Automatic control and WWTPs

PARTIE II : Modelling of bioprocesses for environmental purposes

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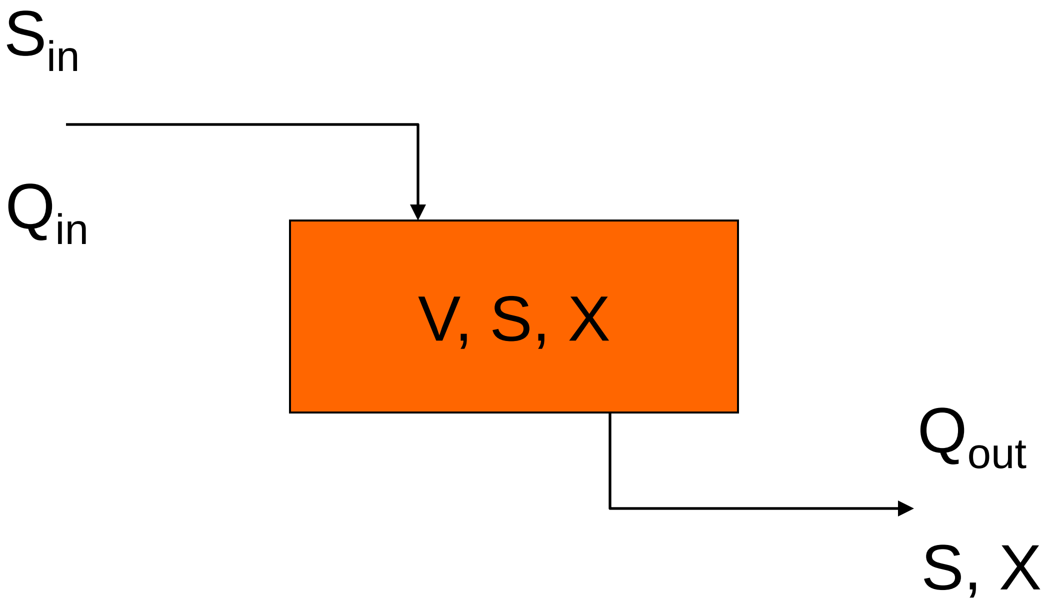
I. Principles of mass-balance modelling



S_{in}

Q_{in}

V, S, X

Q_{out}

S, X

$$\frac{d(SV)}{dt} = \text{"what comes in"} - \text{"what goes out"} + \text{"production"} - \text{"consumption"}$$

I. Principles of mass-balance modelling

Balance =	+ what comes in	- what goes out +	+ what is produced	- what is consumed
$\frac{d(SV)}{dt}=$	$+VS_{in}Q_{in}$	$-VSQ_{out}$		$-kr(x)V$
$\frac{d(XV)}{dt}=$		$-VXQ_{out}$	$+r(x)V$	
$\frac{dV}{dt}=$	$+Q_{in}$	$-Q_{out}$		

with the dimension of $r(x)$ homogeneous to a concentration by time unit and $x=[S,X]^T$ the state vector

I. Principles of mass-balance modelling

However, $\frac{d(SV)}{dt} = V\frac{dS}{dt} + S\frac{dV}{dt}$

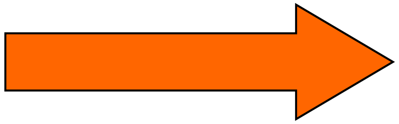
Balance =	+ what comes in	- what goes out	+ what is produced	- what is consumed
$V\frac{dS}{dt} + S\frac{dV}{dt} =$	$+VS_{in}Q_{in}$	$-VSQ_{out}$		$-kr(x)V$
$V\frac{dX}{dt} + X\frac{dV}{dt} =$		$-VXQ_{out}$	$+r(x)V$	
$\frac{dV}{dt} =$	$+Q_{in}$	$-Q_{out}$		

$$\begin{cases} V\frac{dS}{dt} + S\frac{dV}{dt} = V\frac{dS}{dt} + SQ_{in} - \cancel{SQ_{out}} = S_{in}Q_{in} - \cancel{SQ_{out}} - kr(x)V \\ V\frac{dX}{dt} + X\frac{dV}{dt} = V\frac{dX}{dt} + XQ_{in} - \cancel{XQ_{out}} = -\cancel{XQ_{out}} + r(x)V \\ \frac{dV}{dt} = Q_{in} - Q_{out} \end{cases}$$

