Fuzzy and Neuro-Fuzzy Modeling of a Fermentation Process

Chabbi Charef[1], Mahmoud Taibi[1], and Nicole Vincent[2]
[1]Electronics Department, University of Annaba, Algeria
[2]Laboratory CRIP5-SIP, University René Descartes Paris, France

Abstract: *Neuro-fuzzy modeling may be qualified as a grey-box technique, since it combines the transparency of rule-based fuzzy systems with the learning capability of neural networks. The main problem in the identification of non-linear processes is the lack of complete information. Certain variables are, either immeasurable or difficult to measure, the soft sensors are the necessary tools to solve the problem. Those latter can be used via online estimation, and then they will be implemented in fed-batch fermentation processes for optimal production and online monitoring. The process parameters are estimated through a fuzzy logic system. The fuzzy models of takagi-sugeno type suffer of the problem of poor initialization, which can be solved by the trial-and error method Trial-and-error method is used to solve the poor initialization problem of TS models, this deals with identifying the structure of the model, such structure consists on finding the optimum number of rules, which enters in the model cost reduction. The fuzzy model might not capture the process non-linearity, especially if the number of rules is over-optimized. Bioreactors exhibit a wide range of dynamic behaviours and offer many challenges to modeling, as a result of the presence of living micro-organisms whose growth rate is described by complex equations. We will illustrate the fuzzy and the neuro-fuzzy modeling on the identification of such a system. In order to compare the NF model outputs, we use another fuzzy model that does not incorporate the neural network learning capability, to identify the parameters of the same process. Even though, the two models were trained using levenberg-marquardt algorithm, the corresponding simulation results show that a better modeling is achieved using NF technique, especially that we did not employ any involved optimization procedure to identify the NF structure.*

Keywords: *Yeast fermentation, fed-batch, takagi-sugeno model, levenberg-marquardt algorithm.*

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1. Introduction

Real processes in biotechnology are, in their vast majority, non-linear, uncertain and time-varying. The control of such systems is currently driven by a large number of requirements, because of the competition, environmental conditions, costs and furthermore these systems must be robust and fault-tolerant [5]. By considering all these effects, process modeling based on fuzzy logic and neural network techniques is introduced. These two methods imitate human reasoning's. In fuzzy systems [7], the input-output relationships are represented in the form of if-then rules, but in neural networks, the relationships are coded in the network by its parameters. Neuro-fuzzy systems combine the transparency of rule based fuzzy systems with the learning capability of neural networks. Their developments are based on empirical models, heuristics and observed data. They describe systems by using if-then rules represented in a network structure, combined to neural networks learning algorithms. Such a structure is more interpretable than the completely black-box models. In the last decade, different architectures of neuro-fuzzy models were introduced [4, 8]. The ANFIS (adaptive network based fuzzy inference system) proposed by Jang [4], produces fuzzy models consisting of TS type rules. After specifying the number of membership functions for each input variable, the ANFIS algorithm iteratively learns the premise parameters via Levenberg Marquardt (LM) training method and optimizes the consequent parameters via linear least squares estimation. We also use another fuzzy model, trained by LM too, to compare the simulation results. The two fuzzy models are then validated with experimental data. This article is organized as follows. Section 2 discusses the adopted TS model. Thereafter, the description of the fed-batch fermentation process is given in section 3. Section 4 presents the training LM algorithm for premise parameters optimization of the two fuzzy models. Simulation results are discussed in section 5. Finally, conclusion is given in section 6.

