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MODELLING and Parametric IDENTIFICATION of Wastewater Treatment Process

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***Abstract*—This paper deals with the modelling and the identification of parameters applied to biological process of wastewater treatment in a fixed bed within a poultry slaughterhouse. Firstly, the objective of modelling part is to develop a mathematical model of process describing his dynamical behaviour. Next, in identification part we try to synthesize an identification algorithm in order to apply in model. Finally, the validation is concerned with studying the model behaviour.**

***Keywords*—Biological wastewater treatment, Bioprocess, Fixed bed bioreactor, Modelling, Parametric identification.**

I. INTRODUCTION

The main objective of wastewater treatment is to reduce the amount of chemical pollution loaded in water in order to respect the natural water environment.

Indeed there are two types of wastewater treatment the physicochemical and the biological treatment. Compared to the physicochemical treatment the biological is an important and integral sector in the field of wastewater especially considering the economic investment and operating costs [1], [2], [3].

The evolution of research in this domain has been based on the increase of continuous analysis in microbial behaviour and the developing techniques in the basic process [4], [5]. The biological treatment is very important for the conservation of water sources [6].

Despite these advantages and their importance, the bioprocess includes practical problems precisely the prediction and control of the process together with its complexity and nonlinear nature and lock of sensors in biological purification [7], [3], [8]. A dynamic model of wastewater treatment process in fixed bed may be used for prediction of the process through decomposition of process elements that leads the development of the system of monitoring and control to improve the performance and guarantee the stability of wastewater treatment operation [9], [10].

The slaughterhouse heavily produces wastewater loaded with soluble and insoluble organic matter. The quality of wastewater depends on the type of slaughtered animals and the meat transformation including amount of blood capture and water consumption [11], [12], [13].

II. MODELLING

In the first part of this manuscript we are interested in modelling a biological treatment process of wastewater fixed bed. To determine the set of state equations which describes the dynamics of the overall system (biomass, substrate, product volume) within the bioreactor we use the material balance such as [14], [15]:

$$\begin{Bmatrix} Quantity \\ variation \\ in\ the \\ reactor \end{Bmatrix} = \begin{Bmatrix} Brought \\ quantity \end{Bmatrix} - \begin{Bmatrix} Withdrawn \\ quantity \end{Bmatrix} + \begin{Bmatrix} Produced \\ quantity \end{Bmatrix} - \begin{Bmatrix} Consumed \\ quantity \end{Bmatrix}$$

The equations of each components of biological reactions (Biomass, Substrates, Products) is derived from the material balance. The growth of biomass population in an amount of substrate is described by three nonlinear derivatives equations.

$$\begin{cases} \dfrac{d(VX)}{dt} = v_X - Q_{out}X \\ \dfrac{d(VS)}{dt} = -v_S V + Q_{in}(S_{in} - \dfrac{Q_{out}}{Q_{in}}S) \\ \dfrac{dV}{dt} = Q_{in} - Q_{out} \end{cases} \quad (1)$$

The relationship between v_S and v_X is as follows:

$$v_S = Y_{XS}\, v_X \quad (2)$$

The reactor type is continuous, its works at a perfectly homogeneous and constant volume. This model of bioreactor describes the microbiological reaction between the biomass X and two substrates (S_1, S_2) defined by a system of three equations:

$$\begin{cases} \dfrac{dX}{dt} = v_X - DX \\ \dfrac{dS_1}{dt} = -Y_1 v_X + D(S_{1in} - S_1) \\ \dfrac{dS_2}{dt} = -Y_2 v_X + D(S_{2in} - S_2) \end{cases} \quad (3)$$

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This model contains three state equations, the first describes the evolution of biomass, and the other two equations describe the evolution of the substrates S_1 and S_2.

It is necessary to find a relationship between the variables of the system (X, S_1, S_2) and the biomass growth speed v_x to improve the simulation model of the real dynamic for this process and is describe the evolution for the states variables. The second step of modelling is devoted to determining the form adopted for growth speed v_X.

The overall model of the biological process must meet the physical criteria such as positivity of the variables well as the biological properties such as the relationship between reactant and reaction.

The matrix representing of the equations is as follows:

$$\dot{\xi} = K v_x + D(\xi_{in} - \xi) \tag{4}$$

with $\xi = \begin{pmatrix} X \\ S_1 \\ S_2 \end{pmatrix}$; $K = \begin{pmatrix} 1 \\ -Y_1 \\ -Y_2 \end{pmatrix}$; $\xi_{in} = \begin{pmatrix} 0 \\ S_{1in} \\ S_{2in} \end{pmatrix}$; $D = \frac{Q}{V}$

The application of mathematical constraints on the model shows the structure of the speed growth of biomass [16] [17].

$$v_X = S_1 S_2 \, X \, f(.) \tag{5}$$

The unknown function $f(.)$ is defined by the classic functions that represent the biological kinetic such as the classical function of Monod and the classical function of Haldane [16].

