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

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### Abstract

This paper addresses the dynamics of a SHARON reactor, a promising technology for ammonium removal from concentrated wastewater streams. The contraction mapping theorem is used to determine which operating conditions of a SHARON reactor with pH-control result in a unique equilibrium state. However, this approach only identifies the case of very large dilution rates, in practice corresponding with complete biomass wash-out, i.e. with complete loss of biological activity. Practical operation of a SHARON reactor aims at reaching ammonium conversion to nitrite. To identify such interesting operating points, the equilibrium points are subsequently calculated directly in terms of input variables for a simplified SHARON reactor model. The stability of the obtained equilibrium points is assessed and the corresponding phase portraits are analyzed. The influence of slightly varying parameter and input values is investigated as well.

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### 1. Introduction

Biological techniques for nitrogen removal from wastewater have proven their effectiveness and have been widely implemented. In the last few years, several novel nitrogen removal processes with improved sustainability have been developed. An example is the SHARON process (single reactor system for high activity ammonia removal over nitrite), which is ideally suited to remove nitrogen from wastewater streams with high ammonium concentration [1]. In a SHARON reactor, typically a continuous stirred tank reactor (CSTR), ammonium is converted to nitrite while further conversion of nitrite to nitrate is prevented. This is realized by operating the reactor at a suitable dilution rate. 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 controlling the dilution rate. In this way, substantial savings in aeration costs are realized, in comparison with oxidation of ammonium to nitrate. The question arises whether the concentrations obtained in the SHARON process are unique and stable for constant input variables.

This paper addresses the existence, uniqueness and stability of the equilibrium points of a SHARON reactor with pH-control. Operating regions in the control input space for which there exists a unique equilibrium point are identified. For this purpose, the contraction mapping theorem is used, resulting in a sufficient but not necessary uniqueness criterion. Subsequently, the obtained results are verified by direct calculation of the equilibrium points of a simplified SHARON reactor model. Conditions are determined for which the system possesses multiple equilibrium points and their stability is assessed by means of the linearization principle. The analytically obtained results are verified by simulations. Phase trajectories illustrate the process

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behaviour. Finally, it is investigated how slightly varying model parameters and input variables affect the results.

## 2. The SHARON reactor model

### 2.1. State-space model

The simplified SHARON reactor model used in this study considers two nitrification reactions: oxidation of ammonium to nitrite and consecutive oxidation of nitrite to nitrate. Four components are involved in the biological conversion reactions, of which the concentrations ( $x_i(t) \geq 0$ ) are identified as the system's state variables: total ammonium ( $x_1$ ), total nitrite ( $x_2$ ), ammonium oxidizers ( $x_3$ ) and nitrite oxidizers ( $x_4$ ). Ammonium and nitrite oxidations are described by their respective reaction rates:

$$\rho_1 = a_1 \cdot \frac{x_1}{b_1 + x_1} \cdot \frac{c_1}{c_1 + x_2} \cdot x_3 \quad (1)$$

$$\rho_2 = a_2 \cdot \frac{x_2}{b_2 + x_2} \cdot \frac{x_1}{c_2 + x_1} \cdot \frac{d_2}{d_2 + x_2} \cdot \frac{e_2}{e_2 + x_1} \cdot x_4 \quad (2)$$

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. In a SHARON reactor, the maximum growth rate of ammonium oxidizers ( $a_1$ ) is larger than the maximum growth rate of nitrite oxidizers ( $a_2$ ). 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  $d_2$  and  $e_2$ , respectively). It is further assumed that the SHARON reactor is continuously aerated and that oxygen is always present in excess.

The reactor is modelled as a CSTR without biomass retention. The reactor liquid volume is assumed constant. The system's state equations are given by the individual mass balances for the four components:

$$\dot{x}_1 = u_0 \cdot (u_1 - x_1) - a \cdot \rho_1 - b \cdot \rho_2 \triangleq f_1(\mathbf{x}) \quad (3)$$

$$\dot{x}_2 = u_0 \cdot (u_2 - x_2) + c \cdot \rho_1 - d \cdot \rho_2 \triangleq f_2(\mathbf{x}) \quad (4)$$

$$\dot{x}_3 = u_0 \cdot (u_3 - x_3) + \rho_1 \triangleq f_3(\mathbf{x}) \quad (5)$$

$$\dot{x}_4 = u_0 \cdot (u_4 - x_4) + \rho_2 \triangleq f_4(\mathbf{x}) \quad (6)$$

with

$$\mathbf{x} = [x_1 \quad x_2 \quad x_3 \quad x_4]^T \quad (7)$$

and in which  $a, b, c$  and  $d$  represent strictly positive stoichiometric coefficients. Table 1 gives the numerical values for the SHARON model parameters applied in this study.

The input variables ( $u_i(t) \geq 0$ ) are the dilution rate ( $u_0$ ), that equals the ratio of the influent flow rate  $\Phi_{in}$  over the reactor volume  $V$ , besides influent concentrations of (total) ammonium ( $u_1$ ), (total) nitrite ( $u_2$ ), ammonium oxidizing biomass ( $u_3$ ) and nitrite oxidizing biomass ( $u_4$ ).

The state Eqs. (3)–(6) are summarized in the matrix form:

Table 1

Numerical values of the SHARON model parameters (at pH = 7 and  $T = 35^\circ\text{C}$ )

Symbol	Unit	Value
$a_1$	2.1	day <sup>-1</sup>
$b_1$	4.73	mole m <sup>-3</sup>
$c_1$	837	mole m <sup>-3</sup>
$a_2$	1.05	day <sup>-1</sup>
$b_2$	109	mole m <sup>-3</sup>
$c_2$	0.01	mole m <sup>-3</sup>
$d_2$	1000	mole m <sup>-3</sup>
$e_2$	1000	mole m <sup>-3</sup>
$a$	16	mole mole <sup>-1</sup>
$b$	0.2	mole mole <sup>-1</sup>
$c$	58.6	mole mole <sup>-1</sup>
$d$	15.8	mole mole <sup>-1</sup>

$$\dot{\mathbf{x}} = (\mathbf{u} - \mathbf{x}) \cdot u_0 + \mathbf{M} \cdot \boldsymbol{\rho}(\mathbf{x}) \triangleq \mathbf{f}(\mathbf{x}) \quad (8)$$

with

$$\mathbf{u} \triangleq \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{bmatrix}; \quad \mathbf{M} \triangleq \begin{bmatrix} -a & -b \\ c & -d \\ 1 & 0 \\ 0 & 1 \end{bmatrix}; \quad \boldsymbol{\rho}(\mathbf{x}) \triangleq \begin{bmatrix} \rho_1(\mathbf{x}) \\ \rho_2(\mathbf{x}) \end{bmatrix} \quad (9)$$

The question arises whether the concentrations obtained in a SHARON process are unique and stable for constant input variables. Although assuming constant input variables is a simplification of reality, it is very useful for preliminary system analysis, which can be followed by a study for varying input variables in a later stage. In practice, the dilution rate ( $u_0$ ) will be controlled to a more or less constant value to obtain the desired conversion of ammonium to nitrite, at the same time preventing further oxidation of nitrite to nitrate. The influent ammonium concentration ( $u_1$ ) should be seen as an uncontrollable input but is not expected to vary much, as a SHARON reactor is typically fed with the effluent stream of an anaerobic digester, a system that possesses relatively long time constants. The remaining input variables can reasonably be assumed constant as well: the SHARON influent usually does not contain nitrite ( $u_2$ ) and only very small quantities of biomass ( $u_3$  and  $u_4$ ). In this way, the assumption of constant input variables is not considered very restrictive. The subsequent analysis focuses on the existence, uniqueness and stability of associated equilibrium states.

