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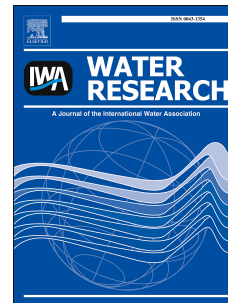
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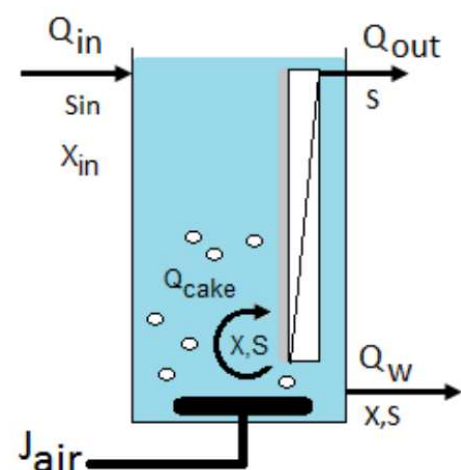
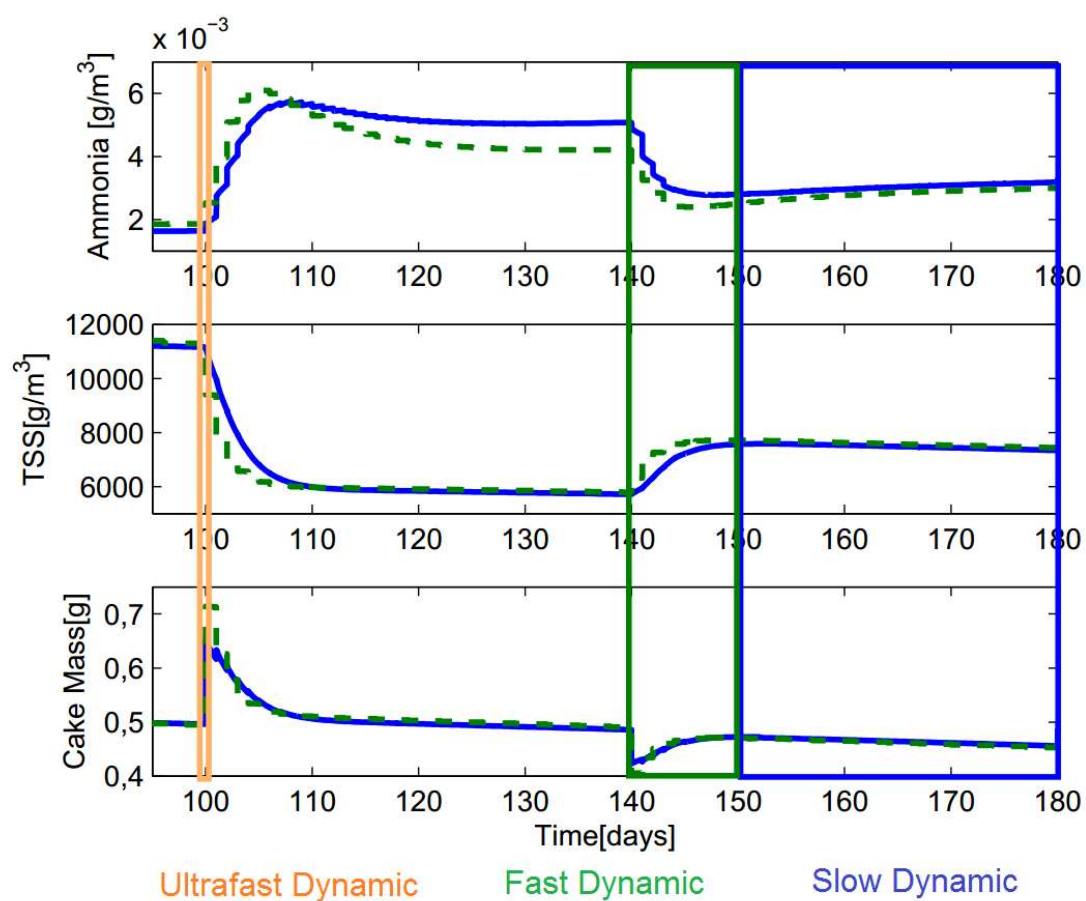
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- For control purposes, a simple dynamic model of a membrane bioreactor is proposed;
- The process behavior is analyzed, showing the existence of slow-fast dynamics;
- A parameter identification procedure exploiting time scale separation is presented.



Design, Analysis and Validation of a Simple Dynamic Model of a Submerged Membrane Bioreactor

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Abstract

In this study, a simple dynamic model of a submerged membrane bioreactor (sMBR) is proposed, which would be suitable for process control. In order to validate the proposed model structure, informative data sets are generated using a detailed simulator built in a well-established environment, namely GPS-X. The model properties are studied, including equilibrium points, stability, and slow/fast dynamics (three different time scales). The existence of slow-fast dynamics is central to the development of a dedicated parameter estimation procedure. Finally, a nonlinear model predictive control is designed to illustrate the potential of the developed model within a model-based control structure. The problem of water treatment in a recirculating aquaculture system is considered as an application example.

Keywords: Mathematical modeling; Singular perturbation; Parameter estimation; Model-based control; Recirculating aquaculture system;

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1 **1. Introduction**

2 Submerged membrane bioreactors (sMBR) are increasingly used for wastew-
3 ater treatment with a relative success (Judd & Judd, 2011). In its simplest con-
4 figuration, a sMBR combines the functions of an activated sludge aerobic sys-
5 tem, secondary clarifier, and tertiary filter in a single tank (Atasi et al., 2006).
6 The advantages are the footprint reduction, high effluent quality and the de-
7 coupling of the hydraulic retention time (HRT) and solid retention time (SRT).
8 Due to filter pore size, particles however start to attach on membrane surface,
9 forming a deposition of solid matter, responsible for fouling. Membrane fouling
10 decreases membrane permeability, increasing operating costs.

11 One of the greatest challenges for process optimization is the development
12 of an integrated model (comprising biological phenomena and filtration mech-
13 anism). In general, sMBR models are stand-alone filtration models includ-
14 ing aeration (Ferrero et al., 2011), cake formation (Li & Wang, 2006), filtration
15 and fouling (Robles et al., 2013a,b; Charfi et al., 2012), physical and biopro-
16 cess description (Bella et al., 2008; Mannina et al., 2011). Regarding the bi-
17 ological phenomena, the activated sludge models (ASM) are widely accepted
18 (Henze et al., 1987). Studies have shown that ASM can be directly imple-
19 mented or modified taking the fouling interference on activated sludge biol-
20 ogy (SMP/EPS) into account (Fenu et al., 2010; Naessens et al., 2012). ASM1,
21 ASM3 and ASM2d have been extensively used to predict the effluent quality re-
22 lated to soluble matter (Sarioglu et al., 2009; Lee et al., 2002; Jiang et al., 2009;
23 Zarragoitia-González et al., 2008). A critical review of sMBR models has been
24 done by Fenu et al. (2010) and Naessens et al. (2012) presenting biokinetics,
25 filtration, hydrodynamics and integrated models intended for process descrip-
26 tion and understanding. These models cover a wide range of phenomena, from
27 empirical to first principles, and have been used mainly for process cognition
28 development (Naessens et al., 2012). In order to compare and evaluate control
29 strategies, an sMBR benchmark for wastewater treatment has been developed
30 by Maere et al. (2011).

31 However, those models include many parameters which can be delicate to
32 estimate from experimental data and they are in general too complex for con-
33 trol purposes. As a general rule, it is always necessary to make a trade-off
34 between model complexity and dynamic predictive capability. For control pur-
35 poses, a model should not be more detailed than required by a specific control
36 task (Kokotović et al., 1986). In this context, there are only a few proposals of
37 SBR models based on empirical approaches (Khan et al., 2009), artificial neu-
38 ral network models (Choi et al., 2012) or black box model to estimate filtration
39 performance (Dalmau et al., 2013).

