A simple model of anaerobic membrane bioreactor integrating toxin effects: preliminary results

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Abstract
In this paper, we propose to modify the simple two-steps AM2 model (cf. [Ber:01]) in order to integrate toxin effects on the bioprocess dynamical behaviour. The model equations are presented on the basis of a mass-balance approach and the main properties of this model are investigated through numerical simulations.

Keywords
Anaerobic Digestion; AM2 model; Modelling; Toxin; Numerical simulation.

INTRODUCTION

Although anaerobic digestion is a suitable bioprocess for wastewater treatment and biogas production, the system can be easily inhibited by external toxins. Retained by the membrane in an Anaerobic Membrane BioReactor (AnMBR) until concentrations that can become high, toxins can affect dramatically the process. When modeled as two step reaction systems (acidogenesis and methanogenesis) [Ber:01], toxins can affect one step or both depending on the capability of the communities to become resistant and/or to degrade them [Wee:12]. It is therefore essential to integrate toxins dynamic into the model of the bioprocess. The aim of this paper is to model the toxin effect on the process behaviour (here phthalates [Zay:14]), by modifying the acidogenesis kinetics function of the two steps model AM2 [Ber:01]. From practical observations, we highlight hypotheses for the model development and we investigate its qualitative behaviour by numerical simulations.

PILOT PLANT AND EXPERIMENTAL DATA

The process considered here is a homogeneous side-stream AnMBR (Fig. 1) installed at the CBS, Sfax, Tunisia. S_1 is the organic matter concentration (COD), S_{1in} is the input COD concentration, S_2 is the Volatile Fatty Acid concentration (VFA), S_{2in} the input VFA concentration, X_1 is the acidogenic biomass, X_2 is the methanogenic biomass, S_{ph} is the toxin concentration and S_{phin} its input concentration. The bioreactor was fed by an increasing Organic Load Rate (OLR) from *4* to *10gCOD/L*. It was monitored during an experimental period of *220 days* (available data are represented in Fig.2). It was observed that for high OLR, biogas production and COD abatement have strongly decreased, while VFA concentration was reasonably low to assume no reactions inhibition. Thus, the observed reactions breakdown is due to the external toxin (phthalates) which had an increasing concentration in the reaction medium over the time. Indeed, these compounds are slightly biodegradable in anaerobic systems.

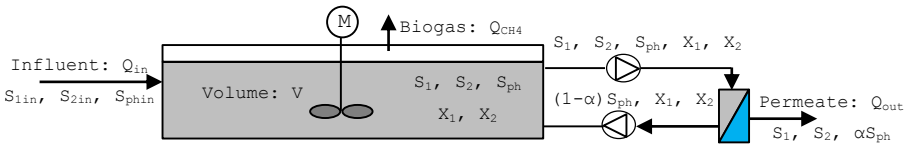

Figure 1. Schematic representation of the proposed model.

The review of experimental data leads us to make the following assumptions for modelling:

- The toxin is slightly present in the influent (S_{phin});
- Only a fraction of the toxin (noted αS_{ph}) leaves the bioreactor, the rest being retained by the membrane;
- The toxin affects only acidogenic bacteria: the acidogenesis kinetics depends both on S_1 and S_{ph};
- One of the two micro-organisms consortia may breakdown the toxin (this is translated in the model as a decay term on S_{ph} dynamics not related to any growth rate).

