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Modelling and Neural Networks of Bioreactors in Wastewater Treatment Process

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Abstract. *The objective of this paper relates to modeling, the estimate of the parameters and the control of a biological process used for waste water treatment. The mathematical models of such process are presented in the form of Distributed parameter system. The numerical resolution of such a system requires the use of the approximation methods. Once the established model, the concepts which are approached in this thesis relates to the modeling of the process considered, the study of identifiability of the model, the estimate and the control by neural network.*

1. Introduction

In the first world report on the "development of the water resources" appeared at the beginning of 2003, UNESCO warns Humanity against the immediate and long-term consequences of the water crisis which touches planet.

We based on the research of M[r.] Docain; the objective of this study relates to the study of dynamic modeling, the analysis and the control of biotechnological processes (fixed bed). This type of engines is used more in practice industrial. The fundamental problem, which appears in the control of such process, is the lack of sensors on line, which are always the weak point of control in real time of the purification processes. In order to better control the operation of the process, it is thus necessary to work out a model of simulation usable in real time in order to predict the evolution of the various concentrations.

Denitrification relates in reducing the reduction of the nitrates NO_3^- in gas nitrogen N_2 with formation of an intermediate compound, the nitrites NO_2^- [1].

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$$NO_3^- \xrightarrow{(1)} NO_2^- \xrightarrow{(2)} N_2 \quad (1)$$

It can be broken up into denitratation (reduction of nitrates) and denitritation (reduction of nitrogen gas nitrites).

Denitrification is an anaerobic reaction (reaction which with place in a medium deprived of oxygen) catalyzed by micro-organisms (of the bacteria whose source of energy is organic carbon).

Our work will be organized in four parts:

1- Modeling of the biotechnological process (biofiltre).

2- Analysis and Identification of the kinetic parameters and other parameters...

3- Estimating and controlling of the biotechnological process.

4- Results of simulations.

2. Modelisation

The process of denitrification which is the subject of our study is an engine length L with fixed granular bed, of ascending type for the liquid. In this type of engine, the micro-organisms are fixed on balls of garnishing, whereas the substrates can circulate freely.

The assessments matters lead to a system described by four partial derivative equations, non-linear, nonstationary, and of hyperbolic type.

$$\begin{cases} \dfrac{\partial s_1(z,t)}{\partial t} = -\dfrac{F}{A\varepsilon}\dfrac{\partial s_1(z,t)}{\partial z} - \dfrac{1}{\alpha_1 \varepsilon}(k_1 - 1)\mu_1(s_1,s_3)\, x(z,t) \\ \dfrac{\partial s_2(z,t)}{\partial t} = -\dfrac{F}{A\varepsilon}\dfrac{\partial s_2(z,t)}{\partial z} + \dfrac{1}{\varepsilon}\left[\dfrac{(k_1-1)}{\alpha_1}\mu_1(s_1,s_3) - \dfrac{(k_2-1)}{\alpha_2}\mu_2(s_2,s_3)\right] x(z,t) \\ \dfrac{\partial s_3(z,t)}{\partial t} = -\dfrac{F}{A\varepsilon}\dfrac{\partial s_3(z,t)}{\partial z} - \dfrac{1}{\varepsilon}\left[k1\,\mu_1(s_1,s_3) + k_2\mu_2(s_2,s_3)\right] x(z,t) \\ \dfrac{\partial x(z,t)}{\partial t} = \left[\mu_1(s_1,s_3) + \mu_2(s_2,s_3) - k_d\right] x(z,t) \end{cases} \quad (2)$$

with $k_{di} = (\mu_{1i} + \mu_{2i})\dfrac{x_i(t)}{x_{\max}}$

for $0 < z \leq 1$

with boundary conditions following:

- $s_l(z = 0, t) = s_{l,in}(t)$ for $l = 1,3$
- $s_2(z = 0, t) = 0$, $x(z = 0, t) = 0$

and following initial conditions:

