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# A RISK MANAGEMENT CRITERION FOR AN UNSTABLE WASTEWATER TREATMENT PROCESS

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Abstract: In this paper we consider an unstable biological process used for wastewater treatment. This anaerobic digestion ecosystem can have 2 locally stable steady states and one unstable steady state. We first study the model and characterise the attraction basin associated to the normal operating mode. In a second step we estimate the size of this attraction basin by using a simplified criterion that turns out to be a good approximation. Finally we apply the approach on a real anaerobic digestion plant, and we show that the proposed criterion allows to rapidly detect the conditions of a destabilisation.

Keywords: Haldane model, Anaerobic digestion, Nonlinear systems diagnosis

## 1. INTRODUCTION AND MOTIVATION

Control of biological systems is a very delicate problem since one has to deal with highly nonlinear systems described by poor quality models. In some cases this control issue can be really crucial when the system is unstable. This is especially the case for the anaerobic digestion process: a biological system in a bioreactor used to treat wastewater. This complex ecosystem involves more than 140 bacterial species (Delbès *et al.*, 2001). It progressively degrades the organic matter into $CO_2$ and methane $CH_4$. However this process is known to be very delicate to manage since it is unstable (Fripiat *et al.*, 1984): an accumulation of intermediate compounds can lead to the crash of the digester.

To solve this problem, many authors have proposed controllers (Perrier and Dochain, 1993; Steyer *et al.*, 1999; Mailleret *et al.*, 2004) that were able to warranty the local or even the global stability of the system using the dilution rate of the bioreactor as input. For various reasons (necessity of a storage tank, lack of online sensors, lack of robustness,...) these control laws are very seldom applied in practice. As a consequence, the controllers are often disconnected at the industrial scale and the plant manager manually operates the process trying both to avoid process destabilisation and wastewater storage.

The approach that we propose has the objective to provide the operator with a risk index associated to his management strategy. The idea is therefore to determine from the global analysis of the nonlinear system whether the process has been triggered to a dangerous working mode. This risk index can also be used in parallel controller.

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The paper is composed as follows:in the second section a dynamical model of an anaerobic digestion process is recalled. The third part puts the emphasis on the analysis of the model dynamics. A simple criterion to assess the stability of the process is set in the fourth section, and finally this criterion is applied to a real experiment to determine its destabilisation risk.

## 2. MODEL PRESENTATION

We consider a simplified macroscopic model of the anaerobic process based on 2 main reactions (Bernard *et al.*, 2001), where the organic substrate ($S_1$) is degraded into volatile fatty acids (VFA denoted $S_2$) by acidogenic bacteria ($X_1$), and then the VFA are degraded into methane $CH_4$ and $CO_2$ by methanogenic bacteria ($X_2$):

- Acidogenesis:

$$k_1 S_1 \overset{\mu_1(S_1)X_1}{\longrightarrow} X_1 + k_2 S_2$$

- Methanogesis:

$$k_3 S_2 \overset{\mu_2(S_2)X_2}{\longrightarrow} X_2 + k_4 CH_4$$

Where $\mu_1(S_1)$ and $\mu_2(S_2)$ represent the bacterial growth rates associated to these 2 bioreactions.

The mass balance model in the CSTR (Continuous Stirred Tank Reactor) can then straightforwardly be derived:

$$\dot{X_1} = \mu_1(S_1)X_1 - \alpha D X_1 \tag{1}$$

$$\dot{S_1} = -k_1\mu_1(S_1)X_1 + D(S_{1in} - S_1) \tag{2}$$

$$\dot{X_2} = \mu_2(S_2)X_2 - \alpha D X_2 \tag{3}$$

$$\dot{S_2} = -k_3\mu_2(S_2)X_2 + k_2\mu_1(S_1)X_1 + D(S_{2in} - S_2) \tag{4}$$

$D$ is the dilution rate, $S_{1in}$ and $S_{2in}$ are respectively the concentrations of influent organic substrate and of influent VFA. The '$k_i$s' are pseudo-stoichiometric coefficients associated to the bioreactions. Parameter $\alpha \in (0\ 1]$ represents the fraction of the biomass which is not attached in the digester. We denote by $\xi = (X_1,\ S_1,\ X_2,\ S_2)^T$ the state vector.

