

Summer School on Mathematical Control Theory
(3 - 28 September 2001)

**Wastewater treatment processes:
Why is it important to control them
and what are the difficulties?**

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These are preliminary lecture notes, intended only for distribution to participants

Wastewater treatment processes : Why is it important to control them and what are the difficulties ?

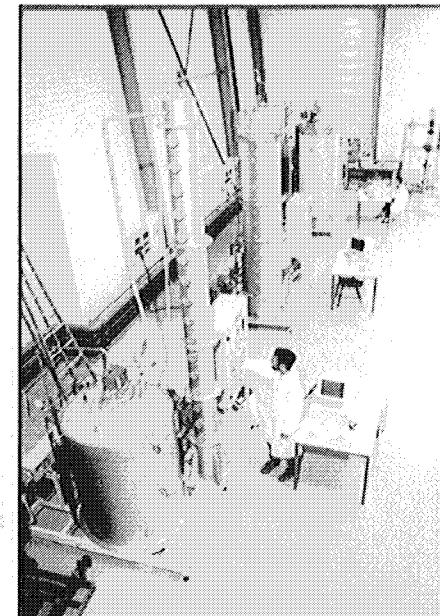
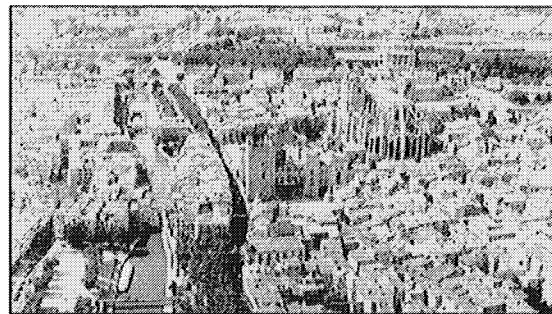
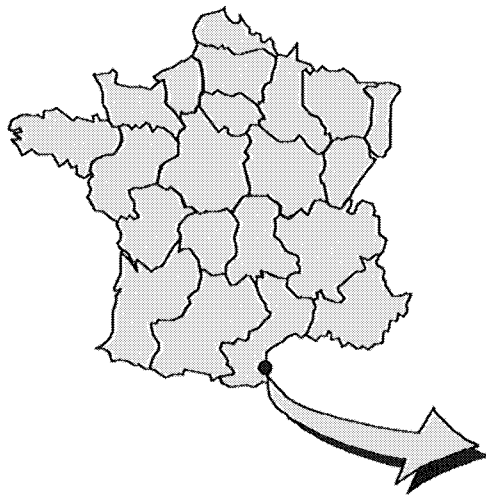
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Contents of the Presentation

- 1) Problem statement***
- 2) Difficulties in Modeling***
- 3) Difficulties in Control***
- 4) An integrated approach***

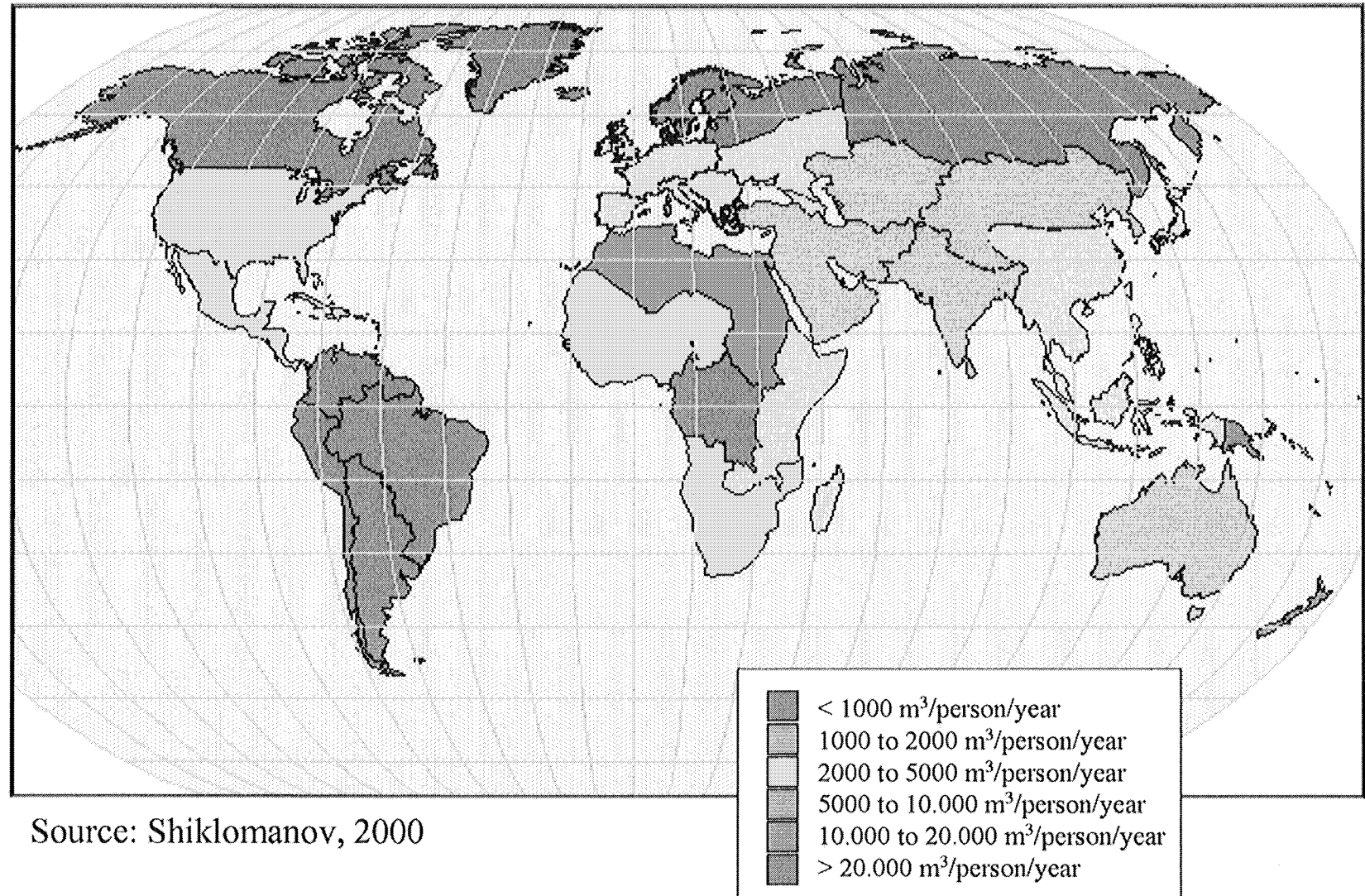
- ↪ Today, in Europe, only 43 % of the entire pollution is removed :
 - ✓ It is better than in the past : 32.5 % in 1981,
 - ✓ But the objective is 65 % in 2002 !...

- ↪ Quantities are enormous, for example :
 - ✓ 40 millions cubic meters of wastewater produced per day in Europe,
 - ✓ 60 billions tons of solid waste produced yearly worldwide,
(e.g., the highest point of the US east coast is the NYC landfill deposit, ...)

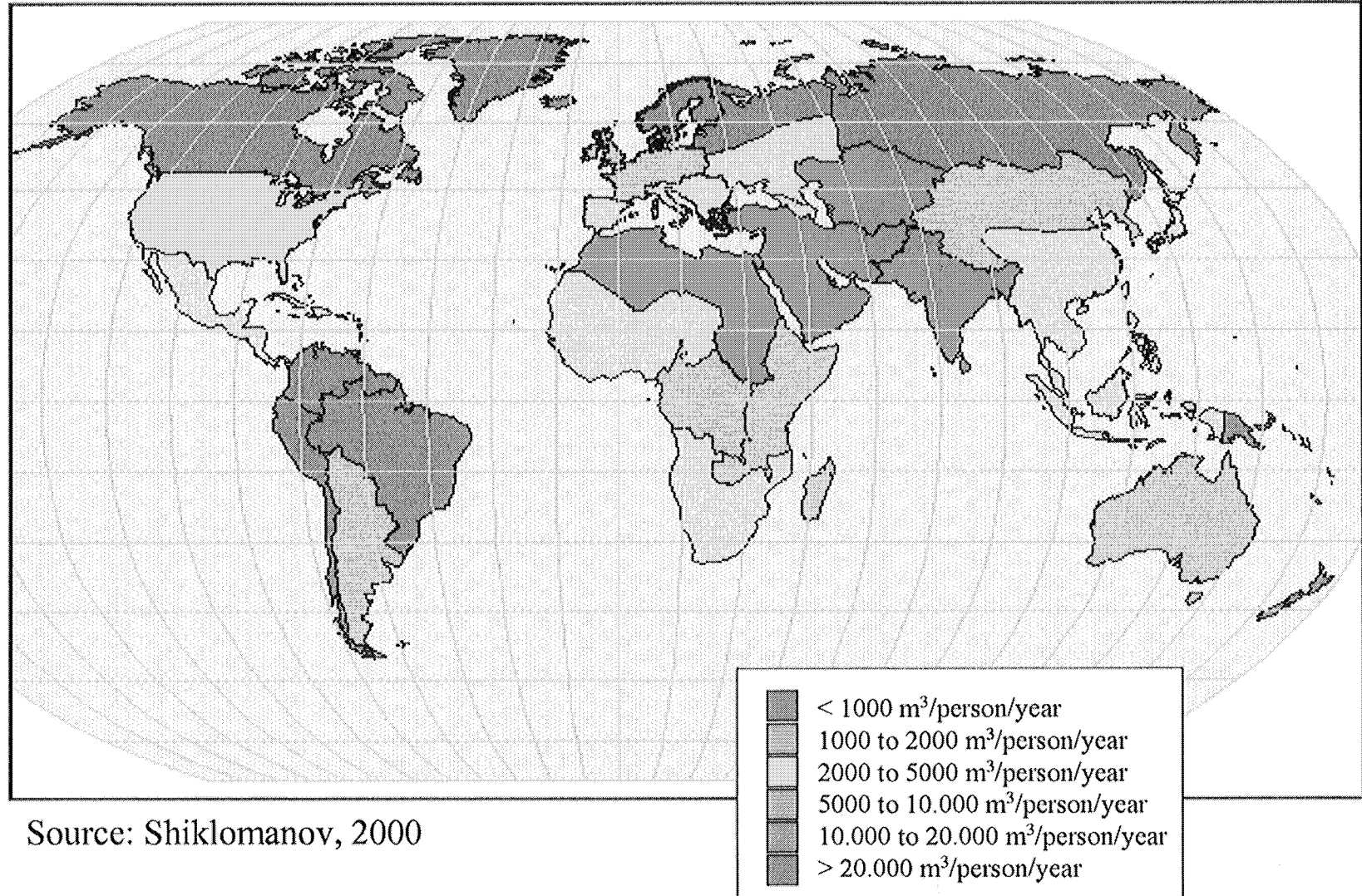
- ↪ High risks for human health :
 - ✓ Loss of fertility of living beings (e.g., birds or bees worldwide)
 - ✓ Loss of fertility of soils (i.e., no more plants in 400 years)
 - ✓ Health problems related to the presence of nitrate, heavy metals, pathogens, ...
*Every year, around 5 million people in developing countries
die from waterborne diseases and polluted air !!!*

- ↪ Legislation is changing :
 - ✓ Thresholds (125 mg/l of COD, 10 mg/l of total nitrogen, 2 mg/l of phosphate)
 - ✓ Results within the limits 95 % of the time

Water Availability in 1995

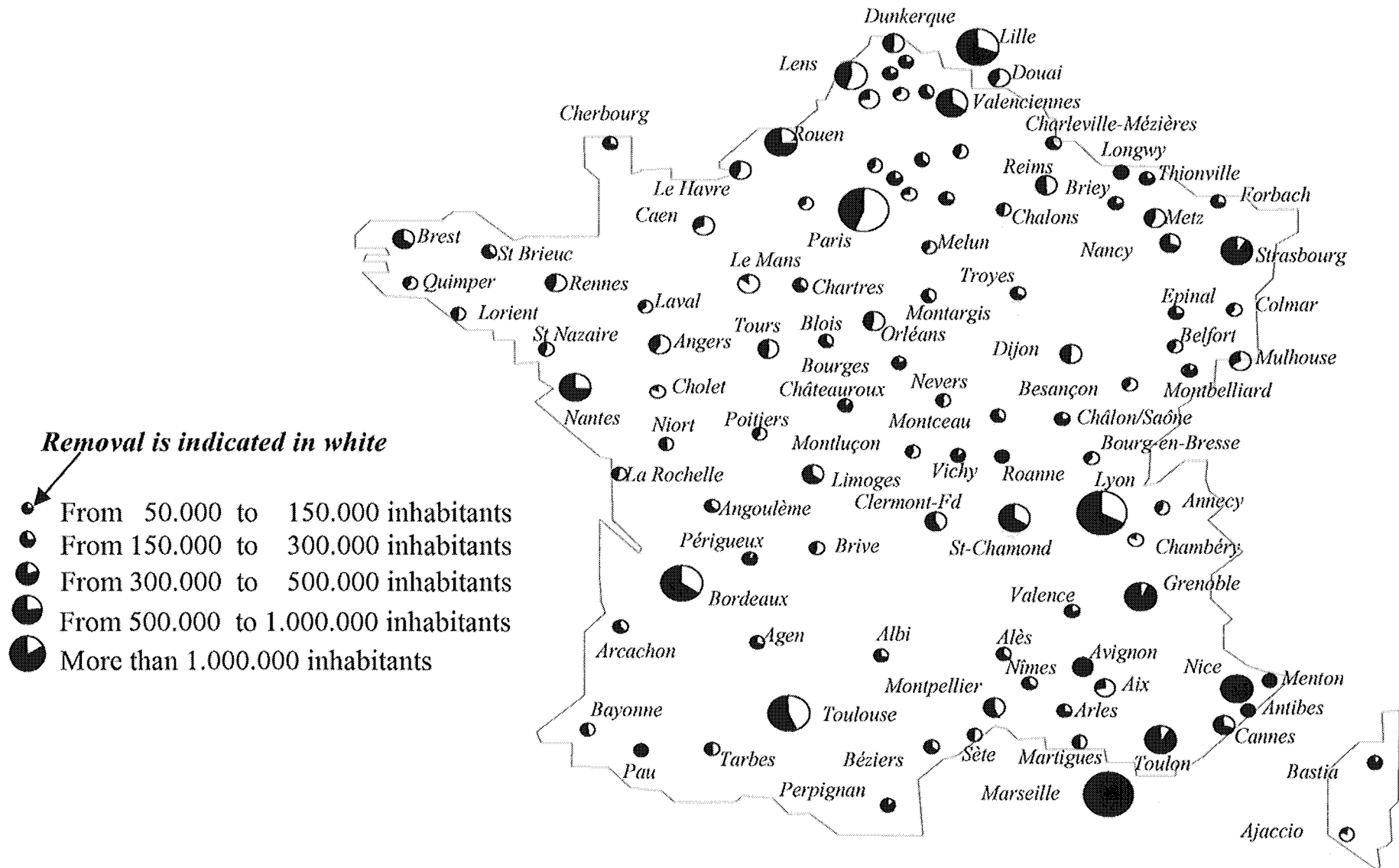


Water Availability Expected in 2025



Source: Shiklomanov, 2000

Performances of urban WWTPs in France



As a consequence ...

There is much to be done !...

BUT :

- ✓ Number of aspects ...
- ✓ Number of solutions ...
- ✓ Number of constraints ...

↳ *Need for pluridisciplinarity !*

Biological Processes : Definition

The growth of the microorganisms (bacteria, yeasts, ...) proceeds by consumption of appropriate nutrients or substrates (involving carbon, nitrogen, oxygen, ...) provided the environmental conditions (temperature, pH, ...) are favourable. The mass of living microorganisms or living cells is called the biomass.

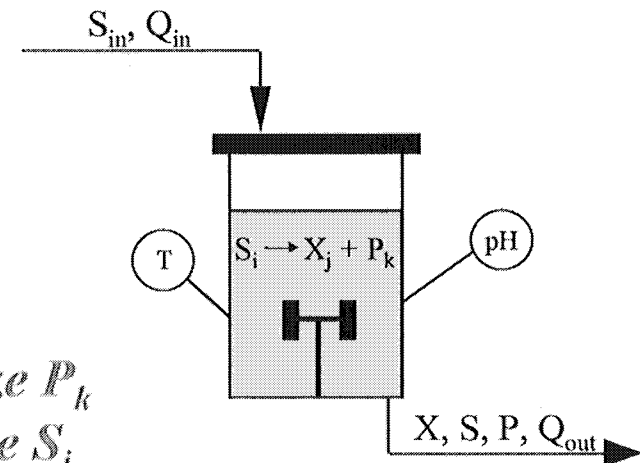
Associated with cell growth, but often proceeding at a different rate, are the enzyme catalysed reactions in which some reactants are transformed into products through the catalytic action of intra or extracellular enzymes.



Objectives :

For pharmaceutical or food processes : *maximize* P_k

For wastewater treatment processes : *minimize* S_i



*A biological wastewater treatment processes
are one solution among others.*

↳ Advantages :

- ✓ Safe for environment,
- ✓ Efficient processes,
- ✓ Economically interesting.