I. Principles of mass-balance modelling

$$\begin{cases} \dfrac{dS}{dt} = (S_{in} - S)\dfrac{Q_{in}}{V} - k\,r(x) \\[2ex] \dfrac{dX}{dt} = r(x) - \dfrac{Q_{in}}{V}X \\[2ex] \dfrac{dV}{dt} = Q_{in} - Q_{out} \end{cases}$$

- $r(S=0)=0$
- $r(X=0)=0$
- $r(\alpha X)=\alpha\, r(X)$



- $r(x)=\mu(S)X$
- $\mu(0)=0$

I. Principles of mass-balance modelling

General case

$$
\begin{cases}
\dfrac{dS}{dt} = \left(S_{in} - S\right)\dfrac{Q_{in}}{V} - k\mu\left(S\right)X \\
\dfrac{dX}{dt} = \mu\left(S\right)X - \dfrac{Q_{in}}{V}X = \left(\mu\left(S\right) - \dfrac{Q_{in}}{V}\right)X \\
\dfrac{dP}{dt} = -\dfrac{Q_{in}}{V}P + k_P\mu\left(S\right)X \\
\dfrac{dV}{dt} = Q_{in} - Q_{out}
\end{cases}
$$

I. Principles of mass-balance modelling

The continuous reactor

$$Q_{in} = Q_{out} = Q$$

V is constant

$$\begin{cases} \dfrac{dS}{dt} = \left(S_{in} - S\right)\dfrac{Q}{V} - k\mu\left(S\right)X \\ \dfrac{dX}{dt} = \mu\left(S\right)X - \dfrac{Q}{V}X = \left(\mu\left(S\right) - \dfrac{Q}{V}\right)X \\ \dfrac{dP}{dt} = -\dfrac{Q}{V}P + k_P\mu\left(S\right)X \end{cases}$$

I. Principles of mass-balance modelling

The fedbatch reactor

$$\begin{cases} Q_{in} \neq 0 \\ Q_{out} = 0 \end{cases}$$

Le reactor work in a sequential mode

$$\begin{cases} \dfrac{dS}{dt} = \left(S_{in} - S\right)\dfrac{Q}{V} - k\mu\left(S\right)X \\ \dfrac{dX}{dt} = \mu\left(S\right)X - \dfrac{Q}{V}X = \left(\mu\left(S\right) - \dfrac{Q}{V}\right)X \\ \dfrac{dP}{dt} = -\dfrac{Q}{V}P + k_P\mu\left(S\right)X \\ \dfrac{dV}{dt} = Q \end{cases}$$

I. Principles of mass-balance modelling

The batch reactor

$$\begin{cases} Q_{in} = 0 \\ Q_{out} = 0 \end{cases}$$

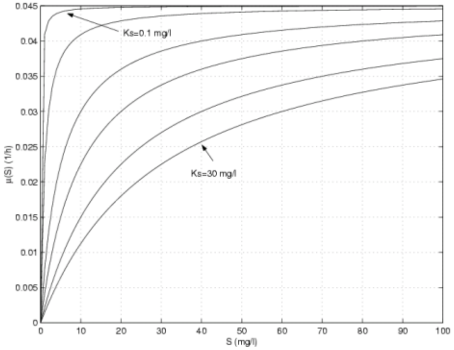
The rteactor works in a sequential mode

$$\begin{cases} \dfrac{dS}{dt} = -k\mu(S)X \\ \dfrac{dX}{dt} = \mu(S)X \\ \dfrac{dP}{dt} = k_P\mu(S)X \end{cases}$$

