèmes dynamiques non linéaires - Applications en biologie et en écologie*, Habilitation à diriger des recherches (en Mathématiques), Univ. Montpellier II, Nov. 2003.

## Articles in referred journals and book chapters

[13] V. ALCARAZ-GONZALEZ, J. HARMAND, A. RAPAPORT, J. STEYER, C. PELAYO-ORTIZ. *Application of a robust interval observer to an anaerobic digestion process.*, in "Developments in Chemical Engineering and Mineral Processing Journal", to appear, 2004.

[14] A. DRAMÉ. *A semilinear parabolic boundary value problem in bioreactors theory*, in "Electronic Journal of Differential Equations", vol. 129, 2004, p. 1-13.

[15] A. DRAMÉ, J. HARMAND, A. RAPAPORT, C. LOBRY. *Multiple steady states profiles in interconected biological systems*, in "Math. Comp. Mod. Dyn. Sys.", to appear, 2004.

[16] J. HARMAND, A. RAPAPORT, A. DRAMÉ. *Optimal design of 2 interconnected enzymatic reactors*, in "Journal of Process Control", vol. 14, n$^o$ 7, 2004, p. 785–794.

[17] C. LOBRY. *Modèles mathématiques et modèles informatiques, sur la théorie du modèle*, in "Annales des Ponts et Chaussées", vol. 107-108, 2004.

[18] C. LOBRY, T. SARI. *Equations différentielles à second membres discontinus*, Ecole du CIMPA, Quelques Questions de Théorie du Contrôle, Hermann, Travaux en cours, 2004.

[19] C. LOBRY, T. SARI. *Introduction à la théorie du contrôle*, Ecole du CIMPA, Quelques Questions de Théorie du Contrôle, Hermann, Travaux en cours, 2004.

[20] C. LOBRY, T. SARI. *Singular perturbations in control theory*, Ecole du CIMPA, Quelques Questions de Théorie du Contrôle, Hermann, Travaux en cours, 2004.

[21] F. MAZENC, S. BOWONG. *Backstepping with bounded feedbacks for time-varying systems*, in "SIAM Journal on Control and Optimization", vol. 43, n$^o$ 3, 2004, p. 856–871.

[22] F. MAZENC, A. IGGIDR. *Backstepping with Bounded Feedbacks*, in "Systems & Control Letters", vol. 51, n$^o$ 3–4, 2004, p. 235–245.

[23] F. MAZENC. *Strict Lyapunov Fonctions for Time-varying Systems*, in "Automatica", vol. 39, 2004, p. 349–353.

[24] F. MAZENC, S. MONDIÉ, R. FRANCISCO. *Global Asymptotic Stabilization of Feedforward Systems with Delay in the Input*, in "IEEE Trans. Aut. Contr.", vol. 49, n$^o$ 5, 2004, p. 844–850.

[25] F. MAZENC, S. MONDIÉ, S. NICULESCU. *Global Stabilization of Oscillators With Bounded Delayed Input*, Lecture Notes in Control and Information Sciences, vol. 38, chap. Advances in time-delay systems, Springer-Verlag, 2004.

[26] F. MAZENC, D. NESIC. *Strong Lyapunov functions for systems satisfying the conditions of La Salle*, in "IEEE Trans. Aut. Contr.", vol. 49, n$^o$ 6, 2004, p. 1026–1030.

[27] A. RAPAPORT, A. ASTOLFI. *A remark on the stability of interconnected nonlinear systems*, in "IEEE Transactions on Automatic Control", vol. 49, n$^o$ 1, 2004, p. 120–124.

[28] A. RAPAPORT, P. CARTIGNY. *Necessary and Sufficient Conditions for Turnpike Optimality : the Singular Case*, Lecture Notes in Control and Information Sciences, vol. 301, chap. Optimal Control, Stabilization and Nonsmooth Analysis, Springer-Verlag, 2004, p. 123–141.

[29] A. RAPAPORT, P. CARTIGNY. *Turnpike Theorems in Infinite Horizon by a Value Function Approach*, in "ESAIM Control, Optimization and Calculus of Variations", vol. 10, 2004, p. 123–141.

[30] A. RAPAPORT, D. DOCHAIN. *Interval Observers for Biochemical Processes with Uncertain Kinetics and Inputs*, in "Mathematical Biosciences", 2004, to appear.

[31] A. Rapaport, M. Maloum. *Design of exponential observers for nonlinear systems by embedding*, in "International Journal of Robust and Nonlinear Control", vol. 14, 2004, p. 273–288.

## Publications in Conferences and Workshops

[32] M. Mabrouk, F. Mazenc, J. Vivalda. *On global observers for some mechanical systems*, in "2nd IFAC Symposium on System, Structure and Control, Oaxaca, Mexico", 2004.

[33] F. Mazenc, S. Mondié, R. Francisco. *Feedforward System with Delay in the Input and Vanishing Perturbations*, in "2nd IFAC Symposium on System, Structure and Control, Oaxaca, Mexico", 2004.

[34] D. Mazouni, J. Harmand, A. Rapaport, H. Hammouri. *Modelling and controlability analysis of an aerobic SBR*, in "CARI'04", November 22-25, Hammamet, Tunisie, 2004.

[35] D. Mazouni, M. Ignatova, J. Harmand. *A simple mass balance model for biological batch reactors used for carbon and nitrogen removal*, in "IFAC Automatic Systems for Building the Infrastructure in developing Countries", 3-5 Oct., Bansko, Bulgarie, 2004.