Nonlinear Dynamics and Systems Theory, **6**(2) (2006) 191–203

Stability Conditions and Stability Boundaries of a SHARON Bioreactor Model with Multiple Equilibrium Points

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Received: December 10, 2005; Revised: May 25, 2006

Abstract: This paper addresses the dynamics of a SHARON bioreactor for ammonium removal from concentrated wastewater streams. It is shown that multiple equilibrium points occur for a simplified reactor model. Conditions are determined for which the system possesses multiple equilibrium points and the corresponding phase portraits are analysed. In case the reactor model possesses two locally asymptotically stable equilibrium points, the stability boundary, that separates their attraction regions, is visualized. Subsequently, it is examined how small parameter changes affect the number of equilibrium points and the corresponding phase portraits. The analytically obtained results are illustrated by means of simulations.

Keywords: *biochemical reactors; nonlinear systems; stability analysis.*

Mathematics Subject Classification (2000): 34A34, 34A50, 34D20.

1 Introduction

Throughout the years, biological nitrogen removal from wastewater has proven its effectiveness and has been adopted widely in favour of the more expensive physicochemical processes. Typically, biological nitrogen removal is performed through nitrification of ammonium (i.e. the main form in which nitrogen is present in wastewater) via nitrite to nitrate, followed by denitrification of nitrate to nitrogen gas.

Several novel nitrogen removal processes have been developed, among which the SHARON process (single reactor system for high activity ammonia removal over nitrite),

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that is ideally suited to remove nitrogen from wastewater streams with high ammonium concentration [5].

The SHARON reactor is operated as a continuously stirred tank reactor (CSTR) without biomass retention. At the prevailing pH (about 7) and high temperature (30-40°C), ammonium oxidizers grow faster than nitrite oxidizers. For this reason, it is possible to establish ammonium oxidation to nitrite only and prevent further oxidation of nitrite to nitrate by setting an appropriate dilution rate. In this way, substantial savings in aeration costs are realized, in comparison with oxidation of ammonium to nitrate. Additional savings can be made when the SHARON reactor is coupled with an Anammox process, in which an almost equimolar mixture of ammonium and nitrite is converted to nitrogen gas [9].

In this paper, the dynamics of the SHARON reactor model with inhibition kinetics is analysed. Starting from a simplified model, conditions under which the reactor exhibits multiple equilibrium points are identified and their importance is discussed from a technological point of view. The global convergence properties of the set of the equilibrium points is discussed and phase trajectories are drawn for the different cases distinguished. In case multiple stable equilibrium points occur at the same time, their stability boundary is visualized by means of a trajectory reversing technique. In order to examine the effect of varying parameter values on the number of equilibrium points, an extended model is considered, that is obtained by small modifications of the simplified model. The equilibrium points are calculated analytically and phase trajectories are drawn to verify the results.

2 The SHARON Reactor Model

For a wide class of biotechnological reaction systems in which n components are involved in m reactions $(n > m)$, the state equations can be written in the general form [1]

$$\dot{\xi} = C\rho(\xi) - D\xi + F. \tag{1}$$

The state ξ, of dimension n, is the vector of reactor concentrations of the various components participating in the process. $F = \operatorname{col}(F_i),\ i = 1, \ldots, n$, represents the supply rates, while D is the dilution rate. F and D are assumed to remain constant and satisfy

$$F_i \geq 0, \quad i = 1, \ldots, n, \quad D > 0. \tag{2}$$

For a CSTR with constant reactor volume, the supply rate can be written as $F = D\xi_{in}$, with ξ_{in} representing the vector of influent concentrations of the various process components.

$\rho(\xi) = \operatorname{col}(\rho_j(\xi)),\ j = 1, \ldots, m$, is the reaction rate function. Let $\rho(\xi) \in \mathcal{C}^1$ (continuous with continuous partial derivatives w.r.t. the components of ξ). This condition ensures the existence and the uniqueness of the solutions of (1) for given initial conditions. For all values of the composition vector $\xi,\ \rho_j(\xi) \geq 0,\ j = 1, \ldots, m$.

$C \in R^{n\times m}$, with $\operatorname{rank} C = m$, is the matrix of yield coefficients. Without loss of generality C can be written as

$$C = \begin{bmatrix} C_b \\ C_a \end{bmatrix} \tag{3}$$

where $C_a \in R^{m\times m}$ is nonsingular.

It has been proven [2, 7] that under some fairly general assumptions, including the principle of mass conservation, the state variables of the system (1) cannot become negative and remain upper bounded for increasing time. Moreover the system (1) can be brought in a canonical form by the state transformation

$$x_b \triangleq A_0\xi_a + \xi_b \in R^{n-m}, \quad x_a \triangleq \xi_a \in {R^+}^m \tag{4}$$

with $A_0 = -C_bC_a^{-1}$. The canonical model consists of a linear part of dimension $(n-m)$ dynamically coupled with a nonlinear part of dimension m.