I. Principles of mass-balance modelling

The microbial kinetics

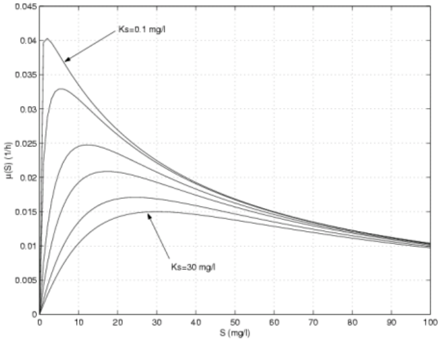
- describe the growth rates,
- captures the nonlinearities and represent the principal limitations in a description of biological phenomena similar to that we can have in physic (presence delays, inaccessibility to measurement, nonlinearity). The kinetics functions remain largely empirical...



The Monod function (1942)

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

The Haldane function (1968)



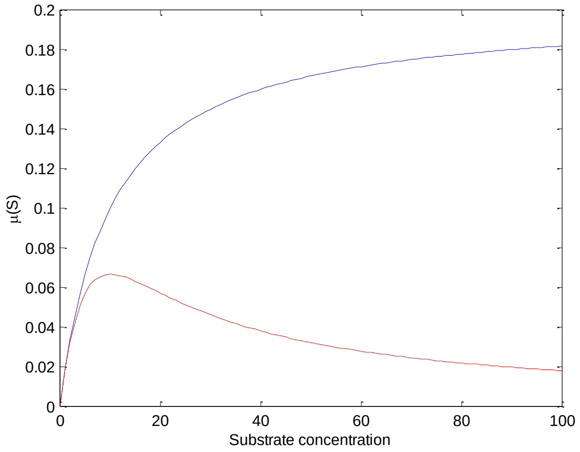
$$\mu(S) = \mu_0 \frac{S}{\left(\frac{S}{K_I}\right)^2 + S + K_S}$$

I. Principles of mass-balance modelling

About the utility of the different operation modes

- *The chemostat*
  - \+ Treats "what comes in at time t" (no storage required),
  - \- Low yields (works at the output substrate concentration),
  - \- The separation phase can be perturbed,
  - \- Contamination risks.

- *The fedbatch reactor*
  - \+ Able to adapt the feeding with respect to the needs of microorganisms,
  - \+ High yields,
  - \+ Allows a better separation than in the chemostat,
  - \- Contamination risks,
  - \- Requires a storage tank.



- *The batch reactor*
  - \+ High yields,
  - \+ No risk of cantamination,
  - \+ Allows a better separation than in the chemostat,
  - \- Requires a storage tank.