- The classical function of MONOD:

$$\mu(S) = \mu_{max} \frac{S}{K_S + S} \tag{6}$$

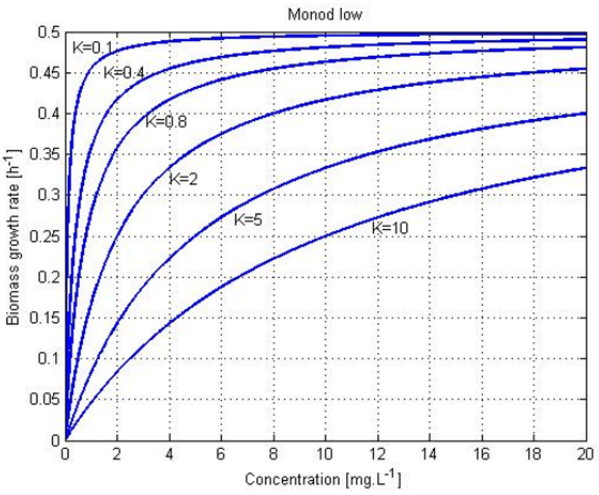

Fig.1 The Monod function for different values of K_S

- The classical function of HALDANE:

$$\mu(S) = \mu_{max} \frac{S}{K_S + S + \frac{S^2}{K_I}} \tag{7}$$

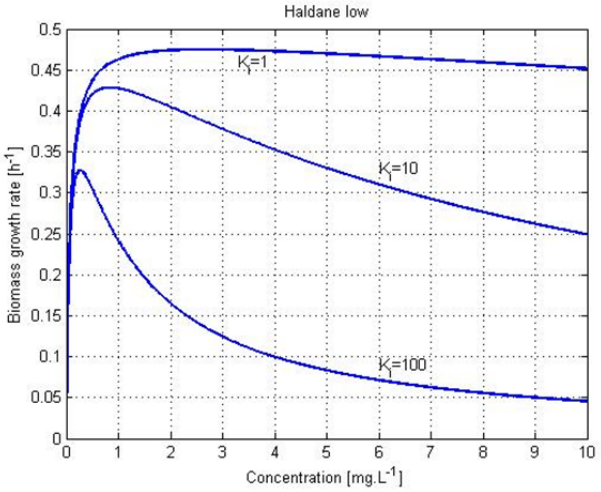

Fig.2 The Haldane function for different values of $\mathbf{K_I}$

The only difference between the two expressions is the term $\frac{S^2}{K_I}$, if we assume that the inhibition constant K_I $[g/L]$ is very large of the substrate concentration S then the Haldane function is equivalent to the Monod function.

We choose the classic function of MONOD to describe the kinetic system.

$$\mu(S_1, S_2) = \mu_{max} \frac{S_1}{Ks_1 + S_1} \frac{S_2}{Ks_2 + S_2} \tag{8}$$

Then the final model to identify is:

$$\begin{cases} \dfrac{dX}{dt} = \left(\mu_{max} \dfrac{S_1}{K_{S_1} + S_1} \dfrac{S_2}{K_{S_2} + S_2} - D \right) X \\ \dfrac{dS_1}{dt} = -Y_1 \mu_{max} \dfrac{S_1}{K_{S_1} + S_1} \dfrac{S_2}{K_{S_2} + S_2} \, X + D(S_{1in} - S_1) \\ \dfrac{dS_2}{dt} = -Y_2 \mu_{max} \dfrac{S_1}{K_{S_1} + S_1} \dfrac{S_2}{K_{S_2} + S_2} \, X + D(S_{2in} - S_2) \end{cases} \tag{9}$$

TABLEI
MODEL'S PARAMETERS

Notation	Signification	Unit
X	Biomass concentration	$g_X.L^{-1}$
S_1, S_2	Substrate concentration	$g_S.L^{-1}$
S_{in}	Substrate concentration in the feed solution	$g_S.L^{-1}$
V	Reactor volume	L
Q_{in}, Q_{out}	Supply flow rate in substrate / Output flow rate	$L.h^{-1}$
D	Dilution rate	h^{-1}
v_X	Biomass growth speed	$g_X.L^{-1}.h^{-1}$
v_S	Speed of substrate consumption	$g_S.L^{-1}.h^{-1}$
Y_{XS}, Y_1, Y_2	Conversion rate of substrate / biomass	$g_X.g_S^{-1}$
μ	Biomass growth rate	h^{-1}
μ_{max}	Maximum biomass growth rate	h^{-1}
K_{S1}, K_{S2}	Half-saturation coefficients in bio-degradable substrate	$g_S.L^{-1}$
K_I	Inhibition constant of HALDANE	$g_S.L^{-1}$
ξ	State vector of system	---
ξ_{in}	Input masse in the bioreactor	---
K	Matrix of pseudo-stoichiometric items	---