40 The main objective of this study is to develop a simplified SBR model,
41 and to validate it by comparison with a well established simulator, e.g., GPS-X
42 (Hydromantis, 2012). In this connection, the detailed simulator is used as an
43 emulation of a real plant to generate realistic data. The advantage of a simu-
44 lator is of course that data can be produced easily and without the operational
45 constraints of a real-life plant. Hence, more informative data sets (i.e. data
46 sets exploring the plant behavior in a wider operating range, and containing
47 sufficient information on the plant dynamics) can be used to test and validate
48 the simplified model. To this end, a dedicated parameter estimation strategy is
49 proposed and applied to fit the reduced model to these data sets. This identifi-
50 cation study is the opportunity to emphasize the need for an appropriate design
51 of experiments to ensure a sufficient level of information. An interesting feature
52 of the system dynamics is the possibility to consider different time scales (fast
53 and slow dynamics), which are evidenced in this study using singular pertur-
54 bation theory. This approach reveals conditions on the model parameters to
55 obtain reduced models at three different time scales. The time scale separation
56 can be used advantageously in system identification, as subsets of parameters
57 can be estimated on different time intervals, and the identification problem can
58 in this way be divided into simpler subproblems. Once the simplified model has
59 been identified, it can be used in model-based control schemes and a "proof of
60 concept" is showed at the end of this study, where nonlinear model predictive
61 control (NMPC) is used as an appealing approach. It is important to stress

62 that model based control could be very delicate if based on complex physical
63 models, due to their large number of variables and parameters, which makes
64 identification, estimation and control difficult or even impossible. In contrast,
65 the simplified model has a much reduced set of variables and parameters and is
66 very convenient for NMPC or other nonlinear model based control approaches.

67 As a particular application example, a recirculating aquaculture system
68 (RAS) is considered, which can be defined as a process that reuses water
69 and has less than 10% of total volume replaced per day (Piedrahita, 2003;
70 Hutchinson et al., 2004). This recirculation however causes accumulation of
71 ammonia, nitrate and organic matter that should be removed before reentering
72 the system. Nitrogen removal for RAS normally includes some filtering tech-
73 nologies such as rotating biological contactors, trickling filters, bead filters and
74 fluidized sand biofilters (Crab et al., 2007). The application of sMBR in this
75 context is still a relatively new prospect.

76 This study is organized as follows. The next section presents the case study
77 related to a recirculating aquaculture process and describes the modeling as-
78 sumptions (Section 2). Section 3 derives the proposed model structure for the
79 sMBR. The model is analyzed considering short-term and long-term evolution
80 in Section 4, and an analysis with regard to the equilibrium points is presented
81 in Section 5. The parameter estimation procedure is discussed in Section 6 and
82 a nonlinear model predictive control is developed in Section 7. Finally, Section
83 8 draws some conclusions and perspectives.

84 2. Process Description

85 A sustainable fish production can be achieved by treating and recirculating
86 the effluent water of the fish tanks, see Figure 1a. This is only achievable if
87 efficient nitrification, denitrification and organic removal can be setup. Nor-
88 mally, fish are susceptible to high concentrations of ammonia, which result from
89 fish feces and excretion, but tolerate higher nitrate concentrations. This is for
90 instance the case for tilapia and trout, as reported in Eding et al. (2006). Based

91 on these classes of fish this work provides a simplified model of the ammonia
92 removal process in sMBR.

93 Figure 1b shows the sketch of the nitrification compartment with membrane
94 bioreactor. This illustration is a simplified representation of the two tanks
95 inside the dashed square in Figure 1a. The advantage of lumping both reactors
96 is to model only the dynamics that are the most important for process control,
97 without considering all the internal variables and parameters of the process.
98 This leads to a simplified input-output black-box model with a “biologically
99 inspired” structure, but with much less variables and parameters.

100 The considered process has a constant trans-membrane pressure and the ef-
101 fluent flow $Q_{out}[m^3/d]$ decreases due to deposition of the particles on the mem-
102 brane surface. To avoid this phenomenon, sMBR are usually equipped with air
103 diffusers in the bottom part. A diffuser produces an air crossflow, $J_{air}[m^3/m^2d]$,
104 that is injected to detach the particle agglomerate from the membrane surface.
105 Figure 2 describes the fouling evolution in time, which can be split in two parts.
106 Initially (t_0), the permeate pump is off and there is no material attached to
107 the membrane. As time goes on (t^+), the permeate pump is active and solid
108 particles are conveyed by the flow towards the membrane surface, resulting in
109 membrane fouling (formation of a “cake”). In the longer term (t^{++}), the ef-
110 fluent flow decreases with time, due to the cake build-up on the membrane
111 surface (considering a process with constant trans-membrane pressure and air
112 crossflow).

113 3. Model Development

114 The particle deposition creates a resistance to the flow through the mem-
115 brane. On inspection of the literature, several descriptions of the total fouling
116 resistance can be found (Busch et al., 2007; E.Remigi, 2008; Lee et al., 2002;
117 Sarioglu et al., 2012). In this work the total fouling resistance ($R_{total}[m^{-1}]$)
118 is represented by equation (1). Based on experiments reported by Lee et al.
119 (2002) and Khan et al. (2009), the cake resistance, $R_{cake}[m^{-1}]$, can be consid-

120 ered as the main responsible for fouling resistance. $R_m[m^{-1}]$ is the intrinsic
 121 resistance and δ_R is used to represent total resistance disturbance, resulting
 122 from pore-blocking, biofilm, concentration polarization and scaling resistances.

$$R_{total} = R_m + R_{cake} + \delta_R \quad (1)$$

123 The effluent rate is given by $Q_{out} = \Delta P / \eta R_{total}$, where $\Delta P[Pa]$ is the
 124 trans-membrane pressure and $\eta[Pa.s]$ is the water apparent viscosity. The cake
 125 resistance is ruled by $R_{cake} = \rho \frac{m+m_0}{A}$, where $\rho[m.g^{-1}]$ is the specific cake resis-
 126 tance, $m_0[g]$ is the initial cake mass, A is the area of the membrane surface and
 127 $m[g]$ is the current cake mass. The latter can be described by equation (2).

$$\frac{dm}{dt} = Q_{cake}X - J_{air}\mu_{air}(m)m, \quad \text{with } \mu_{air}(m) = \beta \frac{m}{K_{air} + m} \quad (2)$$

128 The right hand side of equation (2) has two terms. The first term repre-
 129 sents the attachment of total suspended solids on the membrane surface which
 130 depends on the effluent rate $Q_{cake}[m^3/d]$ and its concentration $X[g/m^3]$. The
 131 flow $Q_{cake} = \psi Q_{out}$ is responsible for the fixation of suspended particle matter
 132 onto the cake. It is assumed that the concentration of substrate that passes
 133 through the membrane is equal to the concentration of the solids that attach
 134 onto it when $\psi = 1$. The time scale is represented in Figure 2 by t^+ , showing
 135 that the particles that are in suspension near the membrane walls are rapidly
 136 forced against the filter. The second term of equation (2) represents the cake
 137 detachment proportional to air crossflow. The parameter $\beta[m^{-1}]$ is linked to
 138 the resistance of the cake to detachment. This latter mechanism is of course
 139 influenced in the first place by J_{air} , but also by the mass of the cake. With
 140 an increasing attached mass, detachment becomes more likely and this is rep-
 141 resented by a ‘Monod law’ like equation, i.e., a monotone law with saturation
 142 (saturation occurrence being adjusted by the half-saturation coefficient K_{air}).
 143 This model structure guarantees that the cake mass will never reach negative
 144 values, that indeed is physically impossible. This time scale dynamic compared
 145 to the other dynamics of the process can be understood as an instantaneous

146 behavior, see more explanation in Section 4.

147 Having proposed a membrane filtration model, the biological activity is de-
 148 scribed using a simple chemostat reactor (Smith & Waltman, 1995), involving
 149 one biomass growing on a limiting substrate, equation (3). It is important
 150 to highlight that this simple biological model structure can be easily extended
 151 to more than one biological reaction, see for instance Dochain & Vanrolleghem
 152 (2001). However, adding details and complexity will make model calibration
 153 more delicate and reduce model suitability to control purposes.

$$\begin{cases} \frac{dS}{dt} = -\frac{1}{Y}\mu(S)X + \frac{Q_{in}}{V}(S_{in} - S) & (3a) \\ \frac{dX}{dt} = \left(\mu(S) - \frac{Q_w}{V}\right)X + \frac{Q_{in}}{V}X_{in} - \frac{Q_{cake}}{V}X + \frac{J_{air}}{V}\mu_{air}(m)m & (3b) \end{cases}$$

154

155 Equation (3a) represents the consumption of the substrate by the free biomass,
 156 ruled by a Monod law $\mu(S) = \mu_{S,max} \frac{S}{K_S+S}$, and the transportation of incoming
 157 and outgoing substrate through the tank. Note that the substrate is not affected
 158 by the membrane, knowing that only solid matter are retained.