II. Modelling of an anaerobic continuous process

2000

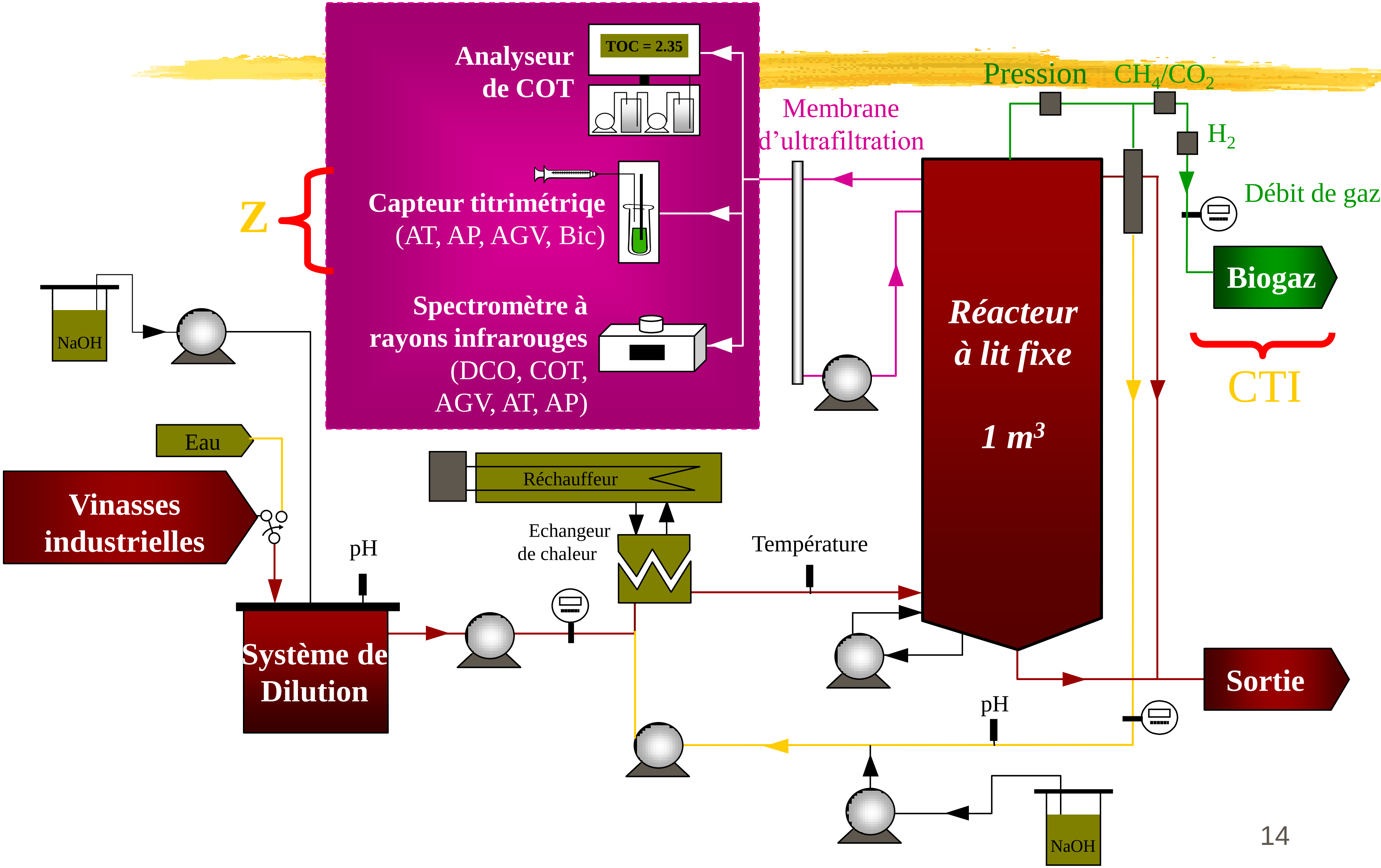
Effluent: **Industrial wine vinasses**

Reactor: **Fixed bed reactors**
circular column

- 3,5 m height,
- 0,6 m diameter,
- 982 liters of total volume.

2006

Process synoptic



Analyseur de COT

TOC = 2.35

Capteur titrimétriqe
(AT, AP, AGV, Bic)

Spectromètre à rayons infrarouges
(DCO, COT, AGV, AT, AP)