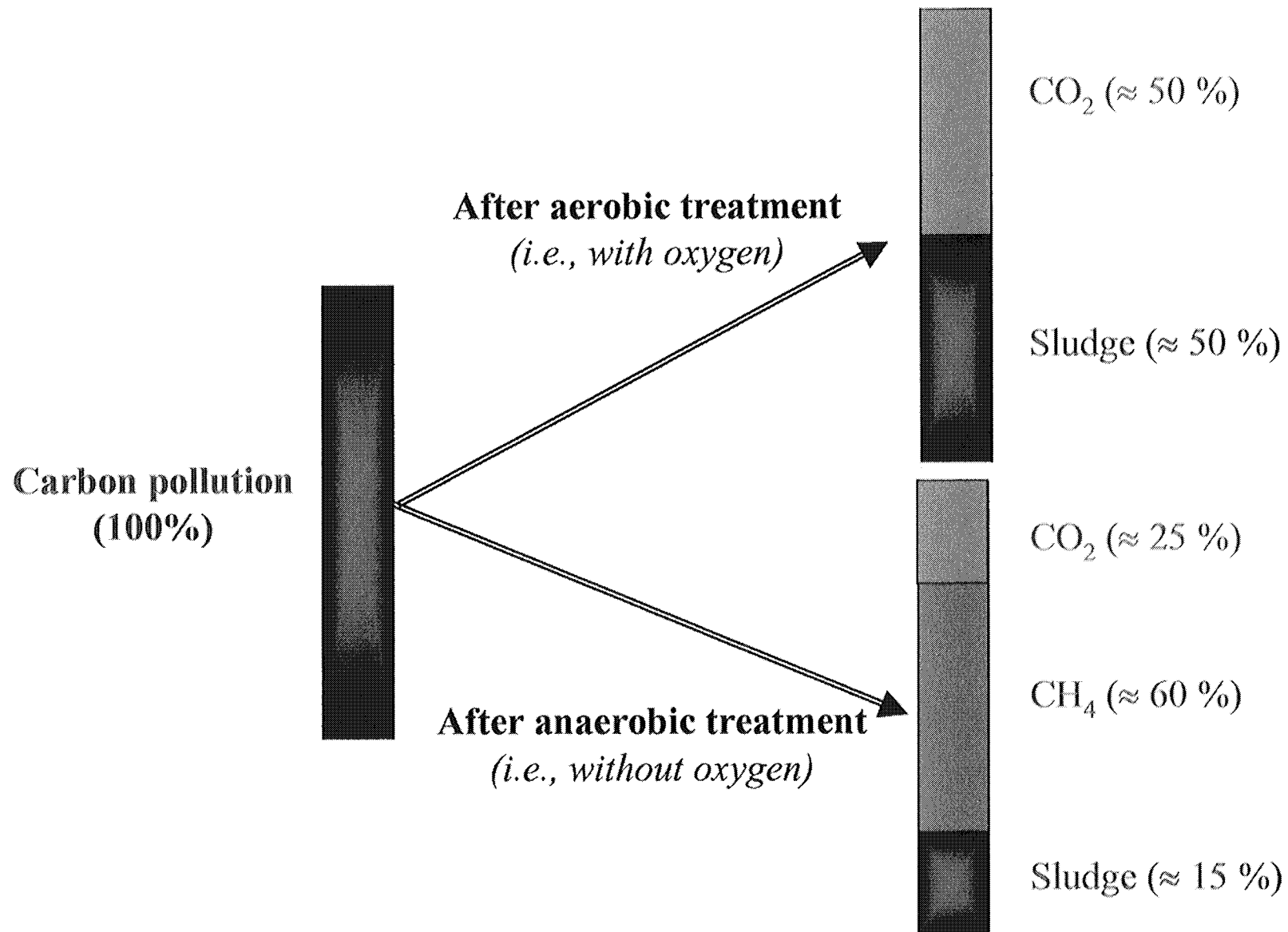
↳ Drawbacks :

- ✓ Very complex pluri-disciplinary systems
- ✓ MIMO non linear systems
- ✓ Difficult to characterize (lack of sensors and actuators)
- ✓ Time delayed systems
- ✓ Time variant systems (non stationary)

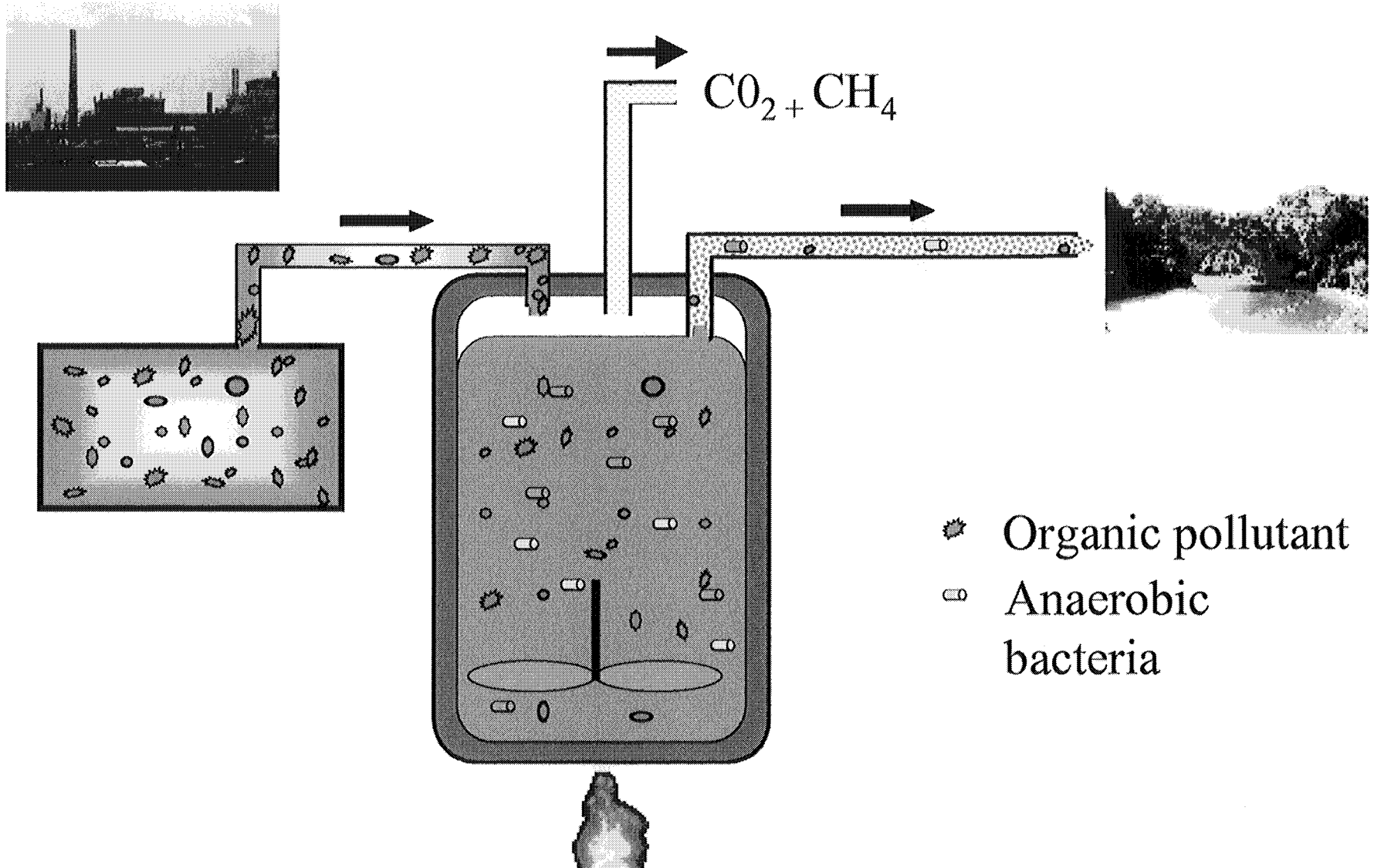
Nature of pollutants in water

- Organic matter (OM)
- Suspended solids (SS)
- Nitrogen (ammonia, nitrate,...)
- Phosphorus (phosphates,...)
- Metals (chromium, lead, copper,...)
- Toxic products (cyanide, chlorophenols,...)

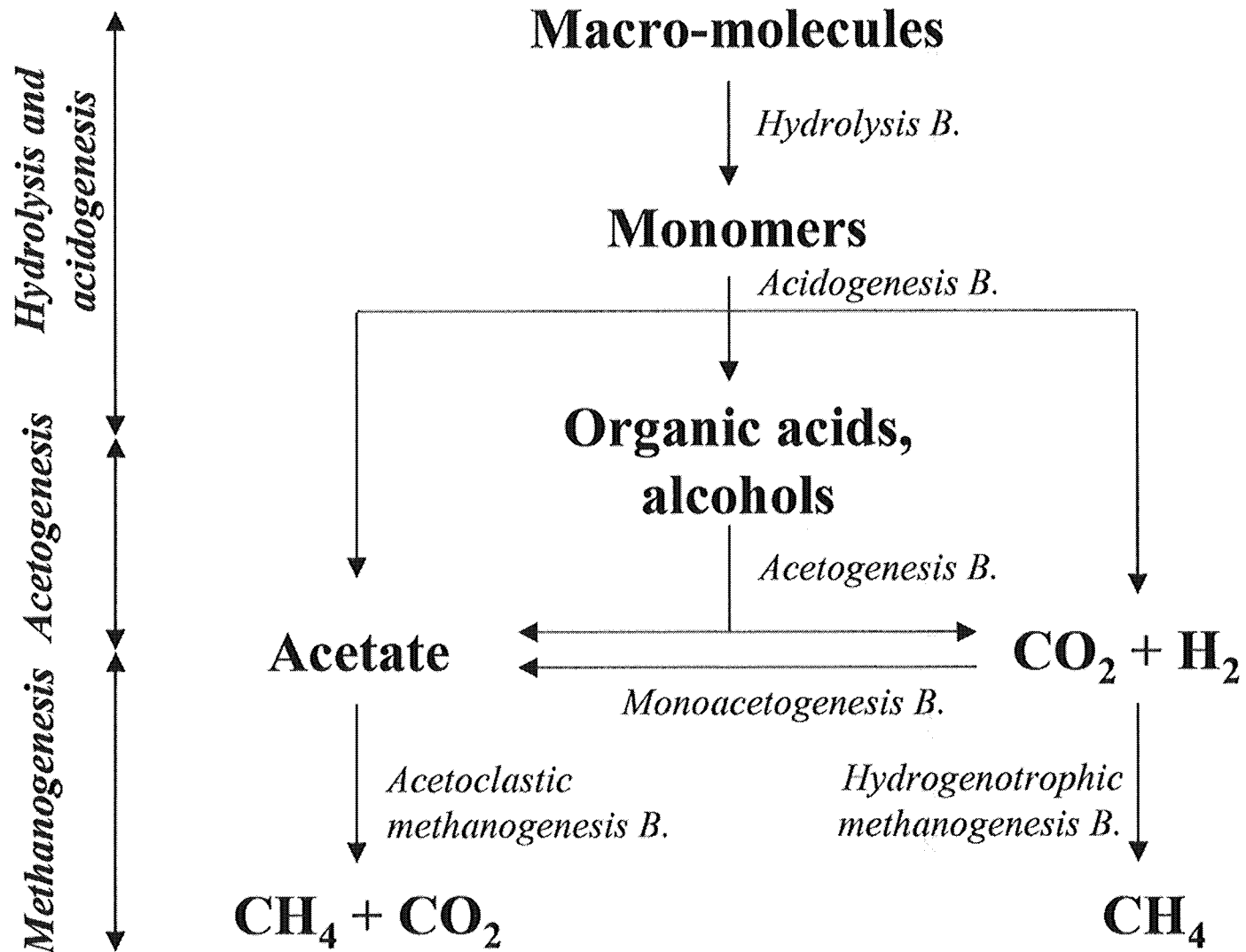
Carbon Removal



Anaerobic Digestion in CSTR



The Anaerobic Digestion Reaction Scheme



How does it work ?

2 main steps

1) Acidogenesis:



Fast

2) Methanogenesis:



Slow

Inhibition



Nitrogen Pollution

Municipal wastewaters :

↳ 30-80 mg/l as organic N (urea)

Industrial wastewaters :

↳ up to several g/l as

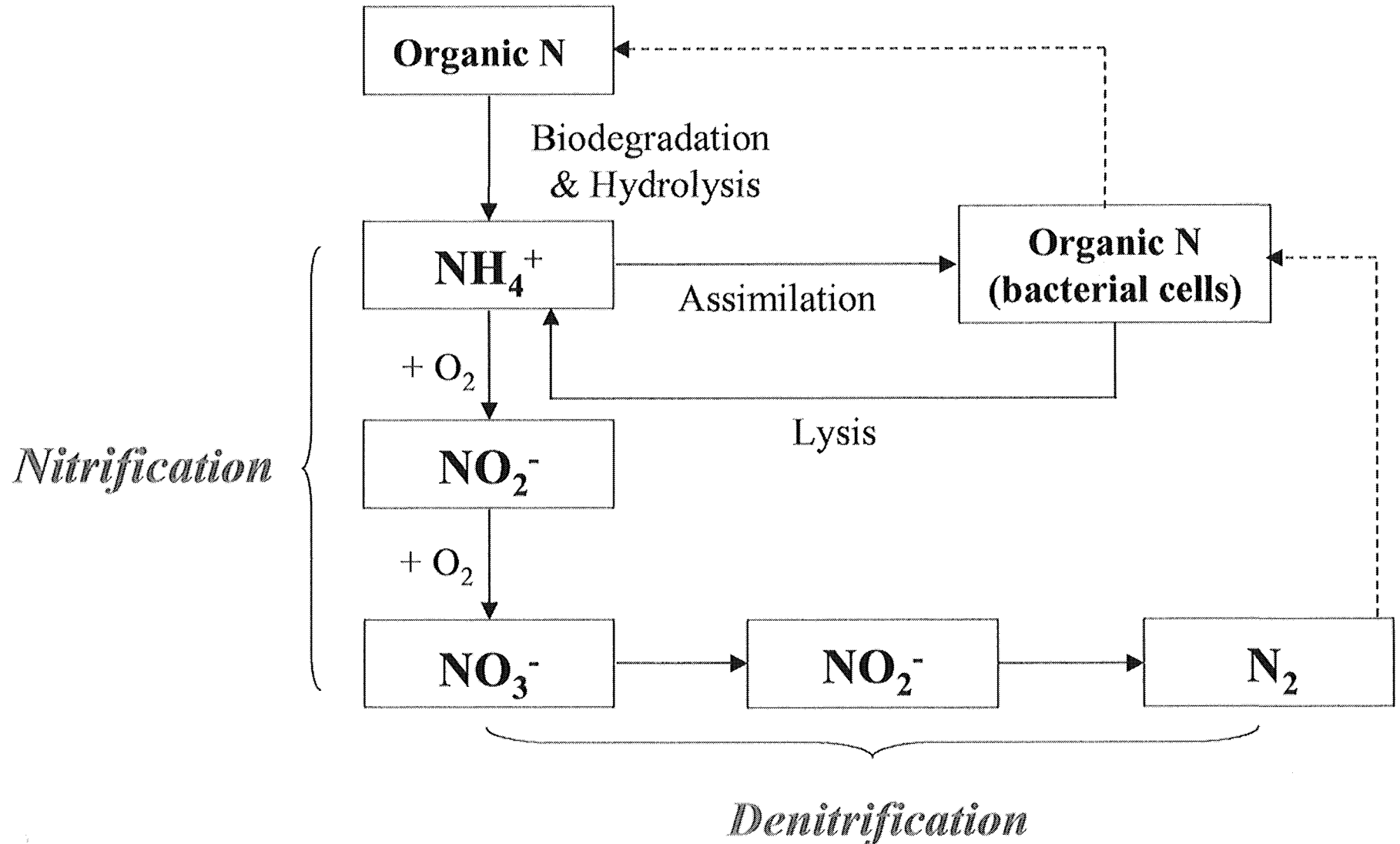
- ✓ organic N (food industry),
- ✓ ammonia (cokery, fertilizer, paper,...)
- ✓ nitrate (explosives, uranium processes, fertilizers)

Problems related to :

- ✓ *Eutrophication of the receiving water*
- ✓ *Health : ammonia \Rightarrow toxic and nitrate \Rightarrow "methemoglobinemy"*

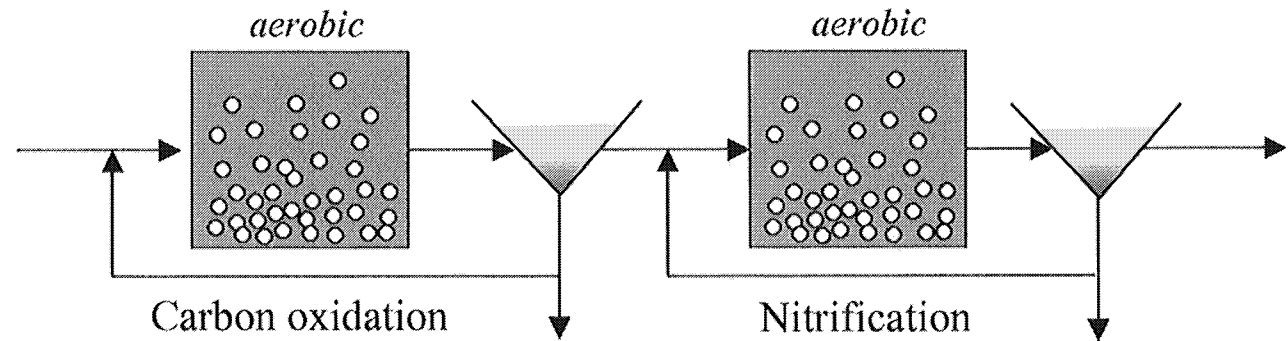
Nitrogen removal by biological treatment

The Nitrogen Cycle

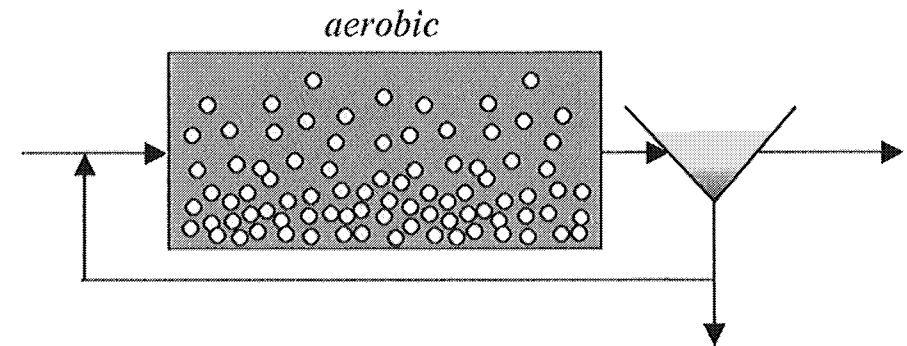


1) Nitrification Processes

Separate-stage
nitrification



Single-stage carbon oxidation
and nitrification
(high HRT and low loading rate)



2) Denitrification

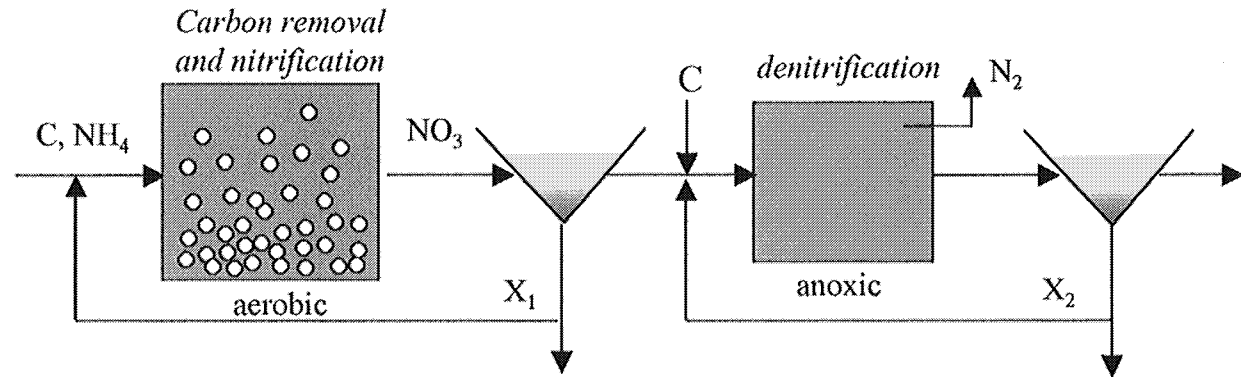
Denitrification is nitrate respiration *in anoxic conditions* by a wide range of bacteria using an organic carbon source as an electron donor :