### 2.2. Equilibrium conditions

The equilibrium states  $x_{ei}$  of the reactor model, corresponding with constant input values  $u_i$ , satisfy

$$0 = (\mathbf{u} - \mathbf{x}_e) \cdot u_0 + \mathbf{M} \cdot \boldsymbol{\rho}(\mathbf{x}_e) \triangleq \mathbf{f}(\mathbf{x}_e) \quad (10)$$

If  $u_0 = 0$ , a number of  $\infty^3 + 2 \cdot \infty^2$  equilibrium solutions are found:

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

In case  $u_0 > 0$ , the equilibrium points cannot easily be calculated directly. However, for an infinitely high dilution rate ( $u_0 \rightarrow \infty$ ), Eq. (10) shows that, in contrast with the case  $u_0 = 0$ , there is a unique equilibrium point  $\mathbf{x}_e$ , corresponding with the influent conditions  $\mathbf{u}$ , i.e. the wash-out point where the reactor fails. Subsequent analysis uses the contraction mapping theorem to identify other regions in the  $(u_0, \mathbf{u})$ -space resulting in a unique equilibrium point. Because of the sufficient but not necessary nature of the derived criteria, the results are verified by direct calculation of the equilibrium points of a simplified reactor model.

### 3. Uniqueness of equilibrium points

In order to determine regions in the input space for which there exists a unique equilibrium point, which are often interesting for practical operation, the contraction mapping theorem is used. Its application to the SHARON model from Section 2, as well as to a reduced equilibrium form, results in two distinct, sufficient but not necessary criteria for the uniqueness of equilibrium states, which are subsequently evaluated through simulation.

#### 3.1. The contraction mapping theorem

Assuming  $u_0 > 0$ , Eq. (10) can be rewritten as

$$\mathbf{x}_e = \mathbf{u} + \frac{1}{u_0} \cdot \mathbf{M} \cdot \rho(\mathbf{x}_e) \triangleq \varphi(\mathbf{x}_e) \quad (11)$$

with

$$\varphi(\mathbf{x}) \triangleq [\varphi_1(\mathbf{x}) \quad \varphi_2(\mathbf{x}) \quad \varphi_3(\mathbf{x}) \quad \varphi_4(\mathbf{x})]^T \quad (12)$$

The mapping  $\mathbf{y} = \varphi(\mathbf{x})$  is defined in the complete metric space  $\mathbb{R}^{4 \times 1}$ , with the Euclidian norm  $\ell$  as distance. If the mapping  $\varphi$  possesses a point  $\mathbf{x}_e$  for which

$$\mathbf{x}_e = \varphi(\mathbf{x}_e) \quad (13)$$

then  $\mathbf{x}_e$  is an equilibrium point of this system.

The uniqueness of equilibrium points can be investigated by means of the principle of contraction mappings, as formulated by [2]: *Every contraction mapping  $\mathbf{g}$  defined in a complete metric space  $\mathbf{X}$  has one and only one fixed point in  $\mathbf{X}$ , that is, there is one and only one point in  $\mathbf{X}$  such that  $\mathbf{x} = \mathbf{g}(\mathbf{x})$ . The value of this fixed point can be determined through the method of successive approximations [2]:*

$$\mathbf{x}_{n+1} = \mathbf{g}(\mathbf{x}_n), \quad n = 0, 1, 2, \dots \quad (14)$$

where the starting value  $\mathbf{x}_0$  is arbitrary. The mapping  $\mathbf{y} = \varphi(\mathbf{x})$  in  $\mathbb{R}^{4 \times 1}$  is a contraction mapping if there exists a positive number  $K < 1$  such that

$$\ell[\varphi(\mathbf{x}), \varphi(\mathbf{w})] \leq K \cdot \ell(\mathbf{x}, \mathbf{w}) \quad \forall \mathbf{x}, \mathbf{w} \text{ in } \mathbb{R}^{4 \times 1} \quad (15)$$

The procedure for determining the conditions under which  $\varphi$  is a contraction mapping, so under which the SHARON model possesses a unique equilibrium point, is summarized in Appendix A.1. It involves the estimation of upper

boundaries for several variables, resulting in a sufficient but not necessary uniqueness criterion:

$$u_0 > \sqrt{s_0 \cdot s_1} \quad (16)$$

where the values of  $s_0$  and  $s_1$  are defined by (A.2) and (A.12).

When equilibrium conditions prevail, two state variables of the SHARON model can be rewritten in terms of the two remaining state variables and the input variables (see Appendix A.2). The model equations are thus rewritten in terms of two state variables instead of four. One could expect that a less restrictive criterion for the existence of a unique equilibrium point would be obtained by applying the contraction mapping to this reduced two-dimensional static model. This results in the criterion (see Appendix A.2)

$$u_0 > \sqrt{\hat{s}_0 \cdot \hat{s}_1} \quad (17)$$

where  $\hat{s}_0$  and  $\hat{s}_1$  are given by (A.25) and (A.26).

Due to relaxations that have been made, both criteria (16) and (17) are of a sufficient but not necessary nature. As it is not possible to determine a priori which condition is the most stringent, they have both been evaluated and the results are compared against each other.

#### 3.2. Simulation results

The criteria (16) and (17) for a unique equilibrium can be evaluated in terms of the dilution rate,  $u_0$ . Fig. 1 depicts the profiles of  $u_0 - \sqrt{s_0 \cdot s_1}$  and  $u_0 - \sqrt{\hat{s}_0 \cdot \hat{s}_1}$  for given  $\mathbf{u}$ -values. The values of  $u_{0,\text{crit}}^{\text{dim}}$  and  $u_{0,\text{crit}}^{2\text{dim}}$  are found as the values of  $u_0$  where these functions become zero, i.e.  $120.1 \text{ day}^{-1}$  and  $7.5 \text{ day}^{-1}$ , respectively. For the given input values, criterion (17) performs better than (16), as it results in a lower (critical) value of the dilution rate above which there exists a unique equilibrium point. This corresponds to what could have been expected intuitively, since it is likely that less relaxations are made in a two-dimensional space compared to a four-dimensional one. It can be concluded that for the given influent conditions, a unique equilibrium will be

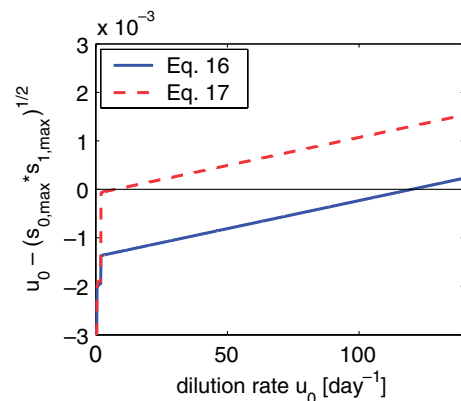


Fig. 1. Evaluation of the criteria for a unique equilibrium in terms of  $u_0$  for  $u_1 = 70 \text{ mole m}^{-3}$ ,  $u_2 = 0 \text{ mole m}^{-3}$ ,  $u_3 = u_4 = 0.01 \text{ mole m}^{-3}$ .

obtained for dilution rates higher than  $7.5 \text{ day}^{-1}$ . It is however known from practice that such a high dilution rate will cause wash-out of both ammonium oxidizing and nitrite oxidizing biomass.