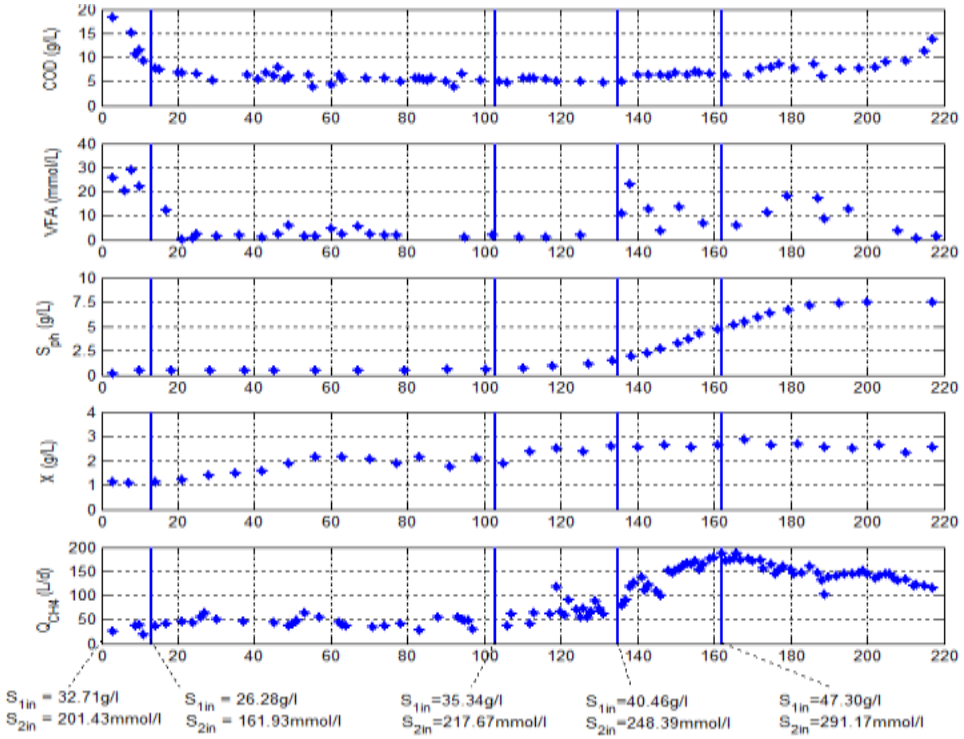

Figure 2. Experimental data from the AnMBR.

MATHEMATICAL MODEL

Taking into account the assumptions introduced in the previous section, the following model is proposed with parameters given in Table 1.

$$\frac{dX_1}{dt} = \left(\mu_1(S_1, S_{ph}) - D_x\right)X_1 \quad (1)$$

$$\frac{dS_1}{dt} = D_s(S_{1in} - S_1) - k_1\mu_1(S_1, S_{ph})X_1 \quad (2)$$

$$\frac{dX_2}{dt} = (\mu_2(S_2) - D_x)X_2 \quad (3)$$

$$\frac{dS_2}{dt} = D_s(S_{2in} - S_2) + k_2\mu_1(S_1, S_{ph})X_1 - k_3\mu_2(S_2)X_2 \quad (4)$$

$$\frac{dS_{ph}}{dt} = D_s\left(S_{phin} - \alpha S_{ph}\right) - K_{ph}S_{ph} \quad (5)$$

$$Q_{ch4} = k_4\mu_2(S_2)X_2 \quad (6)$$

The function $\mu_1(S_1,S_{ph})$ must be chosen with qualitative properties describing the toxin effects (acidogenesis inhibition). In fact, $\mu_1(S_1,S_{ph})$ must have the following properties :

- $\mu_1(S_1, 0)=\mu(S_1)$: no inhibition in the absence of toxin.

- $\mu_1(S_1,\infty)=0$: limit of acidogenesis inhibition at high toxin concentration. As a consequence, the growth rate function should be decreasing with respect to S_{ph}.

The model of [Kis:83] where the acidogenic bacteria growth is inversely proportional to the square of toxins concentration seems appropriate to predict the toxin effects:

$$\mu_1(S_1, S_{ph}) = \mu_1(S_1) * \frac{1}{1+S_{ph}^2} \quad (7)$$

where $\mu_1(S_1)$ can be chosen as a Monod function:

$$\mu_1(S_1) = \frac{\mu_{1max} S_1}{S_1+K_{s1}}. \quad (8)$$

Since S_2 is not inhibitor of methanogenesis reaction as mentioned above, then the function $\mu_2(S_2)$ is chosen as a Monod model:

$$\mu_2(S_2) = \frac{\mu_{2max} S_2}{S_2+K_{s2}}. \quad (9)$$

DYNAMIC BEHAVIOUR

Interesting properties of the model (1)-(9) are now being investigated in simulation. The parameters of the model part without S_{ph} (original AM2 model) have values equal or close to those proposed in [Ber:01]. The other parameters S_{phin}, K_{ph}, D_x and D_s are chosen close to those used to obtain the experimental data. S_{1in} and S_{2in} are stepwise functions (see Fig.3).

Table 1. Nominal values for the parameters of the model (1)-(9)

Parameter	*Value*	*Unit*	*Signification*
S_{phin}	1.5	gCOD/L	The input concentration of the toxin
S_{1in}	Varying by step	gCOD/L	The input concentration of the organic matter (COD_{in})
S_{2in}	Varying by step	mmol/L	The input concentration of the AGV
μ_{1max}	1.2	d^{-1}	Maximum acidogenic biomass growth rate on S_1
K_{s1}	7.1	gCOD/L	Half-saturation constant associated with S_1
μ_{2max}	0.74	d^{-1}	Maximum methanogenic biomass growth rate on S_2
K_{s2}	9.28	mmol/L	Half-saturation constant associated with S_2
K_{ph}	Varying	d^{-1}	The hydrolysis rate of the toxin
α	0.5		The toxin fraction leaving the bioreactor
D_x	0.05	d^{-1}	The decay rate of biomasses
D_s	0.14	d^{-1}	The dilution rate
k_1	42.14		Yield of S_1degradation by X_1
k_2	116.5	mmol/g	Yield of S_2 production from S_1
k_3	268	mmol/g	Yield of S_2 degradation by X_2
k_4	300	mmol/g	Production rate of biogas

