Modeling and improvement of an anaerobic digestion process for the wastewater treatment

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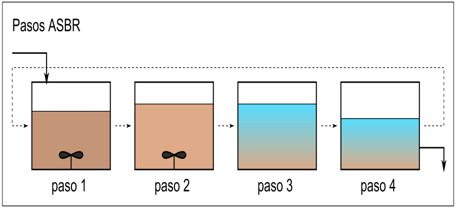

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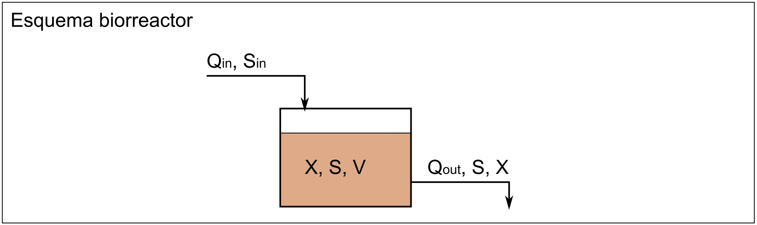
Mass balance model



Volume V : $\frac{dV}{dt} = Q^{\text{in}} - Q^{\text{out}}$

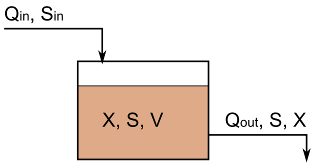
Biomass concentration X : $\frac{d}{dt}(VX) = \mu(S)(VX) - Q^{\text{out}}X$

Substrate concentration S : $\frac{d}{dt}(VS) = Q^{\text{in}}S^{\text{in}} - Q^{\text{out}}S - k\mu(S)(VX)$

Mass balance model

$$\begin{cases} \frac{dX}{dt} = \left(\mu(S) - \frac{Q^{\text{in}}}{V}\right) X \\ \frac{dS}{dt} = \frac{Q^{\text{in}}}{V}(S^{\text{in}} - S) - k\mu(S)X \\ \frac{dV}{dt} = Q^{\text{in}} - Q^{\text{out}} \end{cases}$$

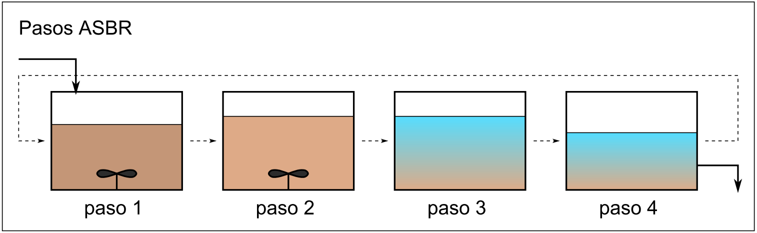
Esquema biorreactor



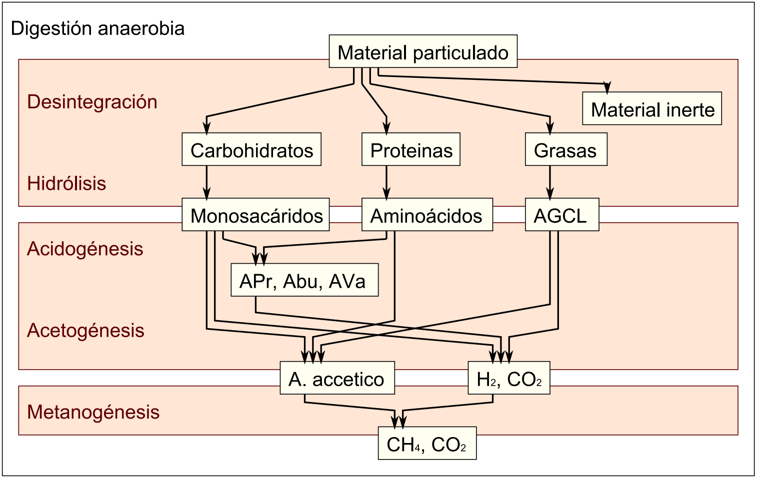
- $Q^{\text{in}} \neq 0$ y $Q^{\text{out}} = 0$; Sequential batch reactor
- $Q^{\text{in}} = Q^{\text{out}} = 0$; Batch reactor
- $Q^{\text{in}} = Q^{\text{out}} \neq 0$; Chemostat or continuous reactor