2. Takagi-Sugeno Fuzzy Model

The considered Fuzzy Logic Systems (FLS) are based on TS type. If the dynamic model is of the form:

$$y = f(x) \quad (1)$$

where the input x is such that $x_k = [x_{1k} \dots x_{nk}]^T$ and the output sample is y_k. The index

$k = 1.....N$ denotes the individual data samples. It is often difficult to find a model that describes the system globally, and one solution might be to construct local linear models around selected operating points. Those local models are represented by fuzzy sets, and each fuzzy set is expressed by a rule; if there are L fuzzy if-then rules, the rule R_i can be written as:

$$\begin{aligned} R_i \;:\; & IF \;\; x_1 \;\; is \;\; A_{i1}(x_1) \;\; and \;\; .... \; x_n \;\; is \;\; A_{in}(x_n) \\ & then \qquad y_i = b_{i0} + b_{i1}x_1 + ... + b_{in}x_n \end{aligned} \tag{2}$$

where A_{ij} are fuzzy sets that are characterized by membership functions $A_{ij}(x_j)$; x_j are input variables; y_i are local output variables; b_{i0} *and* b_{ij} are real parameters. The overall output of the model is given by:

$$\hat{y} = \frac{\sum_{i=1}^{L} \beta_i \, y_i}{\sum_{i=1}^{L} \beta_i} \tag{3}$$

where β_i is the firing strength of the rule R_i, which is computed as:

$$\beta_i = A_{i1}(x_1)\, A_{i2}(x_2) .... A_{in}(x_n) \tag{4}$$

The TS model can describe a highly non-linear system using a small number of rules. It contains the premise parameters (of bell generalized or Gaussian membership functions) and the consequent parameters (b_{i0} ….b_{ij}). If the premise and the consequent parameters are appropriately computed, the above FLS can correctly approximate the underlying non-linear dynamics that generated the given set of input-output data pairs.

3. Yeast Fermentation Process Modeling

Biological well-mixed fed-batch reactor, as shown in Figure 1, includes two models which are the kinetic and the mechanistic models [1]; The yeast cells, of concentration X, are growing in the liquid phase: they are consuming the glucose substrate, of concentration S and the dissolved oxygen, of concentration O_F; they are producing the carbon dioxide, of concentration C_F. Ethanol, of concentration E, can be either a substrate or a product, depending on S and O_F [4].

3.1. Kinetic Model

The saccharomyces cerevisiae yeast is characterized by three metabolic pathways:

- Respiratory growth on glucose:

$$\begin{aligned} & C_6H_{12}O_6 + aO_2 + bNX\;[NH_3] \xrightarrow{\mu_S^O} \\ & bC_l H_{HX} O_{OX} N_{NX} + aCO_2 + dH_2O \end{aligned} \tag{5}$$

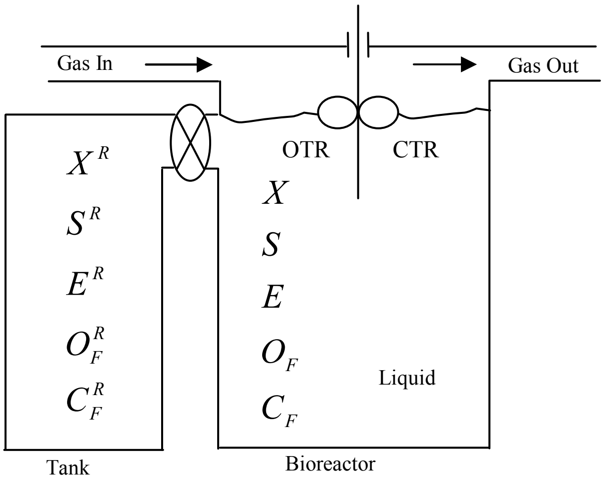


Figure 1. Fedbatch reactor.

- Fermentative growth on glucose:

$$\begin{aligned} & C_6H_{12}O_6 + gNX\;[NH_3] \xrightarrow{\mu_S^F} \\ & gC_l H_{HX} O_{OX} N_{NX} + hCO_2 + iH_2O + jC_2H_6O \end{aligned} \tag{6}$$

- Respiratory growth on ethanol:

$$\begin{aligned} & C_2H_6O + kO_2 + lNX\;[NH_3] \xrightarrow{\mu_E^O} \\ & lC_l H_{HX} O_{OX} N_{NX} + mCO_2 + nH_2O \end{aligned} \tag{7}$$

where μ_S^O, μ_S^F *and* μ_E^O are the specific growth rates (expressed in h^{-1}) for the three metabolisms. Subscripts S and E mean glucose and ethanol respectively.