In the sequel, we will consider the rather generic mappings $\mu_1$ and $\mu_2$, satisfying the following properties:

*Assumption 1.* **$\mu_1$ is an increasing function of $S_1$, with $\mu_1(0) = 0$.**

*Assumption 2.* **$\mu_2$ is a function of $S_2$ which increases until a concentration $S_2^M$ and then decreases, with $\mu_2(S_2^M) = \mu_M$ and $\mu_2(0) = 0$.**

In the mathematical analysis of this system, assumption is made that the environment of the bacteria remains constant and we will thus assume that $D$, $S_{1in}$ and $S_{2in}$ are positive constants. In the same way all the initial conditions are assumed to be positive.

## 3. MODEL ANALYSIS

### *3.1 Analysis of the acidogenic dynamics*

The subsystem (1,2) is close to a classical Monod model but slightly modified by the term $\alpha$. This makes the study of this system less straightforward than for Monod model (with $\alpha = 1$) (Smith and Waltman, 1995). However its behaviour is simple as stated in the following Property:

*Property 1. System (1,2) with initial conditions in $\mathbb{R}_+^2$ admits a single globally stable equilibrium. If $\alpha D < \mu_1(S_{1in})$ this equilibrium is in the interior domain.*

**Proof:** For sake of space limitation only the sketch of the proof is presented here.

The positivity of this system is trivial. To demonstrate the boundedness in a compact set of $\mathbb{R}_+^2$ we consider the quantity $Z = S_1 + k_1 X_1$, and use the positivity of the variables.

The considered system (1,2) has 2 steady states: the trivial washout steady state $X_1^\dagger = 0$, $S_1^\dagger = S_{1in}$ which exists for any $D$, and another steady state in the positive domain if and only if $\alpha D < \mu_1(S_{1in})$ (ensuring $S_1^\star < S_{1in}$ and thus $X_1^\star > 0$) given by:

$$\begin{cases} S_1^\star = \mu_1^{-1}(\alpha D) \\ X_1^\star = \frac{1}{k_1\alpha}\left(S_{1in} - S_1^\star\right) \end{cases} \tag{5}$$

The study of the trace and of the determinant the Jacobian matrix of (1,2) at the two equilibria informs us that only the useful working point $(X_1^\star, S_1^\star)$ is an attractor, the washout steady state being a saddle point.

To conclude the proof and determine the global behaviour of (1,2) we change variables $(X_1, S_1)$ to $(X_1, Z)$. With this reformulation the system becomes :

$$\begin{cases} \dot{X_1} = \mu_1(Z - k_1X_1)X_1 - \alpha D X_1 \\ \dot{Z} = D\left(S_{in} - Z\right) + (1-\alpha)\, k_1 X_1 \end{cases}$$

It follows directly that this system is cooperative. Furthermore the system is asymptotically bounded in a compact closure of $\mathbb{R}_+^2$. Hence from *Theorem* 2.2 in (Smith, 1995) for two-dimensional systems, the limit can only be a stable equilibrium point. Since the washout equilibrium is unstable the system cannot converge towards it.

The useful working point of system (1,2) being globally asymptotically stable we have the following property:

*Property 2. After a transient time $T$, system (1,2) satisfies the inequality* $k_1\,\mu_1(S_1)X_1 \leq DS_{1in}$.

*Remark*: in practice this condition is often met at initial time or the transient time $T$ is small.

### 3.2 Analysis of the methanogenic dynamics

Now we will consider the second system after a period greater than $T$ (*cf. Property 2*). The total concentration of VFA available for the second step of the process is

$$S_{2in} + \frac{k_2}{D}\mu_1\left(S_1\right)X_1 \leq S_{2in} + \frac{k_2}{k_1}S_{1in} = \tilde{S}_{2in}.$$

In order to study the methanogenesis as a stand-alone process we consider $\tilde{S}_{2in}$ as a pessimistic upper bound of the total concentration of VFA in the reactor.