The value of this unique equilibrium point is subsequently determined through the method of successive approximations (Eq. (14)):

$$\mathbf{x}_{n+1} = \varphi(\mathbf{x}_n) = \mathbf{u} + \frac{1}{u_0} \cdot \mathbf{M} \rho(\mathbf{x}_n), \quad n = 0, 1, 2, \dots$$

starting from an arbitrary initial point  $\mathbf{x}_0$ .

The values of the equilibrium states have been obtained for  $u_0 = 7.6 \text{ day}^{-1}$  as

$$\begin{aligned} x_{e1} &= 69.94 \text{ mole m}^{-3} \\ x_{e2} &= 0.0551 \text{ mole m}^{-3} \\ x_{e3} &= 0.135 \text{ mole m}^{-3} \\ x_{e4} &= 0.0100 \text{ mole m}^{-3} \end{aligned}$$

As expected, the equilibrium state indeed corresponds with biomass wash-out. Only a very small amount of ammonium is converted by the ammonium oxidizers present in the influent.

Finally, the influence of the influent ammonium concentration ( $u_1$ ) on the equilibrium points is investigated. The influence of the influent nitrite concentration ( $u_2$ ), and the influent concentrations of ammonium oxidizers ( $u_3$ ) and nitrite oxidizers ( $u_4$ ) is not discussed, as they are not likely to vary much in practice. Both criteria (16) and (17) have been evaluated in terms of the dilution rates ( $u_0$ ) for different values of the ammonium influent concentration ( $u_1$ ). Fig. 2 gives the resulting minimum value of the dilution rate above which there exists a unique equilibrium point,  $u_{0,\text{crit}}$ , in terms of the influent ammonium concentration ( $u_1$ ). In all cases, criterion (17) performs significantly better, i.e. is less restrictive, than (16).

For the range of influent conditions  $u_1$  examined, the minimum value for the dilution rate, above which there exists a unique equilibrium point, is too high to prevent wash-out of ammonium oxidizing biomass. This has been verified by calculation of the equilibrium points for dilution

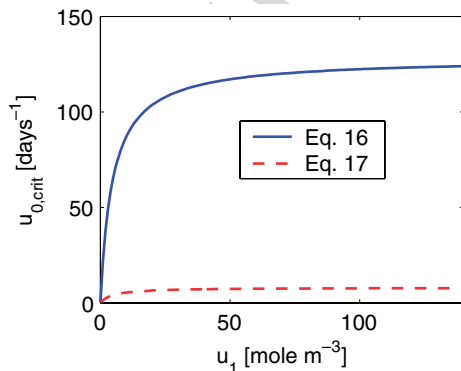


Fig. 2. Minimum dilution rate,  $u_{0,\text{crit}}$ , required for a unique equilibrium point in terms of  $u_1$  ( $u_2 = 0 \text{ mole m}^{-3}$ ;  $u_3 = u_4 = 0.01 \text{ mole m}^{-3}$ ).

rates just above the critical values, that guarantee a unique equilibrium. Each time, the unique equilibrium state has been identified as the wash-out state with negligible ammonium conversion.

#### 4. Analysis of a simplified reactor model

The criteria derived in Section 3 on the basis of the contraction mapping principle identified the wash-out point as unique equilibrium point of the SHARON reactor model for sufficiently high dilution rates. However, because of the ‘sufficient but not necessary’ nature of these criteria, no conclusions can be drawn concerning the uniqueness of equilibrium points for values below the critical dilution rate. For this reason, equilibrium points will now be calculated directly for a simplified reactor model. The latter model is first transformed into a so-called canonical state space representation, which simplifies the subsequent analysis. The multiplicity of the equilibrium points is evaluated in terms of the input variables and their stability is examined as well.

##### 4.1. Canonical state-space model representation

The model of Section 2 is simplified, realistically assuming the incoming stream does not contain any nitrite, ammonium oxidizers or nitrite oxidizers ( $u_2 = u_3 = u_4 = 0$ ). Further, ammonium limitation of nitrite oxidizers is not considered ( $c_2 = 0$ ). Finally, nitrite inhibition of the ammonium oxidation is considered ( $c_1 < +\infty$ ), while the nitrite oxidation is assumed not to be inhibited ( $d_2 = e_2 = +\infty$ ).

By defining new state space variables

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} \triangleq \begin{bmatrix} x_1 + a \cdot x_3 + b \cdot x_4 \\ x_2 - c \cdot x_3 + d \cdot x_4 \\ x_3 \\ x_4 \end{bmatrix} \quad (18)$$

the model is transformed into its so-called canonical state space representation:

$$\dot{y}_1 = u_0 \cdot (u_1 - y_1) \triangleq g_1(\mathbf{y}) \quad (19)$$

$$\dot{y}_2 = -u_0 \cdot y_2 \triangleq g_2(\mathbf{y}) \quad (20)$$

$$\dot{y}_3 = -u_0 \cdot y_3 + \sigma_1(\mathbf{y}) \triangleq g_3(\mathbf{y}) \quad (21)$$

$$\dot{y}_4 = -u_0 \cdot y_4 + \sigma_2(\mathbf{y}) \triangleq g_4(\mathbf{y}) \quad (22)$$

with

$$\sigma_1(\mathbf{y}) = a_1 \cdot \frac{x_1}{b_1 + x_1} \cdot \frac{c_1}{c_1 + x_2} \cdot y_3 \quad (23)$$

$$\sigma_2(\mathbf{y}) = \begin{cases} a_2 \cdot \frac{x_2}{b_2 + x_2} \cdot y_4 & \text{for } x_1 > 0 \\ 0 & \text{for } x_1 = 0 \end{cases} \quad (24)$$

in which

$$x_1 = y_1 - a \cdot y_3 - b \cdot y_4 \quad (25)$$

$$x_2 = y_2 + c \cdot y_3 - d \cdot y_4 \quad (26)$$

Call  $\mathbf{S}_y$  the image of  $\mathbb{R}^+ = \{\mathbf{x} \in \mathbb{R}^4; x_i \geq 0, i = 1, \dots, 4\}$  under the transformation  $\mathbf{x} \mapsto \mathbf{y}$ .  $\mathbf{S}_y$  is the state space of the system (19)–(21). It is defined by the inequalities:

$$x_i \geq 0 \quad \forall i = 1, \dots, 4 \quad (27)$$

Every trajectory that starts at  $t = 0$  in a point  $\mathbf{y}_0$  of  $\mathbf{S}_y$ , stays in  $\mathbf{S}_y$  for  $t \geq 0$ . It subsequently converges to the cross-section  $\Delta$  of  $\mathbf{S}_y$  with the plane  $\{y_1 = u_1, y_2 = 0\}$ , as can be seen from Eqs. (19) and (20).  $\Delta$  is a bounded region, defined by the inequalities

$$u_1 - a \cdot y_3 - b \cdot y_4 \geq 0 \quad (28)$$

$$c \cdot y_3 - d \cdot y_4 \geq 0 \quad (29)$$

$$y_3 \geq 0 \quad (30)$$

$$y_4 \geq 0 \quad (31)$$

After reaching this convergence, the process exhibits a second-order behaviour that is determined by the dynamics of  $y_3(=x_3)$  and  $y_4(=x_4)$ , as can be seen from Eqs. (21)–(26) in which  $y_1 = u_1$  and  $y_2 = 0$ . In the sequel a mathematical equilibrium point  $\mathbf{y}_e$  will be called a physical equilibrium if it lies in  $\mathbf{S}_y$ .

## 4.2. Occurrence of multiple equilibrium states

### 4.2.1. Equilibrium points in case $u_1 = 0$

In case the influent does not contain ammonium ( $u_1 = 0$ ), it follows from Eqs. (19), (20), (25) and (26) that

$$\begin{aligned} \dot{\mathbf{y}} = 0 &\iff y_{e1} = y_{e2} = y_{e3} = y_{e4} = 0 \\ &\iff x_{e1} = x_{e2} = x_{e3} = x_{e4} = 0 \end{aligned}$$

indicating a unique (trivial) equilibrium point corresponding with biomass wash-out.

### 4.2.2. Equilibrium points in case $u_0 > 0$ and $u_1 > 0$

If  $u_0 > 0$  and  $u_1 > 0$ , it results from (23), (24), (21), (22) and (18), that there exists no equilibrium point for which  $x_{e1} = 0$ . Consequently, by Eqs. (19)–(24) the equilibrium points fulfill the following equations:

$$y_{e1} = u_1 \quad (32)$$

$$y_{e2} = 0 \quad (33)$$

$$\left(-u_0 + a_1 \cdot \frac{x_{e1}}{b_1 + x_{e1}} \cdot \frac{c_1}{c_1 + x_{e2}}\right) \cdot y_{e3} = 0 \quad (34)$$

$$\left(-u_0 + a_2 \cdot \frac{x_{e2}}{b_2 + x_{e2}}\right) \cdot y_{e4} = 0 \quad (35)$$

It can be verified that  $y_{e3} = 0$  implies  $y_{e4} = 0$ . As a result, three equilibrium points are obtained:

- (1) Letting  $y_{e3} = y_{e4} = 0$  yields:

$$\mathbf{y}_e^A = \begin{bmatrix} u_1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad (36)$$

This point, corresponding with complete biomass wash-out ( $x_{e3}^A = y_{e3}^A = 0; x_{e4}^A = y_{e4}^A = 0$ ), is always a physical equilibrium point.

- (2) The second equilibrium point corresponds with  $y_{e4} = 0$ , while  $y_{e3} \neq 0$ :

$$\mathbf{y}_e^B = \begin{bmatrix} u_1 \\ 0 \\ \frac{1}{a} \cdot (u_1 - x_{e1}^B) \\ 0 \end{bmatrix} \quad (37)$$

in which  $x_{e1}^B$  is obtained from

$$a_1 \cdot \frac{x_{e1}^B}{b_1 + x_{e1}^B} \cdot \frac{c_1}{c_1 + \frac{a}{a} \cdot (u_1 - x_{e1}^B)} = u_0 \quad (38)$$

This is a physical equilibrium point, i.e. Eq. (27) holds, if and only if

$$u_0 < \frac{a_1 \cdot u_1}{b_1 + u_1} \quad (39)$$

as the left-hand side of Eq. (38) represents a monotonically increasing function of  $x_1$  in  $[0, u_1]$ , with  $u_1$  the upper boundary of  $x_1$ . The point  $\mathbf{y}_e^B$  corresponds with a situation without nitrite oxidizers ( $x_{e4}^B = y_{e4}^B = 0$ ) and consequently without nitrate production. This is exactly the aim of a SHARON reactor. In case  $u_0 = \frac{a_1 \cdot u_1}{b_1 + u_1}$ ,  $\mathbf{y}_e^B$  coincides with  $\mathbf{y}_e^A$ , the wash-out equilibrium point.

- (3) The third equilibrium point corresponds with a situation with both ammonium oxidizers ( $x_{e3} = y_{e3} > 0$ ) and nitrite oxidizers ( $x_{e4} = y_{e4} > 0$ ), so at least part of the formed nitrite is further oxidized to nitrate:

$$\mathbf{y}_e^C = \begin{bmatrix} u_1 \\ 0 \\ \frac{d \cdot (u_1 - x_{e1}^C) + b \cdot x_{e2}^C}{a \cdot d + b \cdot c} \\ \frac{c \cdot (u_1 - x_{e1}^C) - a \cdot x_{e2}^C}{a \cdot d + b \cdot c} \end{bmatrix} \quad (40)$$

in which

$$f(u_0) = u_0 + \frac{b_2 \cdot u_0^2}{c_1 \cdot (a_2 - u_0)} \quad (41)$$

This equilibrium point is a physical equilibrium point if and only if

$$u_1 > \frac{b_1 \cdot f(u_0)}{a_1 - f(u_0)} + \frac{a}{c} \cdot \frac{b_2 \cdot u_0}{a_2 - u_0} \quad (42)$$

It can be verified that the curve defined by Eq. (42) has a horizontal asymptote,  $\hat{u}_0$ , which is the unique solution of

$$(c_1 - b_2) \cdot \hat{u}_0^2 - c_1 \cdot (a_1 + a_2) \cdot \hat{u}_0 + c_1 \cdot a_1 \cdot a_2 = 0 \quad (43)$$

in the interval  $0 < \hat{u}_0 < a_2$  and for which  $a_1 = f(\hat{u}_0)$ .

Note that, for physical  $x_{e2}^C$ ,  $a_2 > u_0$  and consequently also  $f(u_0) > u_0$ . Taking this into account, it is clear that condition (42) is more stringent than condition (39). This means that the occurrence of  $\mathbf{y}_e^C$  implies the occurrence of  $\mathbf{y}_e^B$ ,

while  $\mathbf{y}_e^B$  can be a physical equilibrium point without  $\mathbf{y}_e^C$  being one.  $\mathbf{y}_e^C$  and  $\mathbf{y}_e^B$  coincide if

$$u_1 = \frac{b_1 \cdot f(u_0)}{a_1 - f(u_0)} + \frac{a}{c} \cdot \frac{b_2 \cdot u_0}{a_2 - u_0} \quad (44)$$

In case  $\mathbf{y}_e^C$  and  $\mathbf{y}_e^B$  are distinctive physical equilibrium points, the ammonium concentration at  $\mathbf{y}_e^C$  is slightly lower than at  $\mathbf{y}_e^B$ : as some nitrite is further oxidized to nitrate in  $\mathbf{y}_e^C$ , less nitrite is present, so the corresponding microbial growth rate, that includes nitrite inhibition, is higher, resulting in a (slightly) higher ammonium conversion.