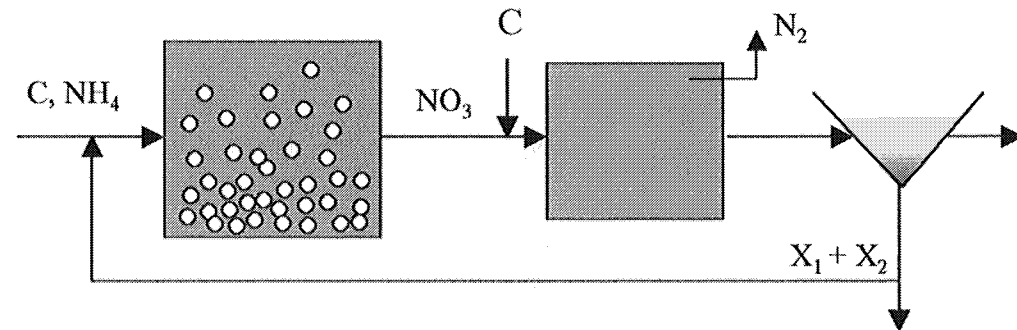
Minimum carbon required : 2.86 mg COD / mg N-NO₃

Carbon and Nitrogen Removal

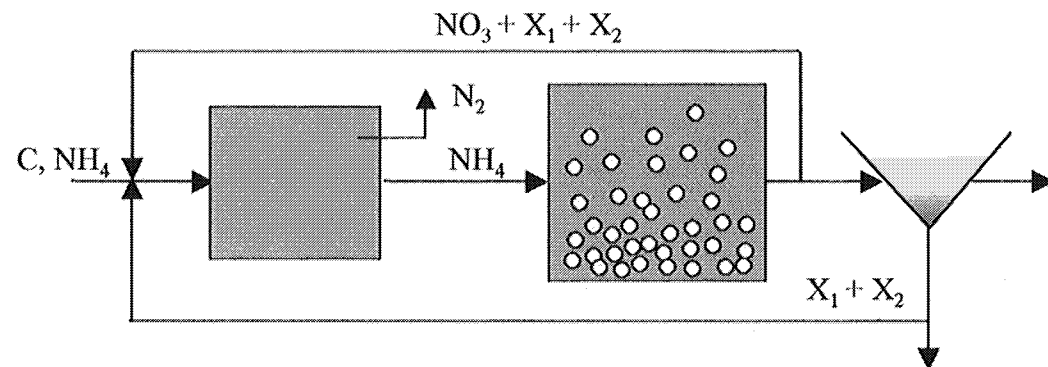
Two-stage biological nitrogen removal



With alternative carbon addition (same biomass)

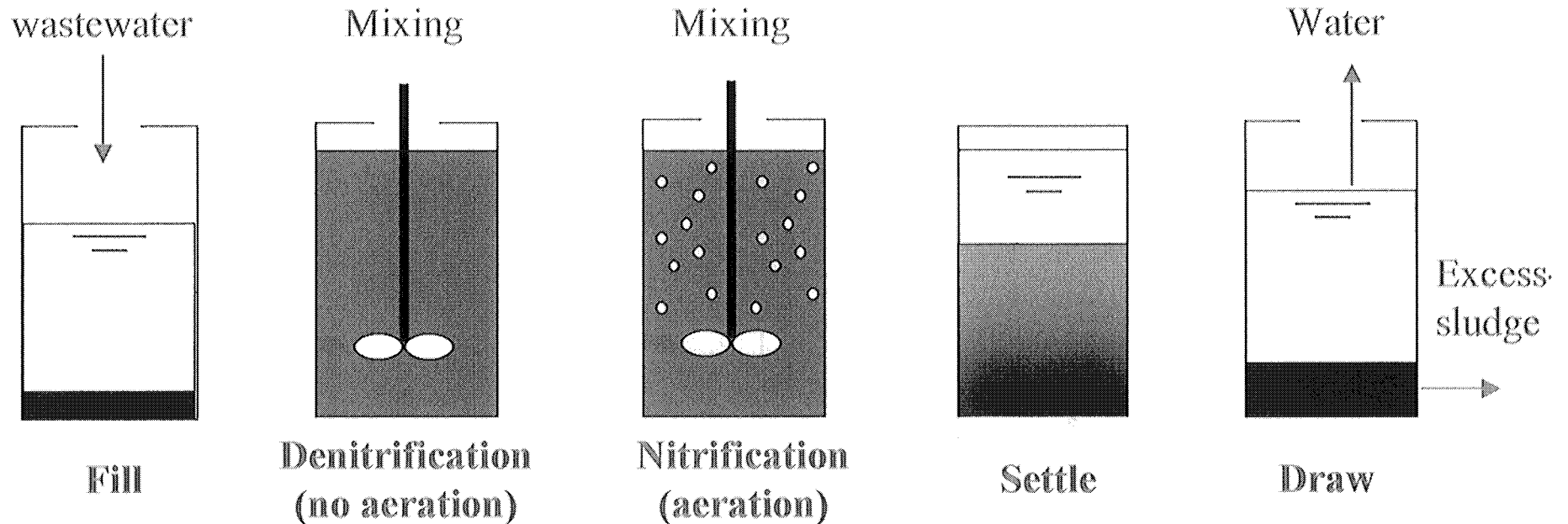


Denitrification using the carbon of the wastewater (*i.e.*, Ludzack-Ettinger configuration)



Biological nitrogen removal in SBR

*SBR : Sequencing Batch Reactor
(i.e., separation in time vs. space)*



Phosphorus Pollution

Municipal wastewaters : 6-25 mg/l as orthophosphate

Industrial wastewaters : Food industry,
Chemical industry,
Surface treatment, ...

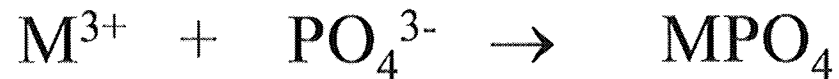
Problem related to eutrophication of the receiving water

Phosphorus removal :

- ✓ Chemical treatment by precipitation*
- ✓ Biological treatment*

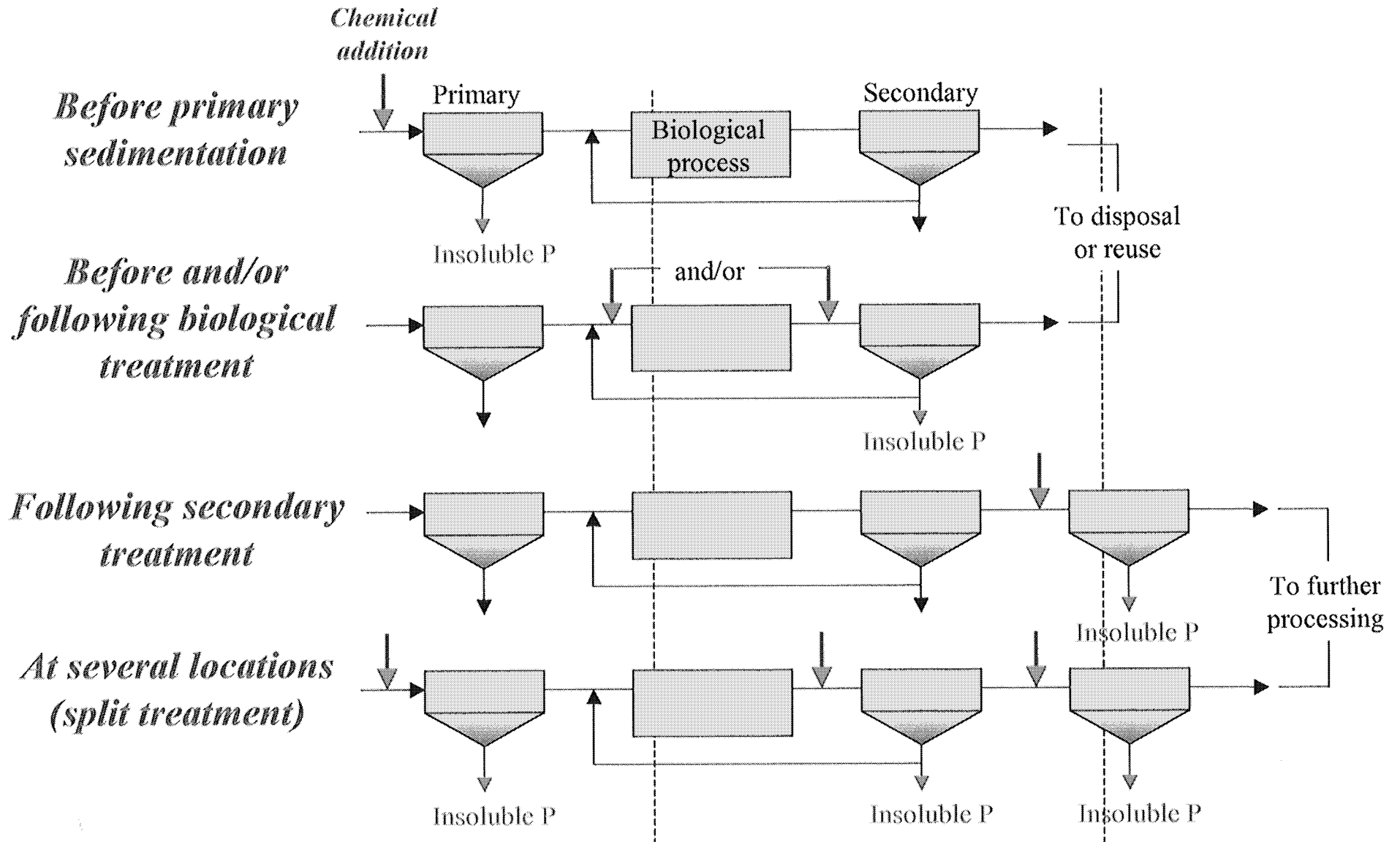
Chemical phosphorus removal

Use of a cation to precipitate phosphate :

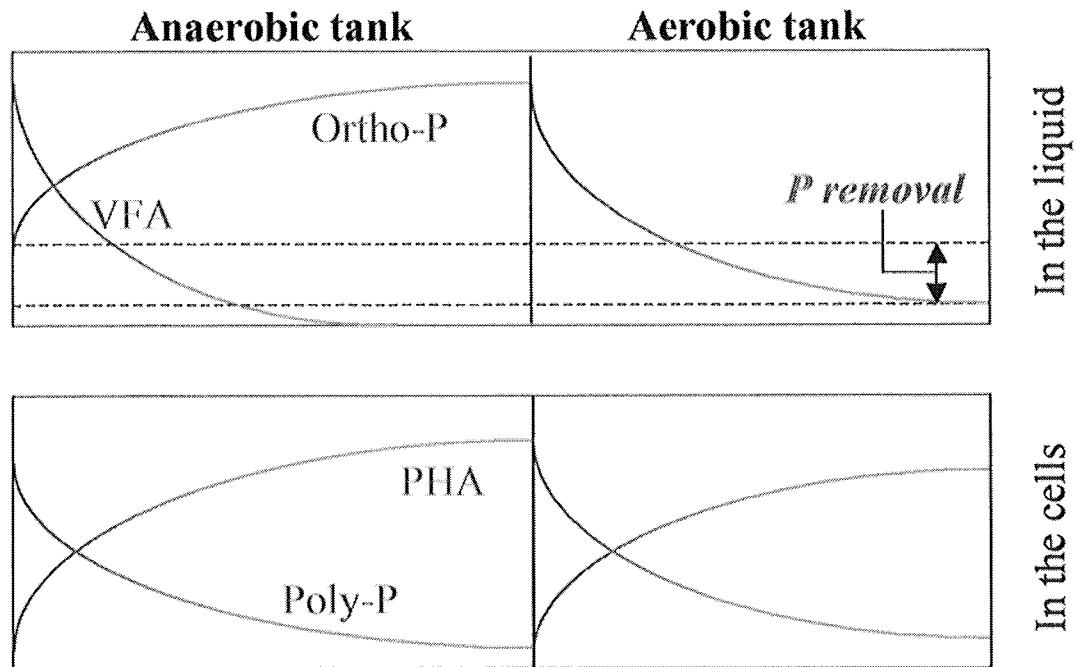
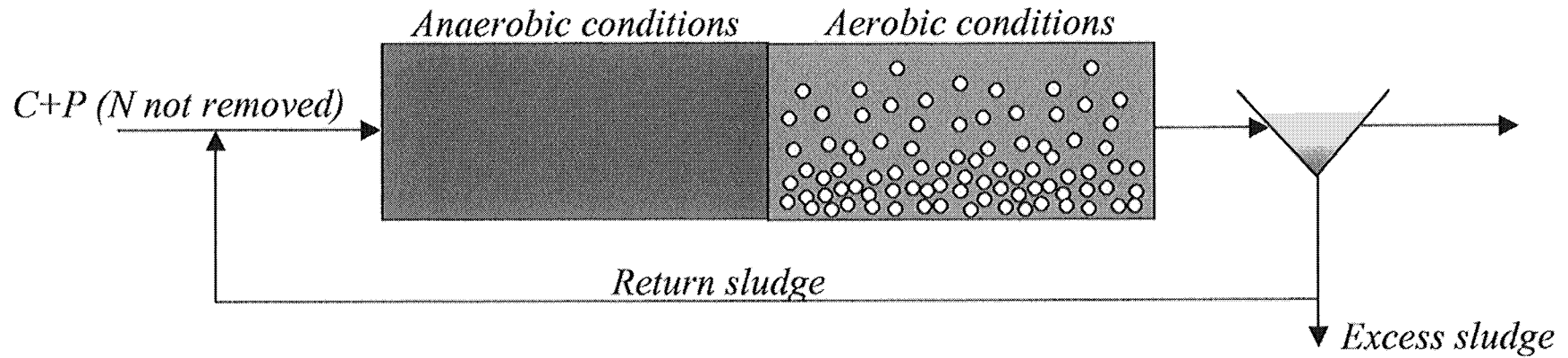


Chemicals used : aluminium salts ($\rightarrow Al(OH)_3 + AlPO_4$)
 iron salts ($\rightarrow FePO_4 + Fe(OH)_3$)
 lime ($\rightarrow Ca_5 (PO_4)_3 OH + CaCO_3$)