Steps of an ASBR

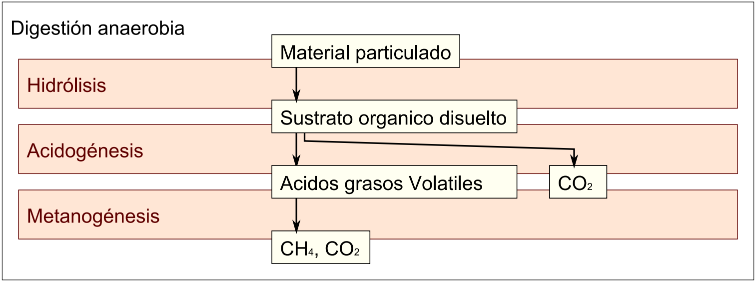
- Filling the reactor with water to be treated
- Reaction
- Settling
- Emptying the clean water from the reactor



Anaerobic digestion

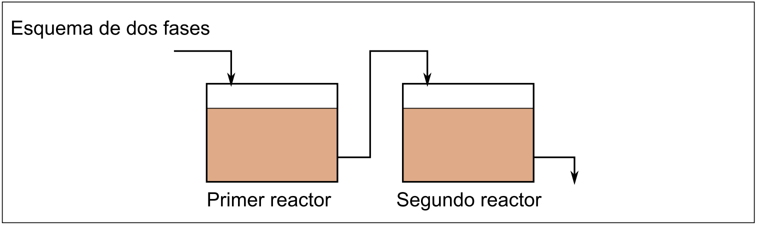


A simplified anaerobic digestion model



- The three main reactions considered: hydrolysis, acidogenesis and methanogenesis
- Two microorganism populations: hidrolitic-acidogenic (X_A) and methanogenic (X_M).
- Three substrates: particulate organic (S_0), dissolved organic (S_1), volatile fatty acids (S_2).

Two steps ASBR system



- First reactor: Hydrolysis - Acidogenic reactions
- Methanogenic reaction

Mass balance model

Reactor 1

(Hidrolitic - Acidogenic)

$$\begin{cases} \dot{X}_A = \left(\mu_1(S_{1A}) - \frac{Q_A}{V_A}\right) X_A \\ \dot{S}_{0A} = \frac{Q_A}{V_A}(S_{0A}^{\text{in}} - S_{0A}) - \mu_0(S_{0A})X_A \\ \dot{S}_{1A} = \frac{Q_A}{V_A}(S_{1A}^{\text{in}} - S_{1A}) - k_1\mu_1(S_{1A})X_A + k_2\mu_0(S_{0A})X_A \\ \dot{S}_{2A} = \frac{Q_A}{V_A}(S_{2A}^{\text{in}} - S_{2A}) + k_3\mu_1(S_{1A})X_A \\ \dot{V}_A = Q_A \end{cases}$$

Reactor 2

(Methanogenic)

$$\begin{cases} \dot{X}_M = \left(\mu_2(S_{2M}) - \frac{Q_M}{V_M}\right) X_M \\ \dot{S}_{0M} = \frac{Q_M}{V_M}(S_{0M}^{\text{in}} - S_{0M}) \\ \dot{S}_{1M} = \frac{Q_M}{V_M}(S_{1M}^{\text{in}} - S_{1M}) \\ \dot{S}_{2M} = \frac{Q_M}{V_M}(S_{2M}^{\text{in}} - S_{2M}) - k_5\mu_2(S_{2M})X_M \\ \dot{V}_M = Q_M \end{cases}$$