III. IDENTIFICATION

A. Structure Identification

The complexity of the dynamic model of bioprocess used is a reflection of the complexity of the process itself. Consequently, it contains a large number of parameters that must be identified.

So it is necessary to determine a simplified identification structure containing a minimum number of parameters and therefore a faster convergence speed.

$$\begin{cases} \mu(S_1,S_2)X = \dot{X} + DX \\ \dot{\Gamma} + D(\Gamma - \Gamma_{in}) = 0 \\ \Gamma(t=0) = \Gamma_{in} \end{cases} \quad (10)$$

with $\Gamma = \varphi + KX$; $\Gamma_{in} = \varphi_{in}$

and $\varphi = \begin{pmatrix} S_1 \\ S_2 \end{pmatrix}$; $K = \begin{pmatrix} Y_1 \\ Y_2 \end{pmatrix}$; $\varphi_{in} = \begin{pmatrix} S_{1in} \\ S_{2in} \end{pmatrix}$

A resolution of the system shows the existence of relationship between a biomass X and substrates (S_1, S_2).

$$\begin{cases} S_1 = S_{1in} - Y_1 X \\ S_2 = S_{2in} - Y_2 X \end{cases} \quad (11)$$

Replacing the two relations in the $\mu(S_1,S_2)$ expression:

$$\mu(S_1,S_2) = \frac{\mu_{max}\left(\frac{S_{1in}}{Y_1} - X\right)\left(\frac{S_{2in}}{Y_2} - X\right)}{\left(\frac{Ks_1+S_{1in}}{Y_1} - X\right)\left(\frac{Ks_2+S_{2in}}{Y_2} - X\right)} \quad (12)$$

The study of dimension of models also serves to reduce the number of input/output vectors in the identification algorithm in order to reduce the computation time.

$$\dot{X} = \left(\frac{\mu_{max}\left(\frac{S_{1in}}{Y_1} - X\right)\left(\frac{S_{2in}}{Y_2} - X\right)}{\left(\frac{Ks_1+S_{1in}}{Y_1} - X\right)\left(\frac{Ks_2+S_{2in}}{Y_2} - X\right)} - D \right) X \quad (13)$$

A formalization of the model equations leads us to write the expression of the identification process as follows:

$$\frac{X(k+1) - X(k)}{T\,X(k)} = \frac{\theta_1(\theta_2 - X(k))(\theta_3 - X(k))}{(\theta_4 - X(k))(\theta_5 - X(k))} - D \quad (14)$$

with $\theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \theta_3 \\ \theta_4 \\ \theta_5 \end{pmatrix}$; $\begin{cases} \theta_1 = \mu_{max} \\ \theta_2 = \frac{S_{1in}}{Y_1} \\ \theta_3 = \frac{S_{2in}}{Y_2} \\ \theta_4 = \frac{K_{S_1}+S_{1in}}{Y_1} \\ \theta_5 = \frac{K_{S_2}+S_{2in}}{Y_2} \end{cases}$

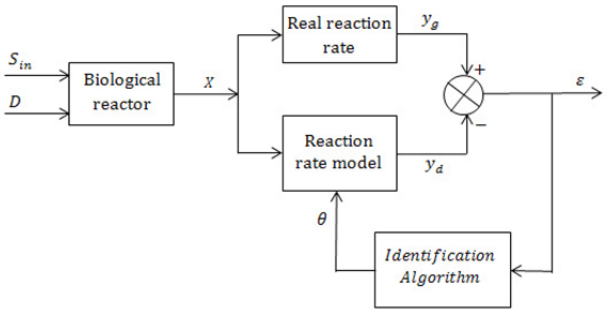

Fig.3 Structure of identification model

Note that the number of input/output vectors is reduced from three vectors (X, S_1, S_2) into a single vector X.

B. Algorithm Of Identification

We used an identification algorithm based on the optimization method of Levenberg-Marquardt.