Chemical phosphorus removal

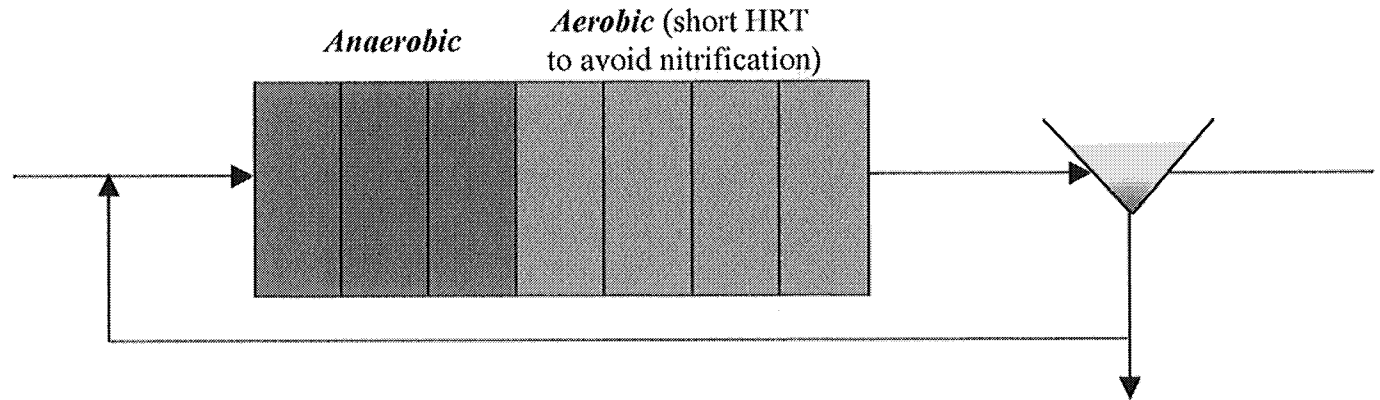


Biological Phosphorus Removal



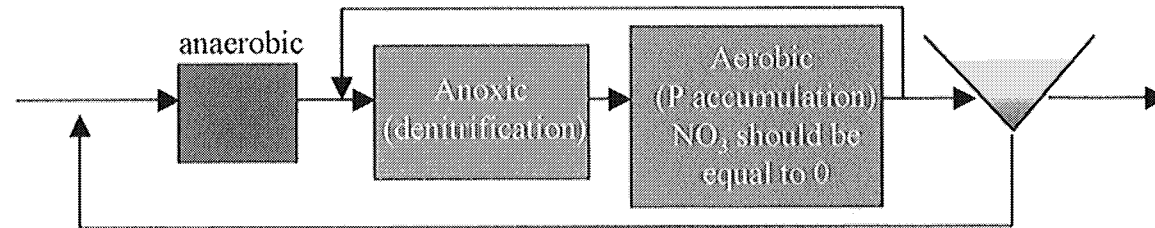
Biological phosphorus removal

A/O process

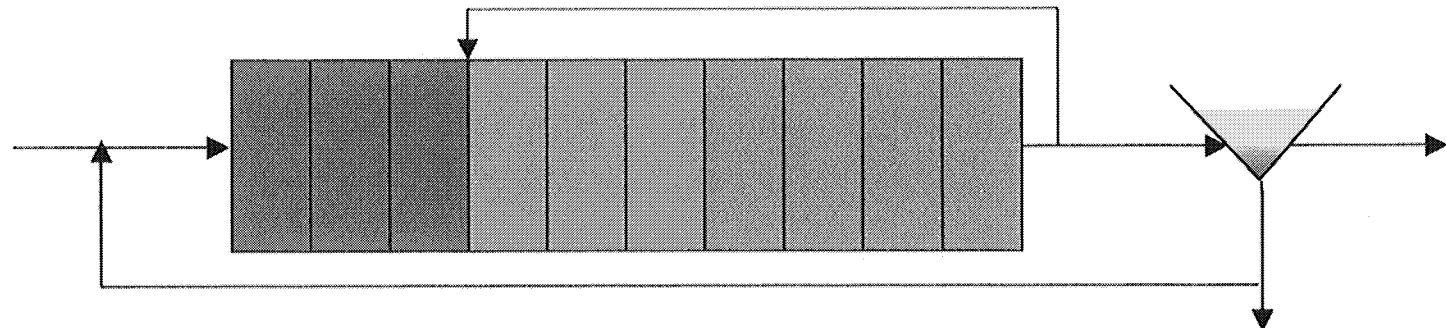


Combined biological carbon, nitrogen and phosphorus removal

Modified Phoredox



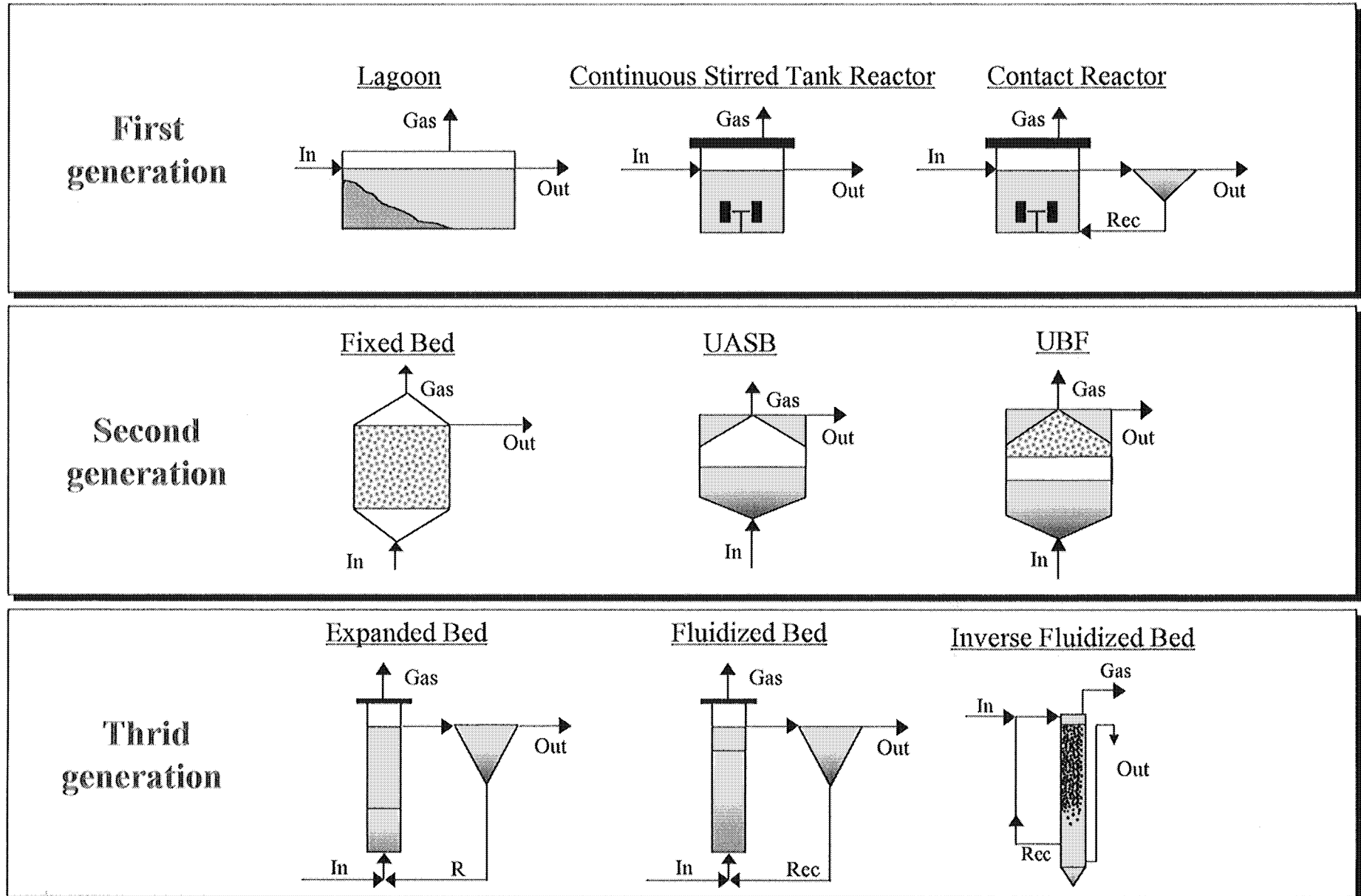
A₂/O



About Biological Treatment ...

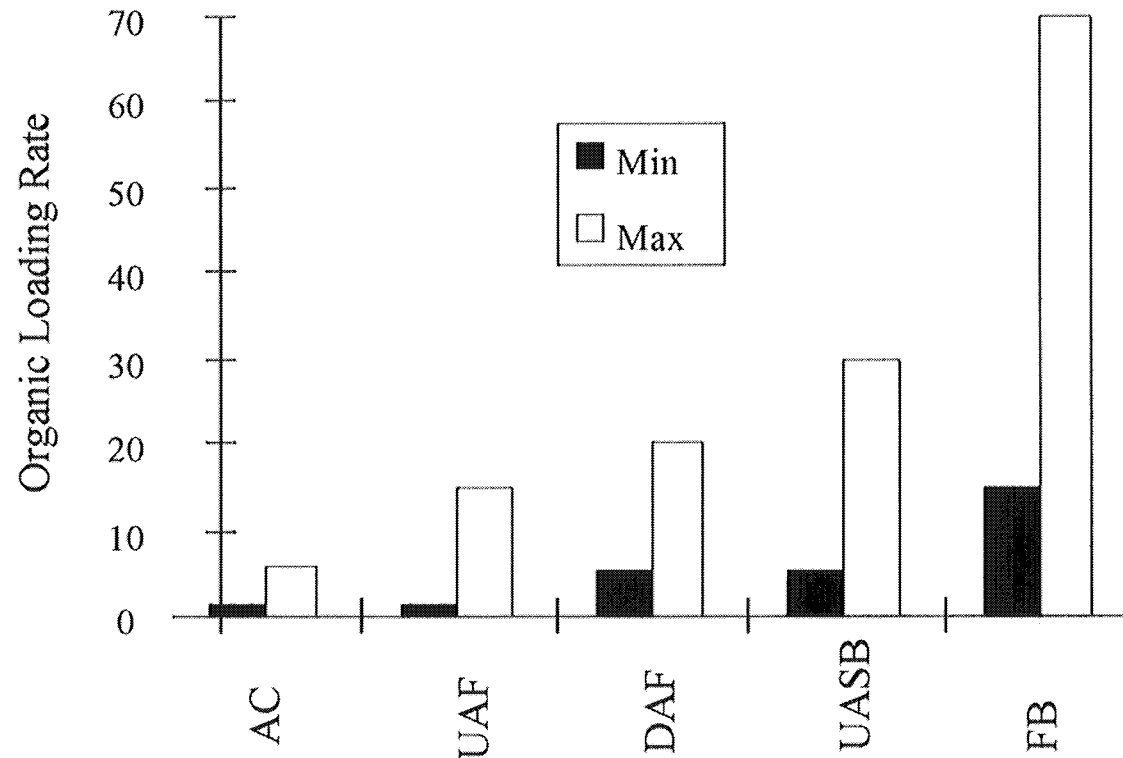
- ⇒ Biological carbon and nitrogen removal is widely adopted.
- ⇒ Phosphorus removal by chemical precipitation is well established and reliable. Biological P-removal processes seem less stable, partly because of a lack of knowledge.
- ⇒ Actual development of high rate processes :
 - Biofilm reactors : biofilters, fluidized bed reactors,
 - Membrane bioreactors.
- ⇒ Need of monitoring and control, especially for P removal processes.
- ⇒ Actual problems to be solved :
 - Sludge management,
 - Availability of carbon sources for denitrification and enhanced biological phosphorus removal.

Characteristics of WWT Processes



Performances of Anaerobic Digestion Processes (from the literature)

Organic Loading Rate : kg COD/m³/d



AC : Anaerobic Contactor

UASB : Up-flow Anaerobic Sludge Blanket

UAF : Upflow Anaerobic Filter

DAF : Down-flow Anaerobic Filter

FB : Fluidized Bed

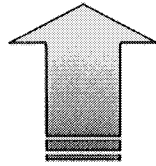
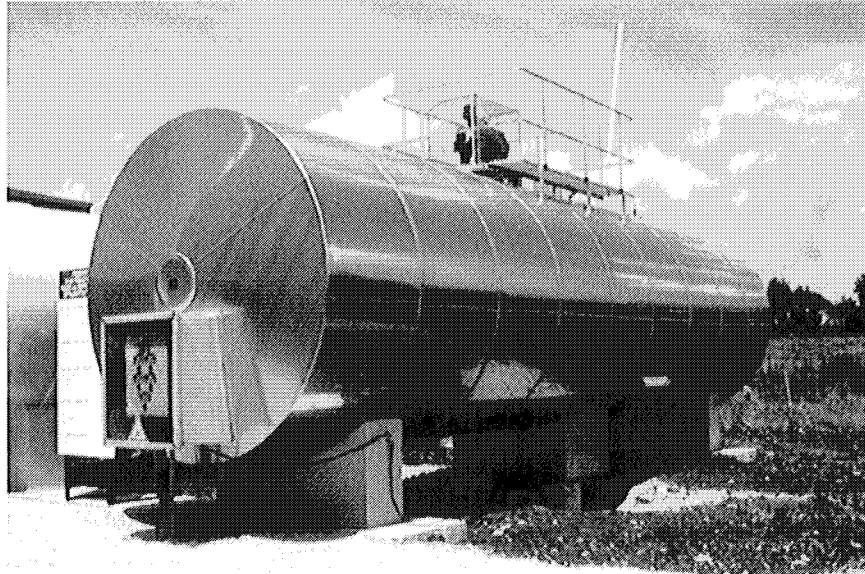
Anaerobic Lagoon

(LBE-INRA, Narbonne)



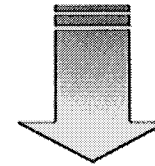
Sequencing Batch Reactor

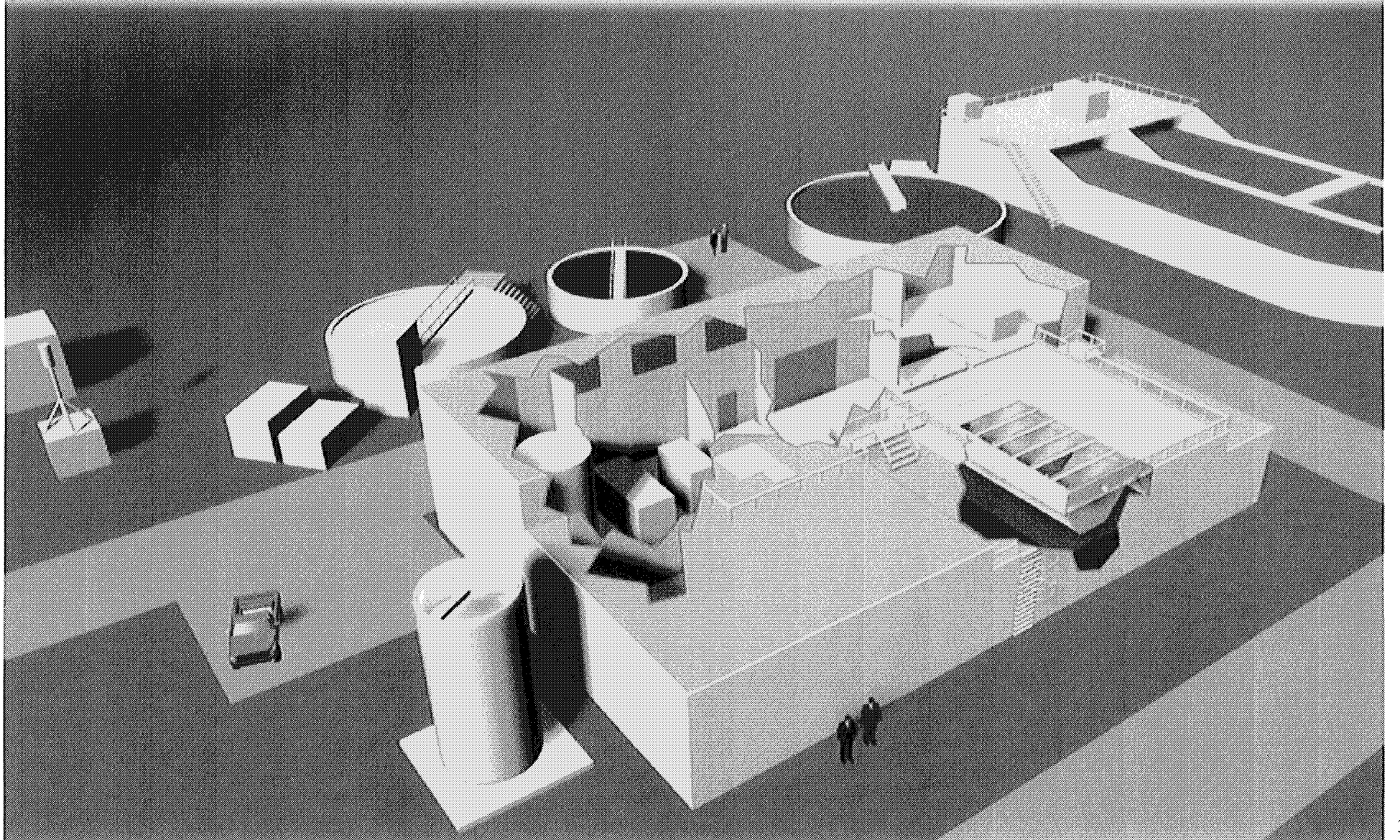
(Narbonne and Le Fied, France)



*For cheese making
wastewater*

*For wine distillery
wastewater*







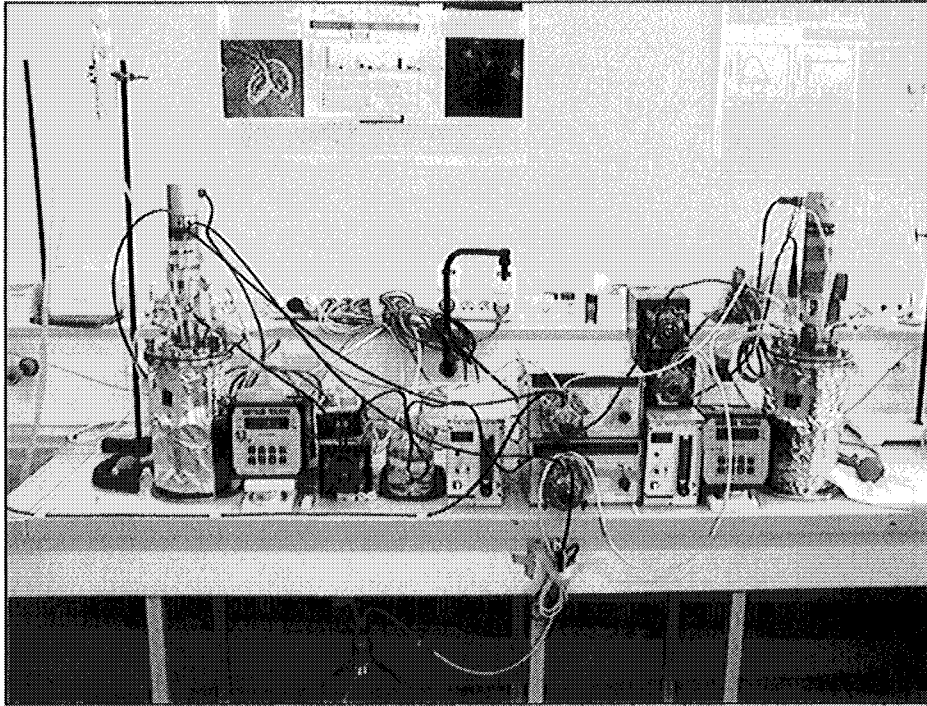
KoSa, Vlissingen

(BIOTHANE Systems International)



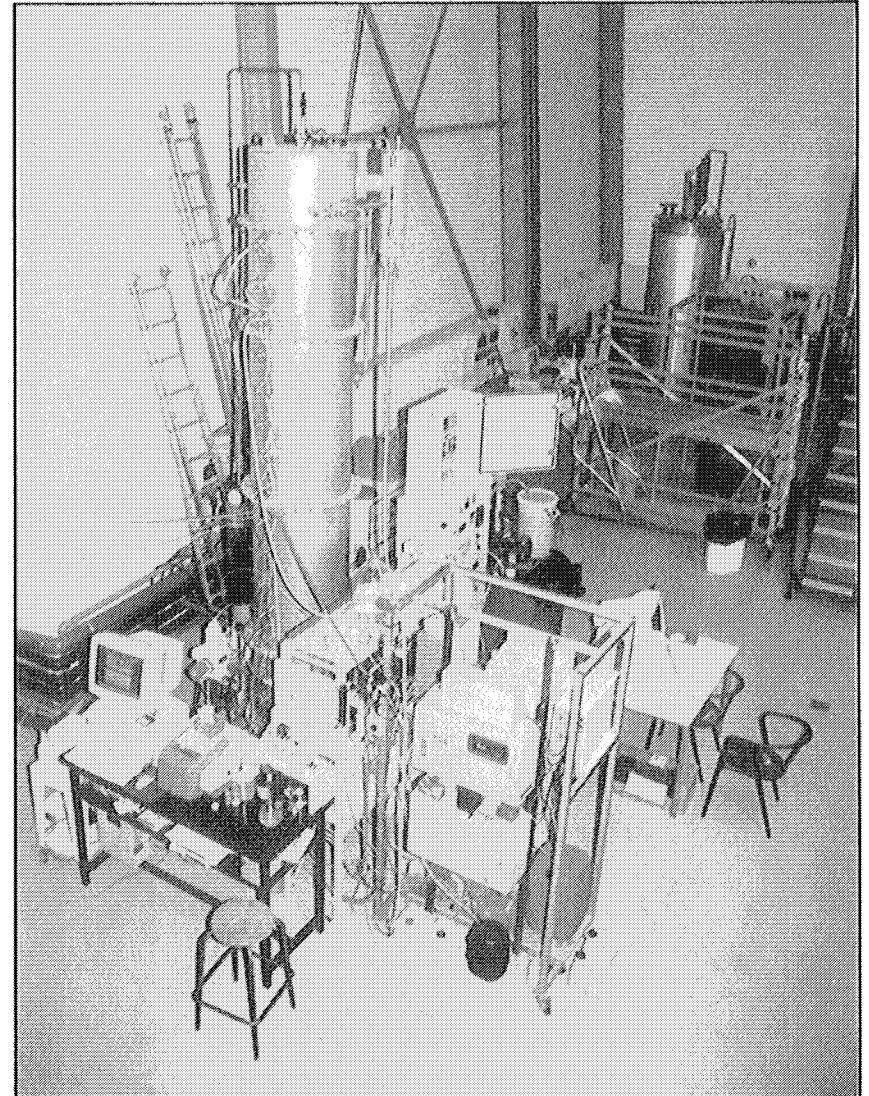
At the Laboratory Scale

(LBE-INRA, Narbonne)



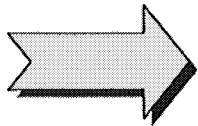
Lab Scale

Pilot Scale



Contents of the Presentation

1) Problem statement



2) Difficulties in Modeling

2.1) Problem Statement

2.2) An Experimental Illustration

3) Difficulties in Control

4) An integrated approach

Model structure and model complexity can only be defined according to the objective we want to achieve :
To elaborate a model without referring to its goal is a nonsense ...