It all depends on the respiratory capacity of the yeast cells. Respiratory pathways (5) and (6) if the respiratory capacity is enough; otherwise pathways (5) and (6) are followed by the yeast growth. Several kinetic models are proposed for yeast growth. In this paper, we considered monod type equations, and used Sonnleitner and Käppeli growth model. If q_S *and* q_{O2} are the specific glucose and oxygen uptake rates respectively, then :

If $aq_s \le q_{02}$, the regime is respiratory;

If $aq_s > q_{02}$, the regime is respiro-fermentative;

where a is the stoichiometric coefficient of the oxygen in the pathway (5).

The specific growth rate μ is related to the corresponding substrates fluxes q and yield coefficients y by:

$$\begin{aligned} \mu = \mu_S^O + \mu_S^F + \mu_E^O = y_{X/S}^O q_S^O + \\ y_{X/S}^F q_S^F + y_{X/E}^O q_E^O \end{aligned} \tag{8}$$

where $y_{X/S}^O$ *and* $y_{X/S}^F$ represent the yield coefficients of biomass X in glucose S in the oxidative and fermentative phases respectively; $y_{X/E}^O$ is the yield coefficient of biomass X in ethanol E in the oxidative way [2].

3.2. Mechanistic Model

Assuming that the yield coefficients y's are constant and the dynamics of the gas phase are neglected, the balances are as follows:

$$\begin{cases} \frac{dX(t)}{dt} = D(t)(X^R(t) - X(t)) + \mu(t)X(t) & (9) \\ \frac{dS(t)}{dt} = D(t)(S^R(t) - S(t)) - q_S(t)X(t) & (10) \\ \frac{dE(t)}{dt} = D(t)(E^R(t) - E(t)) + r_E(t)X(t) & (11) \\ \frac{dO_F(t)}{dt} = D(t)(O_F^R(t) - O_F(t)) - q_{O2}(t)X(t) + OTR(t) & (12) \\ \frac{dC_F(t)}{dt} = D(t)(C_F^R(t) - C_F(t)) + q_{CO2}(t)X(t) - CTR(t) & (13) \end{cases}$$

where r_E and q_{CO2} are the specific ethanol reaction and the specific carbon dioxide production rates respectively; The gas transfer rates are given by:

$$OTR = K_L^O a(O^* - O) \tag{14}$$

$$CTR = K_L^C a(C^* - C) \tag{15}$$

where OTR and CTR are the oxygen and the carbon dioxide transfer rates respectively; $(K_L^i a)$ is the overall mass transfer coefficients (i indicating O or C); O^* and C^* are the equilibrium concentrations of O and C respectively [2].

4. Parameters Optimization Algorithms

As we mentioned in the introduction, we used two FLS, where the first one is of $ANFIS$ type. Both systems are trained using LM algorithm, which is a second order training method based on the modification of Newton's method. In this algorithm, the Hessian matrix H is computed as [6]:

$$H = J^T J \tag{16}$$

and the gradient g is computed as:

$$g = J^T e \tag{17}$$

where J is the Jacobian matrix that contains the first derivatives of the FLS error with respect to the premise parameters, and e is a vector of FLS error. If the performance function is V and the parameter vector is α then:

$$V = \sum_{k=1}^{N} (e_k)^2 \tag{18}$$

where:

$$e_k = y(k) - \hat{y}(k) \tag{19}$$

y and $\hat{y}$ being the desired and the estimated outputs respectively. The update of α is given by: where I is the $(N_p.N_p)$ identity matrix, N_p being the number of FLS adjustable parameters. The parameter μ is

$$\Delta\alpha = \alpha(k+1) - \alpha(k) = -(J^T(\alpha)J(\alpha) + \mu I)^{-1} J^T(\alpha)e \tag{20}$$

increased if $V(\alpha)$ increases and is decreased if $V(\alpha)$ decreases. The aim is to shift toward Newton's method (where $\mu = 0$) as quickly as possible, because Newton's method is faster and more accurate near a minimum.