159 Equation (3b) shows that there is an interaction between the suspended
 160 solid and cake build-up. The first part of the equation represents the growth
 161 of the free biomass that consumes the substrate. Material transportation in-
 162 volves the cake attachment by $\frac{-Q_{cake}X}{V}$ and detachment and the instantaneous
 163 “conversion” in suspended solids by the air crossflow $+\frac{J_{air}}{V}\mu_{air}(m)m$. The free
 164 particle matter is transformed in cake and vice-versa depending on the process
 165 input values. The waste flow is represented by Q_w and the influent is defined
 166 as $Q_{in} = Q_w + Q_{cake}$. The biological time scale is governed by the consump-
 167 tion rate of substrate and consequently the growth of biomass. This rate is
 168 represented by a Monod law equation ($\mu(S)$) and is normally measured in days.

169 In a continuous process a long-term evolution of the cake is observed, which
 170 can be modeled by

$$\frac{d\beta}{dt} = \gamma\beta \quad (4)$$

171 The parameter $\beta[m^{-1}]$ represents the ease (or difficulty) of detaching the
 172 cake from the membrane using an air crossflow. In a process with constant trans-
 173 membrane pressure, the permeate flow decreases with time. Hence β increases,
 174 $\gamma[d^{-1}]$ is positive, meaning that the efficiency of J_{air} increases as a consequence
 175 of the loss of the drag force of the membrane to the particle deposition. In the
 176 other sense, if the process has constant permeate flow, the capacity of J_{air} to
 177 detach the cake decreases, β decreases, thus γ has a negative value. One can
 178 also relate this phenomenon to the cake compression coefficient proposed by
 179 Li & Wang (2006). It is important to highlight that this phenomenon has a long-
 180 term behavior, which is observed on a time scale depending on the process cycles:
 181 Permeate cycle (Q_{cake} is considered as a positive and constant value), relaxation
 182 cycle (where the air crossflow is maintained constant and the permeate flow is
 183 zero, resulting in a zero trans-membrane pressure) and backwash cycle (Q_{cake}
 184 flow is reversed to force the particles detachment). Normally this evolution is
 185 measured in weeks or months (Merlo et al., 2000).

186 Regrouping the previous equations, the integrated model is represented by
 187 (5), where β, S, X and m are always positive and bounded (properties that are
 188 linked to the biological and physical phenomena that rule the process).

$$\left\{ \begin{array}{l} \frac{d\beta}{dt} = \gamma\beta \end{array} \right. \quad (5a)$$

$$\left\{ \begin{array}{l} \frac{dS}{dt} = -\frac{1}{Y}\mu(S)X + \frac{Q_{in}}{V}(S_{in} - S) \end{array} \right. \quad (5b)$$

$$\left\{ \begin{array}{l} \frac{dX}{dt} = \left(\mu(S) - \frac{Q_w}{V} \right) X + \frac{Q_{in}}{V}X_{in} - \frac{Q_{cake}}{V}X + \frac{J_{air}}{V}\mu_{air}(m)m \end{array} \right. \quad (5c)$$

$$\left\{ \begin{array}{l} \frac{dm}{dt} = Q_{cake}X - J_{air}\mu_{air}(m)m \end{array} \right. \quad (5d)$$

$$\text{with } \mu(S) = \mu_{S,max} \frac{S}{K_S + S}, \quad \mu_{air}(m) = \beta \frac{m}{K_{air} + m}$$

189 This dynamic model is generic and could be used in various applications.
 190 In this study, a particular example is considered, so as to demonstrate that the
 191 model structure is appropriate. In this context, assuming there is no oxygen
 192 limitation, the state variables S and X denote the concentrations of ammonia

193 and autotrophic bacteria, respectively. Note that the model could easily be
 194 extended to processes with other species and substrates.

195 4. Fast and Slow Dynamics

196 The simplified model involves three different time scales: cake attachment
 197 and detachment, biology and cake long-term evolution.

198 The simultaneous occurrence of fast and slow phenomena contribute to com-
 199 plex dynamics, stiffness of the model and computational effort for simulation.

200 To simplify the model analysis, the singular perturbation approach is used.
 201 The presence of a small parameter in the description of the dynamic model
 202 that can (regular perturbation) or cannot (singular perturbation) be approxi-
 203 mated by putting the small parameter to zero, reveals the possibility of model
 204 reduction in dimension or in order (Saksena et al., 1984; Kokotović et al., 1986).
 205 Detecting the different time scales results in reduced models, where the slowest
 206 phenomenon is the dominant dynamics. This can be understood as an inner and
 207 outer process loop. The fast dynamics, named also boundary layer, represents
 208 the deviation from the predicted slow behavior. This approach is considered in
 209 more details in the framework of singular perturbations.

210 4.1. Singular Perturbations

211 The mathematical tool used to deal with the different time scales is Tikhonov's
 212 theorem which allows reducing the complexity of the system through suitable
 213 approximations (Khalil, 2002). A slow-fast system is in singular perturbation
 214 form when it can be expressed in suitable coordinates, so as to distinguish two
 215 subsystems with a small positive parameter ϵ .

$$\begin{cases} \dot{x} = f(t, x, z, \epsilon) \\ \epsilon \dot{z} = g(t, x, z, \epsilon) \end{cases} \quad (6)$$

216 The function f and g are continuously differentiable in their arguments for
 217 $(t, x, z, \epsilon) \in [0, t_1] \times D_x \times D_z \times [0, \epsilon_0]$, where $D_x \subset R^n$ and $D_z \subset R^m$ are open
 218 connected sets. Considering $\epsilon = 0$ in (6), the dimension of the state equation

219 reduces from $n + m$ to n because the differential equation degenerates into the
220 algebraic equation.

$$0 = g(t, x, z, 0) \quad (7)$$

221 We assume that (7) admits $k \geq 1$ isolated real roots

$$z = h_i(t, x), \quad i = 1, 2, \dots, k \quad (8)$$

222 defined by $(t, x) \in [0, t_1] \times D_x$. This assumption ensures that a well-defined
223 n -dimensional reduced model will correspond to each root of (7). To obtain
224 the i^{th} reduced model, equation (8) has to be substituted into (6), at $\epsilon = 0$, to
225 obtain

$$\dot{x} = f(t, x, h_i(t, x), 0) \quad (9)$$

226 It will be clear from the context which root of (7) are used. This model is
227 sometimes called a *quasi-steady-state model*, because z , whose velocity $\dot{z} = g/\epsilon$
228 can be large when ϵ is small and $g \neq 0$, may rapidly converge to a root of (7),
229 which is the equilibrium of (6). Equation (9) is called the slow dynamics of the
230 model (Sari, 2005).

231 4.2. Three-time-scale Singular Perturbation

232 In the previous subsection, fast and slow theory is recalled considering two
233 time scales. In the sMBR model, three time scales can be identified: the cake
234 attachment is considered as the ultrafast time scale, the free biomass growth
235 and substrate consumption as the fast time scale and the evolution of the cake
236 as the slow time scale resulting in the following generic representation:

$$\begin{cases} \frac{d\beta}{dt} = \gamma\beta & \longrightarrow \dot{x}_{sl} \\ \frac{dS}{dt} = -\frac{1}{V}\mu(S)X + \frac{Q_{in}}{V}(S_{in} - S) & \longrightarrow \dot{y}_1 \\ \frac{dX}{dt} = (\mu(S) - \frac{Q_w}{V})X + \frac{Q_{in}}{V}X_{in} - \frac{Q_{cake}}{V}X + \beta \frac{J_{air}}{V} \frac{m^2}{K_{air}+m} & \longrightarrow \dot{y}_2 \\ \frac{dm}{dt} = Q_{cake}X - \beta J_{air} \frac{m^2}{K_{air}+m} & \longrightarrow \dot{z} \end{cases} \quad (10)$$

237 where x_{sl} is the slow state variable, y the fast state variable, and z the ultrafast
 238 state variable, and $0 < \epsilon_1 \epsilon_2 \ll \epsilon_1 \ll 1$. The small parameters are assumed to
 239 be $\epsilon_1 = \gamma$ and $\epsilon_2 = \frac{1}{V}$.