The algorithm tries to minimize the function:

$$f(X,\theta) = \frac{\theta_1(\theta_2 - X(k))(\theta_3 - X(k))}{(\theta_4 - X(k))(\theta_5 - X(k))} - D \quad (15)$$

The algorithm is based on the iterative expression such as:

$$\theta_k = \theta_{k-1} + Z_{k-1}\left(y_g(X) - y_d(X,\theta_{k-1})\right) \quad (16)$$

with $Z_{k-1} = \left(\left(J_{k-1}^T.J_{k-1} + \lambda diag(J_{k-1}^T J_{k-1})\right)J_{k-1}^T\right)^{-1}$

and J_{k-1} is the Jacobian matrix of y_d at point θ_{k-1}, such that:

$$J_{k-1} = \frac{\partial y_d}{\partial \theta_k}(\theta_{k-1})$$

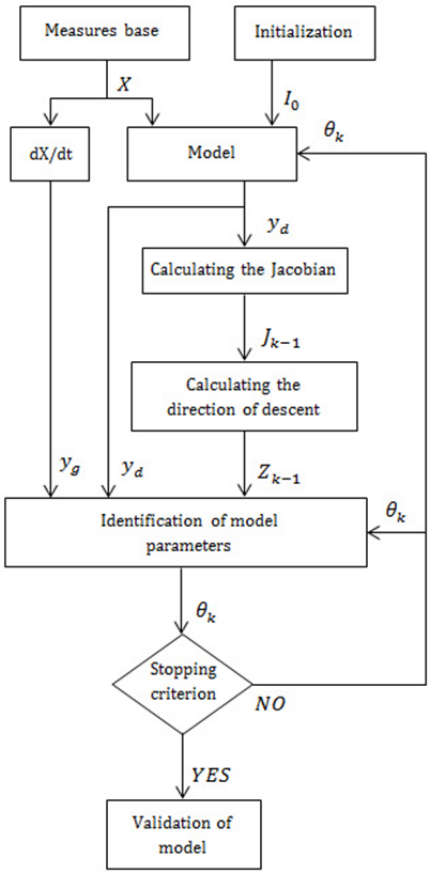

Fig.4 Organization chart of the identification algorithm

The criterion used in our algorithm is the least squares criterion:

$$E^j(\theta) = \frac{1}{N}\sum_{k=1}^{N}\left(y_{g,j}\big(X(k)\big) - y_{d,j}(X(k),\theta)\right)^2 \qquad (17)$$

TABLE II
PARAMETERS USED IN IDENTIFICATION

Notation	Signification	Unit
θ	Vectorof the parameters	---
I_0	Vector of initial parameters	---
ϵ	Identification error	h^{-1}
MES	Suspended matter	$m_g.L^{-1}$
y_g, y_d	The desired output / The model output	---
μ_R	Real reaction rate: $\mu_R = \frac{X(k+1)-X(k)}{TX(k)}$	h^{-1}
μ_I	Identified reaction rate: $\mu_I = \frac{\theta_1(\theta_2 - X(k))(\theta_3 - X(k))}{(\theta_4 - X(k))(\theta_5 - X(k))} - D$	h^{-1}
J_{k-1}	Jacobian matrix of y_d at point θ_{k-1}	---
λ	Learning step	---

IV. EXPERIMENTAL VALIDATION

The validation of the model depends on the database of the measures in the input of the identification algorithm.

In most biological systems the build of measures database is difficult and take a lot of time. Indeed, the set of points in reactor outlet is obtained by the model of indirect measures. Such as, the values of the biomass X are obtained by measurement of MES (suspended matter) of sample levied at the outlet of the station of the slaughterhouse.

We will have to analyze all measures of MES in order to determine the relationship between the biomass X and MES.

$$X = 0.82\, MES \qquad (18)$$

The figure below shows the responses of the real reaction rates μ_R compared to the model reaction rates for a vector of biomass measured at the outlet of station of slaughterhouse poultry.

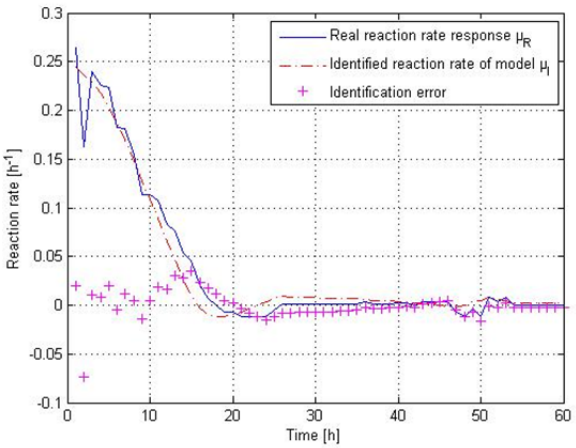

Fig.5 Validation of reaction rate μ_I

The real reaction rate decreases to reach zero, this means that the biomass evolution tends toward a constant limit during time. Indeed:

$$\frac{X(k+1)-X(k)}{TX(k)} = 0 \qquad (19)$$
$$\Longrightarrow X(k+1) = X(k) = X_l \;;\; \forall\, k \geq k_l$$

In figure (Fig.5), one notices that the dynamics as far as the amplitudes of variation is maintained even during the periods when the variation is important due to the stability of identification algorithm which keeps a convergence toward the right direction.