The SHARON reactor model considers two nitrification reactions $(m = 2)$: oxidation of ammonium to nitrite and consecutive oxidation of nitrite to nitrate. Four components $(n = 4)$ are involved in the biochemical reactions: ammonium, nitrite, ammonium oxidizers and nitrite oxidizers. Ammonium and nitrite oxidations are described by their respective reaction rates

$$\rho_1(\xi) = a_1 \cdot \frac{\xi_1}{b_1+\xi_1} \cdot \frac{c_1}{c_1+\xi_2} \cdot \xi_3 \tag{5}$$

and

$$\rho_2(\xi) = a_2 \cdot \frac{\xi_2}{b_2+\xi_2} \cdot \frac{\xi_1}{c_2+\xi_1} \cdot \frac{d_2}{d_2+\xi_2} \cdot \frac{e_2}{e_2+\xi_1} \cdot \xi_4 \tag{6}$$

in which a_1, b_1, c_1, a_2, b_2 c_2, d_2 and e_2 are constant, at least for a SHARON reactor in which temperature and pH are controlled at a fixed level, as is assumed further. The model considers inhibition of ammonium oxidation by nitrite (with inhibition constant c_1), as well as inhibition of nitrite oxidation by ammonium and by nitrite (with inhibition constants e_2 and d_2 respectively). The matrix of yield coefficients has the form:

$$C = \begin{bmatrix} -a & -b \\ c & -d \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{7}$$

Assuming a constant reactor volume, under the state transformation (4), the canonical model of the SHARON reactor becomes:

$$\dot{x}_b = D(w_b - x_b), \tag{8}$$

$$\dot{x}_a = D(w_a - x_a) + C_a\rho(x), \tag{9}$$

where

$$x_a \triangleq \begin{bmatrix} x_3 \\ x_4 \end{bmatrix} \in {R^+}^2, \quad x_b \triangleq \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in R^2, \quad C_a = I_2,$$

$$\rho(x) \triangleq \begin{bmatrix} \rho_1(x) \\ \rho_2(x) \end{bmatrix} \in {R^+}^2; \quad w_a = \begin{bmatrix} w_3 \\ w_4 \end{bmatrix} \triangleq \begin{bmatrix} \xi_{in_3} \\ \xi_{in_4} \end{bmatrix} \in {R^+}^2;$$

$$w_b = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \triangleq \begin{bmatrix} \xi_{in_1} + a\xi_{in_3} + b\xi_{in_4} \\ \xi_{in_2} - c\xi_{in_3} + d\xi_{in_4} \end{bmatrix} \in R^2,$$

$$\rho_i(x) = \rho_i(\xi)|_{\xi_a = x_a;\ \xi_b = x_b + C_bC_a^{-1}x_a}, \quad i = 1, 2.$$

Biochemical reactors are positive systems, which means their state variables ξ_i, $i = 1, \ldots, n$, cannot become negative. Hence the states of the canonical model (8), (9) must fulfill the following physical boundary conditions:

$$w_1 - ax_3 - bx_4 \geq 0, \tag{10}$$
$$w_2 + cx_3 - dx_4 \geq 0, \tag{11}$$
$$x_3 \geq 0, \tag{12}$$
$$x_4 \geq 0. \tag{13}$$

Table 2.1 gives the numerical values/ranges for the SHARON model parameters and input variables, applied in this study. These values are the same as applied in [10], except for the values of a_1 and b_2, that were slightly changed in this study to avoid numerical instabilities, without qualitatively affecting the results.

Table 2.1. Numerical values/ranges SHARON model parameters and input variables.

a_1	1.35×10^{-5}	day^{-1}	a	16	mole mole^{-1}
b_1	4.73	mole m^{-3}	b	0.2	mole mole^{-1}
c_1	837	mole m^{-3}	c	58.6	mole mole^{-1}
a_2	1.22×10^{-5}	day^{-1}	d	15.8	mole mole^{-1}
b_2	60	mole m^{-3}	D	$[0 \quad 3 \times 10^{-5}]$	day^{-1}
c_2	0.01	mole m^{-3}	ξ_{in_1}	$[0 \quad 2000]$	mole m^{-3}
d_2	1000	mole m^{-3}	ξ_{in_2}	0	mole m^{-3}
e_2	1000	mole m^{-3}	$\xi_{in_3} = \xi_{in_4}$	0.01	mole m^{-3}

Since all solutions of the SHARON reactor remain bounded for increasing time, it can easily be established [4], using basic Lyapunov theory, that all trajectories of the canonical model converge to the quarter hyperplane

$$\Delta = \{x_3 \geq 0, \quad x_4 \geq 0, \quad x_b = w_b\}\,. \tag{14}$$

On the hyperplane Δ the dynamics are described by the autonomous second order system (9) in which $x_b \equiv w_b$, whose the solutions remain bounded for $t \to +\infty$. Hence by Poincaré–Bendixson's theorem (see e.g. [6], P. 321) every solution either converges to an equilibrium point or to a closed trajectory (limit cycle). If there are no closed trajectories in the state space of this system then the set of the equilibrium points is globally convergent. More detailed considerations on the convergence of biochemical reactors of rank two can be found in [8]. Here it was concluded that for processes such as the SHARON reactor, working under operating conditions which violate analytical criteria such as Bendixson's negative criterion [6], the absence of limit cycles must be verified by simulation.