- $s_l(z, t = 0) = s_{l,0}(z)$ for $l = 1,2,3$
- $x(z, t = 0) = x_0(z)$

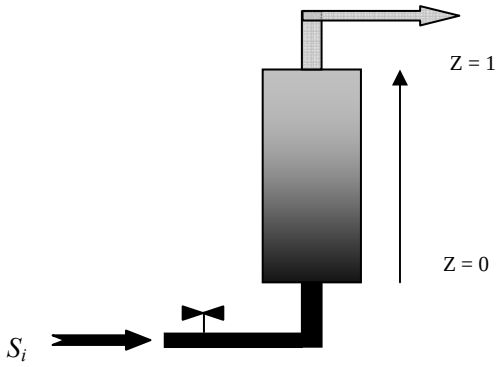

Fig.1.. Diagram of fixed bed reactor

In the equation the preceding ones, z, $s_1(z,t)$, $s_2(z,t)$, $s_3(z,t)$, $x(z,t)$, $s_{1,in}(t)$, $s_{3,in}(t)$ Represent the variable of space(*m)*, the concentrations respectively of nitrate, nitrite, carbon, biomass (g/m^3), the carbon and nitrate concentration at the entry of the reactor(g/m^3); F A k_{iI} k_D and ε rate of feed at the entry of the engine (m^3/*h)*, the section of the biofiltre (m^2) yield coefficients, porosity, μ_i specific rates of growth on nitrate and the nitrite (*g/*m^3*/h)* .

The expression of the specific rate of growth (the model of Monod) is as follows:

$$\mu_i = \eta_g \cdot \mu_{i\max} \cdot \left(\frac{s_i}{s_i + k_{mi}}\right) \cdot \left(\frac{s_3}{s_3 + k_{m3}}\right) \qquad (3)$$

for i = 1, 2

where η_g is the factor of correction for the growth in anaerobic mode; μ_{imax} are the maximum specific rates of growth of the biomass; $k_{m1,}$ $k_{m2,}$ $k_{m3,}$ are the constants of Michaelis-Menten associated respectively with nitrate, nitrite and carbon.

2.1. Transformation of the model with distributed parameters into model with localized parameters

The model is described by partial derivative equations; the variables of state S and X of the system depend not only on time t but also on space z It is a system with distributed parameters.

There are some methods [2] intended to reduce the systems to distributed parameters to transform them into *systems with localised parameters* described rather by ordinary differential equations.

The methods of the balanced residues are largely used in the physique fields, chemical; among, they it method of orthogonal collocation [3].

2.2. Orthogonal collocation method

The orthogonal collocation method makes it possible to build a system of ordinary differential equations corresponding to an approximated model of the process in various points of collocation. The implementation of the method requires the choice of a number N of points of collocation, their position z_i along the engine and the functions of bases making it possible to rebuild the solution approximated to the points of interpolation [4].

It is a question of finding starting from the choice of basic functions $l_i(z)$ an approximate solution $X(z_i\, t)$ in the form:

$$x(t, z) = \sum_{i=0}^{N+1} l_i(z).x_i(t) \qquad (4)$$

with:

N: numbers points of collocation,

$x_i(t) = x(z_i,t)$: value of vector X at the point of collocation z_i This solution not checking exactly the equation (2), one defines a residue $R(x(z,t))$, the problem consists in minimizing $R(x(z,t))$, which is translated in the shape of the scalar product:

$< R(x(z,t)),w_i > = 0 \qquad i = 0,1,2,\ldots N+1$. One will find in [4], [5] a study detailed on these problems.

An approximate solution of the system (2) by the collocation method by taking the polynomial of Lagrange interpolation like basic function, and the zeros of the polynomial of Jacobi like points of collocation and interpolation [6]. If the points of collocation are confused with the points of interpolation, the method is known as of orthogonal collocation.

In [7] one will find that the position of the points of collocations z_j, $j = 1, \ldots, N$ is obtained by checking relations of orthogonality, according to the number N of points of collocation and two parameters α and β.

2.3 Reduction of the denitrification model

With the application of the orthogonal collocation method, the simplified system becomes (Model non-linéare of finished size)