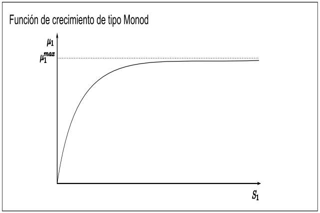
Growth functions

Hydrolysis (linear kinetic)

$$\mu_0(S_0) = K_0 S_0$$

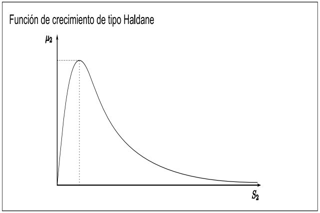
Acidogenesis (Monod kinetic)

$$\mu_1(S_1) = \mu_1^{\mathsf{max}} \frac{S_1}{K_{S1} + S_1}$$

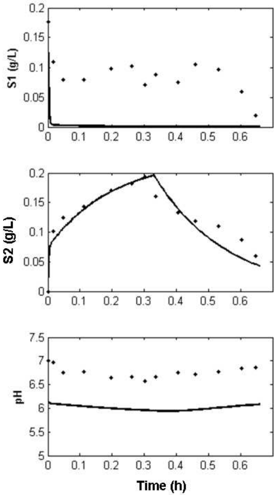


Methanogenesis (Haldane kinetic)

$$\mu_2(S_2) = \mu_2^{\mathsf{max}} \frac{S_2}{K_{S2} + S_2 + \frac{S_2^2}{K_{I2}}}$$



Simulation of one cycle



Optimal control problems

Reactor 1

(Hidrolitic - Acidogenic)

$$\begin{cases} \dot{X}_A = \left(\mu_1(S_{1A}) - \frac{Q_A}{V_A}\right) X_A \\ \dot{S}_{0A} = \frac{Q_A}{V_A}(S_{0A}^{\text{in}} - S_{0A}) - \mu_0(S_{0A})X_A \\ \dot{S}_{1A} = \frac{Q_A}{V_A}(S_{1A}^{\text{in}} - S_{1A}) - k_1\mu_1(S_{1A})X_A + k_2\mu_0(S_{0A})X_A \\ \dot{V}_A = Q_A \end{cases}$$

$$T_A(\xi_A) = \inf_{Q_A(\cdot)} \left\{ t \,|\, S_i^{\xi_A, Q_A}(t) \leq S_i^{\text{out}} \quad i = 0, 1, \right. \\ \left. V_A^{\xi_A, Q_A}(t) = V^{\text{max}} \right\}$$

Recall that μ_0 is linear and μ_1 is increasing

Optimal control problems

Reactor 2

(Methanogenic)

$$\begin{cases} \dot{X}_M = \left(\mu_2(S_{2M}) - \frac{Q_M}{V_M}\right) X_M \\ \dot{S}_{2M} = \frac{Q_M}{V_M}(S_{2M}^{\text{in}} - S_{2M}) - k_5\mu_2(S_{2M})X_M \\ \dot{V}_M = Q_M \end{cases}$$

$$T_M(\xi_M) = \inf_{Q_M(\cdot)} \Big\{ t \mid S_2^{\xi_M, Q_M}(t) \le S_2^{\text{out}}, V_M^{\xi_M, Q_M}(t) = V^{\max} \Big\}$$

The function is non monotonic but it is increasing in $[0, S_{2M}^{\text{in}}]$

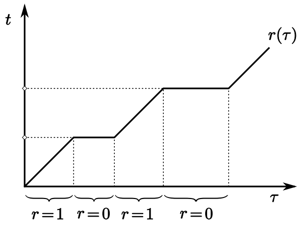
Fictitious time

We include the new control

$$r_j(\tau_j) = \begin{cases} 1 & \text{if the regular pump is manipulated} \\ 0 & \text{if an instantaneous dilution is made.} \end{cases}$$

implying to consider the fictitious time τ

Esquema de la parametrización del tiempo



Optimal control problems

Reactor 1

(Hidrolitic - Acidogenic)

$$\begin{cases} \dot{X}_A = \left(r_A \mu_1(S_{1A}) - \frac{Q_A}{V_A} \right) X_A \\ \dot{S}_{0A} = \frac{Q_A}{V_A}(S_{0A}^{\text{in}} - S_{0A}) - r_A \mu_0(S_{0A}) X_A \\ \dot{S}_{1A} = \frac{Q_A}{V_A}(S_{1A}^{\text{in}} - S_{1A}) - r_A k_1 \mu_1(S_{1A}) X_A + r_A k_2 \mu_0(S_{0A}) X_A \\ \dot{V}_A = Q_A \end{cases}$$

$$T_A(\xi_A) = \inf_{r_A(\cdot), Q_A(\cdot)} \left\{ \int_0^\tau r_A(\theta) d\theta \,|\, S_i^{\xi_A, r_A, Q_A}(t) \leq S_i^{\text{out}} \quad i = 0, 1, \right. \left. V_A^{\xi_A, r_A, Q_A}(t) = V^{\text{max}} \right\}$$