Fig. 3 displays the occurrence of equilibrium points in terms of the dilution rate  $u_0$  and the influent ammonium concentration  $u_1$ . For high dilution rates, only the wash-out equilibrium  $\mathbf{y}_e^A$  is a physical equilibrium point. This corresponds with the findings of Section 3. As the dilution rate decreases, a second equilibrium point  $\mathbf{y}_e^B$  appears, corresponding with only nitrite production. If the dilution rate becomes sufficiently low, a third equilibrium point  $\mathbf{y}_e^C$  appears. The maximum values of the dilution rate below which a second or a third equilibrium point occur, increase with increasing influent ammonium concentration  $u_1$ . This means that  $u_0$  must be sufficiently low and  $u_1$  sufficiently large to obtain a second or a third equilibrium point.

The value of the dilution rate above which the wash-out equilibrium is the unique equilibrium point, obtained by direct calculation, can be compared with the results obtained by applying the uniqueness criterion (17) – resulting from the contraction mapping theorem – to the same simplified model. In this way, the strictness of criterion (17) is evaluated. Fig. 4 depicts the results.

It is clear that criterion (17), obtained by applying the contraction mapping theorem to the reduced (two-dimensional) model, even though in all cases more stringent than criterion (16), obtained by applying the contraction mapping theorem to the original four-dimensional model, is significantly less stringent than the results obtained through direct calculation. Apparently, a lot of information is lost due to the relaxations that have been made.

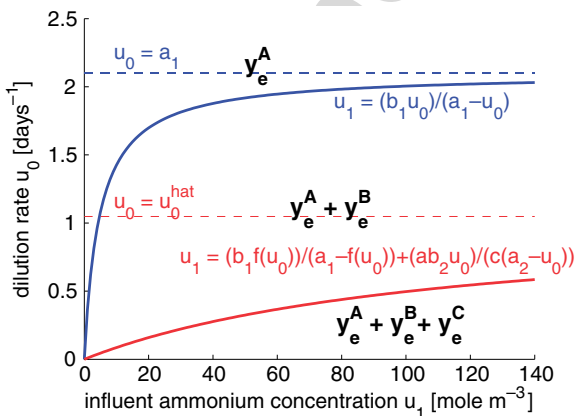


Fig. 3. Equilibrium points of a simplified SHARON model in terms of  $u_0$  and  $u_1$ .

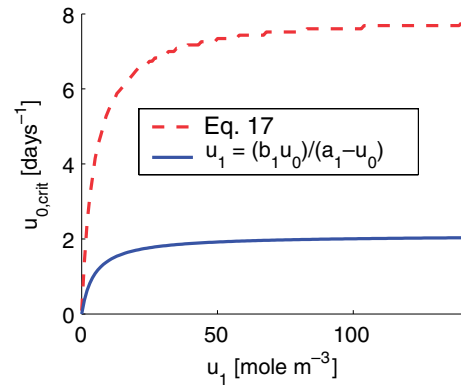


Fig. 4. Evaluation of the uniqueness criterion obtained by the contraction mapping theorem: comparison with results of direct calculation for simplified model.

#### 4.3. Local asymptotic stability of equilibrium points

The local asymptotic stability of the equilibrium points is assessed using the linearization principle. An equilibrium point  $\mathbf{y}_e$  of the system (19)–(22) is locally asymptotically stable if all eigenvalues of the system's Jacobian matrix,

$$\mathbf{J}(\mathbf{y}) = \frac{\partial \mathbf{g}}{\partial \mathbf{y}} \quad (45)$$

evaluated in this equilibrium point  $\mathbf{y}_e$ , are in the open left half plane. It can easily be seen that  $\mathbf{J}(\mathbf{y}_e)$  has a double eigenvalue  $-u_0$  and that its remaining two eigenvalues are the eigenvalues of the two-dimensional matrix:

$$\mathbf{J}_{34}(\mathbf{y}_e) = \begin{bmatrix} \left. \frac{\partial g_3}{\partial y_3} \right|_{\mathbf{y}=\mathbf{y}_e} & \left. \frac{\partial g_3}{\partial y_4} \right|_{\mathbf{y}=\mathbf{y}_e} \\ \left. \frac{\partial g_4}{\partial y_3} \right|_{\mathbf{y}=\mathbf{y}_e} & \left. \frac{\partial g_4}{\partial y_4} \right|_{\mathbf{y}=\mathbf{y}_e} \end{bmatrix} \quad (46)$$

It can be calculated [4] that both eigenvalues of  $\mathbf{J}_{34}(\mathbf{y}_e^A)$  have strictly negative real parts in case (39) is *not* fulfilled. This corresponds with the case in which the wash-out equilibrium point  $\mathbf{y}_e^A$  is the only physical equilibrium point.  $\mathbf{y}_e^A$  is then locally asymptotically stable. An even more general conclusion can be drawn, taking into account that every trajectory of the system's second-order dynamics in the bounded region  $\Delta$  converges to either an equilibrium point, or a limit cycle. According to the theory of the index [3], a limit cycle cannot surround a region containing no equilibrium points. Also, no limit cycle can surround the equilibrium point  $\mathbf{y}_e^A$ , that is lying on the boundary of  $\mathbf{S}_y$ . As a result, in case  $\mathbf{y}_e^A$  is the only equilibrium point, it is also globally asymptotically stable in the sense that every trajectory starting in the interior of  $\mathbf{S}_y$  converges to  $\mathbf{y}_e^A$  as  $t$  tends to  $+\infty$ . On the other hand, in case Eq. (39) is fulfilled, corresponding with a situation in which at least one other physical equilibrium point exists besides  $\mathbf{y}_e^A$ ,  $\mathbf{J}(\mathbf{y}_e^A)$  has one eigenvalue with positive real part, so  $\mathbf{y}_e^A$  is unstable with index 1. In this case only trajectories on the  $y_4$ -axis converge to  $\mathbf{y}_e^A$ . However, except from the equilibrium

point  $\mathbf{y}_e^A$  itself, these trajectories are not located within the physical boundaries of the system.

The equilibrium point  $\mathbf{y}_e^B$ , corresponding with only nitrite production, has been shown [4] locally asymptotically stable in case (42) is *not* fulfilled, i.e. if and only if it is the only physical equilibrium point besides  $\mathbf{y}_e^A$ . In this case,  $\mathbf{y}_e^B$  is also *quasi* globally asymptotically stable, in the sense that all trajectories starting inside  $S_y$  converge to  $\mathbf{y}_e^B$ , except for the trajectory coinciding with the point  $\mathbf{y}_e^A$ . In case the system possesses three equilibrium points,  $\mathbf{y}_e^B$  is unstable with index 1: only trajectories on the  $y_3$ -axis converge to  $\mathbf{y}_e^B$ .