240 **Hypothesis 1.** γ is small.

241 **Hypothesis 2.** The volume V is large.

242 The application of the procedure introduced in the previous subsection there-
 243 fore yields:

244 **First:** The stretched time-scale $\tau_1 = \frac{t}{\epsilon_1}$

$$\frac{dx_{sl}}{d\tau_1} = \epsilon_1 x_{sl} \quad (Slow)$$

$$\epsilon_1 \frac{dy_1}{d\tau_1} = g_1(x_{sl}, y_1, h_2) = \left[-\frac{1}{Y} \mu(y_1) y_2 + \frac{Q_{in}}{V} (S_{in} - y_1) \right] \epsilon_2 \quad (Fast)$$

$$\epsilon_1 \frac{dy_2}{d\tau_1} = g_2(x_{sl}, y_2, h_2) = \left[(\mu(y_1) - \frac{Q_w}{V}) y_2 + \frac{Q_{in}}{V} X_{in} - \frac{Q_{cake}}{V} y_2 + x_{sl} \frac{J_{air}}{V} \frac{z^2}{K_{air} + z} \right] \epsilon_2 \quad (Fast)$$

$$\epsilon_1 \frac{dz}{d\tau_1} = h(x_{sl}, y, z) = Q_{cake} y_2 - x_{sl} J_{air} \frac{z^2}{K_{air} + z} \quad (Fast)$$

$$0 = g_1(x_{sl}, y_1, h_2(x, y_1)) \rightarrow y_1 = \frac{Q_w K_s}{\mu_{max} - Q_w} \quad (11)$$

$$0 = g_2(x_{sl}, y_2, h_2(x, y_2)) \rightarrow y_2 = \frac{Q_{in} Y (S_{in} (V \mu_{max} - Q_w) - Q_w K_s)}{Q_w (V \mu_{max} - Q_w)} \quad (12)$$

$$0 = h(x_{sl}, y, z) \rightarrow z = \frac{\frac{Q_{cake} y_2}{x J_{air}} + \sqrt{(\frac{Q_{cake} y_2}{x_{sl} J_{air}})^2 + \frac{4 K_{air} Q_{cake} y_2}{x_{sl} J_{air}}}}{2} \quad (13)$$

245 **Second:** The stretched time scale $\tau_2 = \frac{\tau_1}{\epsilon_2} = \frac{t}{\epsilon_1 \epsilon_2}$ and x_{sl} is constant.

$$\epsilon_1 \frac{dy_1}{d\tau_2} = -\frac{1}{Y} \mu(y_1) y_2 + \frac{Q_{in}}{V} (S_{in} - y_1) \quad (Fast)$$

$$\epsilon_1 \frac{dy_2}{d\tau_2} = (\mu(y_1) - \frac{Q_w}{V}) y_2 + \frac{Q_{in}}{V} X_{in} - \frac{Q_{cake}}{V} y_2 + x_{sl} \frac{J_{air}}{V} \frac{z^2}{K_{air} + z} \quad (Fast)$$

$$\epsilon_2 \epsilon_1 \frac{dz}{d\tau_2} = h(x_{sl}, y, z) = Q_{cake} y_2 - x_{sl} J_{air} \frac{z^2}{K_{air} + z} \quad (Ultrafast)$$

$$0 = h(x_{sl}, y, z) \rightarrow z = \frac{\frac{Q_{cake}y_2}{x_{Jair}} + \sqrt{\left(\frac{Q_{cake}y_2}{x_{sl}Jair}\right)^2 + \frac{4K_{air}Q_{cake}y_2}{x_{sl}Jair}}}{2} \quad (14)$$

246 5. Model Analysis

247 In this section, we compute the equilibrium points, analyze their stability
248 based on a linearization (Jacobian matrix).

249 5.1. Asymptotic Analysis

250 The filtration process is an unstable process by nature, since solid matter
251 continuously accumulate in an irreversible manner (see the dynamic of β in
252 equation (5)), but it is possible to analyze it on a short time span t , where
253 the process could be considered stable. Analyzing the process in this period,
254 the long-term evolution of the cake is neglected (i.e. it is considered constant).
255 Based on a fast and slow dynamics study, the coupling of the system is simplified
256 and thus when the equilibrium points of S and X are computed, m is considered
257 constant, and reversely, when m is computed, S and X are considered constant.
258 This helps in determining the biomass and cake equilibrium points that are
259 strongly coupled.

$$\bar{S} = \frac{Q_{in}X_{in} - Q_w\bar{X} - Q_{in}S_{in}Y}{Q_{in}} \quad (15)$$

$$\bar{X} = \frac{Q_{in}X_{in}}{Q_w - \mu(S)V} \quad (16)$$

$$\bar{m} = \frac{\frac{Q_{cake}\bar{X}}{\beta J_{air}} + \sqrt{\left(\frac{Q_{cake}\bar{X}}{\beta J_{air}}\right)^2 + \frac{4K_{air}Q_{cake}\bar{X}}{\beta J_{air}}}}{2} \quad (17)$$

260 5.2. Study of the Linearized Dynamics - Short Term

261 The dynamic equations (5) are linearized about the equilibrium point (15),(16),
262 (17) and the long-term dynamic β is considered constant. This is only possible if

263 this analysis is done for a short period of time. Assuming that Jacobian matrix
 264 is given by

$$\begin{bmatrix} -\frac{1}{Y}\mu'(S)X - \frac{Q_{in}}{V} & -\frac{1}{Y}\frac{Q_w}{V} & 0 \\ \mu'(S)X & -\frac{Q_{cake}}{V} & +\beta\frac{J_{air}}{V}\left(\frac{2m(K_{air}+m)-m^2}{(K_{air}+m)^2}\right) \\ 0 & Q_{cake} & -\beta J_{air}\left(\frac{2m(K_{air}+m)-m^2}{(K_{air}+m)^2}\right) \end{bmatrix}$$

265 considering $\mu(S) = \frac{\mu_{max}S}{K_S+S}$, $\mu'(S) = \frac{\mu_{S,max}}{K_S+S} - \frac{\mu_{S,max}S}{(K_S+S)^2}$.

266 A necessary and sufficient condition for a third-order Jacobian to be stable is
 267 to have a negative trace and determinant. Hence, to stabilize the cake dynamics,
 268 J_{air} should be such that $J_{air} > (2m(K_{air} + m) - m^2)/(\beta(K_{air} + m)^2)$ and to
 269 prevent the undesired equilibrium (washout) $0 < Q_w < (S_{in}\mu_{max})/(K_s + S_{in})$.
 270 This strategy is empirically used by the SBR operators that change permeate
 271 flux (i.e. changing directly cake mass (m) attachment (see equation (2))) and
 272 air crossflow set-points to reach an equilibrium point resulting in a constant
 273 cake mass. The Jacobian matrix computation is only valid on a short term,
 274 when the long-term cake evolution phenomenon can be neglected.

275 6. Model Simulation and Identification

276 In this section, we exploit the well-established GPS-X simulator (Hydromantis,
 277 2012), so as to generate realistic simulation data, which can be used as a
 278 database for the estimation of the parameters of our simplified model. Our
 279 objective is to show that the simplified model is able to reproduce the behavior
 280 of a more detailed process representation, implemented in a recognized software
 281 environment.

282 The considered process, which is taken as an application example, has a
 283 membrane permeate flow of $18,75 L/(m^2h)$, resulting in an influent flow of
 284 $0.16284 m^3/d$. The nitrification process is composed of two aerobic tanks, the
 285 first tank has a volume of $0.09 m^3$ and the second, which includes the membrane,
 286 has a volume of $0.045 m^3$. The sludge retention time of the plant is $25 days$,
 287 and the hydraulic retention time $0.5 days$. The total area of the membrane

288 is 0.35 m^2 . The total suspended solids concentration in the membrane com-
 289 partment ranges from 5 to 15 g/L . The influent characteristics are extracted
 290 from Viadero Jr. et al. (2005) with total suspended solids of 10.9 g/m^3 , BOD
 291 of 2.4 g/m^3 and total ammonia nitrogen of 1.5 g/m^3 .

