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Existence, uniqueness and stability of the equilibrium points of a SHARON bioreactor model

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Outline

- Introduction: the SHARON process
- Problem statement - Mathematical model
- Criterion for a unique equilibrium point
- Calculation of the unique equilibrium states
- Local asymptotic stability of the unique equilibrium
- Conclusions – Future work

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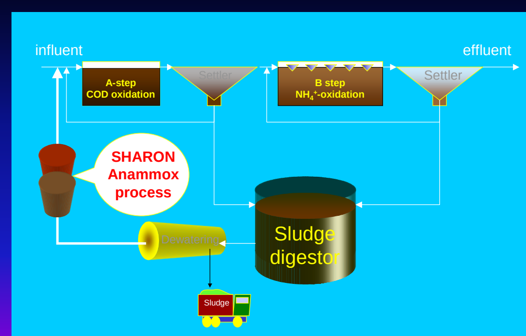
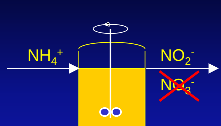
Introduction: a wastewater treatment plant



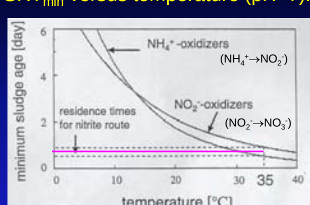
Introduction: the SHARON process



SHARON

- CSTR (chemostat)
- no biomass retention: SRT=HRT
- pH=7 ; T = 35°C

SRT_{min} versus temperature (pH=7):

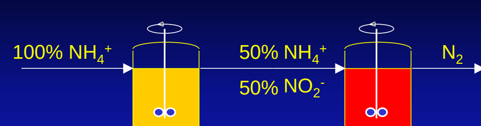


at 35°C: ammonium oxidizers grow faster than nitrite oxidizers

⇒ nitrite oxidizers are washed out by keeping retention time low

⇒ partial nitrification to nitrite is achieved

Introduction: SHARON - Anammox



SHARON

Anammox

Simplified stoichiometry:

$$NH_4^+ + NO_2^- \rightarrow N_2 + 2H_2O$$

⇒ Optimal $NH_4^+/NO_2^- \approx 1/1$

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Problem statement

Is NH_4^+/NO_2^- produced in SHARON reactor

- unique ?
- stable ?

for constant input variables :

- dilution rate : Q/V = u_0 =1/HRT
- (total) influent ammonium concentration : $TNH_{in}=u_1$
- (total) influent nitrite concentration : $TNO2_{in}=u_2$
- (total) influent concentration of ammonium oxidizers: $X_{amm,in}=u_3$
- (total) influent concentration of nitrite oxidizers: $X_{nit,in}=u_4$

OR

constant inputs

$\Rightarrow$ unique and stable equilibrium states?

Mathematical model

Assume SHARON reactor controlled at constant pH

$\Rightarrow$ simplified reactor model:

$$\dot{\mathbf{x}}(t) = (\mathbf{u} - \mathbf{x}(t)) \cdot u_0 + \mathbf{M} \cdot \rho(\mathbf{x}(t))$$

$$\mathbf{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \\ x_3(t) \\ x_4(t) \end{bmatrix} = \begin{bmatrix} TNH(t) \\ TNO2(t) \\ X_{amm}(t) \\ X_{nit}(t) \end{bmatrix} \quad u_0 = \frac{Q}{V} \quad \mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix} = \begin{bmatrix} TNH_{in} \\ TNO2_{in} \\ X_{amm,in} \\ X_{nit,in} \end{bmatrix} \quad \mathbf{M} = \begin{bmatrix} -a & -b \\ c & -d \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\rho = \begin{bmatrix} \rho_1(\mathbf{x}) \\ \rho_2(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} a_1 \cdot \frac{x_1}{b_1 + x_1} \cdot \frac{c_1}{c_1 + x_2} \cdot x_3 \\ a_2 \cdot \frac{x_2}{b_2 + x_2} \cdot \frac{x_1}{c_2 + x_1} \cdot \frac{d_2}{d_2 + x_2} \cdot \frac{e_2}{e_2 + x_1} \cdot x_4 \end{bmatrix}$$

u constant $\Rightarrow$ $\mathbf{x_e}$ unique and stable?