$$\begin{cases} \dfrac{ds_{1i}(t)}{dt} = -\dfrac{F}{A\varepsilon}\left(\sum_{j=1}^{N+1}\dfrac{dl_j(z_i)}{dz}s_{1j}(t) + \dfrac{dl_0(z_i)}{dz}s_{1,in}(t)\right) - \dfrac{(k_1-1)}{\alpha_1\varepsilon}\mu_{1i}\,x_i(t) \\ \dfrac{ds_{2i}(t)}{dt} = -\dfrac{F}{A\varepsilon}\sum_{j=1}^{N+1}\dfrac{dl_j(z_i)}{dz}s_{2j}(t) + \dfrac{1}{\varepsilon}\left[\dfrac{(k_1-1)}{\alpha_1}\mu_{1i} - \dfrac{(k_2-1)}{\alpha_2}\mu_{2i}\right]x_i(t) \\ \dfrac{ds_{3i}(t)}{dt} = -\dfrac{F}{A\varepsilon}\left(\sum_{j=1}^{N+1}\dfrac{dl_j(z_i)}{dz}s_{3j}(t) + \dfrac{dl_0(z_i)}{dz}s_{3,in}(t)\right) - \dfrac{1}{\varepsilon} * [\,k_1\mu_{1i} + k_2\mu_{2i}]\,x_i(t) \\ \dfrac{dx_i(t)}{dt} = [\mu_{1i} + \mu_{2i} - k_{di}]\,x_i(t) \end{cases} \qquad (5)$$

$$\text{with} \quad k_{di} = (\mu_{1i} + \mu_{2i}) \frac{x_i(t)}{x_{\max}}$$

With the following initial conditions:

$s_l(z,0) = s_{l0}$ pour $l = 1, 2, 3$

$x_l(z,0) = x_0$

and :

$$\mu_{1i} = \eta_g . \mu_{1\max} . \left(\frac{s_{1i}}{s_{1i} + k_{m1}} \right) . \left(\frac{s_{3i}}{s_{3i} + k_{m3}} \right)$$

$$\mu_{2i} = \eta_g . \mu_{2\max} . \left(\frac{s_{2i}}{s_{2i} + k_{m2}} \right) . \left(\frac{s_{3i}}{s_{3i} + k_{m3}} \right)$$

Determination of the optimal triplet The criterion chosen to determine N, α and β is a compromise between a good transitory behavior and a good precision of the permanent mode of the solutions. Following several simulations, [5] obtained better results of simulation, with the optimal triplet $N = 4; \alpha = 1; \beta = 1$,

3 Control of the denitrification process

The problem installation is to control with a wished value, the sum of the concentrations of nitrate and of nitrite expressed in equivalent nitrogenizes at exit of the engine.

For that, one defines the variable of exit $y(z,t)$ such as [8]:

$$y_L = y(z = z_L, t) = c_1 s_{1L} + c_2 s_{2L} \tag{6}$$

(c_1=0.226 and c_2=0.304) are the coefficients of conversion into equivalent nitrogenizes nitrite and nitrate concentrations respectively.

the dynamic equation of the variable of state has to control:

$$\frac{dy_L}{dt} = -\frac{u}{\varepsilon} \frac{\partial y(z,t)}{\partial z}_{|z=z_L} + (c_2 - c_1) \frac{k_1 - 1}{\alpha_1 \varepsilon} \mu_{1L} x_{aL} - c_2 \frac{k_2 - 1}{\alpha_2 \varepsilon} \mu_{2L} x_{aL} \tag{7}$$

3.1 The variable of control is *u(t)*

The variable of order can be the rate of flow of the fluid has through the engine *"u(t)",* [5], [9],

The principle of the law of order is to associate the problem of regulation of the variable y_L a dynamics of the loop system closed represented by the following first order linear

$$\frac{dy_L}{dt} = \lambda (y_d - y_l) \text{ with } \lambda > 0 \tag{8}$$

y_d being the desired value of y_L.

By combination of the equation (7) with the equation (8), it comes:

$$u(t) = \frac{-\lambda(y_d - y_l) + (c_2 - c_1)\frac{k_1 - 1}{\alpha_1 \varepsilon}\hat{\mu}_{1L}\hat{x}_{aL} - c_2\frac{k_2 - 1}{\alpha_2 \varepsilon}\hat{\mu}_{2L}\hat{x}_{aL}}{\Psi} \quad \text{with}$$

$$\Psi = \frac{1}{\varepsilon}\frac{\partial y(z,t)}{\partial z}_{|z=z_L} \tag{9}$$

3.2 Estimate of the biomass concentration

That ξ_1 is to say the vector of the measurable state variables: $\xi_1 = \begin{bmatrix} s_1(z,t) \\ s_2(z,t) \end{bmatrix}$