Thus the methanogenic system is reduced to a one-stage process independent of the acidogenic phase:

$$\begin{cases} \dot{X}_2 = \mu_2(S_2)X_2 - \alpha D X_2 \\ \dot{S}_2 = D(\tilde{S}_{2in} - S_2) - k_3\mu_2(S_2)X_2 \end{cases} \tag{6}$$

This system is close to a generic Haldane model but, as for the acidogenic subsystem, it is modified by the term $\alpha$.

*Property 3. System (6) with initial conditions in $\Omega = \mathbb{R}_+^* \times \mathbb{R}_+$ admits a globally exponentially stable equilibrium in the interior domain for $\alpha D < \mu_2\left(\tilde{S}_{2in}\right)$. If $\mu_2\left(\tilde{S}_{2in}\right) < \alpha D < \mu_M$ it becomes locally exponentially stable and the washout equilibrium is also l.e.s. For $\alpha D > \mu_M$ the washout equilibrium becomes g.e.s. (see Tab. 1 for more details)*

**Proof:** For sake of brevity only the main steps are presented here.

We study the boundedness of the variables $X_2$ and $S_2$ in the same way as for the acidogenic phase, considering the quantity $Z_2 = S_2 + k_3X_2$. The trivial steady state corresponding to the bioreactor washout is given by $X_2^\dagger = 0,\ S_2^\dagger = \tilde{S}_{2in}$

Now we are going to explore the other steady states. They are solutions of the following system:

$$\begin{cases} \mu_2(S_2^\star) = \alpha D \\ X_2^\star = \frac{1}{\alpha k_3}(\tilde{S}_{2in} - S_2^\star) \end{cases} \tag{7}$$

Note that they must verify $S_2^\star \leq \tilde{S}_{2in}$ to have $0 \leq X_2^\star$.

First remark that, if $\tilde{S}_{2in} \leq S_2^M$ then $\mu_2$ is an increasing function on the admissible domain $\left[0, \tilde{S}_{2in}\right]$. As a consequence the study of system (6) is identical to the study of equations (1,2). We will then focus now on the other case where $\tilde{S}_{2in} > S_2^M$.

As illustrated on Fig. 1, five cases are possible, depending on parameters values.

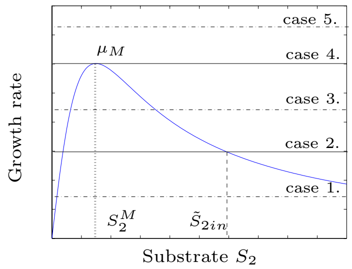


Fig. 1. Possible solutions for $\mu_2(S) = \alpha D$

*cases 1. and 2.* $\alpha D \in \left(0, \mu_2(\tilde{S}_{2in})\right]$: then the equation $\mu_2(S_2) = \alpha D$ has a single solution for $S_2 \in \left[0, \tilde{S}_{2in}\right)$:

$$(X_2^\star, S_2^\star) = \left(\frac{\tilde{S}_{2in} - \mu_2^{-1}(\alpha D)}{\alpha k_3}, \mu_2^{-1}(\alpha D)\right) \text{ (unique)}$$

*case 3.* $\alpha D \in \left(\mu_2(\tilde{S}_{2in}), \mu_M\right)$: here the equation $\mu_2(S_2) = \alpha D$ has two solutions for $S_2 \in \left[0, \tilde{S}_{2in}\right)$. Let us denote $S_2^{1\star}$ and $S_2^{2\star}$ such that $\mu_2(S_2^{1\star}) = \mu_2(S_2^{2\star}) = \alpha D$:

$$0 < S_2^{1\star} < S_2^M < S_2^{2\star} < \tilde{S}_{2in}$$

with $i = 1$ for the useful working point $\left(X_2^{1\star}, S_2^{1\star}\right)$ and $i = 2$ for the unstable equilibrium $\left(X_2^{2\star}, S_2^{2\star}\right)$.