3 Analysis of a Simplified SHARON Reactor Model

In this section, the existence, uniqueness and stability of the equilibrium points is studied for the SHARON reactor model, that is further simplified. The simplified model is obtained by assuming that the inflow does not contain any nitrite, ammonium oxidizers or nitrite oxidizers. Furthermore, nitrite limitation of ammonium oxidizers as well as ammonium inhibition of nitrite oxidizers are not considered. These simplifications are expressed mathematically as

$$\xi_{in_i} = 0, \quad i = 2, \dots, 4, \tag{15}$$

$$c_1 = +\infty, \quad c_2 = 0, \quad e_2 = +\infty. \tag{16}$$

The equilibrium points of the corresponding canonical model satisfy

$$x_1 = w_1 = \xi_{in_1}, \tag{17}$$

$$x_2 = w_2 = 0, \tag{18}$$

$$[-D + \rho_1(x)]\, x_3 = 0, \tag{19}$$

$$[-D + \rho_2(x)]\, x_4 = 0, \tag{20}$$

where

$$\rho_1(x) = a_1 \cdot \frac{\xi_1}{b_1 + \xi_1}, \tag{21}$$

$$\rho_2(x) = a_2 \cdot \frac{\xi_2}{b_2 + \xi_2} \cdot \frac{d_2}{d_2 + \xi_2}, \tag{22}$$

$$\xi_1 = w_1 - a x_3 - b x_4, \tag{23}$$

$$\xi_2 = c x_3 - d x_4. \tag{24}$$

There are three valid possibilities resulting from (19), (20).

Case 1. $x_3 = 0,\ x_4 = 0$.
This gives the equilibrium point:

$$\hat{x}_A = \mathrm{col}\,(\xi_{in_1}, 0, 0, 0). \tag{25}$$

This equilibrium point occurs independently of the choice of dilution rate D and of ammonium concentration in the inflow ξ_{in_1}. It is the wash-out state of the system, in which no biomass remains in the reactor and, consequently, no conversion is realized.

It is worth noting that, if in an equilibrium point there are no ammonium oxidizers present ($x_3 = 0$), then the concentration of nitrite oxidizers (x_4) must also be zero, otherwise the physical boundary $\xi_2 \geq 0$ is violated. This is logical regarding the fact that, in a SHARON reactor, ammonium oxidizers grow faster than nitrite oxidizers.

Case 2. $x_4 = 0,\ \rho_1(x) = D$.
Denoting by $\hat{\xi}_{B_1}$ the solution of $\rho_1(x) = D$,

$$\hat{\xi}_{B_1} = \frac{D b_1}{a_1 - D} \tag{26}$$

the second equilibrium point of the system is found as

$$\hat{x}_B = \mathrm{col}\left(\xi_{in_1},\, 0,\, \frac{\xi_{in_1} - \hat{\xi}_{B_1}}{a},\, 0\right), \tag{27}$$

$\hat{x}_B$ is a physical state of the system only if $D < \dfrac{a_1 \xi_{in_1}}{b_1 + \xi_{in_1}}$. This second equilibrium point corresponds with a situation in which only ammonium oxidizers are present in the reactor, so only nitrite is formed. Nitrate formation is successfully suppressed by keeping out nitrite oxidizers, as is the aim of a SHARON reactor.

Case 3. $\rho_1(x) = D$, $\rho_2(x) = D$.

As before, the first equality results in

$$\hat{\xi}_{C_1} = \frac{Db_1}{a_1 - D} \tag{28}$$

under the condition $D < a_1$, while the second equality will have two solutions $\hat{\xi}_{C_2}$ and $\hat{\xi}_{D_2}$ if $D < a_2 \cdot \dfrac{d_2}{(\sqrt{b_2} + \sqrt{d_2})^2}$. Let $\hat{\xi}_{D_2} > \hat{\xi}_{C_2}$. Then a third physical equilibrium point

$$\hat{x}_C = \begin{bmatrix} \xi_{in_1} \\ 0 \\ \dfrac{d(\xi_{in_1} - \hat{\xi}_{C_1}) + b\hat{\xi}_{C_2}}{ad + bc} \\ \dfrac{c(\xi_{in_1} - \hat{\xi}_{C_1}) - a\hat{\xi}_{C_2}}{ad + bc} \end{bmatrix} \tag{29}$$