For a set of realistic initial conditions, simulations over 250 days of system (1)-(6) are plotted in Fig.3. In particular, S_{1in} and S_{2in} were chosen to cover a large range of concentration values (see Fig.3(G, H)). We assumed that input toxin concentration is nearly zero before *t=110 days*; while it increases significantly after. Since it is partially retained by the membrane, it accumulates more and more (see Fig.3(F)). The presence of high toxin concentration in the bioreactor then increasingly affects the first reaction (acidogenesis), yielding to a decrease of X_1 concentration (Fig.3(A)) and a continuous increase of S_1 which is not degraded anymore (Fig.3(D)). Finally, this undesirable scenario leads to the breakdown of methane production (Fig.3(I)).

The system behaviour (time responses) predicted by the model (1)-(9) has general trend very similar to the real system (experimental data, Fig.2), noting especially: i) the increase of both S_1 and S_{ph} and ii) the breakdown of Q_{CH4} and *VFA* towards the end of the simulation. Perspectives for further work

include: i) an appropriate modelling of toxins effects on the system behaviour by identifying optimal parameter values of the model, ii) the model validation with experimental data and iii) the design of control lows in order to prevent toxic effects and reduce toxicity, to avoid the system breakdown.

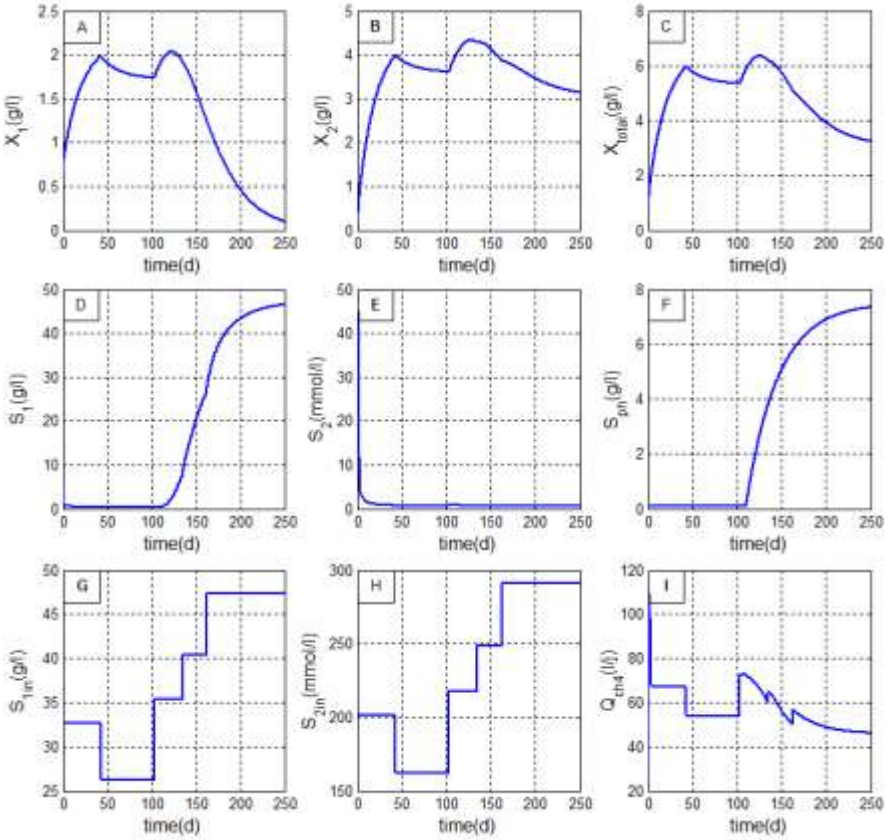

Figure 3. Simulations of the dynamic behaviour of model (1)-(6)

CONCLUSION

In this paper, we propose to modify a simple two steps model of anaerobic digestion to integrate toxin effects on the acidogenesis step in an AnMBR. A first study of model qualitative behaviour was realized through numerical simulations. Perspectives of this work include the confrontation of such model to experimental data and the design of controllers based on this model in order to reduce toxicity.

AKNOWLEDGEMENTS

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