And ξ_2 the vector of the no measurable state variables: $\xi_2 = x_a(z,t)$

Moreover,

$$K_{\xi_1} = \frac{1}{\varepsilon}\begin{bmatrix} \frac{1}{\alpha_1}(k_1 - 1) & 0 \\ -\frac{1}{\alpha_1}(k_1 - 1) & \frac{1}{\alpha_2}(k_2 - 1) \end{bmatrix} \text{ and } K_{\xi_2} = \begin{bmatrix} 1 & 1 \end{bmatrix}$$

There is a transformation of state:

$$\xi = A_0\xi_1 + \xi_2 \quad \textit{that} \quad A_0 K_{\xi_1} + K_{\xi_2} = 0 \text{ si}$$

$$\det\left(K_{\xi_1}\right) \neq 0 \; A_0 = \begin{bmatrix} a_1 & a_1 \end{bmatrix} = \begin{bmatrix} \varepsilon\frac{\alpha_1(k_2 - 1) + \alpha_2}{k_2 - 2} & \varepsilon\frac{\alpha_2(k_1 - 1)}{(k_1 - 1)(k_2 - 2)} \end{bmatrix}$$

This transformation leads to a dynamic equation of observation of ξ, independent of x_a:

$$\frac{\partial \xi(z,t)}{\partial t} = -k_d\xi(z,t) + a_1 s_1(z,t) + a_2 s_2(z,t) - \frac{u}{\varepsilon}\left(a_1\frac{\partial s_1(z,t)}{\partial z} + a_2\frac{\partial s_2(z,t)}{\partial z}\right) \tag{10}$$

$$\hat{x}_a(z_i,t) = \xi(z_i,t) - a_1 s_1(z_i,t) - a_2 s_2(z_i,t) \tag{11}$$

3.3 Estimate of the kinetics of growth

For our model $c_1 = c_2 = 1$ since the nitrite and nitrate concentrations are expressed in equivalent nitrogenizes.

Then the control law is written:

$$u(t) = \frac{-\lambda(y_d - y_l) - \frac{k_2 - 1}{\alpha_2 \varepsilon}\hat{\mu}_{2L}\hat{x}_{aL}}{\Psi} \tag{12}$$

In this case, we will carry out only the estimate of the specific rate of growth relating to the reaction of denitrification. For that, one writes $\mu_2 L$ in the following form:

$$\mu_{2L} = \beta_{2L} s_{2L} \tag{13}$$

β_{2L} is a presumedly unknown parameter and which is estimated by the algorithm of recursive least squares at factor of following lapse of memory:

$$\hat{\beta}_{2L_{t+1}} = \hat{\beta}_{2L_t} - \gamma_t \frac{k_2 - 1}{\alpha_2 \varepsilon} s_{2L_t} \hat{x}_{aL_t} \Delta t (y_{L_{t+1}} - y_{L_t\, 2,in}))$$

$$+ \frac{u_t}{\varepsilon} \Delta t (\Delta s_{1L_t} + \Delta s_{2L_t} + b_{0N+1}(s_{1,in} + s_{2,in})) + \frac{k_2 - 1}{\alpha_2 \varepsilon} \Delta t s_{2L_t} \hat{\beta}_{2L_t} \hat{x}_{aL_t} \quad (14)$$

$$\gamma_t = \frac{\gamma_{t-1}}{\sigma + \gamma_{t-1}^2 \Delta t^2 (\frac{k_2 - 1}{\alpha_2 \varepsilon})^2 s_{2L_t}^2 \hat{x}_{aL_t}^2} \quad 0 \le \sigma \le 1 \quad (15)$$

3.4 Neuronal control model

The purpose of the neural networks hereafter is to provide at every moment the control increment $\Delta u(t) = u(t) - u(t-1)$. The future variations of the output $\Delta y(t+1)$ will make it possible to carry out a one step ahead prediction. [10], [11]**.**

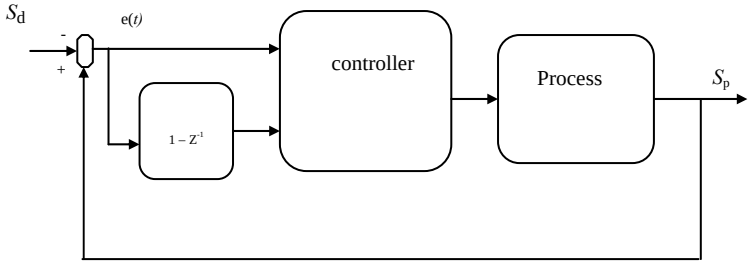

Fig.2. Functional scheme of the control strategy

The training of the network consists in modifying, with each step of training, the weights and skews in order to minimize the sum of the squares of the errors at exit. The method of retropropagation is based on the technique of the gradient. The weights and skews are initialized with random values. Of uniform distribution -0.5 and 0.5, the profit of adaptation is selected equal to 0.8. We chose 7 cells in the layer of entry 6 cells in the hidden layer and a cell in the layer of exit fig 3. [10], [12].