292 The simulator makes use of specific GPS-X modules (and not of our proposed
 293 model at this stage) with ASM1 as biological model and the TMP computation
 294 for the membrane. Standard conditions of $20 \text{ }^\circ\text{C}$, at sea level with barometric
 295 pressure of one *atm* are set. To illustrate the previous discussion, the process
 296 trajectory is computed over a period of 150 days: the first 100 days with an air
 297 crossflow of 2.86 m/d and the next 50 days with a reduced flow of 1.43 m/d .
 298 Figure 3 clearly shows the existence of at least three time scales, ultrafast, fast
 299 and slow, thus confirming our observation in the previous section. The ultrafast
 300 behavior of the cake mass is evident when air flow is changed. A fast time scale
 301 is then observed which corresponds to the transient of the substrate and free
 302 biomass. Finally, a slow evolution of the cake is apparent (the evolution of the
 303 cake has been reported by Merlo et al. (2000) with a fouling rate constant of
 304 0.001 d^{-1}).

305 In Figure 4, a phase plane plot of three GPS-X simulations with different
 306 initial conditions are presented. Note that the system rapidly converges to
 307 the equilibrium point, which confirms our analysis of a fast evolution of the
 308 suspended solids to the cake.

309 The proposed model has been solved using ode45 (a variable-step explicit
 310 Runge-Kutta method) and ode15s (an implicit solver for stiff ODEs based on
 311 numerical differentiation formulas) as implemented in Matlab, using a Intel
 312 Celeron 2.20GHz processor, and the simulation times are respectively 211.65
 313 seconds and 3.08 seconds, demonstrating the process stiffness.

314 In order to fit the response of the simplified model to the experimental data
 315 collected from the GPS-X simulator, the weighted least-squares cost function

$$J(\theta) = \sum_{i=1}^{n_t} ((\xi_{sim}(i) - \xi_{GPS-X}(i)))^T \Omega^{-1} ((\xi_{sim}(i) - \xi_{GPS-X}(i))) \quad (18)$$

316 is minimized, where $\xi_{GPS-X} = [S \ X \ m]$, $\xi_{sim} = [S_{sim} \ X_{sim} \ m_{sim}]$, $\theta =$
 317 $[\beta_0, K_{air}, Y, \mu_{S,max}, \gamma]$, n_t is the number of measurements and Ω is defined as a
 318 scaling matrix that is selected as a diagonal matrix of the square of the maxi-
 319 mum values corresponding to each state. The optimization is performed in this
 320 study using a *Nelder Mead* algorithm as implemented in *fminsearch* in *Matlab*.

321 A lower bound on the covariance matrix \hat{P} of the parameter estimates is
 322 obtained by the inverse of the Fisher Information Matrix (FIM):

$$\hat{P} = F^{-1}(\hat{\theta}) \quad (19)$$

323 The FIM is computed by:

$$F(\hat{\theta}) = \sum_{i=1}^{n_t} \left[\frac{\partial Y_m}{\partial \theta} \right]_{(t_i, \hat{\theta})}^T \Omega^{-1} \left[\frac{\partial Y_m}{\partial \theta} \right] \quad (20)$$

324 The square root σ_j of the j^{th} diagonal element of \hat{P} is an estimate of the
 325 standard deviation of $\hat{\theta}$, which is used to obtain the parameters confidence
 326 intervals of 2.56σ corresponding to a probability of 99%.

327 Based on the fast and slow dynamics analysis, parameter identification can
 328 be organized in three steps corresponding to the three time scales. Indeed, a
 329 direct identification of all the parameters at once is delicate and leads to the
 330 occurrence of several local minima. A divide and conquer approach is therefore
 331 used, where subsets of parameters are estimated first, and the full set of param-
 332 eters is then re-estimated starting from the previous estimates, which are then
 333 much closer to the optimum and severely decrease the computation efforts.

334 Figure 5 shows simulation results corresponding to step-changes in the mem-
 335 brane aeration at day 100 and 140 with values of $1.43m/d$ and $2m/d$, respec-
 336 tively. The ultrafast (orange), fast (green) and slow (blue) time windows are
 337 shown. The parameters related to ultrafast dynamics β_0 which is considered
 338 constant and K_{air} are first estimated using the data collected on a period of
 339 0.02 days, while all the other parameters are fixed (to some initial values that
 340 can be randomly chosen in the parameter space using the latin hypercube strat-
 341 egy - see later). Then, the biological parameters that are linked to the fast

342 dynamics (Y and $\mu_{S,max}$) are estimated from data collected on a period of six
343 days (all the other parameters being fixed) and finally, the remaining slow dy-
344 namics parameter (γ) is estimated from data on a period of 33 days (again
345 all the other parameters being fixed to their last estimated values). The three
346 successive parameter identification steps are followed by an identification of all
347 parameters at once, starting from the current parameter estimates, and using
348 the full data set. The resulting vector of parameters θ is the starting point
349 for a new sequence of ultrafast, fast, slow partial identification and identifica-
350 tion of all parameters. This process can be iterated as necessary, but for this
351 application it is observed that after two iterations the minimization algorithm
352 converges to one single point. The results are shown in Table 2.

353 Following the identification procedure, it is important to test the predic-
354 tive capability of the model with a set of data that has not been used in the
355 identification procedure, i.e., the so-called model cross-validation. This step is
356 important to check if the parameters that have been inferred from the experi-
357 mental data, indeed translate the process behavior, and not only some specific
358 and restricted operating conditions. In this study, the initial conditions and
359 air crossflow are changed, e.g., to $2.29m^3/d$, $2.86m^3/d$, $2m^3/d$ and $1.43m^3/d$,
360 at days 100, 120, 160 and 180, respectively. Figure 6 shows the satisfactory
361 cross-validation results.

362 The correlation matrix of the estimated parameters is presented in Table
363 3. It is apparent that β_0 is correlated with Y and $\mu_{S,max}$, since the value
364 of β_0 affects biomass and in turn the substrate concentration. The pair of
365 parameters Y and $\mu_{S,max}$ are strongly correlated, which is often the case in
366 bioprocess identification. Note that K_{air} is the short-term detachment factor
367 and is correlated with γ that rules the behavior of the long-term detachment,
368 proving again the three time scales behaviors.

369 Accurate correlation coefficients (R^2) of 0.98, 0.94 and 0.93 are obtained for
370 the substrate, free suspended solids and cake build-up outputs. Figure 7 repre-
371 sents the L1-norm of the normalized parametric sensitivities (Muñoz Tamayo et al.,

2009). The matrix is computed by $\sum_{i=1}^{nt} \left| \frac{\hat{\theta}_j}{y_m(t_i, \hat{\theta})} \left[\frac{\partial y_{m_k}}{\partial \theta} \right]_{(t_i, \hat{\theta})} \right|$ and shows the interaction between the identified parameters and states. Note that the brown color denotes that the parameter is more susceptible to the state variation, meaning that this parameter is strongly linked to this state and the opposite for parameters with the dark blue color.

In addition, a multi-start strategy using the Latin Hypercube Sampling (LHS) is used (McKay et al., 1979). The LHS method is a form of stratified sampling, which allows to achieve a reasonably accurate random distribution, while reducing the computational costs associated with Monte Carlo techniques. The parameter bounds defining the exploration space are fixed at plus 50% and minus 50% of the nominal values found after identification in Table 2. Parameter estimation is repeated 80 times using LHS. The minimum costs for all trials are summarized in Table 4, showing that the minimum found has a relatively large region of attraction.

One can observe that, some parameters presented in Table 2 do not totally converge with the standard parameters of the ASM1 model (Henze et al., 1987). This can be explained, due to the simple fact that simplified model is used to fit a complex data behaviour. Nonetheless, GPS-X uses detailed models, such as the full ASM1 (Henze et al., 1987) for the biological compartment, and this study demonstrates that under standard operating conditions, a simple model can capture the main dynamics.

7. sMBR Process Control

The main motivation behind the development of a simple dynamic model is the potential of applying advanced model-based control. Especially, simple models involve a reduced set of state variables, which can be measured by on-line probes or estimated on-line using observers (or software sensors). State feedback can therefore be developed efficiently. Large models, on the contrary, often lead to measurement and observability problems that cannot so easily be alleviated.

401 The purpose of this paper is mostly to present and validate such a simple model,
 402 and not to enter in details in the problematic of process control. However, we
 403 show by an example that our proposed model is indeed appropriate for model-
 404 based control. One of the most straightforward control approaches, in wide
 405 use in industrial process, is Nonlinear Model Predictive Control (NMPC). The
 406 advantage of this control technique is its ability to handle model nonlinearity
 407 and various types of constraints on the actuators and state variables. In this
 408 application the control strategy has three main tasks: (i) maintain cake build-up
 409 inside a certain region; (ii) minimize the ammonia effluent concentration; (iii)
 410 maximize the effluent. It is important to highlight that these tasks can only be
 411 fulfilled based on a model describing biology and filtration, but with a simple
 412 structure, so as to reduce the computational effort.