4.1. ANFIS Algorithm

The ANFIS is an adaptive fuzzy Sugeno model that facilitates the learning and the adaptation. The ANFIS modeling is more systematic and less dependant on a priori process information. The ANFIS architecture ncludes five layers which are described in the following:

- Layer 1: its outputs are the membership functions of the inputs,

$$O_i^1 = \mu_{Ai}(OUR),\ i = 1,2,3,4. \tag{21}$$

$$O_j^1 = \mu_{Bj}(CPR),\ j = 1,2,3,4. \tag{22}$$

- Layer 2: each of its nodes computes the firing strengths of the associated rules. Its nodes outputs are given by:

$$O_j^2 = \omega_i = \mu_{Ai}\,\mu_{Bm},\ i = 1,2,\ldots,16 \tag{23}$$

$$1 \le i \le 4,\ j = 1,\ m = i$$

$$5 \le i \le 8,\ j = 2,\ m = i - 4$$

$$9 \le i \le 12,\ j = 3,\ m = i - 8$$

$$13 \le i \le 16,\ j = 3,\ m = i - 12$$

- Layer 3: its outputs are the normalization of the rules firing strengths,

$$O_i^3 = \overline{\omega}_i = \frac{\omega_i}{\sum_{i=1}^{16} \omega_i},\ i = 1,2,\ldots,16 \tag{24}$$

- Layer 4: its outputs are:

$$O_i^4 = \overline{\omega}_i\, f_i = \overline{\omega}_i\,(p_i\, OUR + q_i\, CPR + r_i) \tag{25}$$

f_i are the rules outputs; $\{p_i, q_i, r_i\}$ are the consequent parameters that are determined during the training procedure.

- Layer 5: its output is the overall output of the model which is given by :

$$O_i^5 = \sum_{i=1}^{16} \overline{\omega}_i \, f_i \tag{26}$$

For this architecture, the first and the fourth layers are adaptive, the first layer premise parameters are determined using the LM algorithm; the fourth layer consequent parameters are identified using the least squares method. The Membership Functions (MF) are of type generalized bell membership functions and are of the form:

$$\mu_{Ai} = \frac{1}{1 + (\frac{x - c_i}{a_i})^{2b_i}} \tag{27}$$

where $\{a_i \, , b_i \, , c_i\}$ is the antecedent parameter set; A_i is the linguistic label; c_i determines the center of MF; a_i is the half width and b_i (together with a_i) control the slope at the points where MF value is 0.5.

The Jacobian matrix is computed through the back propagation algorithm, where the error propagates from the output, in a backward pass, toward the inputs

$$\frac{de_k}{d\alpha} = \sum_{O \in S} \frac{de_k}{dO} \frac{dO}{d\alpha} \tag{28}$$

where S is the set of nodes whose outputs depend on α . Then for the overall error e , we get:

$$\frac{de}{d\alpha} = \sum_{k=1}^{N} \frac{de_k}{d\alpha} \tag{29}$$

and the update equation 20.

4.2. Fuzzy Algorithm

The $MF's$ are gaussians and are of the form[3]:

$$\mu_{A_i} = \exp(-0.5((x - c_i)/a_i)^2) \tag{30}$$

where $\{a_i \, , c_i\}$ is the antecedent parameters set, c_i determines the center of the MF , a_i is the half-width. Using equation 3, the error e is written as:

$$e = y - \frac{\sum_{i=1}^{L} \beta_i y_i}{\sum_{i=1}^{L} \beta_i} \tag{31}$$

then

$$\frac{d\mu_{A_i}}{dc_i} = \frac{(x - c_i)}{a_i^2} \mu_{A_i}(x) \tag{32}$$

$$\frac{d\mu_{A_i}}{da_i} = \frac{(x - c_i)^2}{a_i^3} \mu_{A_i}(x) \tag{33}$$

and

$$\frac{de}{dc_i} = - \frac{d\beta_i}{dc_i} \cdot \frac{y_i - \hat{y}}{\sum_{i=1}^{N} \beta_i} \tag{34}$$

$$\frac{de}{da_i} = - \frac{d\beta_i}{da_i} \cdot \frac{y_i - \hat{y}}{\sum_{i=1}^{N} \beta_i} \tag{35}$$

The overall error E is computed through equation 23, and the update formula i given by equation 5.