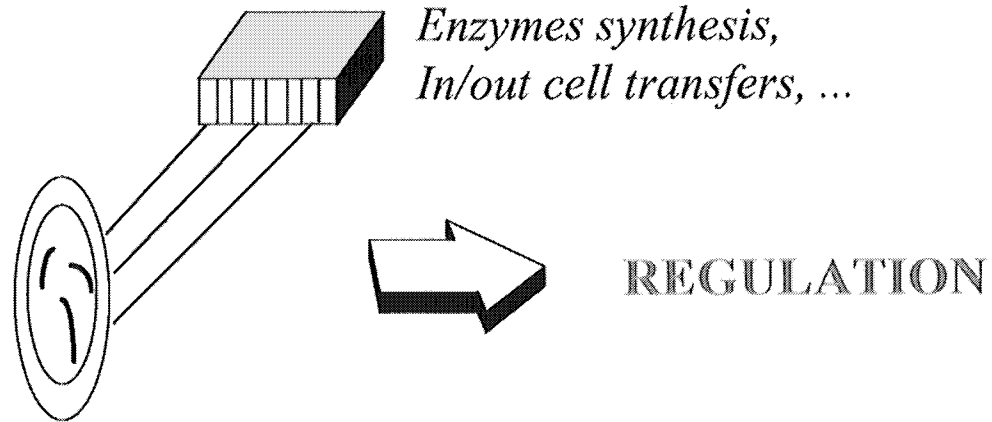
Among other advantages, mathematical modeling is useful and helpful :

- To minimize the number of experiments to be run,
- To improve the process design,
- To optimize process operations,
- To test and validate different control strategies.

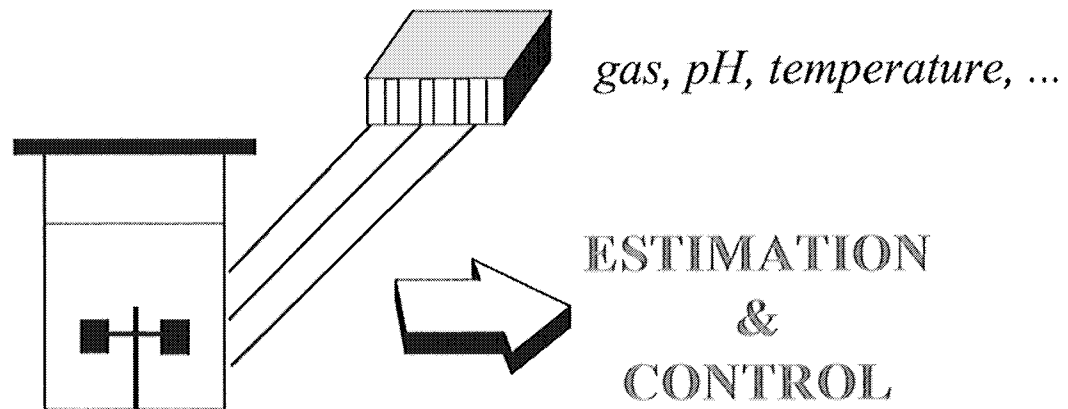
⇒ *Need of pluridisciplinarity in order to get closer to micro-organisms just knowing what happens in their surrounding*

"Ideal" measurements are not always available

In reality :



In practice :

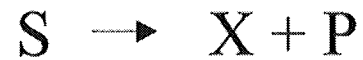


Variation of the quantity in the reactor

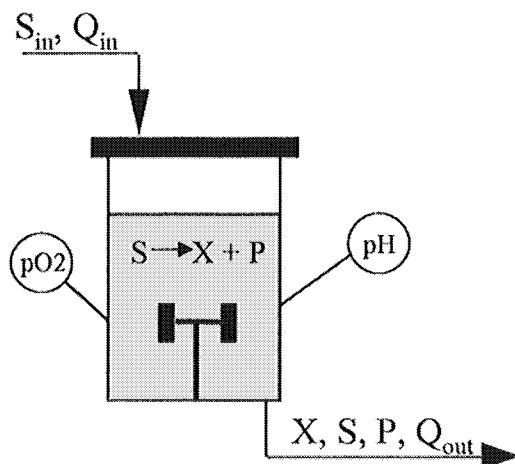
=

input - output + production - consumption

Biological Reaction Scheme :



In a CSTR :



Structure of the model

From :

$$\begin{cases} \frac{d(XV)}{dt} = 0 & -Q_{out}X & +r_XV & -0 \\ \frac{d(SV)}{dt} = +Q_{in}S_{in} & -Q_{out}S & +0 & -r_SV \\ \frac{dV}{dt} = +Q_{in} & -Q_{out} & & \end{cases}$$

To :

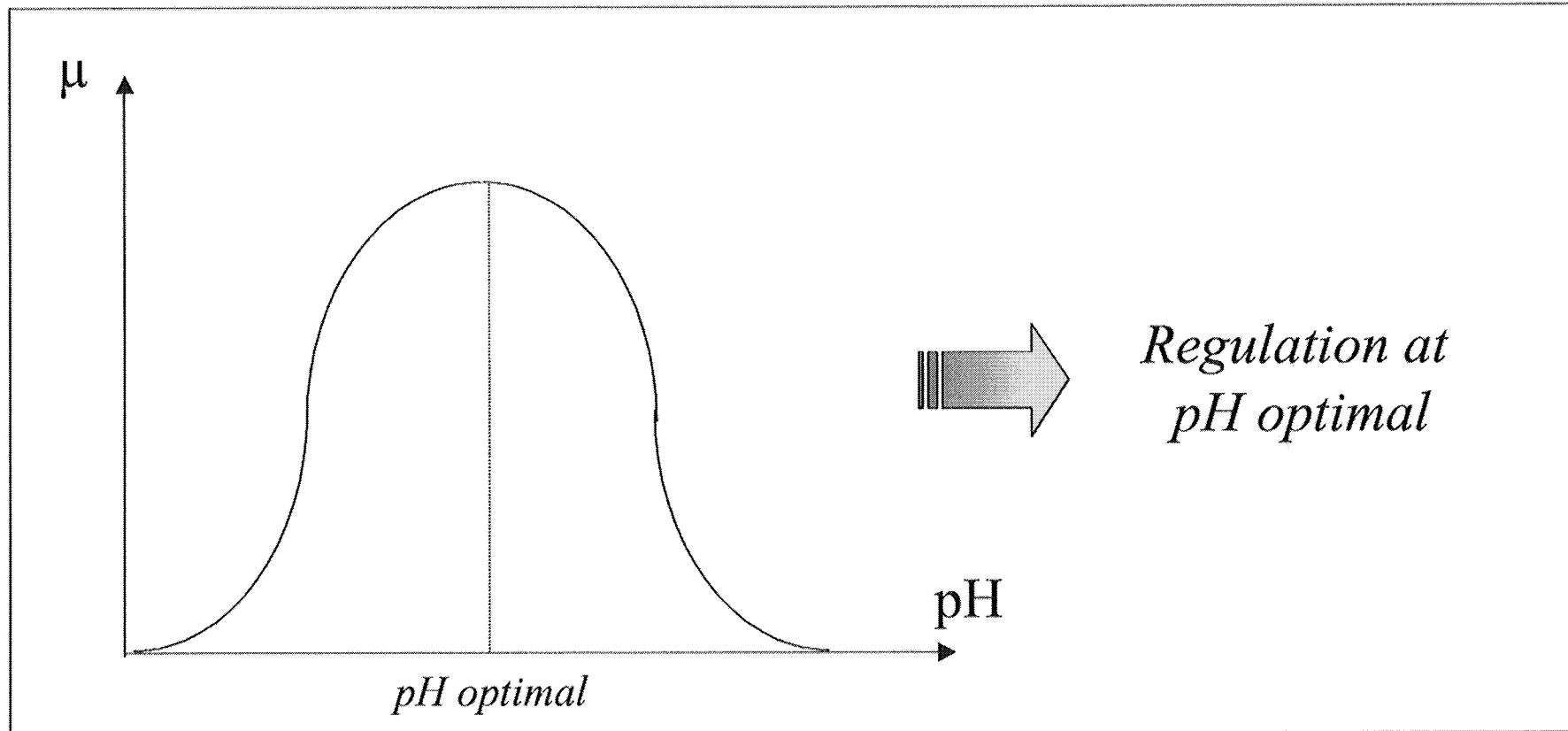
$$\begin{cases} \frac{dX}{dt} = (\mu - D)X \\ \frac{dS}{dt} = -\frac{\mu X}{Y_{X/S}} + D(S_{in} - S) \\ \frac{dV}{dt} = Q_{in} - Q_{out} \end{cases}$$

With D : dilution rate, $Y_{X/S}$: yield coefficient
and μ : specific growth rate

$$\mu = \frac{1}{XV} \frac{d(XV)}{dt} \Rightarrow \mu = f(X, S, P, T, pH, \dots)$$

Modeling of the Specific Growth Rate

Specific Growth rate : $\mu = f(X, S, P, T, pH, \dots)$



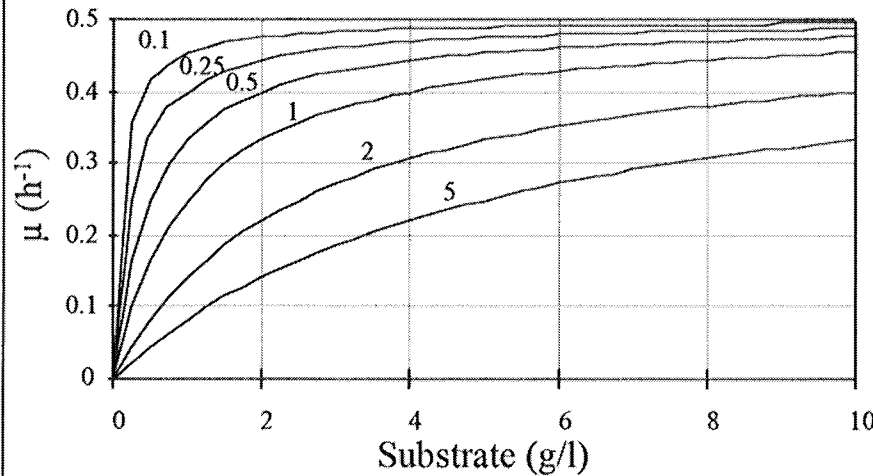
$\mu = f(X, S, P, T, pH, \dots)$ is usually restricted to $\mu = f(S)$

Modeling of the Specific Growth Rate

When $\mu = f(X, S, P, T, pH, \dots)$ is restricted to $\mu = f(S)$

**With only limitation by the substrate :
the Monod law**

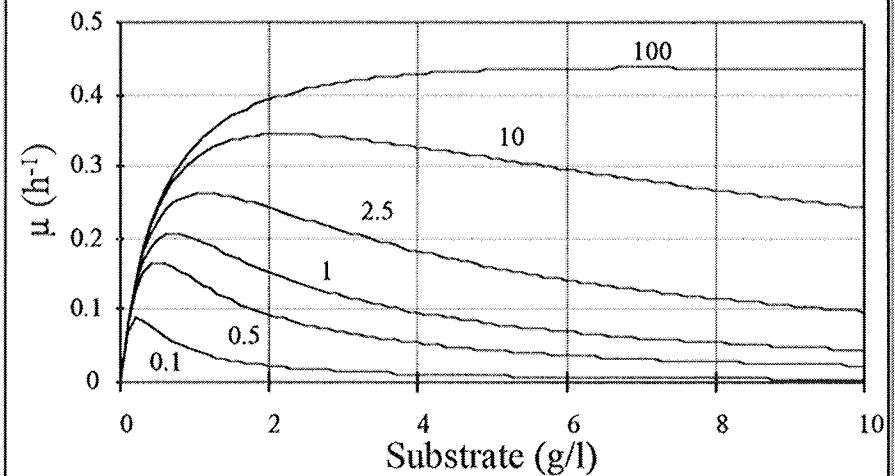
$$\mu = \mu_{\max} \frac{S}{K_S + S}$$



Example with $\mu_{\max} = 0.5 \text{ h}^{-1}$ and $K_S \in [0.1, 5]$

**With limitation and inhibition :
the Haldane law**

$$\mu = \mu_{\max} \frac{S}{K_S + S + \frac{S^2}{K_I}}$$



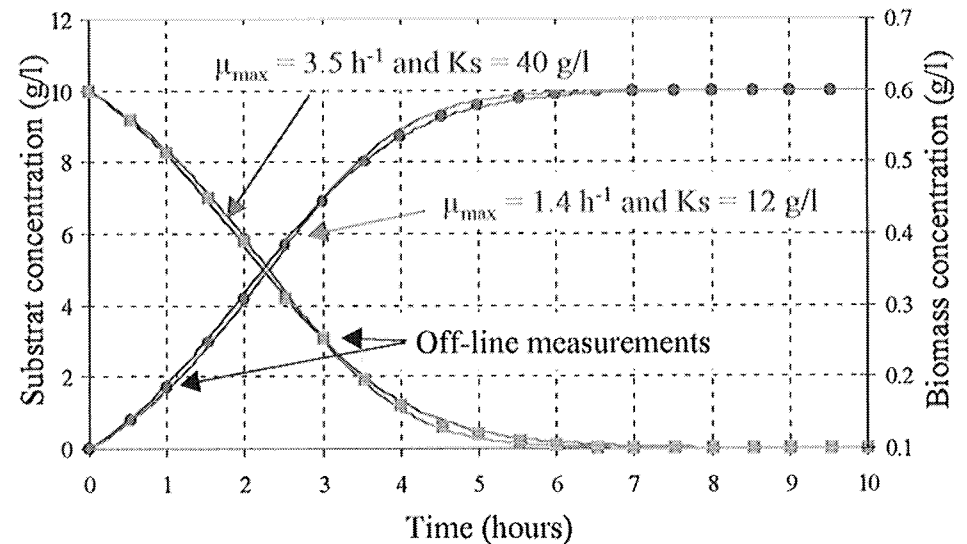
Example with $\mu_{\max} = 0.5 \text{ h}^{-1}$, $K_S = 0.5 \text{ g/l}$
and $K_I \in [0.1, 100] \text{ g/l}$

In practice, the identifiability of the kinetic is far from being guaranteed !...

For example :
$$\mu = \mu_{\max} \frac{S}{K_s + S}$$

Cultivation	Initial substrate So (g/l)	Estimated Kinetic Coefficient	
		μ^* (h ⁻¹)	Km (g/l)
1	11.6	1.0 +/- 2.0	16.8 +/- 22.3
2	7.0	1.1 +/- 0.8	1.8 +/- 2.2
3	18.2	0.7 +/- 0.2	12.9 +/- 14.6
4	25.0	0.3 +/- 0.2	7.0 +/- 11.9

Identification results of the kinetic coefficient μ^* and Km



Simulation with two different sets of kinetic coefficients

From A. Holmberg (1983) : *On the accuracy of estimating the parameters of models containing Michaelis-Menten type nonlinearities*, in G.C. Vansteenkiste and P.C. Young (Eds.), *Modelling and Data Analysis in Biotechnology and Medical Engineering*, North-Holland

Hydrolysis

$$\begin{aligned} & \rightarrow K_h \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \frac{X_S / X_H}{K_X + X_S / X_H} X_H \\ & \rightarrow K_h \eta_{NO_3} \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{X_S / X_H}{K_X + X_S / X_H} X_H \\ & \rightarrow K_h \eta_{Fe} \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{X_S / X_H}{K_X + X_S / X_H} X_H \end{aligned}$$

Heterotrophic Organisms

$$\begin{aligned} & \rightarrow \mu_H \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \frac{S_F}{K_F + S_F} \frac{S_F}{S_F + S_A} \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \frac{S_{PO_4}}{K_P + S_{PO_4}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_H \\ & \rightarrow \mu_H \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \frac{S_A}{K_A + S_A} \frac{S_A}{S_F + S_A} \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \frac{S_{PO_4}}{K_P + S_{PO_4}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_H \\ & \rightarrow \mu_H \eta_{NO_3} \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \frac{S_F}{K_F + S_F} \frac{S_F}{S_F + S_A} \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \frac{S_{PO_4}}{K_P + S_{PO_4}} X_H \\ & \rightarrow \mu_H \eta_{NO_3} \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \frac{S_A}{K_A + S_A} \frac{S_A}{S_F + S_A} \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \frac{S_{PO_4}}{K_P + S_{PO_4}} X_H \\ & \rightarrow q_{Fe} \frac{K_{O_2}}{K_{O_2} + S_{O_2}} \frac{K_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{S_F}{K_{Fe} + S_F} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_H \\ & \rightarrow b_H X_H \end{aligned}$$

Phosphorus Accumulating Organisms

$$\begin{aligned} & \rightarrow q_{PHA} \frac{S_A}{K_A + S_A} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \frac{X_{PP} / X_{PAO}}{K_{PP} + X_{PP} / X_{PAO}} X_{PAO} \\ & \rightarrow q_{PP} \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \frac{S_{PO_4}}{K_{PS} + S_{PO_4}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \frac{X_{PHA} / X_{PAO}}{K_{PHA} + X_{PHA} / X_{PAO}} \frac{K_{MAX} - X_{PP} / X_{PAO}}{K_{IPP} + K_{MAX} - X_{PP} / X_{PAO}} X_{PAO} \\ & \rightarrow \mu_{PAO} \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \frac{S_{PO_4}}{K_P + S_{PO_4}} \frac{X_{PHA} / X_{PAO}}{K_{PHA} + X_{PHA} / X_{PAO}} X_{PAO} \\ & \rightarrow b_{PAO} X_{PAO} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \\ & \rightarrow b_{PP} X_{PP} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \\ & \rightarrow b_{PHA} X_{PHA} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \end{aligned}$$

Autotrophics Nitrifying Organisms

$$\begin{aligned} & \rightarrow \mu_{AUT} \frac{S_{O_2}}{K_{O_2} + S_{O_2}} \frac{S_{NH_4}}{K_{NH_4} + S_{NH_4}} \frac{S_{PO_4}}{K_P + S_{PO_4}} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} X_{AUT} \\ & \rightarrow b_{AUT} X_{AUT} \end{aligned}$$

Simultaneous Precipitation of Phosphorus with Fe(OH)₃

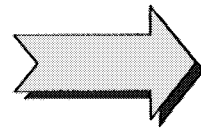
$$\begin{aligned} & \rightarrow k_{PRB} S_{PO_4} X_{MeOH} \\ & \rightarrow b_{RBD} X_{MeP} \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \end{aligned}$$