For the equilibrium point  $\mathbf{y}_e^C$ , corresponding with nitrate formation, the eigenvalues of the associated Jacobian matrix always have strictly negative real parts [4], so the equilibrium point  $\mathbf{y}_e^C$  is always locally asymptotically stable. In case  $\mathbf{y}_e^C$  is not surrounded by a limit cycle (this will be verified through simulation), all solutions that start in  $S_y$  will converge to  $\mathbf{y}_e^C$ , except for the trajectories on  $y_4 = 0$ . The latter converge to  $\mathbf{y}_e^B$ , except for the trajectory coinciding with  $\mathbf{y}_e^A$ . In this sense,  $\mathbf{y}_e^C$  is quasi globally asymptotically stable.

#### 4.4. Phase trajectories

Fig. 5 shows the system boundaries, the equilibrium points and trajectory fields in the set  $A$  for different values of the dilution rate  $u_0$  and a fixed value of the influent ammonium concentration  $u_1$ . Three different cases are distinguished.

For high values of the dilution rate (e.g.  $u_0 = 2.5 \text{ day}^{-1}$ ) or low influent ammonium concentrations  $u_1$ , for which Eq. (39) is not fulfilled, only the equilibrium point  $\mathbf{y}_e^A$ , corresponding with biomass wash-out, is a physical equilibrium point and is globally asymptotically stable.

For moderately high dilution rates  $u_0$  and not too high influent ammonium concentrations  $u_1$  (e.g.  $u_0 = 1 \text{ day}^{-1}$  and  $u_1 = 70 \text{ mole m}^{-3}$ ), that fulfill Eq. (39) but not Eq. (42), the system possesses two physical equilibrium points. The wash-out equilibrium point  $\mathbf{y}_e^A$  is now unstable. Within the physical boundaries of the system, there are no nontrivial trajectories converging to  $\mathbf{y}_e^A$ . This point corresponds with a situation in which initially no biomass is present in the reactor. The second equilibrium point  $\mathbf{y}_e^B$  corresponds with only nitrite formation. It is lying on the  $y_3$ -axis

since no nitrite oxidizers are present. This equilibrium point is quasi globally asymptotically stable, in the sense that all trajectories within the physical boundaries of the system converge to this point, except from the equilibrium point  $\mathbf{y}_e^A$ .

In a third case, for sufficiently low dilution rates  $u_0$  and corresponding influent ammonium concentrations  $u_1$  (e.g.  $u_0 = 0.3 \text{ day}^{-1}$  and  $u_1 = 70 \text{ mole m}^{-3}$ ), that fulfill Eq. (42), the SHARON reactor model possesses three physical equilibrium points. The wash-out equilibrium point  $\mathbf{y}_e^A$  is still unstable in the same sense as above. The equilibrium point  $\mathbf{y}_e^B$ , corresponding with only nitrite formation, now also becomes unstable: only trajectories on the  $y_3$ -axis converge to  $\mathbf{y}_e^B$ . This corresponds with a reactor in which initially only ammonium oxidizers are present (note that the reactor influent does not contain biomass). A third equilibrium point,  $\mathbf{y}_e^C$ , corresponding with nitrate formation, appears. Simulation results have indicated that no limit cycle occurs around  $\mathbf{y}_e^C$ , which means that this equilibrium point is quasi globally asymptotically stable, in the sense that all trajectories within the physical boundaries of the system converge to this point, except from the equilibrium point  $\mathbf{y}_e^A$  and the trajectories on the  $y_3$ -axis.

The main advantages of a SHARON reactor are established when only nitrite and no nitrate is formed. To obtain this result, one needs to control the dilution rate  $u_0$  (according to the influent ammonium concentration  $u_1$ , which mostly cannot be controlled) in such a way that the equilibrium point  $\mathbf{y}_e^B$  is the only equilibrium point and is then also quasi globally asymptotically stable.

#### 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, the input values may be uncertain. Therefore, in this section, the effect of changing parameter and input values on the number of physical equilibrium points and their stability is assessed.

Consider the model described in Section 4.1, but now assume that  $u_2, u_3, u_4, c_2, d_3 \triangleq \frac{1}{d_2}$  and  $e_3 \triangleq \frac{1}{e_2}$  do deviate *slightly* from zero, i.e. have *small* positive values. It is important to note that the index of the equilibrium points (i.e. the number of eigenvalues of the associated Jacobian

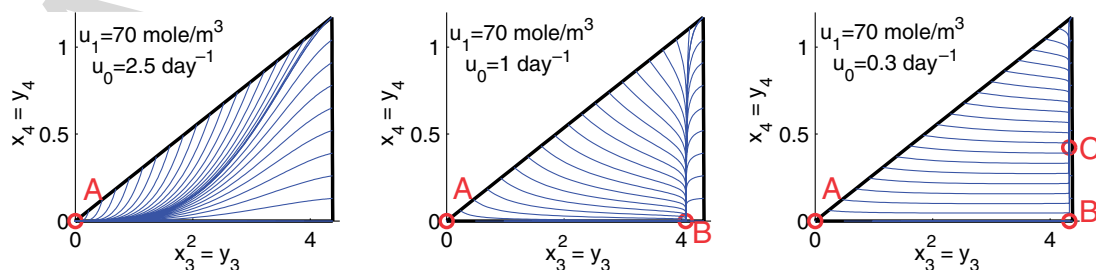


Fig. 5. Trajectory fields for a simplified SHARON model in terms of  $u_0$  and  $u_1$ .



matrix with strictly positive real parts) and thus the local asymptotic stability properties of the equilibrium points are not affected by these small parameter changes as the associated Jacobian matrix does not possess any eigenvalues on the imaginary axis.

The equilibrium points of the resulting model have been calculated as variations of the equilibrium points of the simplified model of Section 4.1:

$$\mathbf{y}_e^{X,m} = \mathbf{y}_e^X + \Delta \mathbf{y}_e^X \quad \text{for } X = A, B, C \quad (47)$$

each time neglecting higher order terms in the variations of the parameters and variables ( $\Delta y_{e3}^X$ ,  $\Delta y_{e4}^X$ ,  $u_2$ ,  $u_3$ ,  $u_4$ ,  $c_2$ ,  $d_3$  and  $e_3$ ). The results of these calculations (for details see [4]) are summarized below.

The equilibrium point  $\mathbf{y}_e^{A,m}$ , now corresponds with (almost complete) biomass wash-out:

$$\mathbf{y}_e^{A,m} = \begin{bmatrix} u_1 + a \cdot u_3 + b \cdot u_4 \\ u_2 - c \cdot u_3 + d \cdot u_4 \\ \frac{u_0 \cdot u_3}{u_0 - a_1 \cdot \frac{u_1}{b_1 + u_1}} \\ u_4 \end{bmatrix} \quad (48)$$

The only conversion realized in this equilibrium point is caused by the biomass present in the influent. Unlike for the model considered in Section 4.1, this equilibrium point does not always occur but is a physical equilibrium point if and only if Eq. (39) is *not* fulfilled, which is exactly the same condition as for  $\mathbf{y}_e^{A,m}$  to be the only equilibrium point. This condition arises from the assumption that  $u_3 > 0$ : in case ammonium oxidizers are present in the influent, the wash-out equilibrium point only occurs for high dilution rates  $u_0$ . The equilibrium point is then globally asymptotically stable.