then the two possible equilibria are:

$$\begin{cases} S_2^{1\star} < S_2^M \\ X_2^{1\star} = \frac{1}{\alpha k_3}(\tilde{S}_{2in} - S_2^{1\star}) \end{cases} \text{ and } \begin{cases} S_2^{2\star} > S_2^M \\ X_2^{2\star} = \frac{1}{\alpha k_3}(\tilde{S}_{2in} - S_2^{2\star}) \end{cases}$$

*case 4.* $\alpha D = \mu_M$: there is a unique solution to equation $\mu_2(S_2) = \alpha D$:

$$(X_2^\star, S_2^\star) = \left(\frac{\tilde{S}_{2in} - S_2^M}{\alpha k_3}, S_2^M\right)$$

*case 5.* $\alpha D > \mu_M$: here there is no solution to the equation $\mu_2(S_2) = \alpha D$. In this case there is no other equilibrium than the washout point.

### 3.3 Study of equilibria stability

The stability of system (6) is easy to assess by computing the trace and the determinant of the Jacobian matrix for all the considered cases:

- For the interior steady states $X_2^\star > 0$:

$$\mathrm{trace}(\mathcal{J}) = -D - k_3 X_2^\star \frac{\partial \mu_2}{\partial S_2}(S_2^\star)$$
$$\det(\mathcal{J}) = k_3 \alpha D X_2^\star \frac{\partial \mu_2}{\partial S_2}(S_2^\star)$$

- For the washout steady states $X_2^\star = 0$:

$$\mathrm{trace}(\mathcal{J}) = \mu_2(\tilde{S}_{2in}) - (1+\alpha)D$$
$$\det(\mathcal{J}) = -D(\mu_2(\tilde{S}_{2in}) - \alpha D)$$

It straightforwardly leads to the classification proposed in Table 1 [2].

Table 1. Possible equilibria together with parameter values

| Case # | Conditions | int. | wash. |
|---|---|---|---|
| 1) | $\alpha D < \mu_2(\tilde{S}_{2in})$ | g.e.s. | un. |
| 2) | $\alpha D = \mu_2(\tilde{S}_{2in})$ | l.e.s. | un$^\dagger$. |
| 3) | $\alpha D \in ]\mu_2(\tilde{S}_{2in}), \mu_M[$ | $S_2^{1\star}$ l.e.s.<br>$S_2^{2\star}$ un. | l.e.s. |
| 4) | $\alpha D = \mu_M$ | un$^\dagger$. | l.e.s. |
| 5) | $\alpha D > \mu_M$ | / | g.e.s. |

*Remark:* the 2 cases denoted by 'un$^\dagger$.' corresponding to non hyperbolic equilibria are:

- Case 2: $\left(0, \tilde{S}_{2in}\right)$ for $\alpha D = \mu_2(\tilde{S}_{2in})$. Let us remark that the region $\{S_2 \leq \tilde{S}_{2in},\ X_2 \geq 0\}$ is positively invariant. Moreover $X_2$ is increasing in the sub-domain $\{X_2 > 0,\ S_2^{1\star} \leq S_2 \leq \tilde{S}_{2in}\}$. The only way to reach the washout $X_2^\star = 0$ from the region $\{S_2 \leq \tilde{S}_{2in}\}$ is thus to start with a zero initial condition. This proves that $\left(0, \tilde{S}_{2in}\right)$ is unstable.
- Case 4: $(X_2^\star, S_2^\star)$ for $\alpha D = \mu_M$. It is clear that in this case $\dot{S}_2 \leq 0$, and therefore the point is unstable (there is however a region above $X_2 = X_2^\star$ converging toward this steady-state).