5. Simulations

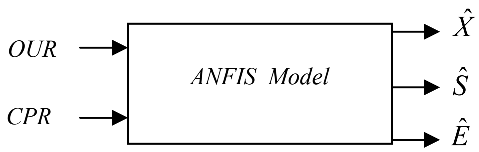


Figure 2. ANFIS model.

The $ANFIS$ model is as shown in Figure 2. The inputs are OUR *and* CPR , which are oxygen uptake rate and carbon dioxide production rate respectively, and they are expressed in $(g/l/h)$. OUR of 1g/l/h is defined as 1 gram of oxygen consumed per 1 liter of solution per 1 hour; CPR of 1g/l/h is defined as 1 gram of carbon dioxide produced per 1 liter of solution per 1 hour; In this work, OUR varies up to 5.8g/l/h and CPR varies up to 14g/l/h. The outputs are X, S *and* E are as defined in section 3. For $ANFIS$ algorithm, we use 16 rules, where each input is assigned 4 MFs of bell type; then 24 premise parameters and 48 consequent parameters are to be determined; The sixteen rules of ANFIS model are of the form:

If $OUR\ (k)$ *is* $\mu_{Aj}(OUR\ (k))$ *and* $CPR\ (k)$ *is* $\mu_{Bm}(CPR\ (k))$, *then* $(k) = p_i OUR + q_i CPR + r_i$

where stands for any output; the indices i, j *and* m are as defined before. The eight rules of the FS model are of the form:

If $OUR\ (k)$ *is* $\mu_{An}(OUR\ (k))$ *and* $CPR\ (k)$ *is* $\mu_{Bn}(CPR\ (k))$, *then* $(k) = p_n OUR + q_n CPR + r_n$

The index n is such that $n = 1,2,...8$. The number of epochs is 100. The outputs of the $ANFIS$ model are as shown below:

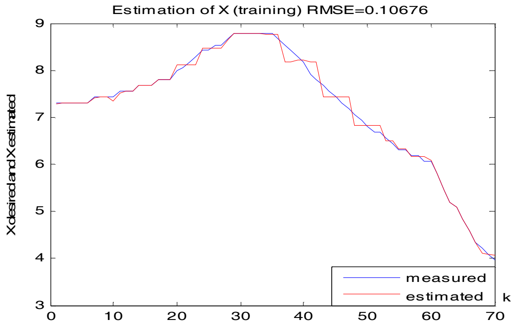


Figure 3. Estimation of X (training).

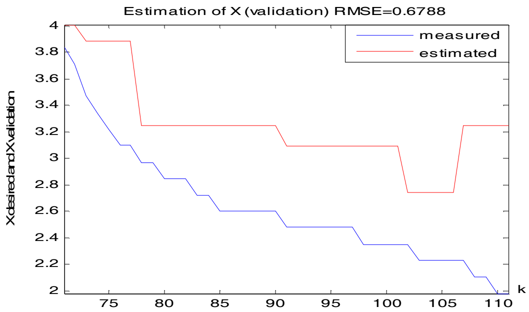


Figure 4. Estimation of X (validtion).

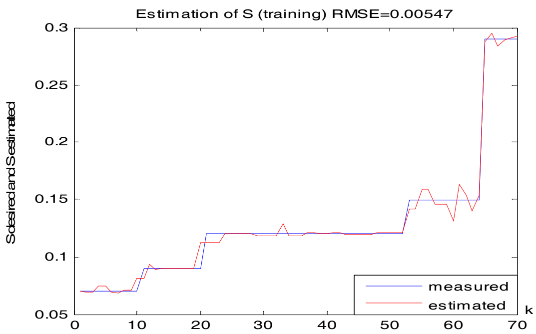


Figure 5. Estimation of S (training).