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Calculation of equilibrium states

The equilibrium states are obtained from

$$0 = (\mathbf{u} - \mathbf{x}_e) \cdot u_0 + \mathbf{M} \cdot \rho(\mathbf{x}_e)$$

Case $u_0 = 0$ (i.e. no flow) :

- $x_{e1}=0$; x_{e2}, x_{e3}, x_{e4} arbitrary
- $x_{e2} = x_{e3} = 0$; x_{e1}, x_{e4} arbitrary
- $x_{e3} = x_{e4} = 0$; x_{e1}, x_{e2} arbitrary

$\Rightarrow$ number of equilibrium solutions: $\infty^3 + 2\ \infty^2$

Case $u_0 \neq 0$:

$$\mathbf{x}_e = \mathbf{u} + \frac{1}{u_0} \cdot \mathbf{M} \cdot \rho(\mathbf{x}_e)$$

$\Rightarrow$ principle of contraction mappings

Criterion for a unique equilibrium

Contraction mapping theorem :

every contraction mapping φ, defined in a complete metric space X, has one and only one fixed point in X, i.e. for which $\mathbf{x} = \varphi(\mathbf{x})$

Case $u_0 \neq 0$:

$$\mathbf{x}_e = \mathbf{u} + \frac{1}{u_0} \cdot \mathbf{M} \cdot \rho(\mathbf{x}_e) \equiv \varphi(\mathbf{x}_e)$$

Define mapping φ in the complete metric space $\mathbf{R}^{4\text{x}1}$

with the Euclidian norm as distance: $\ell(\mathbf{x},\mathbf{w}) = |\mathbf{x} - \mathbf{w}|$

IF φ is a contraction mapping

i.e. there exists a K < 1 such that

$\ell(\varphi(\mathbf{x}),\varphi(\mathbf{w})) \leq K \cdot \ell(\mathbf{x},\mathbf{w}) \qquad \forall \mathbf{x},\mathbf{w} \text{ in } \mathbf{R}^{4\text{x}1}$

THEN φ possesses a unique fixed point $\mathbf{x}_e = \varphi(\mathbf{x}_e)$

that is the *unique equilibrium point* for the SHARON model

Criterion for a unique equilibrium

Is φ a contraction mapping?

$$\ell^2[\varphi(\mathbf{x}),\varphi(\mathbf{w})] = \frac{1}{u_0^{\,2}}[\rho(\mathbf{x})-\rho(\mathbf{w})]^T\mathbf{M}^T\mathbf{M}[\rho(\mathbf{x})-\rho(\mathbf{w})]$$

$$\le \frac{s_0}{u_0^{\,2}}\cdot[\rho(\mathbf{x})-\rho(\mathbf{w})]^T[\rho(\mathbf{x})-\rho(\mathbf{w})]$$

$$\le \frac{s_0}{u_0^{\,2}}\cdot[\mathbf{x}-\mathbf{w}]^T\mathbf{J}^T\mathbf{J}[\mathbf{x}-\mathbf{w}]$$

$$\mathbf{J}=\begin{bmatrix} \left.\frac{\partial\rho_1}{\partial x_1}\right|_{x=\hat{x}_{11}} & \left.\frac{\partial\rho_1}{\partial x_2}\right|_{x=\hat{x}_{12}} & \left.\frac{\partial\rho_1}{\partial x_3}\right|_{x=\hat{x}_{13}} & \left.\frac{\partial\rho_1}{\partial x_4}\right|_{x=\hat{x}_{14}} \\ \left.\frac{\partial\rho_2}{\partial x_1}\right|_{x=\hat{x}_{21}} & \left.\frac{\partial\rho_2}{\partial x_2}\right|_{x=\hat{x}_{22}} & \left.\frac{\partial\rho_2}{\partial x_3}\right|_{x=\hat{x}_{23}} & \left.\frac{\partial\rho_2}{\partial x_4}\right|_{x=\hat{x}_{24}} \end{bmatrix} = \begin{bmatrix}\delta_1 & \delta_2 & \delta_3 & 0\\ \delta_5 & \delta_6 & 0 & \delta_8\end{bmatrix}$$

Criterion for a unique equilibrium

Is φ a contraction mapping?

$$\ell^2[\varphi(\mathbf{x}),\varphi(\mathbf{w})] \le \frac{s_0}{u_0^{\,2}}\cdot[\mathbf{x}-\mathbf{w}]^T\mathbf{J}^T\mathbf{J}[\mathbf{x}-\mathbf{w}]$$

$$\le \frac{s_0\cdot s_1}{u_0^{\,2}}\cdot\ell^2[\mathbf{x},\mathbf{w}]$$

YES, IF

$$\frac{s_0\cdot s_1}{u_0^{\,2}}\le 1$$

$$u_0 \ge \sqrt{s_0\cdot s_1} \equiv u_{0,crit}^{4dim}$$

= criterion for a unique equilibrium ('4dim') !!!