### 3.4 Concluding remarks on stability

This study highlighted a special case of interest, for $\tilde{S}_{2in} > S_2^M$ and $\alpha D \in \left(\mu_2(\tilde{S}_{2in}), \mu_M\right)$. Here there are 2 steady states in the interior domain, one of which together with the washout are stable. In this case, illustrated on Fig. 2a), the asymptotic state of the system is *a priori* not predictable, and depends on the initial state. The set of initial conditions leading to the interior steady state $\xi_2^{1\star} = (X_2^{1\star}, S_2^{1\star})$ corresponds to the **basin of attraction**.

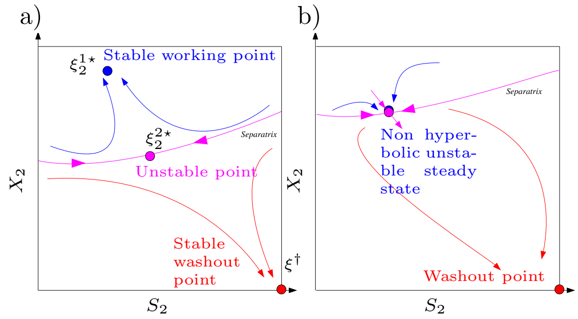


Fig. 2. Possible orbits in the phase plan: a) case 3, b) case 4

The next section will consist in characterising the size of the attraction basin in this specific case.

## 4. ATTRACTION BASIN OF THE NORMAL OPERATING MODE AND STABILITY CRITERIA

We still focus on the methanogenic step to establish a stability criterion associated to a process control action. In this part we assume the following specific forms for $\mu_1(S_1)$ and $\mu_2(S_2)$ satisfying *Assumptions* 1 and 2:

$$\mu_1(S_1) = \bar{\mu}_1 \frac{S_1}{S_1 + K_{S1}} \quad (Monod)$$
$$\mu_2(S_2) = \bar{\mu}_2 \frac{S_2}{S_2 + K_{S2} + \frac{S_2{}^2}{K_{I2}}} \quad (Haldane) \qquad (8)$$

In the sequel $\xi$ denotes the state vector of the methanogenic phase $(X_2, S_2)$.

### 4.1 Definition of the Attraction Basin and of the stability criterion

We have shown in the previous section that $\xi$ remains bounded. We thus consider the acceptable domain as follows:

$$\mathcal{K} = \left(0, \frac{\tilde{S}_{2in}}{\alpha k_3}\right] \times \left[0, \tilde{S}_{2in}\right] \qquad (9)$$

For $\xi^{1\star} = \left(X_2^{1\star}, S_2^{1\star}\right)$, the interior critical point of system (6), we define its basin of attraction $\Lambda$ as the set of initial conditions in $\mathcal{K}$ converging asymptotically towards it.

$$\Lambda\,(D, \xi_{in}) = \left\{\xi_0 \in \mathcal{K} \mid \lim_{t \to +\infty} \xi(\xi_0, t) = \xi^{1\star}\right\},$$

The main idea of this paper is to characterise the stability of the system by the area of the attraction basin $\Lambda$. The process stability can then be assessed by the relative surface of $\Lambda$ in $\mathcal{K}$ (10).

However, from the previous study (see Tab. 1) it is worth noting that there still exists a non empty

[2] (ss: steady state, l.e.s.: locally exp. stable, g.e.s.: globally exp. stable, un.: unstable, int.: interior, wash: washout).

attraction basin $\Lambda^{\star} = \Lambda\left(\frac{\mu_M}{\alpha}, \xi_{in}\right)$ associated to case 4 ($\alpha D = \mu_M$) where the interior equilibrium is unstable (see Fig. 2b). This case should correspond to a zero stability index. For this reason we define the following criterion, which is simply the relative area of the attraction basin on the domain $\mathcal{K} \setminus \Lambda^{\star}$:

$$\mathcal{I}_{\mathcal{S}}\left(D, \tilde{S}_{in}\right) = \frac{\mathcal{S}\left(\Lambda\left(D, \xi_{in}\right) \setminus \Lambda^{\star}\right)}{\mathcal{S}\left(\mathcal{K} \setminus \Lambda^{\star}\right)} \qquad (10)$$

Where application $\mathcal{S}$ is the area of the considered domain.