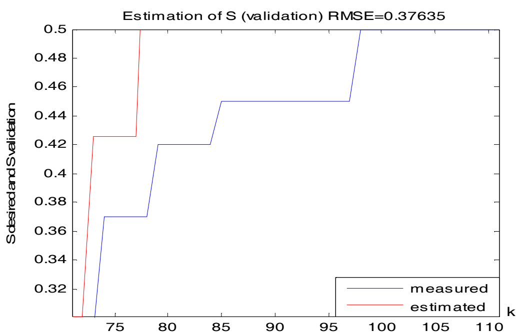


Figure 6. Estimation of S (validtion).

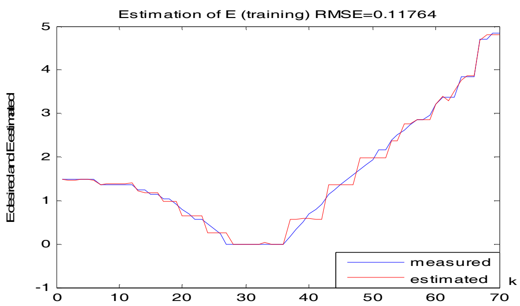


Figure 7. Estimation of E (traning).

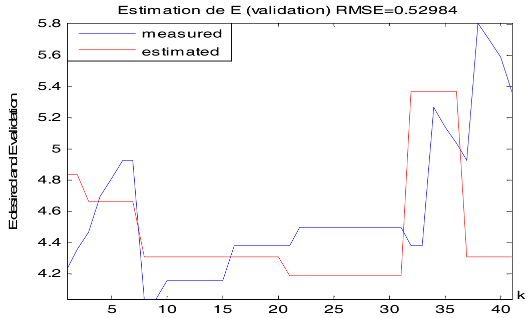


Figure 8. Estimation of E (validation).

For the fuzzy method, we use eight rules, where each input is assigned 8 membership functions of gaussian type; then 32 premise parameters and 24 consequent parameters are to be determined. The fuzzy model is as shown in Figure 9.

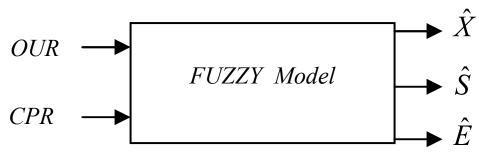


Figure 9. Fuzzy model.

The outputs of the fuzzy model are as shown below:

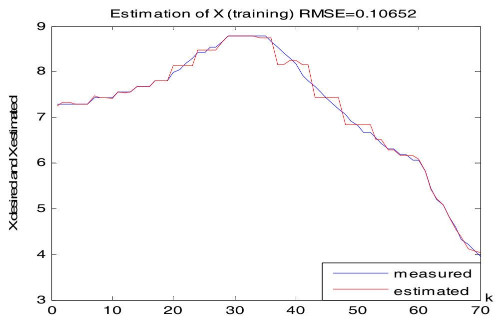


Figure 10. Estimation of X (traning).

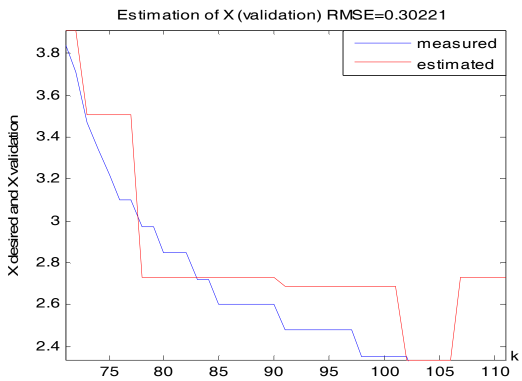


Figure 11. Estimation of X (validation).