will occur if in addition $\hat{\xi}_{C_2} < \dfrac{c}{a}(\xi_{in_1} - \hat{\xi}_{C_1})$. Moreover, if also $\hat{\xi}_{D_2} < \dfrac{c}{a}(\xi_{in_1} - \hat{\xi}_{D_1})$, where $\hat{\xi}_{D_1} = \hat{\xi}_{C_1}$ then the fourth equilibrium point

$$\hat{x}_D = \begin{bmatrix} \xi_{in_1} \\ 0 \\ \dfrac{d(\xi_{in_1} - \hat{\xi}_{D_1}) + b\hat{\xi}_{D_2}}{ad + bc} \\ \dfrac{c(\xi_{in_1} - \hat{\xi}_{D_1}) - a\hat{\xi}_{D_2}}{ad + bc} \end{bmatrix} \tag{30}$$

is also a physical equilibrium point of the system. The equilibrium points $\hat{x}_C$ and $\hat{x}_D$ correspond with situations in which nitrite oxidizers are present, so in which at least part of the nitrite is further oxidized to nitrate. This is mostly not desirable in a SHARON reactor, as more oxygen is consumed. Also for coupling with an Anammox process, nitrate formation should be avoided. Note that, as $\hat{\xi}_{D_2} > \hat{\xi}_{C_2}$, more ammonium oxidizers and less nitrite oxidizers are present, which means that less nitrate is produced in $\hat{x}_D$ than in $\hat{x}_C$.

Summarizing, depending on the values of the dilution rate D and the ammonium concentration in the influent ξ_{in_1}, the simplified model of the SHARON reactor may possess one, two, three or four equilibrium points. The boundaries delimiting the regions with various numbers of equilibrium points are illustrated in Figure 3.1. For high dilution rates

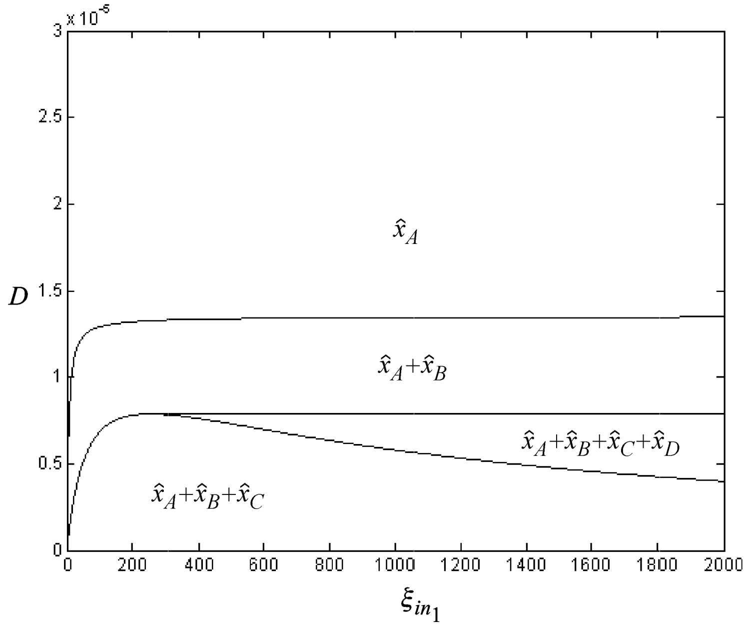

Figure 3.1. Boundaries of regions with various numbers of equilibrium points.

D, the wash-out equilibrium point $\hat{x}_A$, in which both ammonium and nitrite oxidizers are washed out of the reactor, is the only equilibrium point. In case the dilution rate is set lower so that ammonium oxidizers can maintain themselves in the reactor, but still high enough so that nitrite oxidizers are washed out, the equilibrium point $\hat{x}_B$, corresponding with only nitrite formation, occurs besides the wash-out equilibrium point $\hat{x}_A$. If the dilution rate becomes so low that also nitrite oxidizers can grow in the reactor, a third equilibrium point $\hat{x}_C$ appears, and even a fourth equilibrium point $\hat{x}_D$, depending on the influent ammonium concentration ξ_{in_1}. Note, however, that the influent ammonium concentration often cannot be set by the user but should rather be seen as a process disturbance.