### *4.2 Numerical computation of the stability index*

The separatrix can be computed numerically by integrating System (6) in inverse time along the stable direction of the saddle point $\left(X_2^{2\star}, S_2^{2\star}\right)$ starting very close to it. The computation of the attraction basin area follows straightforwardly.

However the numerical computation of $\mathcal{I}_{\mathcal{S}}$ does not provide any analytical expression of the stability index that would base a management strategy. In the following section we seek a simpler criterion related to $\mathcal{I}_{\mathcal{S}}$.

### *4.3 Overloading tolerance of the process: a simple criterion*

If the dilution rate is increased from zero, the interior equilibrium will remain g.e.s. until $D = \frac{\mu_2(\tilde{S}_{2in})}{\alpha}$. Then the second (unstable) steady state appears in the interior domain together with a separatrix associated to the attraction basin $\Lambda\left(D, \xi_{in}\right)$ that does no longer occupy all the domain. The size of $\Lambda\left(D, \xi_{in}\right)$ will then decrease and finally vanish for $D \geq \frac{\mu_M}{\alpha}$. It is worth noting that the distance between the 2 interior steady states follows a rather comparable scheme: it will decrease from a maximum distance when $D = \frac{\mu_2(\tilde{S}_{2in})}{\alpha}$ to zero for $D \geq \frac{\mu_M}{\alpha}$.

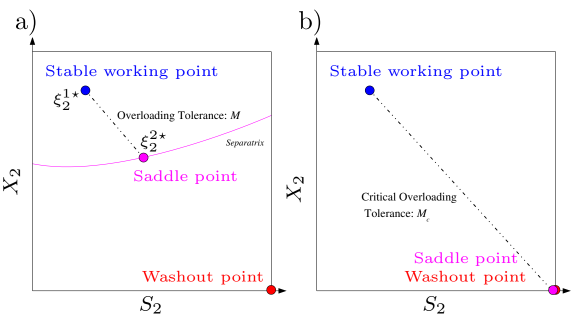


Fig. 3. Definition of a) the Overloading and b) the Critical Overloading Tolerance in the phase plan

From this consideration we define, for $\alpha D \in \left[\mu_2(\tilde{S}_{2in}), \mu_M\right]$, the notion of **Overloading Tolerance (OT)**, $\boldsymbol{M}$ which is simply the distance between the 2 interior steady states (see Fig 3a):

$$M\left(D\right) = \|\xi_2^{2\star} - \xi_2^{1\star}\| \qquad (11)$$

We also define the **Critical Overloading Tolerance (COT)** $M_c$, which is the maximum value of the overloading tolerance obtained for $D = \frac{\mu_2(\tilde{S}_{2in})}{\alpha}$.

The approximate stability criterion that we will consider (named **Relative Overloading Tolerance, ROT**) is then defined as follows:

$$m(D, \xi_{in}) = \begin{cases} 0 & \text{for } \alpha D > \mu_M \\ \frac{M(D)}{M_c(\xi_{in})} & \text{for } \alpha D \in [\mu_2(\tilde{S}_{2in}), \mu_M] \\ 1 & \text{for } \alpha D < \mu_2(\tilde{S}_{2in}) \end{cases} .$$

The distance $M$ between the 2 interior steady states can be computed straightforwardly from equations (7) and (8):

$$M(D) = 2\sqrt{1 + \frac{1}{\alpha^2 {k_3}^2}}\sqrt{\left(\frac{K_{I2}}{2}\left(\frac{\bar{\mu}_2}{\alpha\, D} - 1\right)\right)^2 - K_{I2}K_{S2}}$$

From this relation, we can see that the OT is a strictly decreasing function of the dilution rate and that it is independent from conditions $(S_{1in}, S_{2in})$. The COT is then:

$$M_c\left(\xi_{in}\right) = \sqrt{1 + \frac{1}{\alpha^2 {k_3}^2}}\left(\tilde{S}_{2in} - \frac{K_{I2}\, K_{S2}}{\tilde{S}_{2in}}\right)$$

### *4.4 Comparison between stability index and relative tolerance*

Using model parameters presented in (Bernard *et al.*, 2001), we have computed the stability index $\mathcal{I}_{\mathcal{S}}$ and the ROT associated with many working conditions (D, $S_{1in}$ and $S_{2in}$).