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1) Problem statement

2) Difficulties in Modeling

2.1) Problem Statement

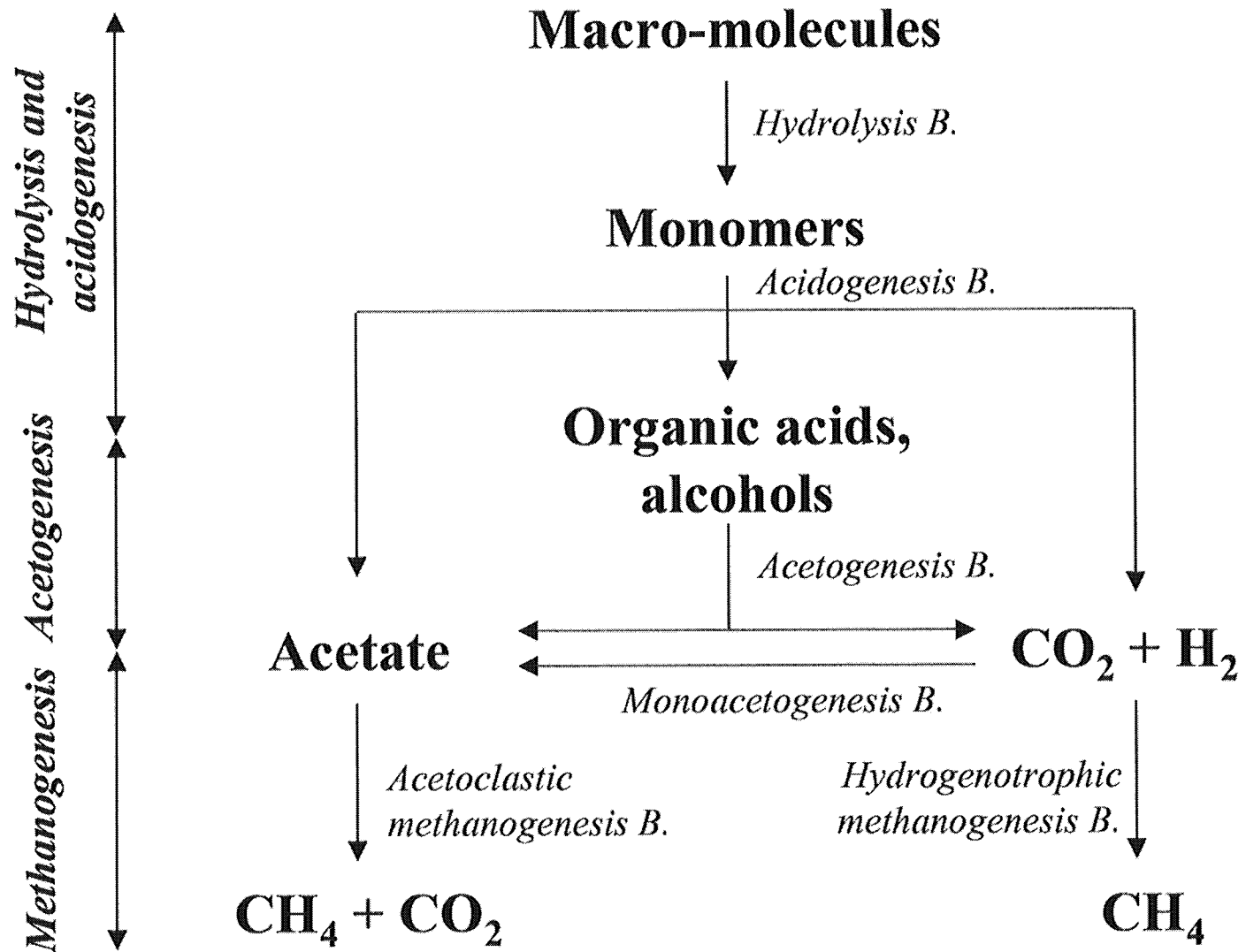


2.2) An Experimental Illustration

3) Difficulties in Control

4) An integrated approach

The Anaerobic Digestion Reaction Scheme



The process used in Narbonne

Influent : **Raw industrial distillery vinasses**

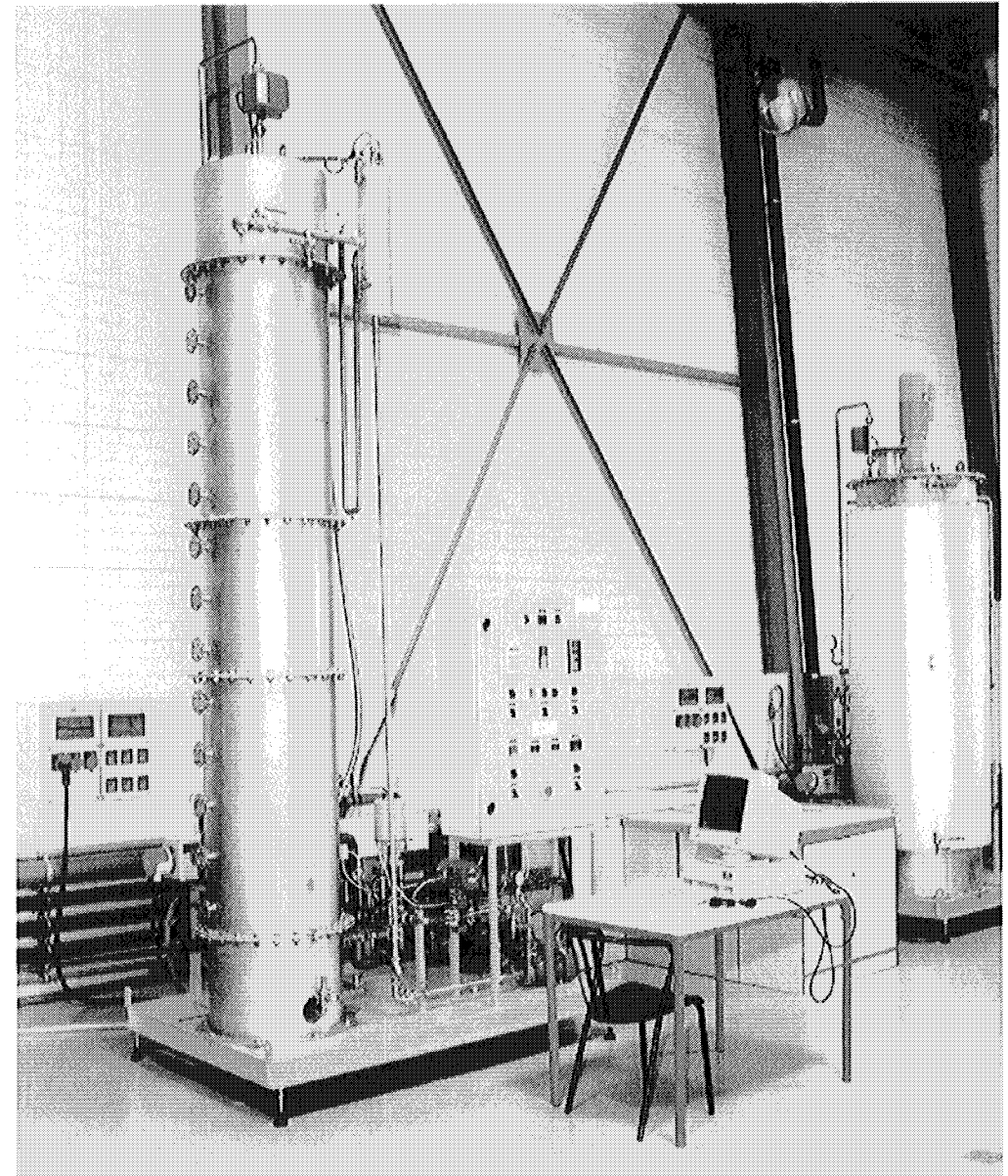
Reactor : **Circular column
Up-flow fixed bed reactor**

- 3.5 m height,
- 0.6 m diameter,
- 982 liters of total volume.

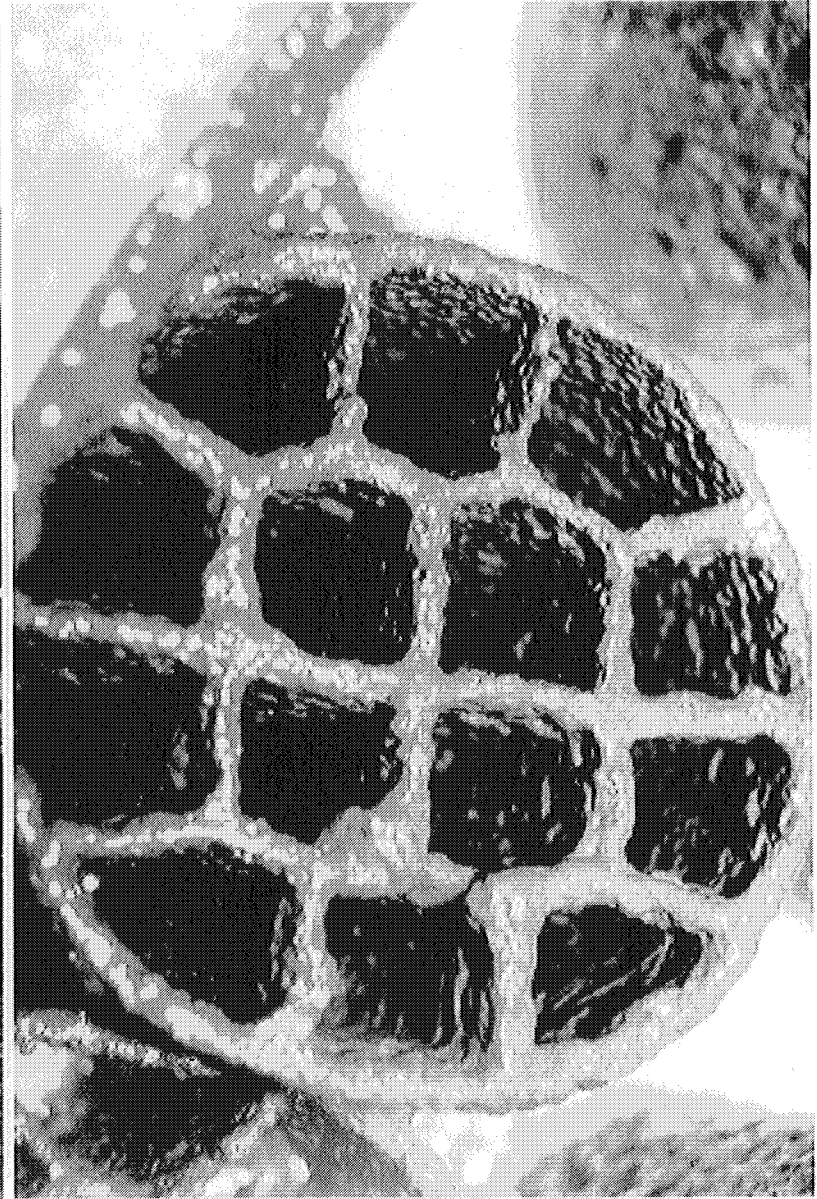
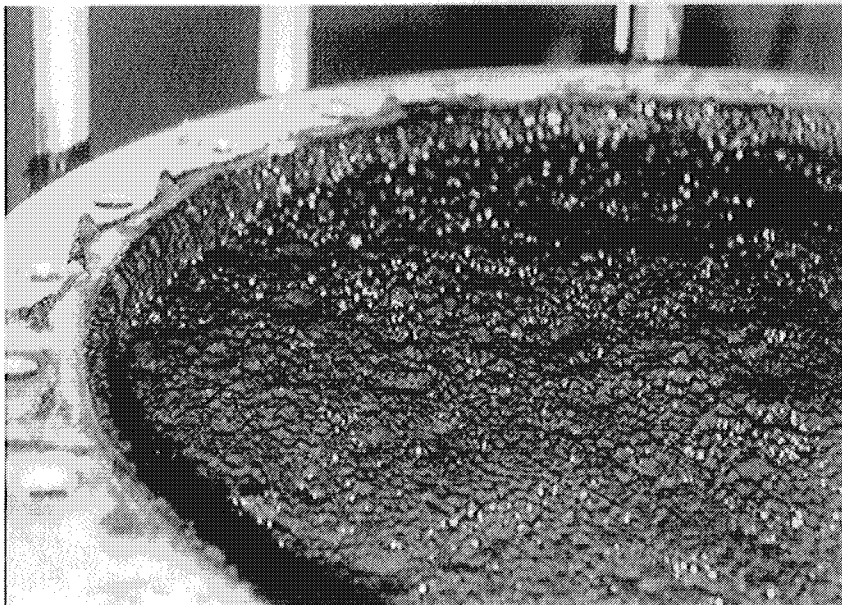
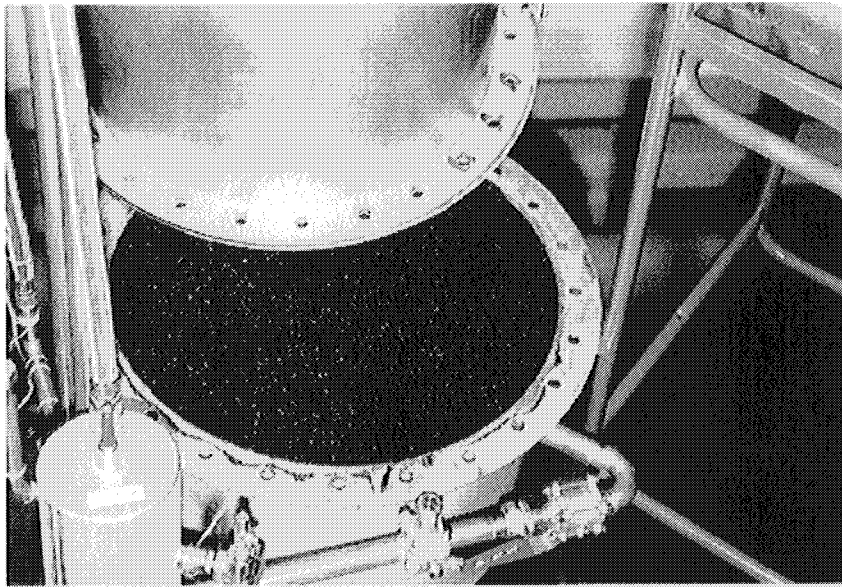
Media : **Cloisonyl**

- Specific surf. : $180 \text{ m}^2/\text{m}^3$
- Volume : 33.7 liters

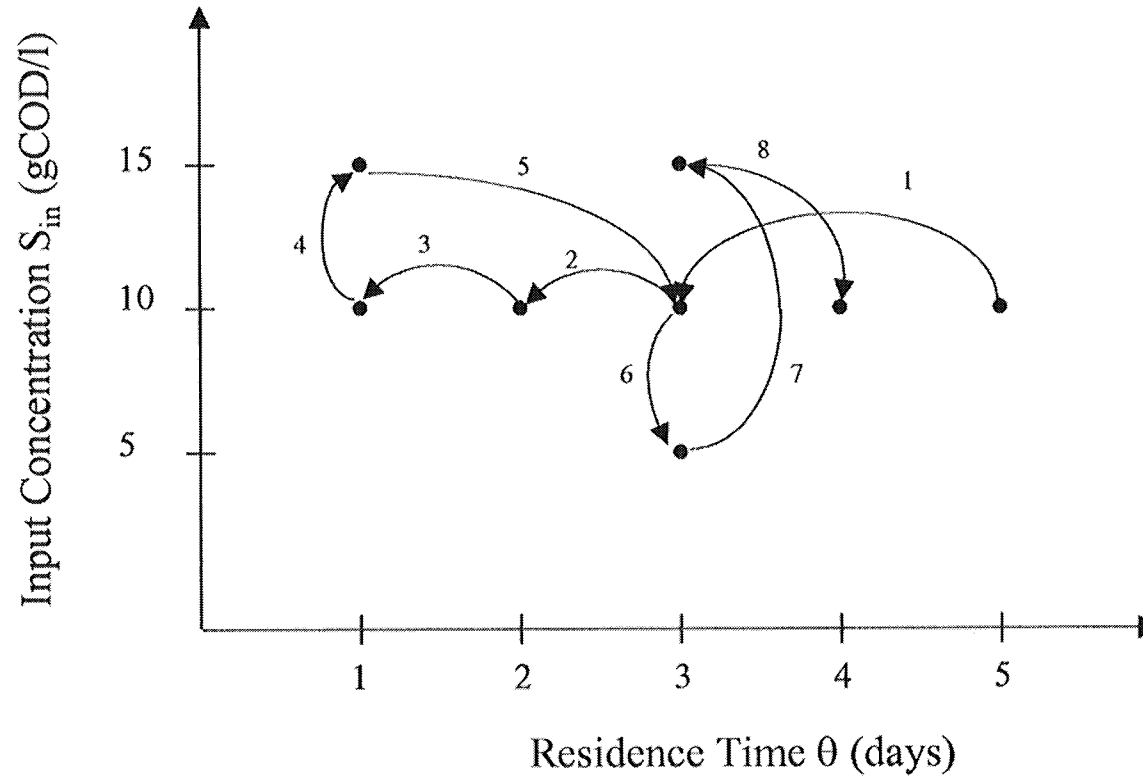
Total effective volume : **948 liters**



Media for Microorganisms (Cloisonnyl)

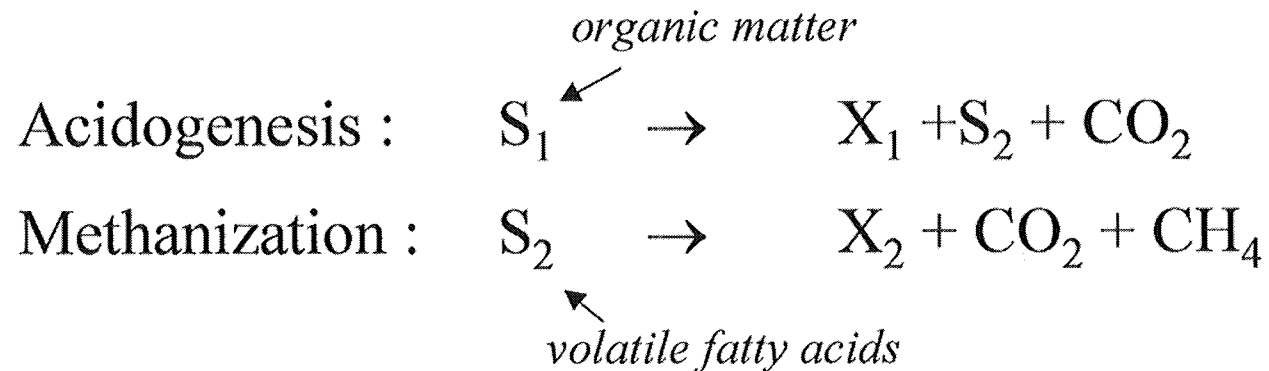


Experimental Protocol for the Modeling of the Process

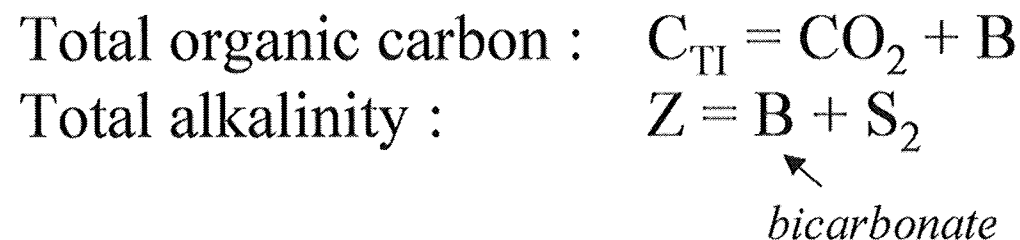


8 transient changes and ... 1 year of heavy experimental work !