Optimal control problems

Reactor 2

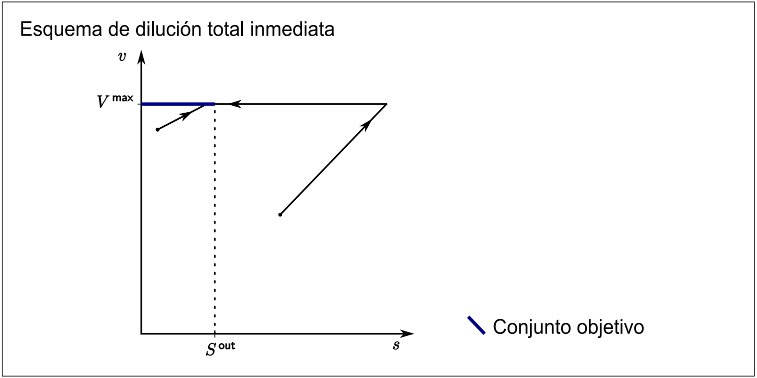
(Methanogenic)

$$\begin{cases} \dot{X}_M = \left(r_M \mu_2(S_{2M}) - \frac{Q_M}{V_M} \right) X_M \\ \dot{S}_{2M} = \frac{Q_M}{V_M}(S_{2M}^{\text{in}} - S_{2M}) - r_M \mu_2(S_{2M}) X_M \\ \dot{V}_M = Q_M \end{cases}$$

$$T_M(\xi_M) = \inf_{r_M(\cdot), Q_M(\cdot)} \left\{ \int_0^\tau r_M(\theta) d\theta \,|\, S_2^{\xi_M, r_M, Q_M}(t) \leq S_2^{\text{out}}, \right. \left. V_M^{\xi_M, r_M, Q_M}(t) = V^{\text{max}} \right\}$$

Immediate One Impulse (IOI)

Total dilution at the beginning



Theorem (G, Ramírez C., Rapaport 2008)

In the reactor 2 (methanogenic: 1 microorganism & 1 substrate) the strategy IOI is optimal due to the growth function is increasing in the operating range.

Singular arc strategy

Reactor 1

(Hidrolitic - Acidogenic)

$$\begin{cases} \dot{X}_A = \left(r_A \mu_1(S_{1A}) - \frac{Q_A}{V_A} \right) X_A \\ \dot{S}_{0A} = \frac{Q_A}{V_A}(S_{0A}^{\text{in}} - S_{0A}) - r_A \mu_0(S_{0A}) X_A \\ \dot{S}_{1A} = \frac{Q_A}{V_A}(S_{1A}^{\text{in}} - S_{1A}) - r_A k_1 \mu_1(S_{1A}) X_A + r_A k_2 \mu_0(S_{0A}) X_A \\ \dot{V}_A = Q_A \end{cases}$$

$$T_A(\xi_A) = \inf_{r_A(\cdot), Q_A(\cdot)} \left\{ \int_0^\tau r_A(\theta) d\theta \,|\, S_i^{\xi_A, r_A, Q_A}(t) \leq S_i^{\text{out}} \quad i = 0, 1, \right. \\ \left. V_A^{\xi_A, r_A, Q_A}(t) = V^{\text{max}} \right\}$$