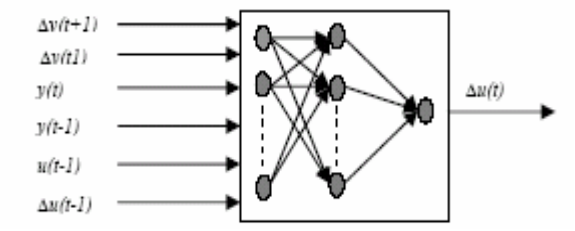

Fig.3. The neural network controller

4 Results of digital simulations

Simulations are carried out for the initial conditions following: $\forall\, i = 1,\ldots,\ N + 1$

- $s_1(z_i,\ t = 0)$ = 16.93 $g[N]/m^3$
- $s_2(z_i,\ t = 0)$ = 0 $g[N]/m^3$
- $s_3(z_i,\ t = 0)$ = 101.5 $g[N]/m^3$
- $x_a(z_i,\ t = 0)$ = 625 $g[N]/m^3$

The rate of flow of the fluid is equal to:

$u = 9\ m/h$
$Y_{h1} = 0.51$, $Y_{h2} = 0.42$, $\mu_{1max} = 0.35\ h^{-1}$,
$\mu_{2max} = 0.27\ h^{-1}$.
$K_1 = 1.5\ g[N]/m^3$, $K_2 = 1\ g[N]/m^3$,
$K_3 = 40\ g[N]/m^3$.
$\eta_g = 0.8$, $\varepsilon = 0.52$, $x_{amax} = 675\ g[DCO]/m^3$, $\lambda = 4$, $\sigma = 0.98$, $\gamma_0 = 10$.

Figure 5- showed that the exit of the process (concentration in substrate of the effluent) reached the set point at the end of a few days at the price of a light oscillation in the transitional stage. As we considered in the calibration, it is noticed that the exit of the cascade converges nevertheless towards the instruction. This proves that the action of integration of the error at the entry of the regulator is actually carried out thanks to the estimator of $\hat{\mu}_2$ intended to gauge the outputs of the cascade.

The estimated values of the concentration in biomass $\hat{x}_a$ using the asymptotic observer converges quickly towards the effective concentrations in the effluent as show it the figure 6. The results of simulation are satisfactory; they show that the regulator functions well and present of good performances from the point of view of the regulation.