Z

Membrane d'ultrafiltration

Pression

CH_4/CO_2

H_2

Débit de gaz

Biogaz

CTI

Réacteur à lit fixe

1 m^3

NaOH

Eau

Vinasses industrielles

pH

Système de Dilution

Réchauffeur

Echangeur de chaleur

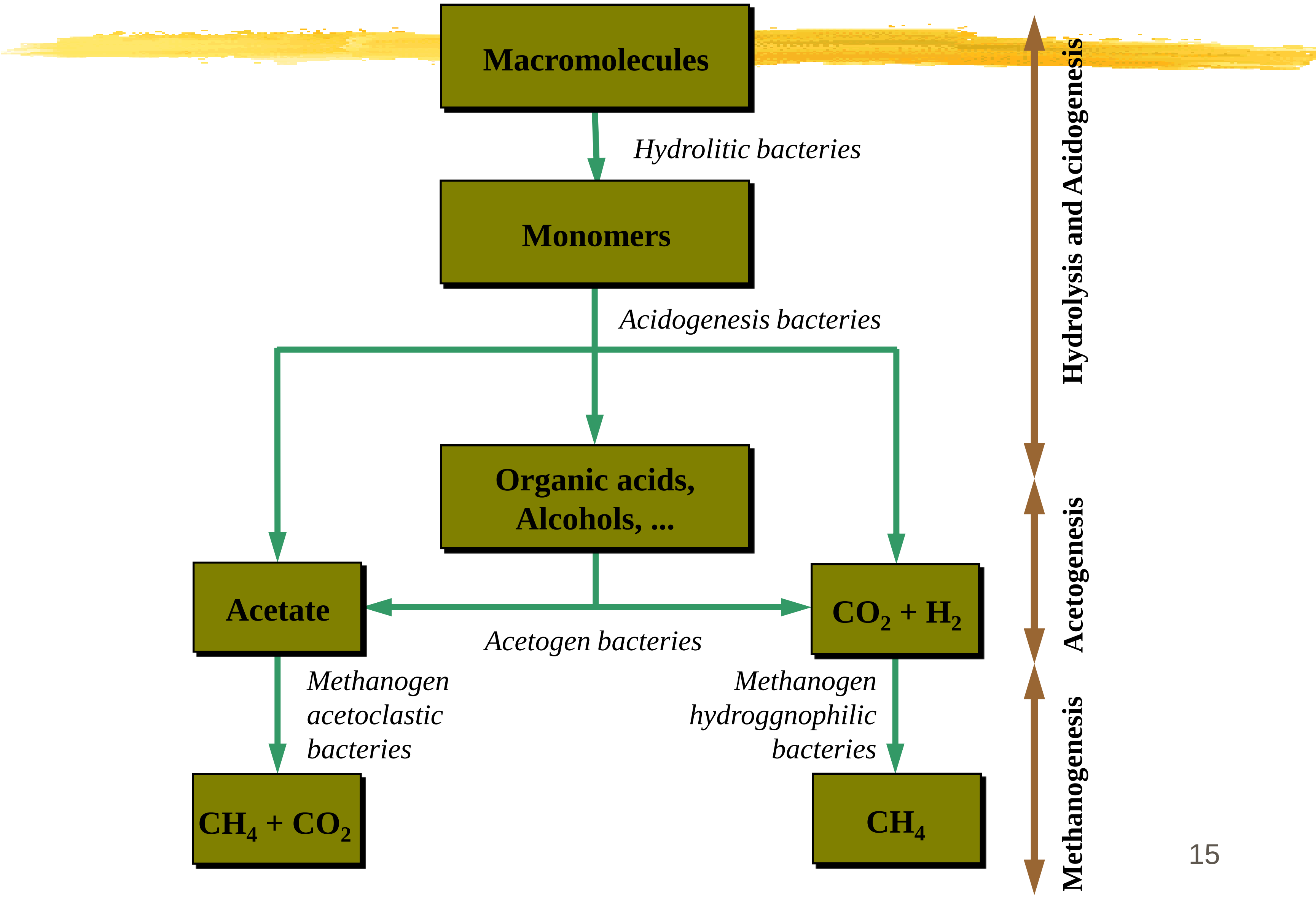
Température

Sortie

pH

NaOH

The anaerobic digestion



Macromolecules

Hydrolitic bacteries

Monomers

Acidogenesis bacteries

Organic acids, Alcohols, ...