The analytically obtained results for the simplified reactor model have been checked by simulations. Figure 3.2 shows the obtained phase portraits of the system on the hyperplane Δ for different combinations of dilution rate and influent ammonium concentration. One combination was selected in each one of the four regions in the $\xi_{in_1} - D$ plane:

1. $D = 2 \times 10^{-5}\,\text{day}^{-1},\ \xi_{in_1} = 1000$ mole m^{-3}.
   In this case the system has only one equilibrium point, $\hat{x}_A$, which is globally asymptotically stable (Figure 3.2a). All trajectories of the system converge to $\hat{x}_A$, where all ammonium and nitrite oxidizers are washed out of the bioreactor.
2. $D = 1.33 \times 10^{-5}\,\text{day}^{-1},\ \xi_{in_1} = 1000$ mole m^{-3}.
   For this choice of inputs the simplified reactor model possesses two equilibrium points (Figure 3.2b): the wash-out state $\hat{x}_A$ which is unstable and a desired operating point $\hat{x}_B$ which is asymptotically stable. All trajectories, except for the wash-out state, converge to the operating point $\hat{x}_B$.
3. $D = 0.786 \times 10^{-5}\,\text{day}^{-1},\ \xi_{in_1} = 275$ mole m^{-3}.
   Three equilibrium points occur in this situation (Figure 3.2c): two unstable ones

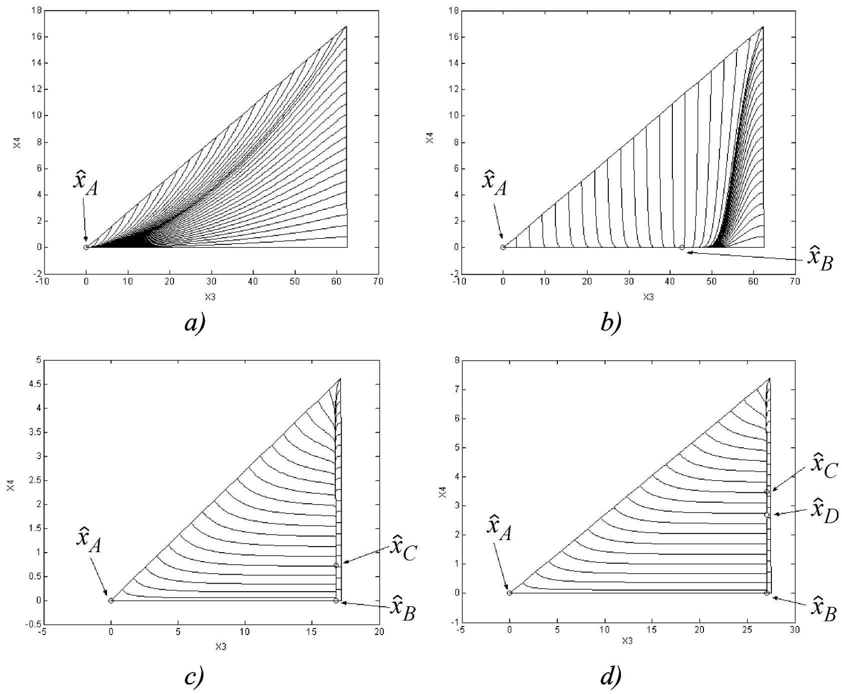

Figure 3.2. Phase portraits in the $x_3 - x_4$ plane.

$(\hat{x}_A, \hat{x}_B)$ and an asymptotically stable operating point $\hat{x}_C$. All trajectories, except those starting with $x_4(0) = 0$, converge to $\hat{x}_C$.

4. $D = 0.786 \times 10^{-5}\,\text{day}^{-1}$, $\xi_{in_1} = 440$ mole m^{-3}.
This situation corresponds to the occurrence of four equilibrium points (Figure 3.2d). There are two unstable equilibrium points ($\hat{x}_A$ and $\hat{x}_D$) and two locally asymptotically stable equilibrium points ($\hat{x}_B$ and $\hat{x}_C$). Because $\hat{\xi}_{B_2} > \hat{\xi}_{C_2}$ and $\hat{\xi}_{B_1} = \hat{\xi}_{C_1}$, in practice $\hat{x}_B$ is a better operating point than $\hat{x}_C$.

4 Estimation of a Stability Boundary

For the practical situation, in which two stable equilibrium points occur at the same time, as in Case 4 of the previous section, it is essential to forecast from which initial states the process will converge to the desired operating point $\hat{x}_B$, corresponding with only nitrite formation, and which initial conditions will lead the system to the operating point $\hat{x}_C$, in which nitrate is formed. This corresponds to estimating the stability boundary

$$\partial\Omega(\hat{x}_B) = \partial\Omega(\hat{x}_C) \tag{31}$$

separating the regions of attraction $\Omega(\hat{x}_B)$ and $\Omega(\hat{x}_C)$ of the stable equilibria. For systems such as the SHARON reactor, algorithms to find an estimate of the stability boundary $\partial\Omega_{est}(\hat{x}_B)$ that approaches the true stability boundary $\partial\Omega(\hat{x}_B)$ as some algorithmic parameter $\varepsilon \to 0$, have been described in [8]. In the present case