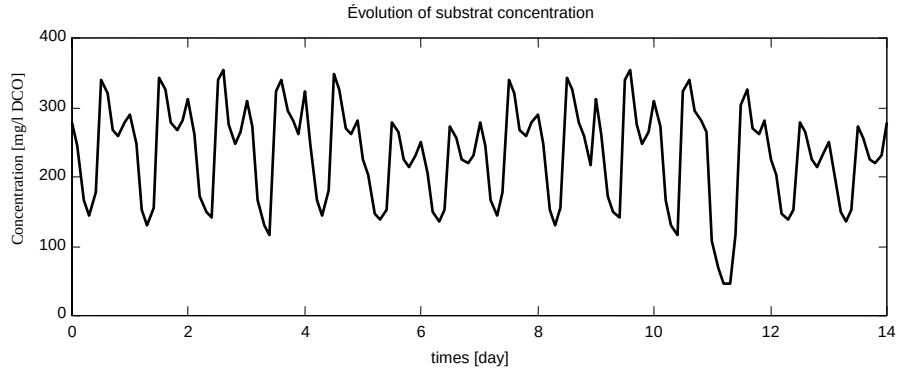

Fig.4. Evolution of the substrate at the entry

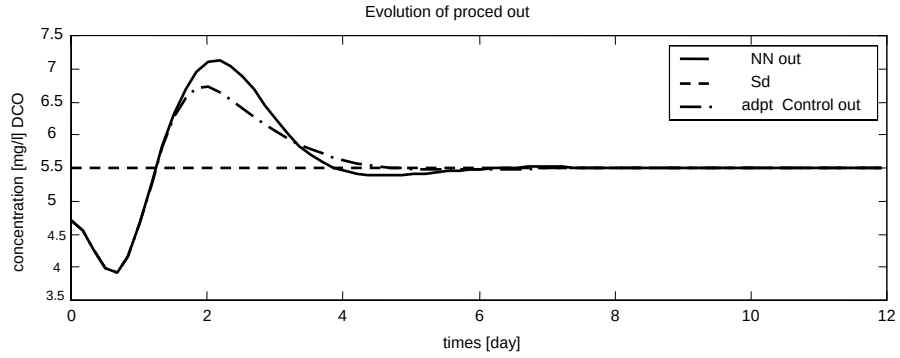

Fig.5. Evolution of the exit

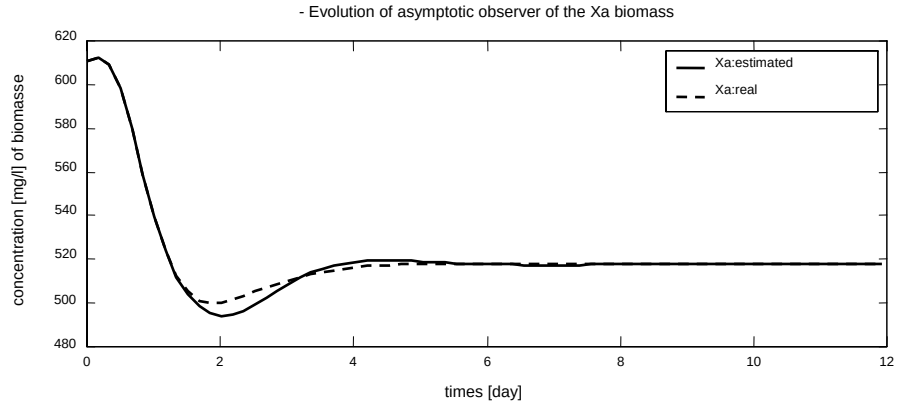

Fig.6. Evolution of estimated biomass

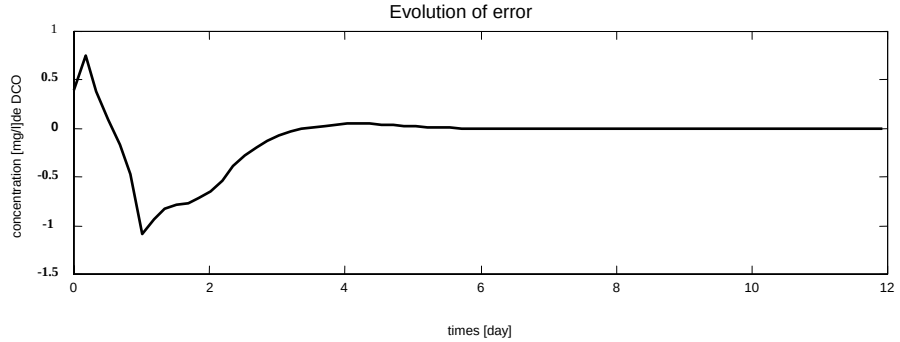

Fig.7. Evolution of error

5 Conclusion

In this work the matter flow and transformation in the collector of sewer were modeled by an engine piston in which the substrate is degraded by the micro-organisms which multiply. One, obtains in any rigour, a system with distributed parameters hyperbolic governs by a system of differential equations to the derivative partial. These stages of modeling, analysis and identification were of primary importance for the development of algorithms of estimate. The objective of our study being to regulate the sum of the concentrations of the substrate to a standard fixes at exit of the biofiltre while acting on the rate of flow of the fluid. As the kinetic term of the process is related to the variation of the operating conditions, an algorithm of adaptive control was adopted.

We studied the possibility of considering an improvement an improvement of the structure of order of the process by implementing an Order of the bioreactor by networks of neurons. One showed; that it is possible to establish a controller by neuronal opposite model in the process to ensure the waste water treatment in the biofiltre.

The simulations carried out thanks to data (I.N.S.A. of Toulouse) show that the adopted regulator presents of the satisfactory performances

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