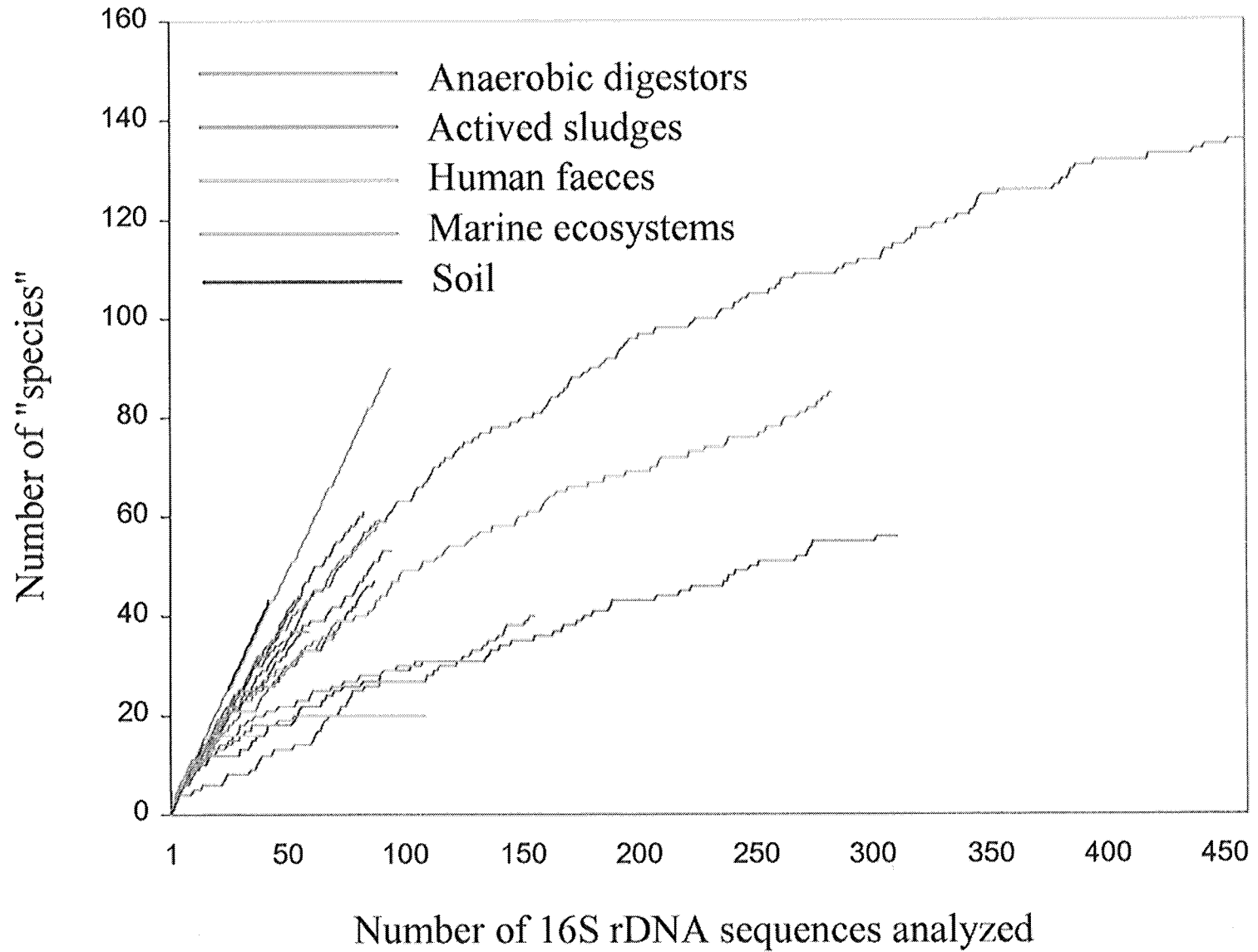
- Starting point : reaction network



- Alkalinity assumptions : $6 \leq \text{pH} \leq 8$ and temperature $\approx 38 \text{ C}$



Anaerobic Digestion is a Complex Ecosystem



The "AMOCO" Anaerobic Digestion Model

(EU FAIR Project CT 1198)

From Mass Balance

$$\left\{ \begin{array}{l} \dot{X}_1 = (\mu_1 - \alpha D) X_1 \\ \dot{X}_2 = (\mu_2 - \alpha D) X_2 \\ \dot{Z} = D(Z^i - Z) \\ \dot{S}_1 = D(S_1^i - S_1) - k_1 \mu_1 X_1 \\ \dot{S}_2 = D(S_2^i - S_2) + k_2 \mu_1 X_1 - k_3 \mu_2 X_2 \\ \dot{C}_{TI} = D(C_{TI}^i - C_{TI}) + k_7 (k_8 P_{CO_2} + Z - C_{TI} - S_2) + k_4 \mu_1 X_1 + k_5 \mu_2 X_2 \end{array} \right.$$

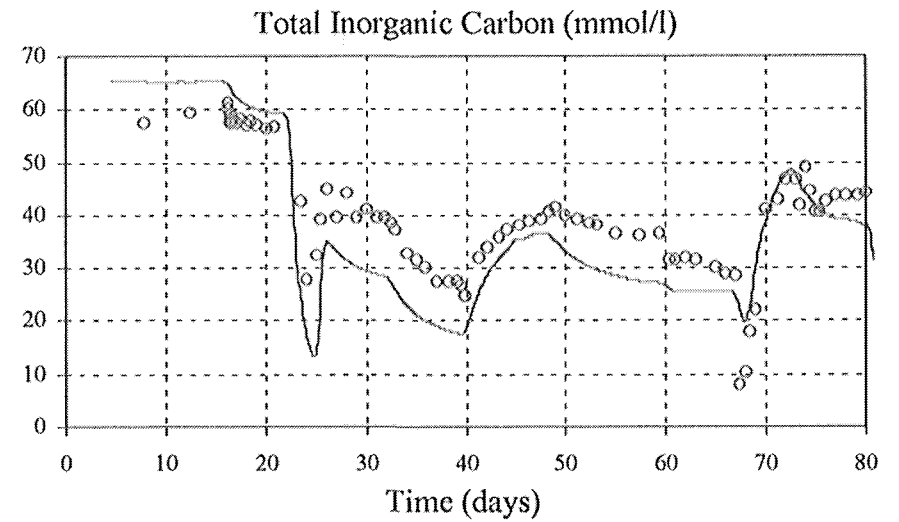
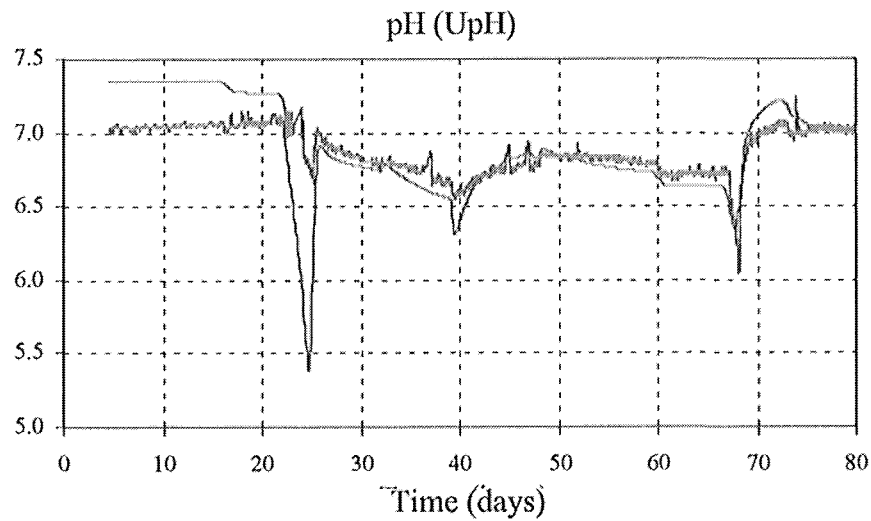
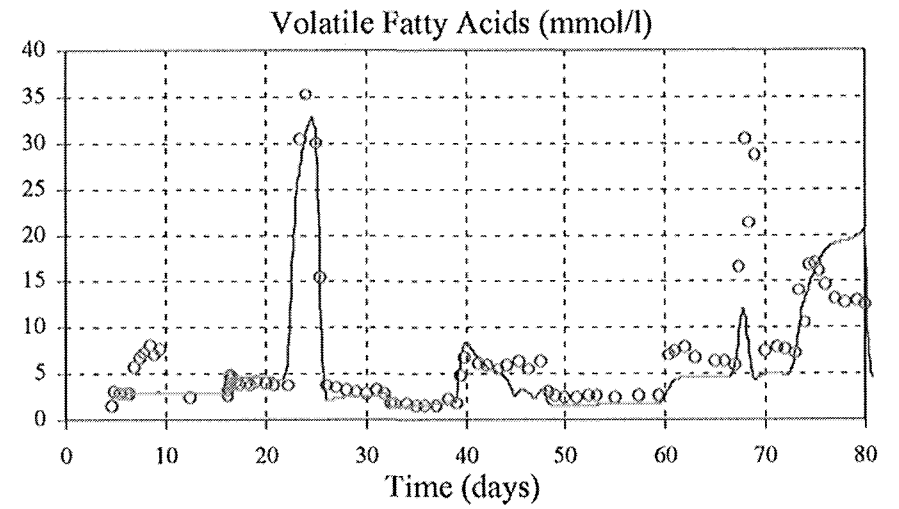
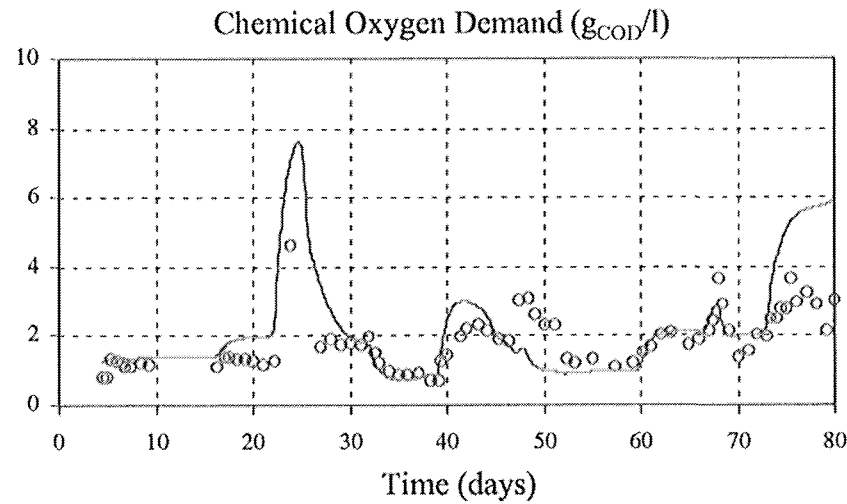
With $\mu_1 = \mu_{\max 1} \frac{S_1}{K_{S_1} + S_1}$ (i.e., limitation by organic matter)

and $\mu_2 = \mu_{\max 2} \frac{S_2}{K_{S_2} + S_2 + \left(\frac{S_2}{K_{I_2}} \right)^2}$ (i.e., limitation and inhibition by VFA)

Process parameters of the "AMOCO" model

Parameter	Meaning	Value
k_1	Yield coefficient for COD degradation	6.6 kg COD/kg X_1
k_2	Yield coefficient for fatty acid production	7.8 ml VFA/kg X_1
k_3	Yield coefficient for fatty acid consumption	611.2 ml VFA/kg X_2
α	Proportion of dilution rate for bacteria	0.5
μ_{max1}	Maximum acidogenic biomass growth rate	1.2 day ⁻¹
μ_0	Maximum methanogenic biomass growth rate	0.69 day ⁻¹
K_{S_1}	Saturation parameter associated with S_1	4.95 kg COD/m ³
K_{S_2}	Saturation parameter associated with S_2	9.28 ml VFA/m ³
K_{I_2}	Inhibition constant associated with S_2	20 (ml VFA/m ³) ^{1/2}

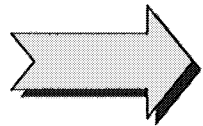
Dynamic simulations vs. experimental data



Contents of the Presentation

1) Problem statement

2) Difficulties in Modeling



3) Difficulties in Control

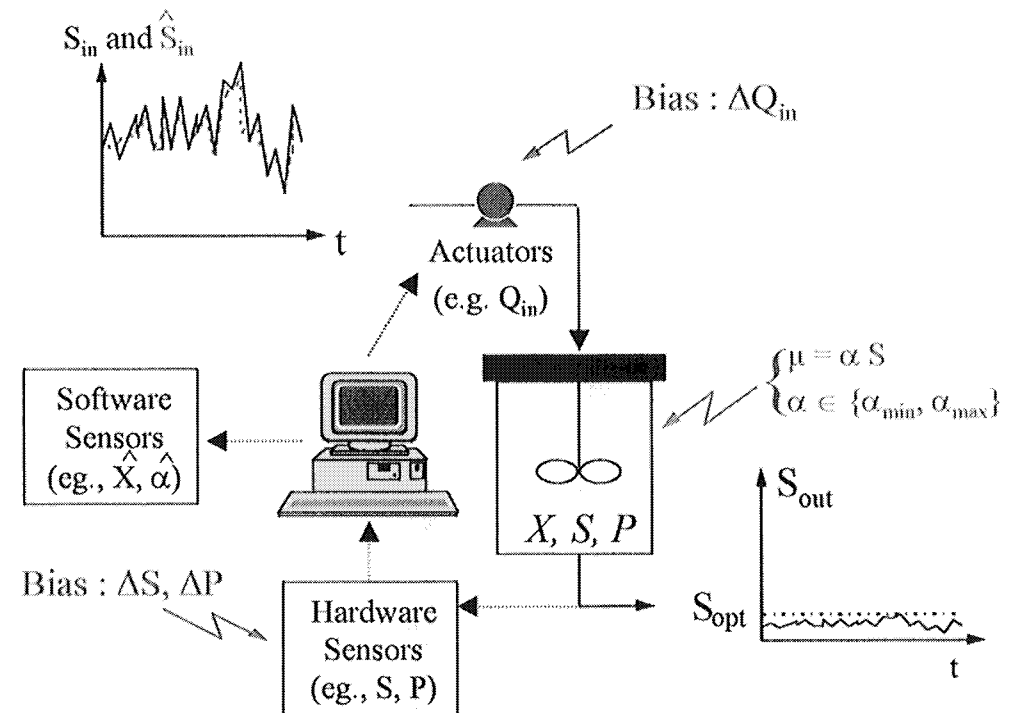
4) An integrated approach

Main Requirements for Process Control

- ✓ Insensitivity to unmodeled or approximated phenomena,
- ✓ Insensitivity to variations of model parameters,
- ✓ Both short and long time scale disturbances rejection,
- ✓ Handling of constraints for state and control variables.

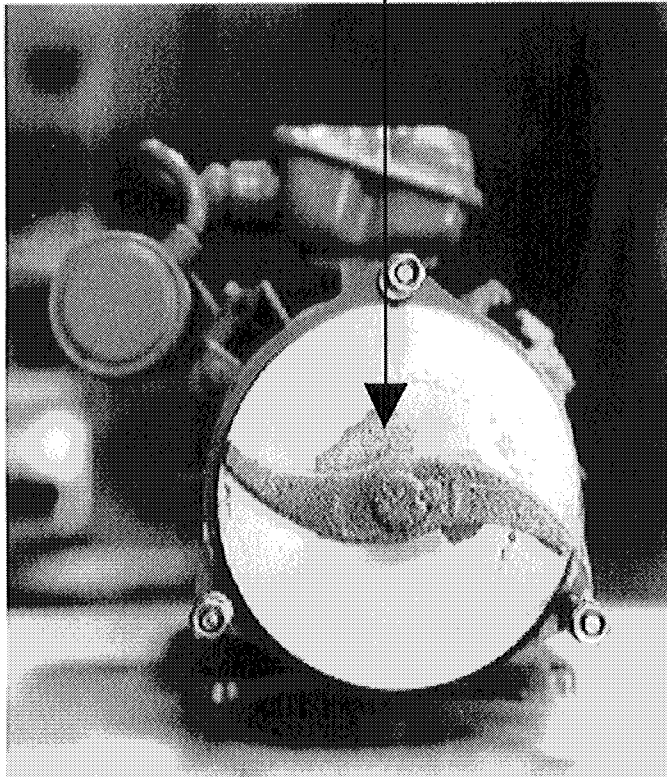
Objectives :

Process regulation in the presence of internal/external disturbances and uncertainty