$$\partial\Omega(\hat{x}_B) = W^s(\hat{x}_D) \tag{32}$$

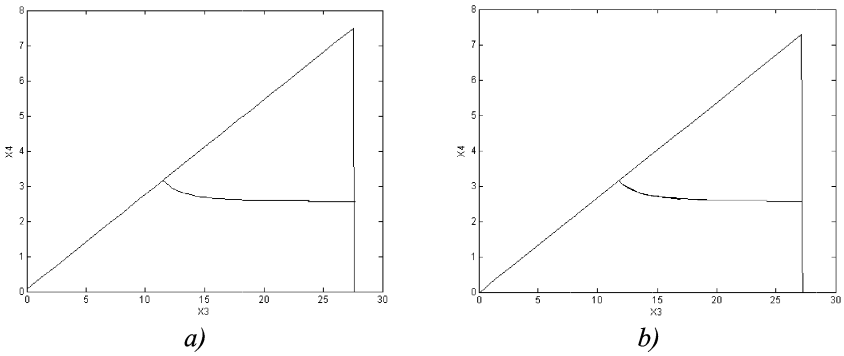

Figure 4.1. Intersections of the stability boundary with the planes H_1, H_2.

where the right hand side of (32) denotes the stable manifold of $\hat{x}_D$. An estimate $W^s_{est}(\hat{x}_D)$ can be found by a trajectory reversing technique such as described e.g. in [3].

The extent of the stability boundary in the four-dimensional state space of the system can be visualized by computing intersections of $\partial\Omega_{est}(\hat{x}_B)$ with the set $H = \{x_b = \eta\}$ for constant vectors $\eta = [\eta_1, \eta_2]^{\mathrm{T}}$. For a numerical technique to accomplish such visualizations see [8].

Figure 4.1 presents the intersection of the estimated stability boundary with the planes H_1 and H_2 corresponding respectively to $\eta_1 = \hat{x}_{D_1} + 2$, $\eta_2 = \hat{x}_{D_2} + 4$ and $\eta_1 = \hat{x}_{D_1} - 4$, $\eta_2 = \hat{x}_{D_2} - 2$. The obtained intersections practically coincide with the curve $W^s(\hat{x}_D)$ on the Δ hyperplane (Figure 3.2d). If the initial conditions of the process are chosen in such a way that the states x_3 and x_4 are below this intersection line (e.g. by ensuring that the initial amount of nitrite oxidizers, $x_4(t = 0)$ is small) and inside the physical boundaries, then the SHARON reactor will converge to the desired operating point $\hat{x}_B$, in which only nitrite is formed.

Summarizing, even for high dilution rates, stable nitrite formation is possible, as long as the influent ammonium concentration is sufficiently high to have four equilibrium points (see Figure 3.1) and if the initial concentration of nitrite oxidizers is sufficiently low.

5 Effect of Changing Parameter and Input Values

For biological systems, it is often difficult to determine exact parameter values. Also, parameter values may change in time e.g. because of biomass adaptation. Besides, also the input values may be uncertain. For this reason, the effect of changing parameter and input values is assessed by the analysis of an extended model of the SHARON reactor. Let

$$c_3 \triangleq \frac{1}{c_1}, \quad e_3 \triangleq \frac{1}{e_2} \tag{33}$$

and suppose that ξ_{in_i}, $i = 2, \ldots, 4$, c_2, c_3 and e_3 have small positive values. We investigate the effect of these values on the position of equilibrium points. Note that the index, hence the local asymptotic stability or instability, of the equilibrium points are not affected by these small parameters because all the equilibrium points of the reactor are hyperbolic. The equilibrium points of the extended model are the solutions of:

$$x_1 = w_1, \tag{34}$$

$$x_2 = w_2, \tag{35}$$

$$[-D + \rho_1(x)]\, x_3 + D\xi_{in_3} = 0, \tag{36}$$

$$[-D + \rho_2(x)]\, x_4 + D\xi_{in_4} = 0, \tag{37}$$

where

$$\rho_1(x) = a_1 \cdot \frac{\xi_1}{b_1 + \xi_1} \cdot \frac{1}{1 + c_3\xi_2}\,, \tag{38}$$

$$\rho_2(x) = a_2 \cdot \frac{\xi_2}{b_2 + \xi_2} \cdot \frac{d_2}{d_2 + \xi_2} \cdot \frac{\xi_1}{c_2 + \xi_1} \cdot \frac{1}{1 + e_3\xi_1}\,. \tag{39}$$

We calculate the equilibrium points of the extended model as variations of the solutions of the simplified model, neglecting higher order terms in the small parameter values.

Case 1. $\tilde{x}_A = \hat{x}_A + \Delta\hat{x}_A$. This equilibrium point is given by

$$\tilde{x}_A = \begin{bmatrix} \xi_{in_1} + a\xi_{in_3} + b\xi_{in_4} \\ \xi_{in_2} - c\xi_{in_3} + d\xi_{in_4} \\ \dfrac{D\xi_{in_3}}{D - a_1 \frac{\xi_{in_1}}{b_1 + \xi_{in_1}}} \\ \xi_{in_4} \end{bmatrix}. \tag{40}$$

It is a physical equilibrium point if $D > a_1 \dfrac{\xi_{in_1}}{b_1 + \xi_{in_1}}$. This corresponds to the case in which $\hat{x}_B$ is not a physical equilibrium point of the simplified model.