The function of Monod tends toward the dilution rate during the system evolution.

$$\frac{\theta_1(\theta_2 - X(k))(\theta_3 - X(k))}{(\theta_4 - X(k))(\theta_5 - X(k))} = D \;;\; \forall\, k \geq k_l \qquad (20)$$

The length of the evolution of biomass goes through a last phase of adapting to new environment in the bioreactor.

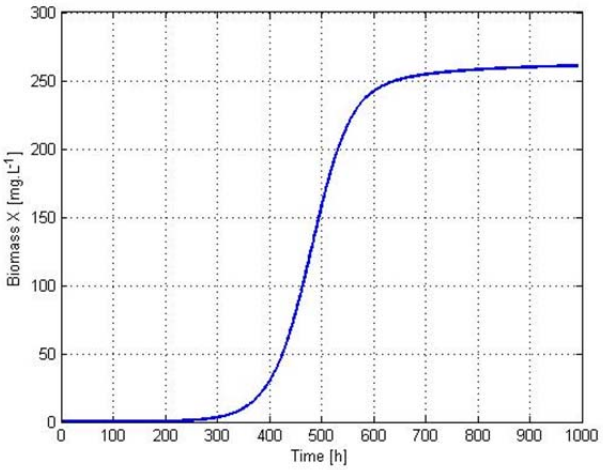

Fig.6 Biomass growth

The evolution follows an exponential growth, in which growth rate is maximum before it is null when the biomass reaches the stationary phase.

During simulation the system dynamics (Biomass, Substrates) is practically the same. The system keeps the convergence to equilibrium point.

In (Fig.7), during its growth, the biomass feeds on the substrate readily biodegradable at the same time it reacts for degrading the substrate hardly biodegradable. The reaction unfolds for 25 days in order that the system attains its equilibrium state.

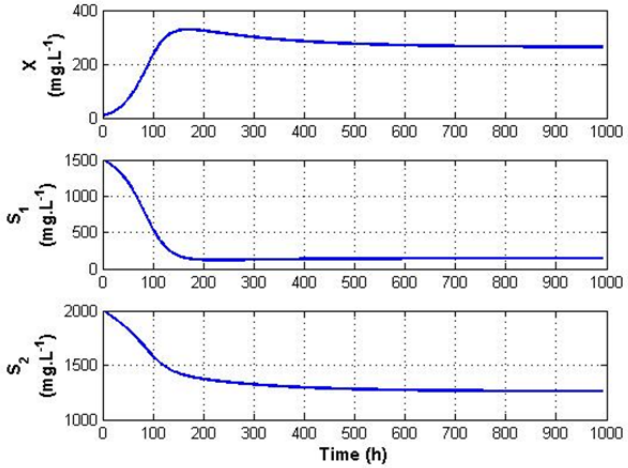

Fig.7 Identified model response

Only, the system response time varies depending on the initial concentration. A summary table shows the variation of response time compared to the initial concentration of biomass.

TABLE III
VARIATION OF THE RESPONSE TIME OF BIOPROCESS

$\mathbf{X_0}$ $(\mathbf{mg_X L^{-1}})$	System response time	
	τ (h)	**τ (j)**
0.1	600	25
10	400	17
100	300	13
200	300	13
400	400	17
500	500	25

There may be mentioned a relationship between $|X_0 - X_e|$ and the response time τ.

$$\tau = f(|X_0 - X_e|) \tag{21}$$

with X_0 the starting concentration and X_e the equilibrium concentration.

V. CONCLUSIONS

Most of biological processes such as the method of wastewater treatment, fixed bed is a subject to many natural change and structural complexity may be due to the architecture of living organisms.

As a result, the modeling of such system is been made through many steps such as structural decomposition into simple elements and dimensions of the model that seeks to reduce the number of equation and parameters.

The objective is to develop an algorithm identification based on an optimization criterion whose purpose into validate the model.

The modeling allows us to know the dynamics and evolution of the bioprocess. But in reality, the main purpose of the modeling is a bioprocess control and its study can be one of the plausible perspectives.

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