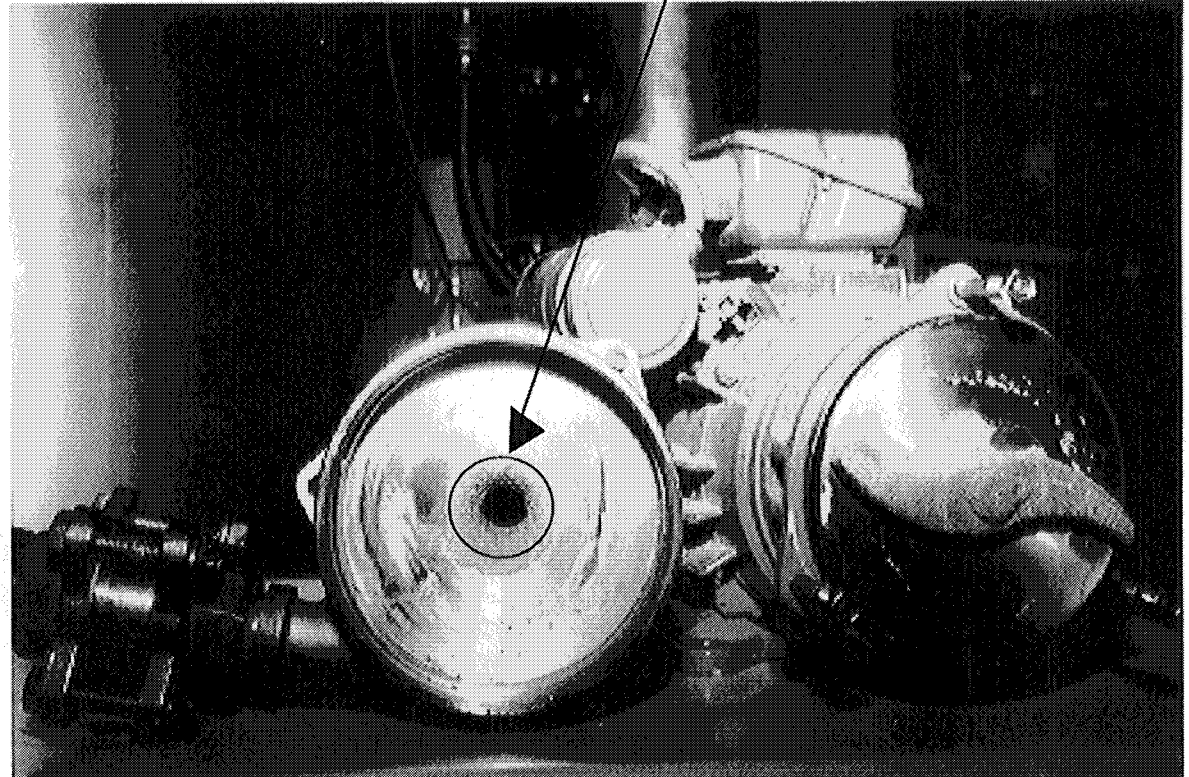


There are also Technical Problems

Pure Struvite appears on the pump

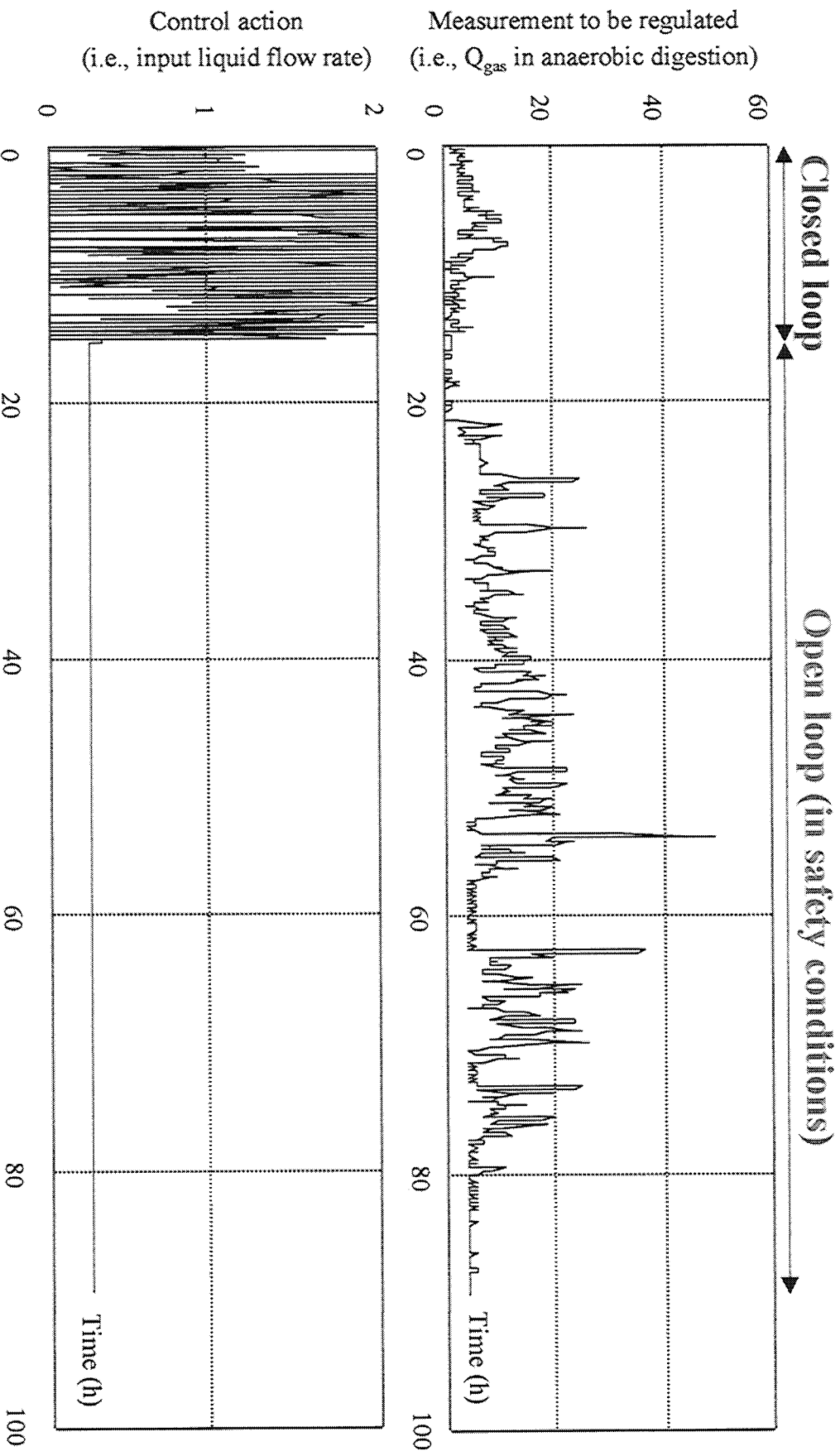


Original hole for the pipe



Pipe Clogging due to Struvite Formation
(and pumps are very often used as main actuators)

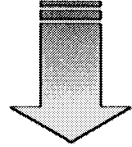
Consequences of the Unappropriate Tuning of a Control Law



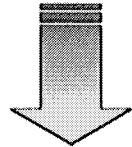
*It took more than a week for the process to recover
(i.e., during this time, the wastewater was not treated !...)*

Consequences of a Technical Problem

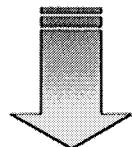
Birds on wires



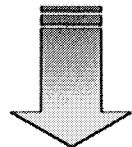
Electricity shutdown



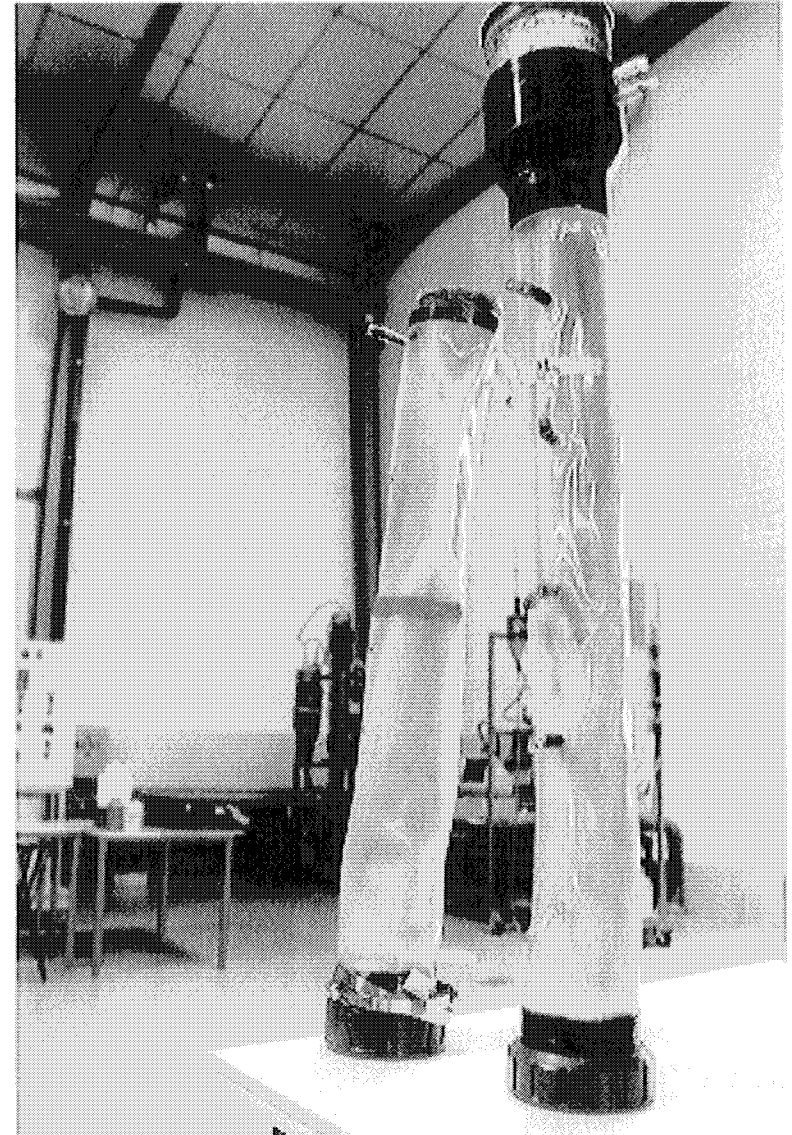
*Problem with temperature regulation
(boiling water in the jacket)*



Melted reactors !!!



Everything is lost ...

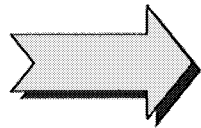


Contents of the Presentation

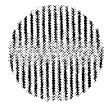
1) Problem statement

2) Difficulties in Modeling

3) Difficulties in Control

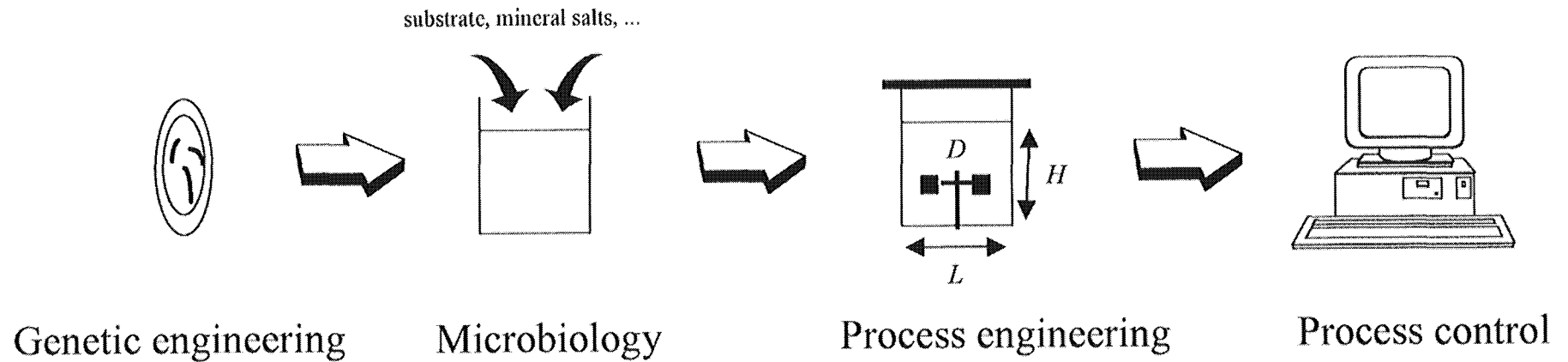


4) An integrated approach

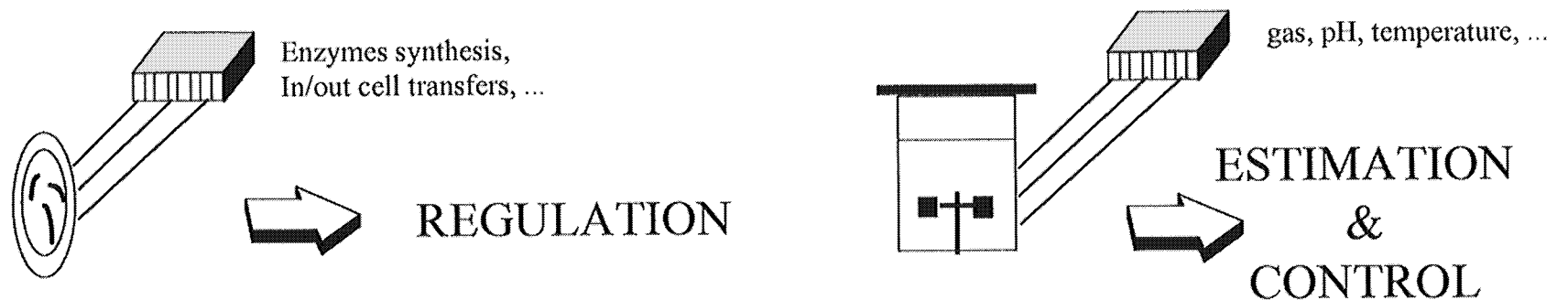


INRA *Bioprocesses from the process control "point of view"*

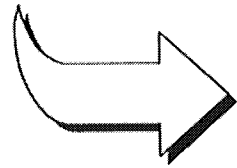
- Process control is usually assumed to be helpful *at the end* of the bioprocess



- "Ideal" measurements are not always available



Step 1 : Selection of the microorganism(s)



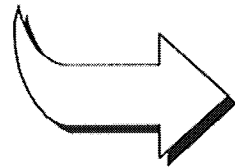
GENETIC ENGINEERING

- What are the most appropriate species ?
- Change (if possible) of the genetics of the cells

Reactor size : the cell

On the usual design of a bioprocess

Step 2 : Choice of the optimal conditions

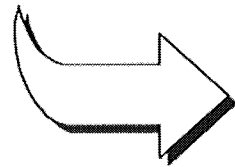


MICROBIOLOGY

- What substrates should be used ?
- What are the best conditions (pH, temperature, ...) ?

Reactor size : 1 ml to 10 liters

Step 3 : Analysis of the hydrodynamics

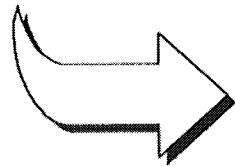


PROCESS ENGINEERING

- What is the best appropriate reactor design ?
- How to improve the mass transfer ?

Reactor size : 1 liter to few cubic meters

Step 4 : Monitoring of the process



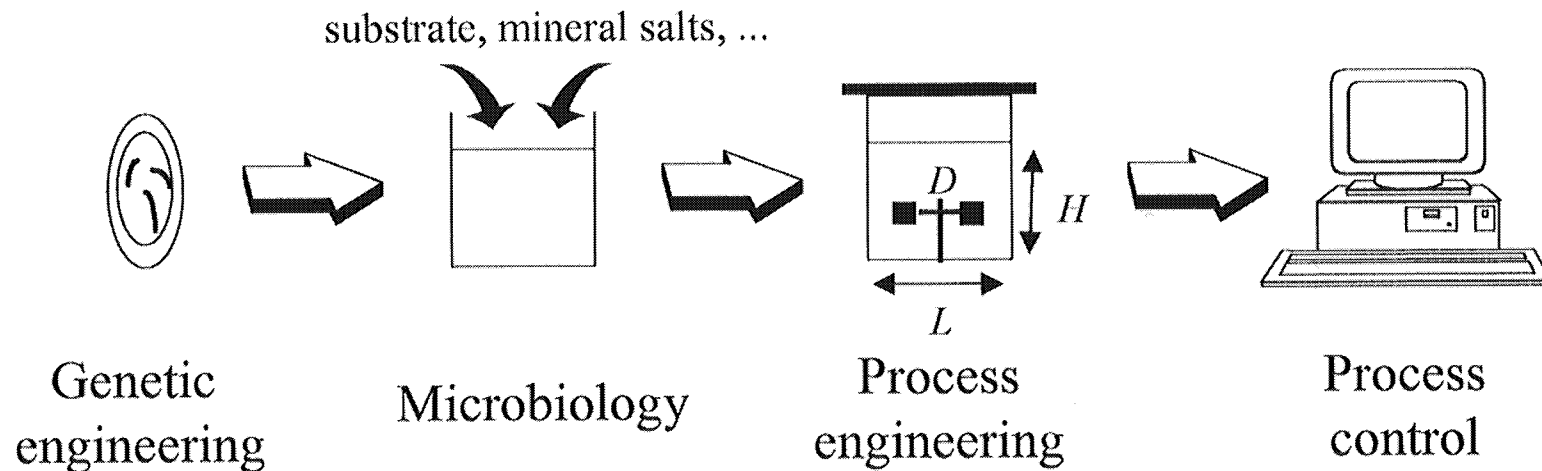
PROCESS CONTROL

- How to improve the available measurements ?
- What is the control law to be applied ?

Reactor size : several liters to few cubic meters

The usual design of a bioprocess is ...

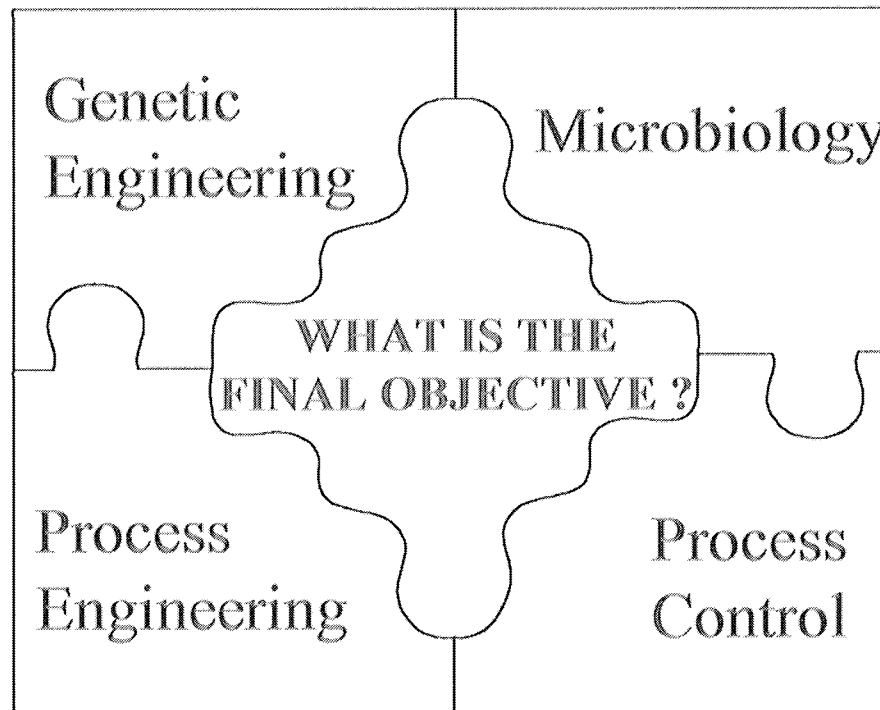
... an "open loop" process



THIS IS FAR FROM BEING OPTIMIZED !...

On a better way to design a bioprocess ...

Every step is of equal importance and should be done accordingly (i.e., in "closed loop")

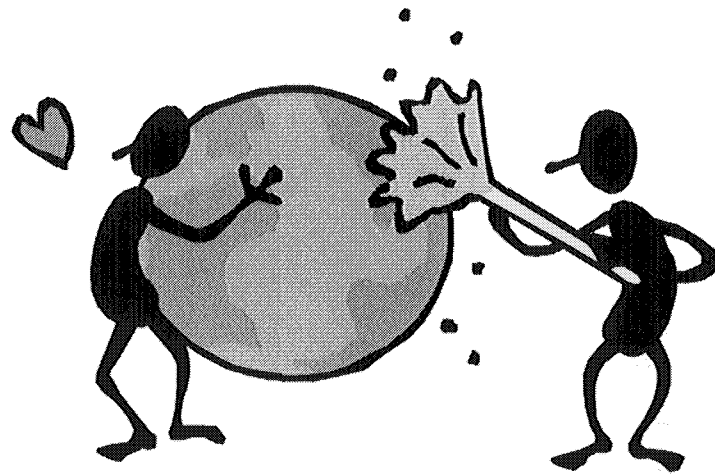


Need for pluridisciplinarity !

$$\frac{d \left[\text{Earth} \right]}{dt} = F \left(\text{Moon}, \text{Space Station}, \text{Control Room} \right)$$

The diagram illustrates the concept of pluridisciplinarity using a mathematical analogy. On the left, the derivative of Earth with respect to time is shown. This is equated to a function F that depends on three variables: the Moon, a Space Station, and a Control Room. Each variable is represented by a small image within a large bracketed structure.

Thank you very much for your attention !



I will be very happy to answer your questions