5.1. Comments

- Biomass of concentration *X*: the process is started at a dilution rate D=0.2h^{-1} for a duration of 10 hours; the sampling interval is 15 minutes, OUR is relatively high, the biomass growth is oxidative on glucose and is also oxidative on ethanol; *X* then increases while S is kept constant and E decreases. Stationary operation is reached at t =8h, in this phase, the estimation is working well; at t =10h, D is increased to $0.32h^{-1}$, the biomass growth is now fermentative, but the crabtree effect represses the growth and X then decreases; the ethanol production rate is higher; at t=15h, OUR is reduced, X continues to decrease and E continues to increase; the growth is strongly oxygen limited [1].

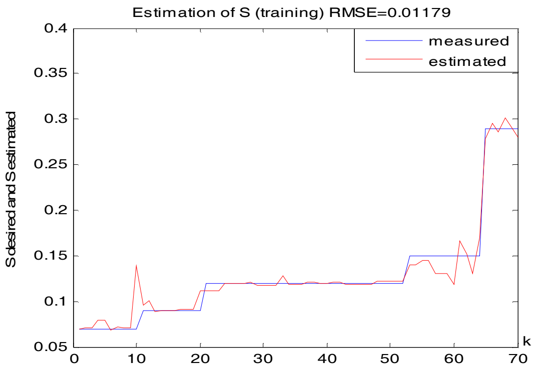


Figure 12. Estimation of S (traning).

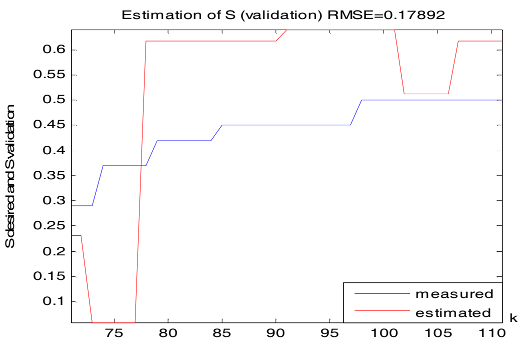


Figure 13. Estimation of S (validation).

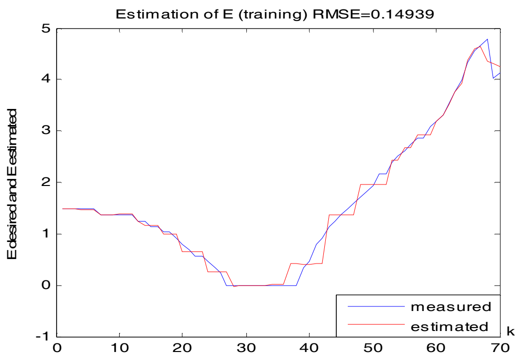


Figure 14. Estimation of E (traning).

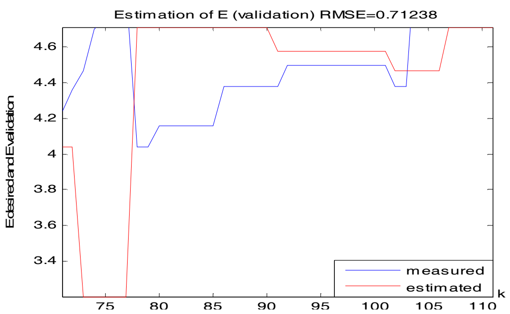


Figure 15. Estimation of E (validation).

- Glucose of concentration S: Baker's yeast is capable of oxidizing glucose when the glucose concentration is below a critical value. Above that value, the yeast will not be able to oxidize all the glucose. In this fedbatch experiment, the glucose concentration is kept at a very low value, for optimization of the biomass production.
- Ethanol of concentration E: the ethanol is reduced at first, because it enters in the oxidative growth of the biomass, then it increases again because of the fermentative growth of the biomass; where it is produced in big quantities, the ethanol production rate is high.