Acetate

Acetogen bacteries

$CO_2 + H_2$

Methanogen acetoclastic bacteries

Methanogen hydroggnophilic bacteries

$CH_4 + CO_2$

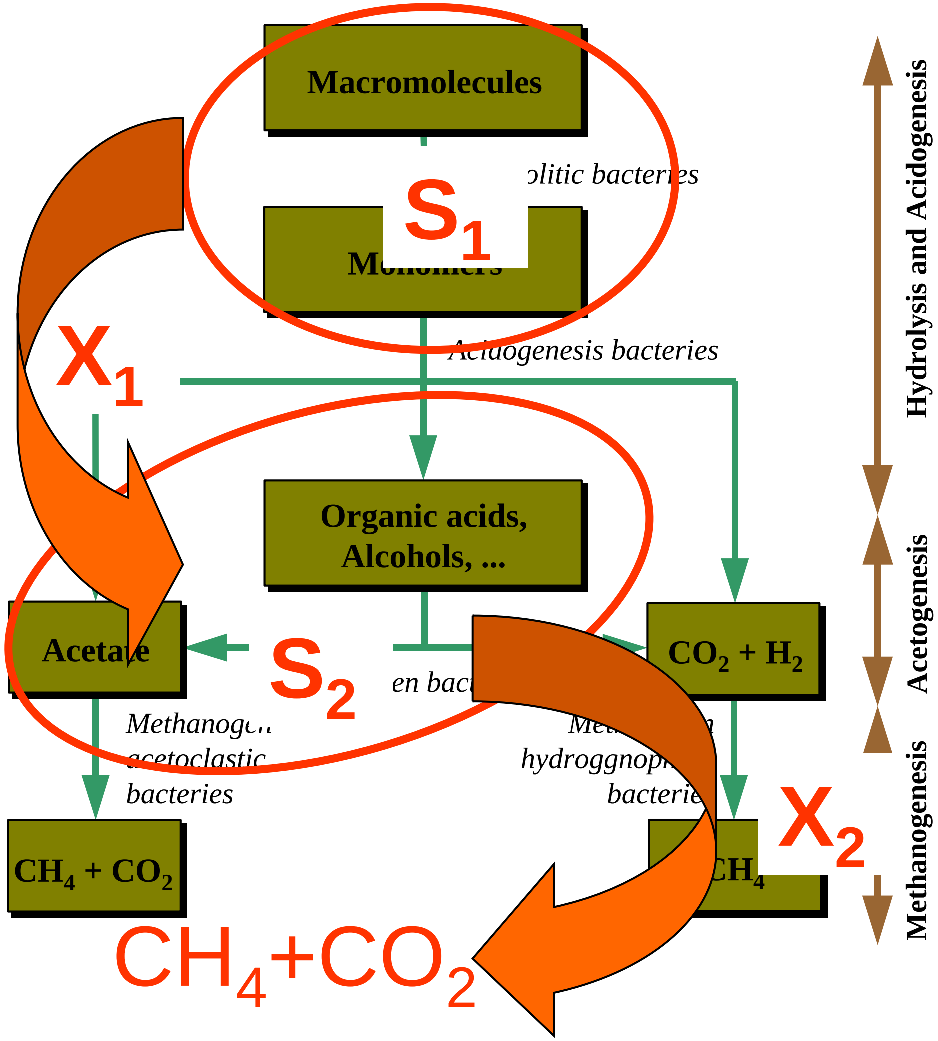
CH_4

Hydrolysis and Acidogenesis

Acetogenesis

Methanogenesis

The anaerobic digestion



$$\begin{cases} S_1 \xrightarrow{\mu_1} X_1 + S_2 \\ S_2 \xrightarrow{\mu_2} X_2 + P_i \end{cases}$$

$$\mu_1(S_1) = \mu_{\max 1} \frac{S_1}{K_{S1} + S_1}$$

$$\mu_2(S_2) = \mu_{\max 2} \frac{S_2}{K_{S2} + S_2 + \left(\frac{S_2}{K_I}\right)^2}$$

The "AMOCO" model

(Bernard, et coll., 1997)

Hypotheses :

a) $6 \leq pH \leq 8$

b) Acetic acid is the dominant acid

c) P_{CO_2} is always at equilibrium

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

Experimental evaluation of the model (2001)