Case 2. $\tilde{x}_B = \hat{x}_B + \Delta\hat{x}_B$,

$$\tilde{x}_B = \begin{bmatrix} \xi_{in_1} + a\xi_{in_3} + b\xi_{in_4} \\ \xi_{in_2} - c\xi_{in_3} + d\xi_{in_4} \\ \hat{x}_{B_3} + \Delta\hat{x}_{B_3} \\ \Delta\hat{x}_{B_4} \end{bmatrix} \tag{41}$$

where

$$\Delta\hat{x}_{B_3} = \frac{1}{a\hat{x}_{B_3}\frac{b_1}{b_1 + \hat{\xi}_{B_1}} + c_3\hat{\xi}_{B_2}\hat{\xi}_{B_1}}\, \hat{x}_{B_3} \left[-c_3\hat{\xi}_{B_2}\hat{\xi}_{B_1} + \frac{b_1}{b_1 + \hat{\xi}_{B_1}} (a\xi_{in_3} + b\xi_{in_4} - b\Delta\hat{x}_{B_4}) \right],$$

$$\Delta\hat{x}_{B_4} = \frac{D\xi_{in_4}}{D - a_2 \frac{\hat{\xi}_{B_2}}{b_2 + \hat{\xi}_{B_2}} \cdot \frac{d_2}{d_2 + \hat{\xi}_{B_2}}}. \tag{42}$$

It can be shown that $\tilde{x}_B$ is a physical equilibrium point of the extended model in the region where the simplified model has two equilibrium points $(\hat{x}_A, \hat{x}_B)$ and also in the region where the simplified model possesses four equilibrium points $(\hat{x}_A, \hat{x}_B, \hat{x}_C, \hat{x}_D)$.

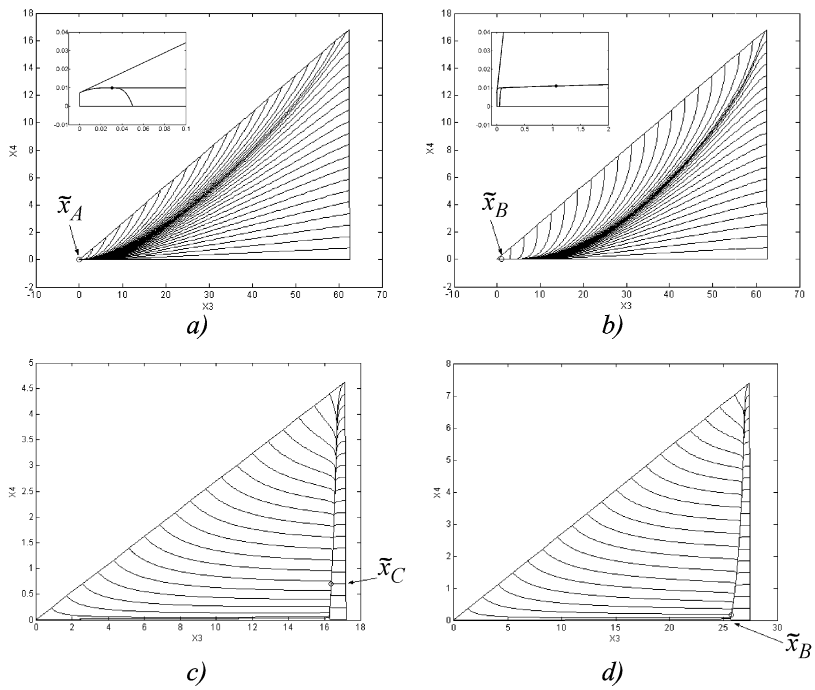

Figure 5.1. Phase portraits in the $x_3 - x_4$ plane for the extended model. a) $\tilde{x}_A = [0.03 \quad 0.01]^T$; b) $\tilde{x}_B = [1.06 \quad 0.01]^T$; c) $\tilde{x}_C = [16.37 \quad 0.7]^T$; d) $\tilde{x}_B = [25.71 \quad 0.16]^T$.

Case 3. $\tilde{x}_C = \hat{x}_C + \Delta\hat{x}_C$ and $\tilde{x}_D = \hat{x}_D + \Delta\hat{x}_D$,

$$\tilde{x}_C = \begin{bmatrix} \xi_{in_1} + a\xi_{in_3} + b\xi_{in_4} \\ \xi_{in_2} - c\xi_{in_3} + d\xi_{in_4} \\ \hat{x}_{C_3} + \Delta\hat{x}_{C_3} \\ \hat{x}_{C_4} + \Delta\hat{x}_{C_4} \end{bmatrix}, \qquad \tilde{x}_D = \begin{bmatrix} \xi_{in_1} + a\xi_{in_3} + b\xi_{in_4} \\ \xi_{in_2} - c\xi_{in_3} + d\xi_{in_4} \\ \hat{x}_{D_3} + \Delta\hat{x}_{D_3} \\ \hat{x}_{D_4} + \Delta\hat{x}_{D_4} \end{bmatrix}. \tag{43}$$

These equilibrium points can be determined in a similar way as $\tilde{x}_A$ and $\tilde{x}_B$. They are lying in the neighborhood of $\hat{x}_C$ and $\hat{x}_D$ and therefore they are physical equilibrium points.