As it can be seen on Fig. 4 the ROT represents a good approximation of the stability index $\mathcal{I}_{\mathcal{S}}$ based on the real computation of the attraction basin size.

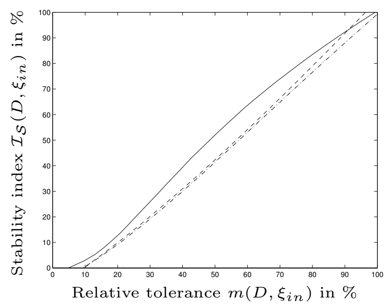


Fig. 4. Relation between $S_{BA^{\star}}$ and the ROT $m$ for various couples $(S_{1in}, \tilde{S}_{2in})$: (3,30), (0,25), (15,20), (30,30)

The relative tolerance appears then as a simple but relevant criterion to assess the stability of an anaerobic digester.

From this criterion we define now the **"risk index"** which is simply $r = 1 - m$, and which will on-line indicate to the operator the destabilisation risk he is taking.

In the next section we use this operational criterion to assess the management strategy of a real anaerobic digester.

## 5. APPLICATION TO THE ON-LINE DETERMINATION OF THE DESTABILISATION RISK

In this section we apply the proposed index to a real experiment performed at the LBE-INRA in Narbonne, France. The process is an up-flow anaerobic fixed bed reactor with a useful volume of 0.948 $m^3$. The reactor is highly instrumented and many variables were measured during the experiments (Bernard *et al.*, 2001). The experiments were performed with raw industrial wine distillery vinasses.

The risk index has been computed with parameters of (Bernard *et al.*, 2001). Nevertheless, in order to favour a prudent strategy, and in the framework of a "worst case analysis" the parameter $K_{I2}$ defining the inhibition level has been multiplied by a security constant $\delta$ (we have chosen $\delta = 0.7$).

The risk estimation is presented on Fig. 5 for an experiment conducted on the pilot scale fixed bed reactor at the LBE.

It is worth noting that the regimes associated with acid accumulation are all characterised by a very high risk. More surprising, some a priori less dangerous working mode are indeed also associated to a non zero risk. A very important point is that the risk index increases immediately while it takes time for the VFA to accumulate and even more time for the pH to decrease (not shown here).

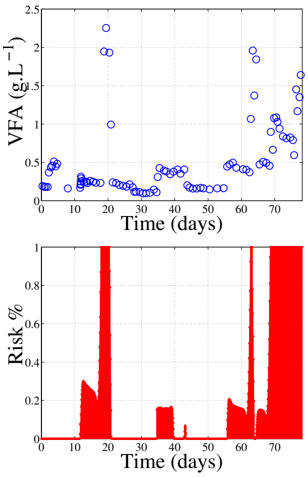


Fig. 5. Measured VFA and computed risk for an experiment performed at INRA LBE.

## 6. CONCLUSION

From the analysis of the nonlinear system describing the anaerobic process we have proposed a criterion that assesses the risk associated to an operating strategy. This index is highly correlated to the relative size of the normal working mode attraction basin.

The criterion turns out to be relevant to diagnose an operation strategy since it can predict very early a future accumulation of acids. It can thus be run as an indicator that helps an operator, or even diagnoses the strategy of an automatic controller which would not ensure global stability.

Next step would consist in estimating on-line the parameters in order to take into account the biological evolution of the system in the risk index computation.

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