Criterion for unique equilibrium:alternative

The SHARON reactor model *in equilibrium* can be rewritten in 2 state variables (instead of 4)

The equilibrium states are now obtained from

$$\mathbf{y}_e = \mathbf{w} + \frac{1}{u_0}\cdot\hat{\mathbf{M}}\cdot\hat{\rho}(\mathbf{y}_e) \equiv \hat{\varphi}(\mathbf{y}_e)$$

$$\mathbf{y}=\begin{bmatrix}x_1\\x_2\end{bmatrix}\quad \mathbf{w}=\begin{bmatrix}u_1\\u_2\end{bmatrix}\quad \hat{\mathbf{M}}=\begin{bmatrix}-a & -b\\ c & -d\end{bmatrix}$$

The reactor has a unique equilibrium $\mathbf{y}_e=\hat{\varphi}(\mathbf{y}_e)$

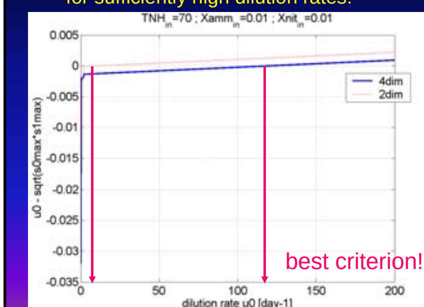
if $\hat{\varphi}$ is a contraction mapping

$$\Leftrightarrow u_0 \ge \sqrt{\hat{s}_0\cdot\hat{s}_1} \equiv u_{0,crit}^{2dim}$$

= '2 dim' criterion for a unique equilibrium !!!

Criterion for a unique equilibrium

The SHARON reactor possesses a unique equilibrium for sufficiently high dilution rates:



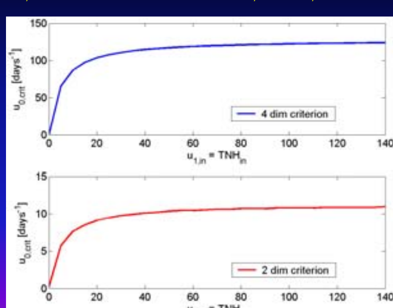
$$u_0 \ge \sqrt{s_0\cdot s_1} \equiv u_{0,crit}^{4dim} = 120\ \text{day}^{-1}$$

or

$$u_0 \ge \sqrt{\hat{s}_0\cdot\hat{s}_1} \equiv u_{0,crit}^{2dim} = 10.63\ \text{day}^{-1}$$

Criterion for a unique equilibrium

$u_{0,crit}$ in terms of TNH_{in} ($X_{amm,in}$= $X_{nit,in}$ 0.01 mole/m³):



$u_1 = TNH_{in}\uparrow$
$\Rightarrow u_{0,crit}\uparrow$

2-dim criterion gives best results

In practice:
$u_0 = 0.5 – 1\ \text{day}^{-1}$
$<< u_{0,crit}$

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Calculation of unique equilibrium states

The unique fixed point $x_e = \varphi(x_e)$ of a contraction mapping φ is obtained by the method of successive approximations:

$$x_{n+1} = \varphi(x_n) \qquad n = 0,1,2,\ldots$$

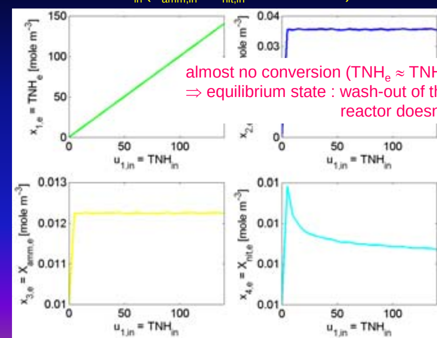
for an arbitrary starting value x_0

Application to the SHARON process model:

- calculate x_e for different values of $u_1 = TNH_{in}$
- choose $x_0 = u$ (e.g.)