The equilibrium point  $\mathbf{y}_e^{B,m}$  corresponds with (almost) only nitrite production, besides a little nitrate production by nitrite oxidizers present in the influent:

$$\mathbf{y}_e^{B,m} = \begin{bmatrix} u_1 + a \cdot u_3 + b \cdot u_4 \\ u_2 - c \cdot u_3 + d \cdot u_4 \\ y_{e3}^B + \Delta y_{e3}^B \\ \Delta y_{e4}^B \end{bmatrix} \quad (49)$$

It can be shown [4] that the equilibrium point  $\mathbf{y}_e^{B,m}$  is a physical equilibrium point if  $\mathbf{y}_e^B$  is a physical equilibrium point (Eq. (39)) and if at the same time condition (42) is *not* fulfilled, so  $\mathbf{y}_e^C$  is not a physical equilibrium point. The latter condition arises from the assumption that  $u_4 > 0$ : if nitrite oxidizers are present in the influent, the equilibrium point  $\mathbf{y}_e^{B,m}$  only occurs in the range of dilution rates  $u_0$  and influent ammonium concentrations  $u_1$  determined by Eqs. (39) and (42) (the latter not being fulfilled). In this case,  $\mathbf{y}_e^{B,m}$  is also the only equilibrium point and is globally asymptotically stable.

The third equilibrium point corresponds with substantial nitrate production:

$$\mathbf{y}_e^{C,m} = \begin{bmatrix} u_1 + a \cdot u_3 + b \cdot u_4 \\ u_2 - c \cdot u_3 + d \cdot u_4 \\ y_{e3}^{C,m} \\ y_{e4}^{C,m} \end{bmatrix} \quad (50)$$

This equilibrium point is a physical equilibrium point if  $\mathbf{y}_e^C$  is a physical equilibrium point (condition (42)), since the small parameter differences between both models will not significantly affect the position of the equilibrium point, that lies in the interior of the state space boundaries of the system.

It is important to note that the parameters  $c_2$ ,  $c_3$  and  $d_3$ , which values are assumed small, do not appear in the (approximate) expressions that determine the position of the equilibrium points  $\mathbf{y}_e^{A,m}$  and  $\mathbf{y}_e^{B,m}$  (for the latter, see [4]). Their effect vanishes by neglecting higher order terms in the variations of the parameters and input variables, that are assumed small. When the values of these parameters become relatively high, their effect on the position of the equilibrium points cannot be neglected any longer. The occurrence of additional inhibition terms in the kinetic rate expressions  $\sigma_1(\mathbf{y})$  and  $\sigma_2(\mathbf{y})$  may even give rise to additional equilibrium points, as is shown by [5,6]. For this reason, in case additional inhibition terms occur, it is advisable to explicitly calculate the number of equilibrium points for the corresponding model structure.

## 6. Conclusion

In this paper, the existence, uniqueness and stability of the equilibrium points of a SHARON reactor model for constant pH have been studied on theoretical grounds. The contraction mapping theorem has been applied to identify regions in the input space for which the system possesses a unique equilibrium point. However, only the wash-out equilibrium point could be identified, occurring at high values of the dilution rate. Subsequently, the equilibrium points of the SHARON reactor have been calculated directly for a simplified reactor model. It has been shown that up to three physical equilibrium points can occur, although in all cases only one equilibrium point is (quasi) globally asymptotically stable. The effect of slightly changing parameter and input values on the number of equilibrium points and their stability has also been examined. Although the position of the equilibrium points is only slightly affected, the equilibrium points on the state space boundaries may now shift outside these boundaries. As a result, only one equilibrium point occurs at a time.

From an operating point of view, the situation in which the equilibrium point with only nitrite formation is quasi globally asymptotically stable, is clearly the most interesting. This can be established by suitably controlling the dilution rate for the given influent ammonium concentrations, in such a way that the conditions determined in this study, are fulfilled. These requirements for the dilution rate include an upper limit, above which the wash-out state is

reached, as well as a lower limit, below which nitrate is formed.

## Appendix A. Derivation of a criterion for uniqueness of equilibrium points

### A.1. Applying the contraction mapping theorem to the four-dimensional model

The SHARON reactor model possesses a unique equilibrium point in case the mapping  $\varphi(\mathbf{x}_e)$  in  $\mathbb{R}^{4 \times 1}$  is a contraction mapping, i.e. if Eq. (15) is fulfilled.

From Eq. (11) the distance between two elements  $\mathbf{x}$  and  $\mathbf{w}$  in  $\mathbb{R}^{4 \times 1}$  satisfies:

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

The largest eigenvalue of the real-symmetric matrix  $\mathbf{M}^T \mathbf{M}$  is

$$s_0 = \frac{(\alpha + \beta) + \sqrt{(\alpha - \beta)^2 + 4 \cdot \gamma^2}}{2} \quad (\text{A.2})$$

with

$$\alpha \triangleq a^2 + c^2 + 1 \quad (\text{A.3})$$

$$\beta \triangleq b^2 + d^2 + 1 \quad (\text{A.4})$$

$$\gamma \triangleq a \cdot b - c \cdot d \quad (\text{A.5})$$

For a real-symmetric matrix  $\mathbf{A} \in \mathbb{R}^{n \times n}$  with largest eigenvalue  $\lambda_{\max}$  and for every vector  $\mathbf{x} \in \mathbb{R}^{n \times 1}$ :

$$\mathbf{x}^T \mathbf{A} \mathbf{x} \leq \lambda_{\max} \cdot \mathbf{x}^T \mathbf{x} \quad (\text{A.6})$$

Hence Eq. (A.1) implies that

$$\ell^2[\varphi(\mathbf{x}), \varphi(\mathbf{w})] \leq \frac{s_0}{u_0^2} \cdot [\rho(\mathbf{x}) - \rho(\mathbf{w})]^T [\rho(\mathbf{x}) - \rho(\mathbf{w})] \quad (\text{A.7})$$

According to the mean value theorem, there exist vectors  $\tilde{\mathbf{x}}_{ij}$  in the hyperrectangle with opposite corners  $\mathbf{x}$  and  $\mathbf{w}$  for which

$$\rho(\mathbf{x}) = \rho(\mathbf{w}) + \mathbf{J}(\mathbf{x} - \mathbf{w}) \quad (\text{A.8})$$

with

$$\mathbf{J} = \begin{bmatrix} \left. \frac{\partial \rho_1}{\partial x_1} \right|_{\mathbf{x}=\tilde{\mathbf{x}}_{11}} & \left. \frac{\partial \rho_1}{\partial x_2} \right|_{\mathbf{x}=\tilde{\mathbf{x}}_{12}} & \left. \frac{\partial \rho_1}{\partial x_3} \right|_{\mathbf{x}=\tilde{\mathbf{x}}_{13}} & \left. \frac{\partial \rho_1}{\partial x_4} \right|_{\mathbf{x}=\tilde{\mathbf{x}}_{14}} \\ \left. \frac{\partial \rho_2}{\partial x_1} \right|_{\mathbf{x}=\tilde{\mathbf{x}}_{21}} & \left. \frac{\partial \rho_2}{\partial x_2} \right|_{\mathbf{x}=\tilde{\mathbf{x}}_{22}} & \left. \frac{\partial \rho_2}{\partial x_3} \right|_{\mathbf{x}=\tilde{\mathbf{x}}_{23}} & \left. \frac{\partial \rho_2}{\partial x_4} \right|_{\mathbf{x}=\tilde{\mathbf{x}}_{24}} \end{bmatrix} \triangleq \begin{bmatrix} \delta_1 & \delta_2 & \delta_3 & 0 \\ \delta_5 & \delta_6 & 0 & \delta_8 \end{bmatrix} \quad (\text{A.9})$$