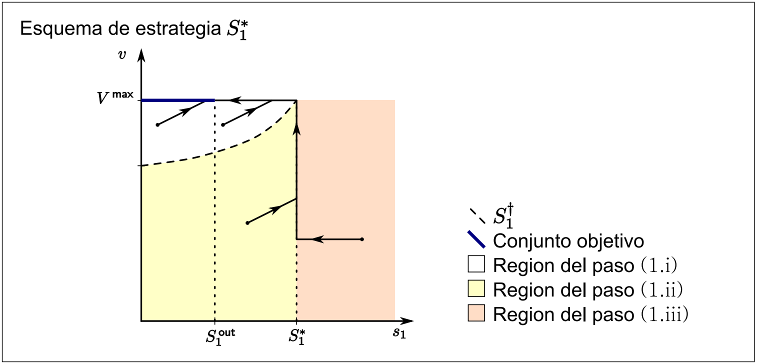
Theorem (G, Ramírez C., Rapaport 2008)

For two species (with increasing growth functions) & one substrate there are only two optimal strategies:

- *IOI*
- *Singular arc*

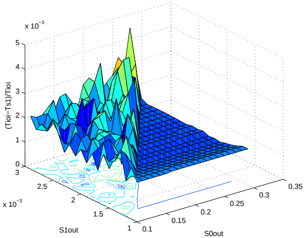
Singular arc strategy

First reactor



Idea: To evaluate arc singular arc strategies keeping constant the substrate level S_1^*

Strategy S_1^* constant



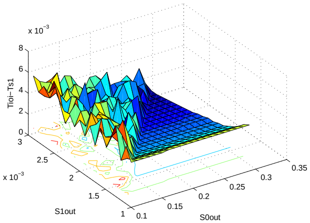


Figura: Superficies de respuesta variando las concentraciones de salida S_0^{out} y S_1^{out}

Strategy S_1^* constant

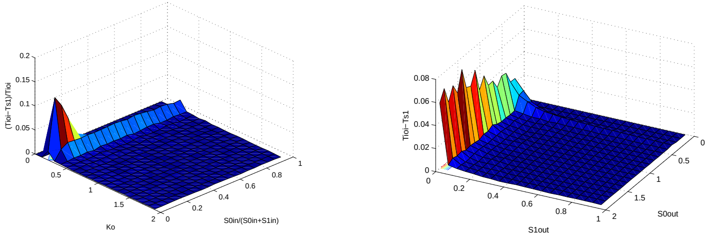


Figura: Superficie de respuesta variando la fracción de material particulado y la constante de hidrólisis

Strategy S_1^* constant

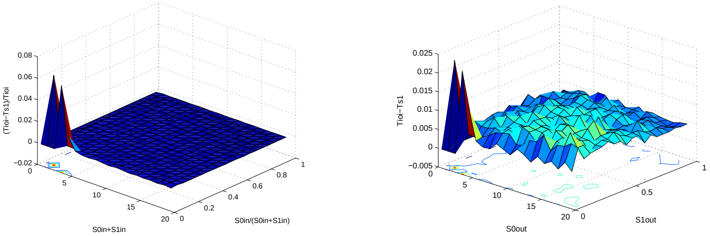


Figura: Superficie de respuesta variando la fracción de material particulado y concentración de materia orgánica total

Strategy S_1^* constant

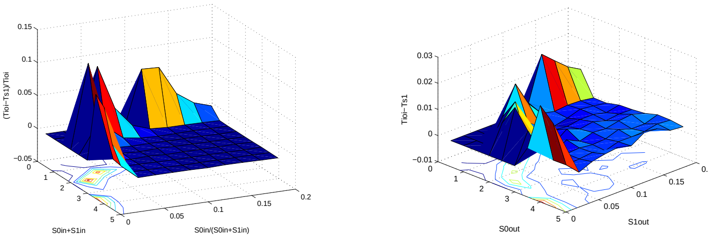


Figura: Superficie de respuesta variando la fracción de material particulado y concentración de materia orgánica total

Conclusiones

- Se adaptó un modelo ASBR para un esquema de operación de dos fases.
- Se realizó una identificación del parámetro de sedimentación de S_0.
- Se mostró que la estrategia optima de llenado para el reactor metanogénico es IOI.
- Se encontró una estrategia de menor tiempo que IOI para el reactor acidogénico.
- Se estudió mediante simulación, para cuales configuraciones la estrategia alternativa presenta mayor reducción del tiempo de operación.

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