The equilibrium points of the extended model can also be determined using a numerical search algorithm. Figure 5.1 displays the phase portraits in the $x_3 - x_4$ plane of the extended model for the same combinations of dilution rate and ammonium concentration in the inflow as considered for the simplified model. For the selected parameter values and inputs the analytical calculation of the equilibrium points proved to be reasonably accurate. Similar values for the equilibria were obtained from the simulation of the phase portraits. While in the cases 1, 3 and 4 the phase portrait of the extended model is very similar to the phase portrait of the simplified model, this is not true however in case 2. Here small variations of the component concentration in the inflow and a more detailed reaction rate function have a great impact on the technological relevance of the equilibrium point: $\hat{x}_B$ changes from a desirable operating point in the case of the simplified model to a non-desirable equilibrium point in the case of the extended model.

More specifically, in the first situation (Figure 5.1a), the globally asymptotically stable wash-out state $\tilde{x}_A$ moves into the interior of the physical state space, however the change is not sufficiently significant to make $\tilde{x}_A$ a desirable operating point. For the second choice of inputs (Figure 5.1b), $\tilde{x}_A$ moves out of the physical state space. Only one physical equilibrium point occurs, namely $\tilde{x}_B$, which changes from a desired operating point to an almost wash-out state, that is undesirable. Apparently, the assumed parameter and input variations affect the model behavior significantly.

In the third situation (Figure 5.1c) both $\tilde{x}_A$ and $\tilde{x}_B$ move out of the physical state space. Now the extended reactor model possesses only one physical equilibrium point $\tilde{x}_C$, where the rate of conversion to nitrite is smaller than in the case of Figure 3.2. The last situation presents a particularity of the SHARON reactor: although the calculations indicate the occurrence of three physical equilibrium points ($\tilde{x}_B$, $\tilde{x}_C$, $\tilde{x}_D$), while $\tilde{x}_A$ has moved out of the physical state space, the phase portrait (Figure 5.1d) shows $\tilde{x}_B$ as a globally asymptotically stable equilibrium point, while it was expected to be only locally asymptotically stable. Due to numerical limitations, the equilibrium points $\tilde{x}_C$ and $\tilde{x}_D$ could not be detected. This is due to the fact that for the extended reactor model the equilibrium points $\tilde{x}_C$ (locally asymptotically stable) and $\tilde{x}_D$ (unstable) move so close to each other that they practically cancel each other and do not noticeable affect the phase portrait. The remaining equilibrium point $\tilde{x}_D$ corresponds with good reactor operation, as only nitrite is formed.

6 Conclusion

In this paper, the dynamic behavior of a SHARON reactor with constant volume, considering two consecutive nitrification reactions, is assessed. The reactor models that have been studied, are valid for constant temperature and pH.

First, the behavior of a simplified reactor model is analysed. The only inhibition effect considered in this model, is nitrite inhibition of nitrite oxidation. It is further assumed that the reactor influent does not contain biomass. It was shown that multiple equilibrium points occur, depending on the dilution rate and the influent ammonium concentration. For the case in which two stable equilibrium points occur at the same time, the stability boundary has been estimated, to determine the initial states which will lead the reactor to the most desirable operating point. Four situations are identified, corresponding to the occurrence of one, two, three or four equilibrium points respectively. From a technological point of view, the SHARON reactor should be operated in such a way that only nitrite is produced and nitrate formation is suppressed. Good operation of the SHARON reactor is ensured in case the dilution rate is sufficiently low to make sure the ammonium oxidizers can maintain themselves in the reactor, while nitrite oxidizers are washed out (case 2), but also for lower dilution rates and at the same time sufficiently high ammonium influent concentrations, provided a rather low concentration of nitrite oxidizers initially present in the reactor (case 4).

Subsequently, an extended reactor model has been studied to determine the effect of changing parameter and input values. Small influent biomass concentrations were considered, as well as additional inhibition effects in in the reaction rate functions. However, even the slight modifications applied, significantly affect the reactor performance. The moderate dilution rate and influent ammonium concentration corresponding with case 2, that allow good performance of the simplified reactor model, now corresponds with almost wash-out of biomass. On the other hand, the relatively high dilution rate, high influent ammonium concentration and low initial concentration of nitrite oxidizers, corresponding with case 4, still allow good operation of the SHARON reactor.

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