413 7.1. Nonlinear Model Predictive Control

NMPC uses a model to predict the trajectory of the system on a prediction horizon, and computes an optimal control sequence on a control horizon (Allgöwer et al., 2004). The first important element is therefore a nonlinear model in the form:

$$\dot{x} = f(x(t), u(t)), \quad x(0) = x_0, \quad (21)$$

414 together with constraints in the form $u(t) \in \mathbf{U}, \forall t \geq 0, x(t) \in \mathbf{X}, \forall t \geq 0$
 415 where $x(t) \in \mathbb{R}^n$ and $u(t) \in \mathbb{R}^m$ are the vector of states and inputs, re-
 416 spectively. The sets \mathbf{U} and \mathbf{X} are compact and can be represented by $\mathbf{U} :=$
 417 $u \in \mathbb{R}^m | u_{min} \leq u \leq u_{max}, \mathbf{X} := x \in \mathbb{R}^n | x_{min} \leq x \leq x_{max}$ with the constant
 418 vector u_{min}, u_{max} and x_{min}, x_{max} .

The NMPC control moves are usually given by the solution of a finite horizon open-loop optimal control problem, which is solved at every sampling instant.

In generic notation, the NMPC problem can be expressed as:

$$\min_{\phi_u(\cdot)} J_{NMPC}(x(t), \phi_u(\cdot))$$

$$\text{s.t. } \dot{\phi}_x(\tau) = f(\phi_x(\tau), \phi_u(\tau)), \phi_x(t) = x(t), \quad (22a)$$

$$\phi_u(\tau) = \phi_u(t + T_c), \forall \tau \in [t + T_c, t + T_p], \quad (22b)$$

with the cost function

$$J_{NMPC}(x(t), \phi_u(\cdot)) := \int_t^{t+T_p} F(\phi_x(\tau), \phi_u(\tau)) d\tau;$$

419 where $\phi_u(\tau) \in \mathbf{U}$, $\forall \tau \in [t, t + T_c]$, $\phi_x(\tau) \in \mathbf{X}$, $\forall \tau \in [t, t + T_p]$, T_p and T_c are the
 420 prediction and control horizon with $T_c \leq T_p$. $\phi_x(\cdot)$ denotes the new value of the
 421 state $x(\cdot)$ computed by the closed loop equation $\dot{\phi}_x$ using the new input value
 422 ϕ_u found by the optimization problem for each instant over the moving finite
 423 horizon T_c .

The cost function, equation (23), is chosen based on the process desired performance. Often the first choice for the cost function is the quadratic function. Positive weighting matrices (Ω_1 and Ω_2) can also be included in the cost function.

$$F(x, u) = (x - x_{ref})^T \Omega_1 (x - x_{ref}) + (u - u_{ref})^T \Omega_2 (u - u_{ref}). \quad (23)$$

424 where x_{ref} and u_{ref} are the desired reference of a state and input, respectively.

425 7.2. Application to sMBR Model

426 NMPC, equations (22), are applied to the model equation (5) with the
 427 parameter identified in Section 6. The cost function is defined as $F(x, u) =$
 428 $(S)^2 + (1/Q_{cake})^2$ meaning that ammonia concentration minimization and permeate
 429 flow maximization are desired. The following constraints are added:
 430 (i) $0 \leq m \leq 1.0$ [g] to avoid reaching the maximum membrane pressure;(ii)
 431 $0 \leq Q_{cake} \leq 4.3$ [m^3/d] for the physical range of the permeate pump. The

432 methodology is applied using the Matlab code developed by Grüne & Pannek
433 (2011).

434 The results presented in Figure 8 are obtained assuming that all the state
435 variables are measured. NMPC uses a sampling time of 0.1 day, a prediction
436 horizon $T_p = 10$ days and a control interval of $T_c = 0.1$ day (so we consider a
437 very simple scenario with only one control move on the control horizon). On the
438 left plot of Figure 8 are represented the ammonia concentration, total particle
439 matter and cake mass. Note that the cake mass is maintained around 1.0 [g]
440 because the input (Q_{cake} on the right of the Figure) oscillates to keep the desired
441 response using the detachment propriety of J_{air} , that is constant in this case.

442 This short application demonstrates that our dynamic model can be used
443 as an effective predictor in a NMPC scheme and that NMPC could probably
444 be applied with success to sMBR processes. Of course, more work would be
445 required to fully explore this option, also with real data. This is currently the
446 subject of further investigations.

447 8. Conclusion and Perspectives

448 The main contributions of this study are: (i) the development of a simplified
449 dynamic model of a submerged membrane bioreactor, and its validation in the
450 framework of a particular application example, using simulation data generated
451 with the well-established GPS-X environment; (ii) the study of the equilibrium
452 points of the system (stability analysis) which aims at giving a clue to sMBR
453 process operator about the values of air crossflow and permeate flow to main-
454 tain a good process efficiency, (theses values are nowadays set by operators on
455 an empirical basis); (iii) the investigation of the fast/slow dynamics of the pro-
456 cess (using singular perturbation theory) based on the simplified model, that
457 captures the three main process time scales under conditions of slow evolution
458 of the maximal specific speed of detachment (parameter γ) and large volume
459 of the reactor (parameter V). These time scales correspond to short-term phe-
460 nomena linked to cake formation, defined as ultrafast dynamics, and mid- and

461 long-term phenomena linked to biology and fouling, defined as fast and slow dy-
462 namics, respectively;(iv) the proposal of an identification procedure, that could
463 easily be applied to a real process, taking account of the time scale separation;
464 and finally (v) a short “proof of concept” showing that the dynamic model can
465 be the basis for the design of nonlinear control laws, using either analytical
466 techniques to derive globally stabilizing feedback law or numerical techniques,
467 such as model-based predictive control for optimizing the production of treated
468 water (maximizing Q_{out}) and at the same time reducing energy consumption
469 (minimizing J_{air}).

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Table 1: Symbols and Notations

Symbol	Meaning
Y	yield coefficient of the substrate consumption [-]
μ	Monod's Law [1/d]
$\mu_{S,max}$	maximum growth rate[1/d]
K_s	half saturation of substrate[g/m ³]
X	solid matter concentration [g/m ³]
Q_{in}	inflow[m ³ /d]
V	tank volume[m ³]
S_{in}	input substrate concentration [g/m ³]
S	substrate concentration [g/m ³]
Q_w	waste flux [m ³ /d]
β	resistance of detachable cake by air crossflow [m ⁻¹]
J_{air}	air crossflow [m ³ /m ² d]
m	mass cake state [g]
K_{air}	half saturation of airflow[g]
Q_{cake}	permeate flux ($Q_{cake} = \psi Q_{out}$)[m ³ /d]

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Table 2: Parameters with their standard deviation.

	β_0	K_{air}	Y
Ultrafast [0.02 Days]	(48198.348 ± 0.175)	(47.733 ± 0.0002)	fixed value
Fast [6 Days]	fixed value	fixed value	(0.897 ± 0.0424)
Slow [20 Days]	fixed value	fixed value	fixed value
All Parameters	(55310.548 ± 0.534)	$(45.965 \pm 1.12e - 6)$	(0.898 ± 0.0173)
	$\mu_{S,max}$	γ	$min(J(\theta))$
Ultrafast [0.02 Days]	fixed value	fixed value	53.55
Fast [6 Days]	(2 ± 0.094708)	fixed value	0.8592
Slow [20 Days]	fixed value	(0.0010081 ± 0.80756)	6.42
All Parameters	(2.2654 ± 0.04371)	(0.0014025 ± 0.53516)	22.79

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Table 3: Correlation matrix of the parameters

	β_0	K_{air}	Y	$\mu_{S,max}$	γ
β_0	1	-0.52018	0.74435	0.74407	-0.99999
K_{air}		1	-0.52101	-0.52084	0.52322
Y			1	1	-0.74489
$\mu_{S,max}$				1	-0.74489
γ					1