Consequently,

$$[\rho(\mathbf{x}) - \rho(\mathbf{w})]^T [\rho(\mathbf{x}) - \rho(\mathbf{w})] = [\mathbf{x} - \mathbf{w}]^T \mathbf{J}^T \mathbf{J} [\mathbf{x} - \mathbf{w}] \quad (\text{A.10})$$

Substitution of Eq. (A.10) in Eq. (A.7) yields

$$\ell^2[\varphi(\mathbf{x}), \varphi(\mathbf{w})] \leq \frac{s_0}{u_0^2} \cdot [\mathbf{x} - \mathbf{w}]^T \mathbf{J}^T \mathbf{J} [\mathbf{x} - \mathbf{w}] \quad (\text{A.11})$$

The largest eigenvalue of the real-symmetric matrix  $\mathbf{J}^T \mathbf{J}$  is found as

$$s_1 = \frac{(\mu + \nu) + \sqrt{(\mu - \nu)^2 + 4 \cdot \zeta^2}}{2} \quad (\text{A.12})$$

with

$$\mu \triangleq \delta_1^2 + \delta_2^2 + \delta_3^2 \quad (\text{A.13})$$

$$\nu \triangleq \delta_5^2 + \delta_6^2 + \delta_8^2 \quad (\text{A.14})$$

$$\zeta \triangleq \delta_1 \cdot \delta_5 + \delta_2 \cdot \delta_6 \quad (\text{A.15})$$

So Eq. (A.11) becomes

$$\ell^2[\varphi(\mathbf{x}), \varphi(\mathbf{w})] \leq \frac{s_0 \cdot s_1}{u_0^2} \cdot \ell^2[\mathbf{x}, \mathbf{w}] \quad (\text{A.16})$$

Hence  $\varphi$  is a *contraction mapping* according to the definition (Eq. (15)) if

$$\frac{s_0 \cdot s_1}{u_0^2} < 1 \iff u_0 > \sqrt{s_0 \cdot s_1} \quad (\text{A.17})$$

In order to evaluate the condition (A.17) for a unique equilibrium,  $s_0$  and  $s_1$  must be known. While the calculation of  $s_0$  is straightforward, the calculation of  $s_1$  is more complicated since the values of  $\mu$ ,  $\nu$  and  $\zeta$  depend on the values of  $\delta_i^2$  and thus on the absolute values of the partial derivatives  $\frac{\partial \rho_i}{\partial x_j}$ , evaluated in the unknown  $\tilde{\mathbf{x}}_{ij}$  (see Eq. (A.9)). However, it is possible to define maximum absolute values for the partial derivatives (so there is no need to know the values of  $\tilde{\mathbf{x}}_{ij}$ ) and in this way also maximum values for  $\mu$ ,  $\nu$  and  $\zeta$ . More details on the estimation of these upper boundaries can be found in [4].

### A.2. Applying the contraction mapping theorem to a reduced two-dimensional static model

Under equilibrium conditions, a reduced two-dimensional reactor model can be set-up, from which an alternative criterion for the existence of a unique equilibrium point is deduced. In case  $u_0 > 0$ , the equilibrium concentrations of ammonium oxidizers ( $x_{e3}$ ) and nitrite oxidizers ( $x_{e4}$ ) can easily be eliminated from the equilibrium conditions. Some manipulations yield

$$x_{e3} = u_3 + \frac{1}{a \cdot d + b \cdot c} \cdot [d \cdot (u_1 - x_{e1}) - b \cdot (u_2 - x_{e2})] \quad (\text{A.18})$$

$$x_{e4} = u_4 + \frac{1}{a \cdot d + b \cdot c} \cdot [c \cdot (u_1 - x_{e1}) + a \cdot (u_2 - x_{e2})] \quad (\text{A.19})$$

Redefine  $\mathbf{y}$  and define  $\mathbf{w}$  as

$$\mathbf{y} \triangleq \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}; \quad \mathbf{w} \triangleq \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \quad (\text{A.20})$$

Then using Eqs. (A.18) and (A.19), the equilibrium values of  $\mathbf{y}$  can be verified to satisfy a relationship of the form

$$\mathbf{y}_e = \mathbf{w} + \frac{1}{u_0} \cdot \widehat{\mathbf{M}} \hat{\rho}(\mathbf{y}_e) \triangleq \hat{\phi}(\mathbf{y}_e) \quad (\text{A.21})$$

in which

$$\hat{\phi}(\mathbf{y}_e) \triangleq \begin{bmatrix} \hat{\phi}_1(\mathbf{y}_e) \\ \hat{\phi}_2(\mathbf{y}_e) \end{bmatrix}; \quad \widehat{\mathbf{M}} \triangleq \begin{bmatrix} -a & -b \\ c & -d \end{bmatrix}; \quad \hat{\rho}(\mathbf{y}_e) \triangleq \begin{bmatrix} \rho_1(\mathbf{y}_e) \\ \rho_2(\mathbf{y}_e) \end{bmatrix} \quad (\text{A.22})$$

Every fixed point of the mapping

$$\mathbf{y}_e = \hat{\phi}(\mathbf{y}_e) \quad (\text{A.23})$$

yields an equilibrium point of the system. If the mapping  $\hat{\phi}$  is a contraction mapping, the unique fixed point of the mapping is a unique equilibrium point for the SHARON model.

The procedure for determining the conditions under which  $\hat{\phi}$  is a contraction mapping, is completely analogous as the one in [Appendix A.1](#). This results in the criterion (for details, see [\[4\]](#)):

$$\frac{\hat{s}_0 \cdot \hat{s}_1}{u_0^2} < 1 \quad \iff \quad u_0 > \sqrt{\hat{s}_0 \cdot \hat{s}_1} \quad (\text{A.24})$$

where

$$\hat{s}_0 = \hat{s}_0(a, b, c, d) \quad (\text{A.25})$$

$$\hat{s}_1 = \hat{s}_1 \left( \left. \frac{\partial \hat{\rho}_1}{\partial x_{e1}} \right|_{y=\hat{y}_{11}}, \left. \frac{\partial \hat{\rho}_1}{\partial x_{e2}} \right|_{y=\hat{y}_{12}}, \left. \frac{\partial \hat{\rho}_2}{\partial x_{e1}} \right|_{y=\hat{y}_{21}}, \left. \frac{\partial \hat{\rho}_2}{\partial x_{e2}} \right|_{y=\hat{y}_{22}} \right) \quad (\text{A.26})$$

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