From the simulations results obtained, the training of ANFIS model is conducted with lower RMS errors, but the validation of FS model is better achieved, meaning that for this application, the FS model is capable of better forecasting the future behavior of the process. Also, we have sixteen fuzzy regions for the ANFIS model inputs, against only eight regions for FS model inputs.

The reference [9] uses FS by means of fuzzy clustering to implement a soft sensor of the biomass concentration; the MSE is between 0.5 and 0.7.

6. Conclusion

One problem which appears in control of biotechnical processes is the difficulty to measure the important state variables. The required specific sensors are either not available, or costly. The soft sensors provide a solution to overcome this problem, but their performance depends on both the measurement quality delivered by the sensor and the associated estimation algorithms [9].

The simulations show that satisfactory training estimation results could be obtained through ANFIS because of the learning capability of the neural networks. For the training case, the RMSE for ANFIS is lower than for the other fuzzy model. For the validation of the model, need to have sufficient and accurate data for the training of the network. By the simulations, we can see that the RMSE for validation is lower by using the fuzzy model. Furthermore, the soft sensors could replace the specific and sophisticated sensors if we improve the measurement quality and assess the estimation algorithms.

References

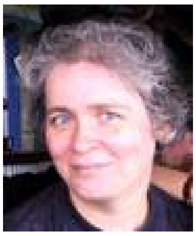
[1] Bellgardt H., " Application of an EKF for State Estimation of a Yeast Fermentation," *in IEE Proceedings*, Germany, pp. 226-234, 1986.

[2] Celina L. and Filomena S., "Heuristic Sensitivity Analysis of Baker's Yeast Model Parameters," *in Proceedings of Investigacio Operacional*, Portugal, pp. 247-263, 2004.

[3] Euntai K., "A Transformed Input-Domain Approach to Fuzzy Modeling," *Computer Journal of IEEE Transactions on Fuzzy System*, vol. 6, no. 4, pp. 596-604, 1998.
[4] Jang R., "ANFIS: Adaptive Network Based Fuzzy Inference System," *in Proceedings of IEEE Transactions on Syststem Man Cybeern,* USA, pp. 665-685, 1993.
[5] Oliveira R., "Supervision, Control and Optimization of Biotechnological Processes," *PhD Thesis*, Martin-Luther University, Portugal, 1998.
[6] Panchariya C., "Nonlinear System Identification Using Takagi-Sugeno Type Neuro-Fuzzy Model," *in Proceedings of the Second IEEE International Conference on Intelligent Systems*, India, pp. 76-81, 2004.
[7] Takagi T. and Sugeno M., "Fuzzy Identification of Systems and its Applications to Modeling and Control," *in Proceedings of IEEE Transactions on Syststem Man Cybern,* Japan, pp. 116-132, 1985.
[8] Tzafestas G. and Zikidis C., "On-Line Neuro Fuzzy ART Based Structure and Parameter Learning TSK Model," *in Proceedings of IEEE Transactions on Syststem Man Cybeern*, Greece, pp. 797-802, 2001.
[9] Xiong Z., "On Line Estimation of Concentration Parameters in Fermentation Processes," *Journal of Zhejiang University SCIENCE,* vol. 6, no. 3, pp. 530-534, 2005.

Chabbi Charef received his BSc in electrical engineering from USTO University, Algeria in 1981, his MSc from Ohio University, USA in 1985, and currently, preparing his PhD in electrical engineering. Currently, he is an assistant professor at BadjiMokhtar University, Algeria since 1988.

Mahmoud Taibi received his BSc in electrical engineering from USTO University, Algeria in 1980, and his MSc from Badji-Mokhtar University, Algeria in 1996. Currently, he is an assistant professor at Badji-Mokhtar University, Algeria since 1983. His interests are in intelligent systems.



Nicole Vincent is full professor since 1996. She presently heads the Center of Research in Computer Science (CRIP5) and the team Systèmes Intelligents de Perception (SIP) in the University Paris Descartes, France. After studying in Ecole Normale Supérieure and graduation in mathematics, and graduation in mathematics, Nicole Vincent received a PhD in computer science in 1988 from Lyon Insa.