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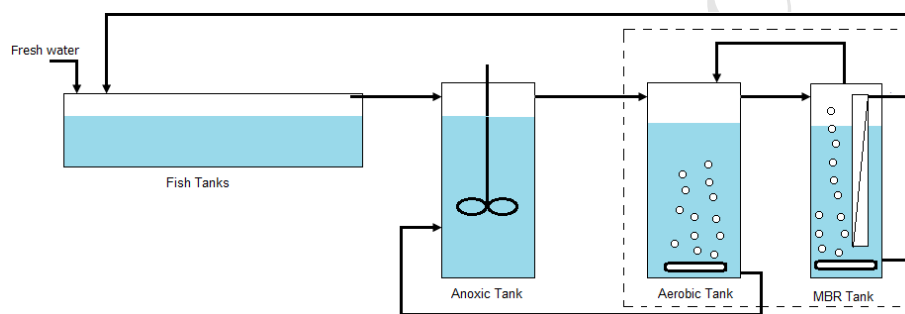
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Table 4: Minimized Cost Function values with standard deviation. First and second iterations of the full procedure

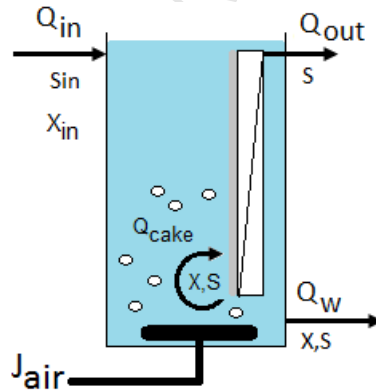
	$\min(J(\theta))_1$	$\min(J(\theta))_2$
Ultrafast [0.02 Days]	(77.49 ± 145.3)	(52.63 ± 2.35)
Fast [6 Days]	(0.8595 ± 0.0014)	(0.8592 ± 0.0013)
Slow [20 Days]	(6.58 ± 2.16)	(6.50 ± 0.36)
All Parameters	(22.86 ± 1.42)	(22.79 ± 0.39)

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(a) Recirculating aquaculture system fitted with an sMBR.



(b) sMBR process sketch

Figure 1: sMBR process structure.

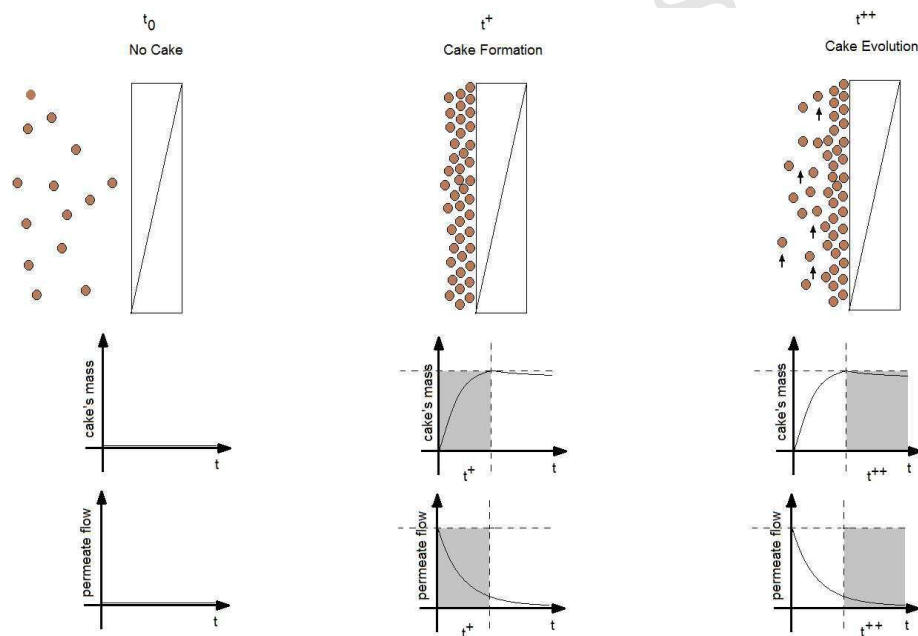


Figure 2: Time evolution of cake mass and effluent flow: at t_0 , $Q_{out} = 0$; at t^+ , the cake is formed; the time interval up to t^{++} shows the further cake evolution

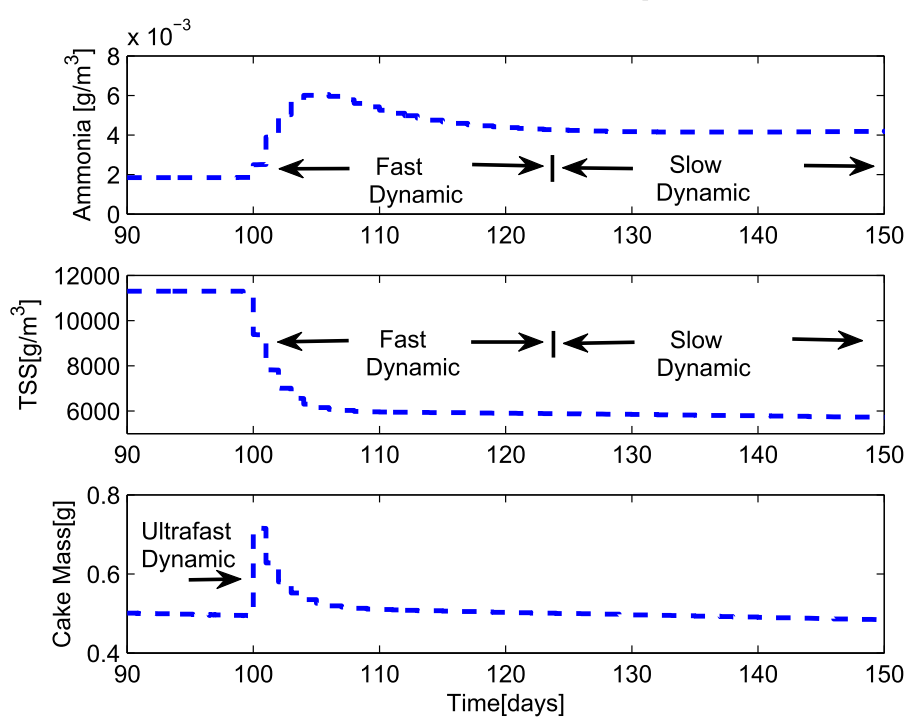


Figure 3: GPS-X simulation.

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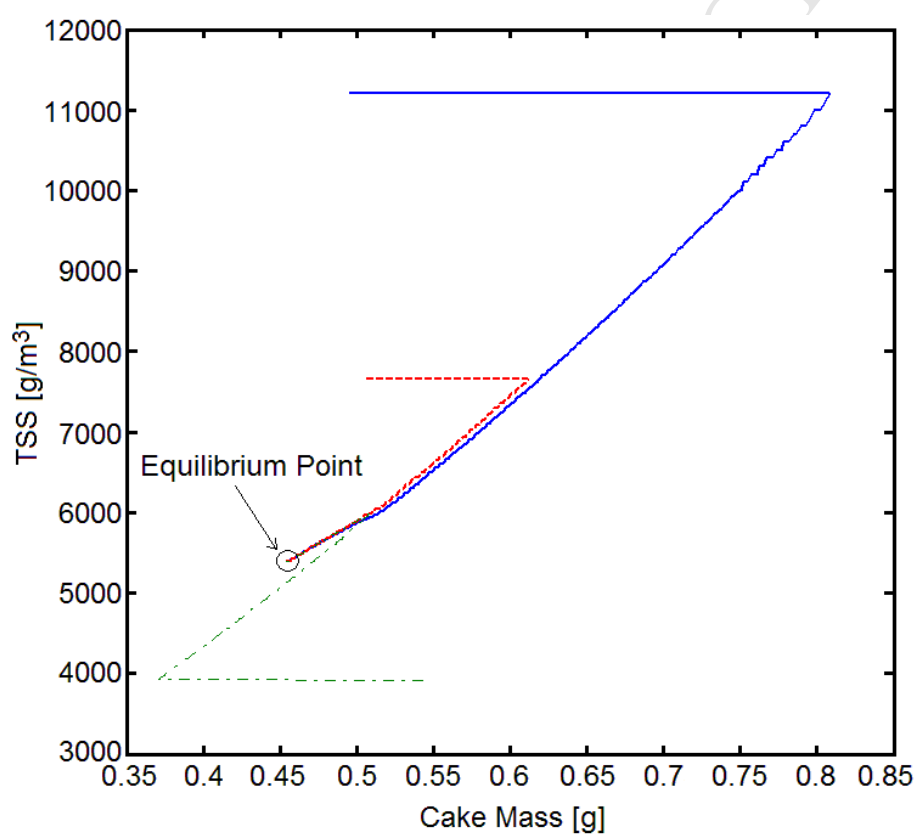


Figure 4: GPS-X simulation: Phase plane plot. Trajectories from three different initial conditions.