Calculation of the equilibrium states

In terms of TNH_{in} ($X_{amm,in} = X_{nit,in}$ 0.01 mole/m³):



almost no conversion ($TNH_e \approx TNH_{in}$)
⇒ equilibrium state : wash-out of the biomass
reactor doesn't work!

e.g. for TNH_{in} = 70 mole/m³:

TNH_e = 69.96
$TNO2_e$ = 0.035
$X_{amm,e}$ = 0.122
$X_{nit,e}$ = 0.010
[mole/m³]

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LAS of the unique equilibrium

Linearization principle:

The SHARON reactor model

$$\dot{\mathbf{x}}(t) = (\mathbf{u} - \mathbf{x}(t))\cdot u_0 + \mathbf{M}\cdot\rho(\mathbf{x}(t)) = \mathbf{f}(\mathbf{x})$$

is locally asymptotically stable if the eigenvalues of the Jacobian matrix

$$\left.\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}_e} = \begin{bmatrix} \left.\frac{\partial f_1}{\partial x_1}\right|_{\mathbf{x}=\mathbf{x}_e} & \cdots & \left.\frac{\partial f_1}{\partial x_4}\right|_{\mathbf{x}=\mathbf{x}_e} \\ \vdots & & \vdots \\ \left.\frac{\partial f_4}{\partial x_1}\right|_{\mathbf{x}=\mathbf{x}_e} & \cdots & \left.\frac{\partial f_4}{\partial x_4}\right|_{\mathbf{x}=\mathbf{x}_e} \end{bmatrix}$$

all have a strictly negative real part (are in the open left phase plane)

LAS of the unique equilibrium

Eigenvalues of the Jacobian matrix:

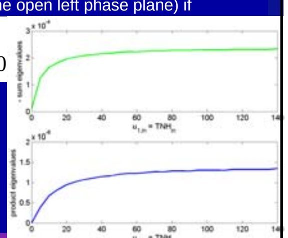
$$s = -u_0 \qquad (2\times)$$

$$s^2 + (2\cdot u_0 - \alpha - \delta)\cdot s + (u_0 - \alpha)(u_0 - \delta) - \beta\cdot\gamma = -u_0$$

all have a negative real part (are in the open left phase plane) if

$$\text{-sum} = (2\cdot u_0 - \alpha - \delta) > 0$$

$$\text{product} = (u_0 - \alpha)(u_0 - \delta) - \beta\cdot\gamma > 0$$



fulfilled for all values of TNH_{in}
⇒ unique (wash-out) equilibrium is locally asymptotically stable !

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Conclusions

- A simplified mathematical model for a SHARON reactor with constant pH was constructed
- A criterion for a unique equilibrium point was deducted and the equilibrium states were calculated using a contraction mapping theorem
- A unique equilibrium point is only obtained for high values of the dilution rate corresponding with wash-out of the biomass and almost no conversion
- The unique equilibrium point is locally asymptotically stable

Future work

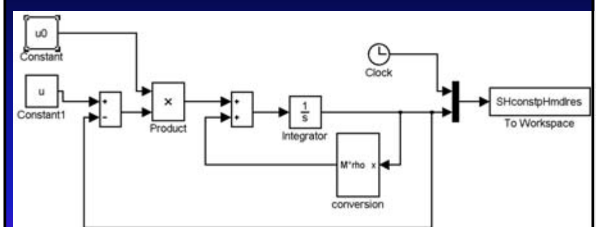
For realistic (low) values of the dilution rate u_0 :

- calculate all equilibrium points
- show that the system converges to one of the equilibrium points, regardless the initial condition
- define attraction regions for each equilibrium point

using Liapunov's theory

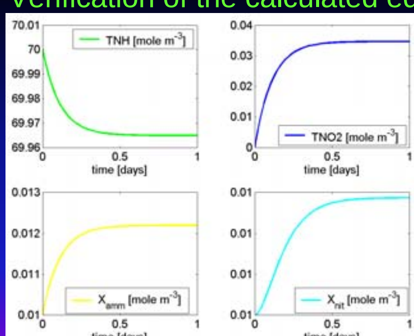
Verification of the calculated equilibrium

Simulation of the SHARON reactor in Simulink



TNH_{in} = 70 mole/m^3; $X_{amm,in}$= $X_{nit,in}$ 0.01 mole/m^3;

Verification of the calculated equilibrium



TNH_e = 69.96
$TNO2_e$ = 0.035
$X_{amm,e}$ = 0.122
$X_{nit,e}$ = 0.0100

The same equilibrium values are obtained!

System dynamics

The characteristic equation

$$s^2+(2\cdot u_0-\alpha-\delta)\cdot s+(u_0-\alpha)(u_0-\delta)-\beta\cdot\gamma=-u_0$$

can also be written as

$$s^2+2\cdot\varsigma\cdot\omega_n\cdot s+\omega_n^{\ 2}=0$$

ς and ω_n determine the system dynamics

- non-oscillating transient behaviour