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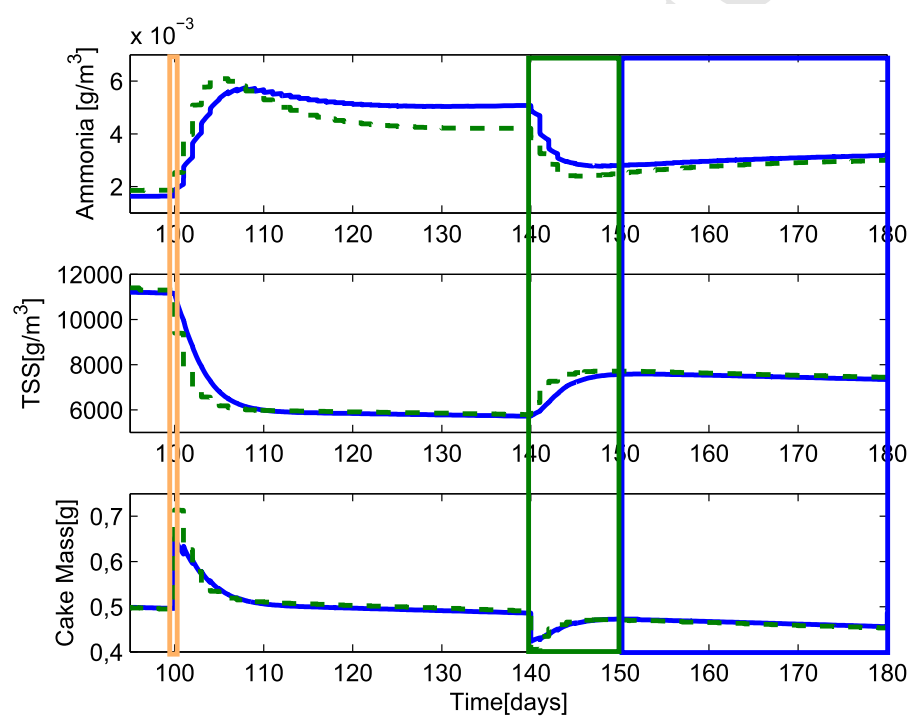


Figure 5: Dotted line: GPS-X with full ASM1 model; solid line: proposed simplified model. Orange window - Ultrafast; Green window - Fast; Blue window - Slow.

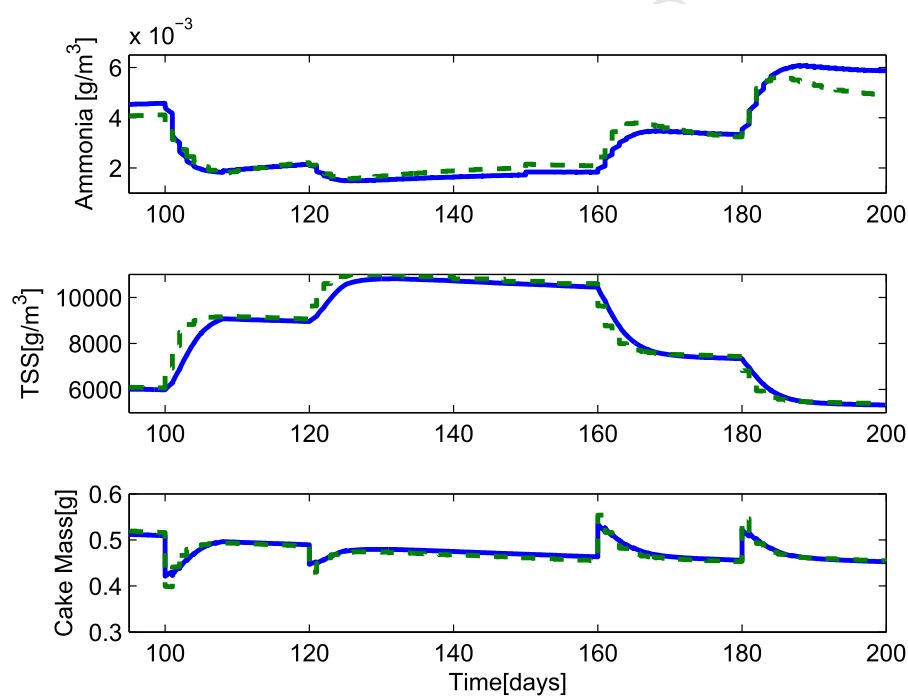


Figure 6: Cross-validation with different initial values and setpoints. Dotted line: GPS-X with full ASM1 model; solid line: proposed simplified model.

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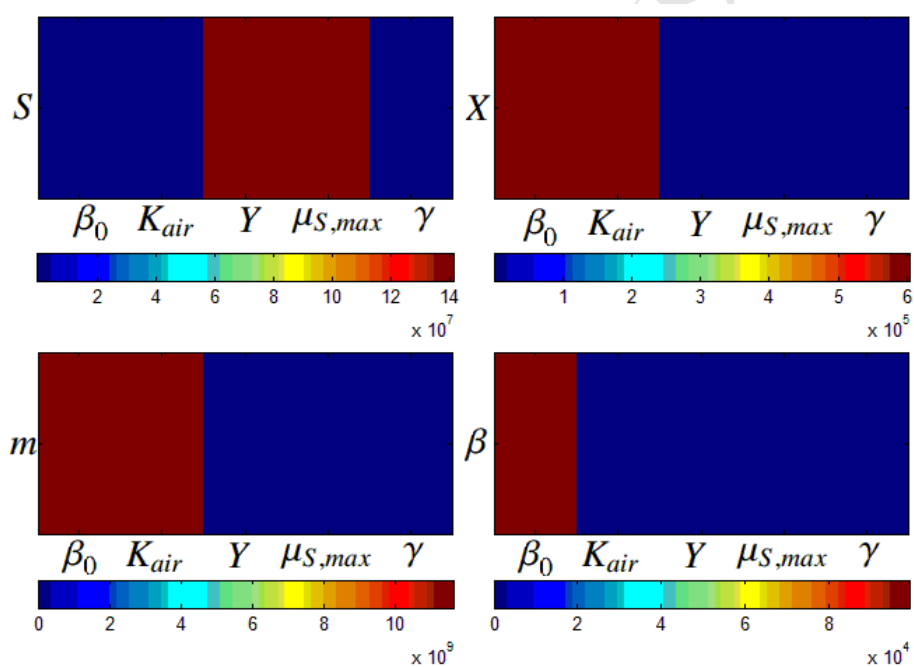


Figure 7: L1-norm of parametric sensitivities

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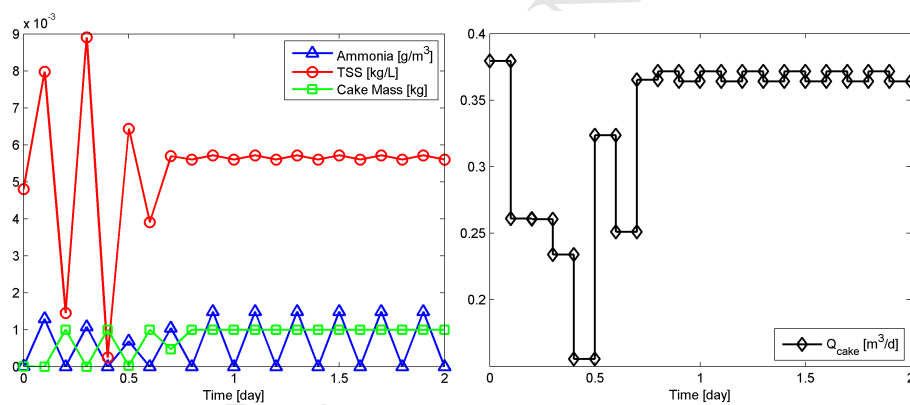


Figure 8: NMPC applied to MBR model: state evolution (left) and control moves (right)

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