A Hybrid Neural Network Approach for Batch Fermentation Simulation

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A Hybrid Neural Network Approach for Batch Fermentation Simulation

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Abstract: The paper aims the simulation of a batch fermentation process. This phenomenon is very complex and challenging to monitor. To achieve this purpose, a hybrid neural network model is presented. Data used to derive and validate the model was obtained from experiments. The neural network whose architecture is combined to differential equations has shown good ability to simulate the batch fermentation process with predictive error less than 0.030.

Key words:

INTRODUCTION

Fermentation is a complex phenomenom intensively investigated (Psichogios and Ungar, 1992; Marin, 1999; Assidjo *et al.*, 2006; Coleman and Block, 2006). Modelling such phenomenon is difficult and challenging (Assidjo *et al.*, 2006). Nevertheless, many mathematicals models were proposed to monitor and control different reactions that occur (Psichogios and Ungar, 1992; Andrés-Toro et al., 2004; Assidjo *et al.*, 2006; Coleman and Block, 2006). These equations based on mass balance give results not always expected. In order to better the fermentation process modelling, some empirical models like artificial neural networks are sometimes proposed (Linko, 1998; Sinha et al., 2002; Andrés-Toro et al., 2004; Assidjo *et al.*, 2006; Coleman and Block, 2006).

Artificial Neural Network:

The artificial neural network concept is used for describing a particular type of model that emulates the human brain behavior (Werbos, 1990; Haykin, 1994). Generally, neural networks processing corresponds to a weighted sum of the neuron input values with their weights, which will be the argument of a function, usually the sigmoid or logistic function, whose value constutes the neuron output. Parameters in the net, weight factors and biases are fitted in the training process.

The prediction capability of a neural network depends on the quality of data used for training and on the training algorithm (Savkovic-Stevenovic, 1994).

Alcoholic fermentation is a complex process occuring when yeast are in presence of simple sugar like glucose. This challenging phenomenom can take advantage of capability of ANN (black-box) for describing complex functions in the mathematical models derived from first principles (white-box).

Indeed, in the case in which mathematical relationship is available describing different kinetics of fermentation process, this expression usually contains one or more parameters that have to be estimated (Bazaei and Majd, 2003). In hybrid model, system equations and neural network are used simultaneously to describe the behavior of the system. Generally in these models, neural networks are used to approximate the parameters of the first principle, balance equations (Lee *et al.*, 2002; Laursen *et al.*, 2007).

Artificial neural network is more and more used in hybrid models which provide better performance for interpolation and extrapolation properties of ethanol production by *Saccharomyces cerevisea* concentration (Pramanik, 2004; Riviera et al., 2006), for instance. Therefore, hybrid models combine more than one approach for simulating the behavior of a given system, as presented in figure 1.

The purpose of this work is to use the artificial neural network for computing the kinetics and avoid therefore one of the steps to establish relationship between the different variables that affect the kinetics models.

The experimental data was used to derive and validate the hybrid neural network model that simulates system behavior under the different conditions tested.

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MATERIAL AND METHODS

Experimental System:

The neural network modeling technique was employed in batch fermentation in which, the yeast consume glucose to produce alcohol and carbon dioxyde (CO_2) The substrate was glucose from Prolabo (Villeurbanne, France).

The fermentations were performed using a Brunswick microferm fermentor (New Brunswick Scientific co inc., New Jersey, USA), in batch mode at constant initial temperature and pH.

Firstly, the wort was produced by crushing the malt into coarse flour that was then mixed with water. The resulting porridge-like mash was heated to a selected temperature that permitted the malt enzymes to partially solubilize the ground malt. The resulting sugar-rich aqueous extract (wort), was separated from the solids and boiled. The wort was then clarified, cooled and poured in the vessel of the micro-fermentor for inoculation. Inoculated ferments were traditionally produced by female brewers that use it for a well-known local beer (tchapalo or dolo) making. This ferment is in fact a mixture of micro-organisms containing different species (e.g. *Saccharomyces cerevisae, Candida* …). During the fermentation process (t=0 to 18 hours), different parameters (pH, biomass, substrate, ethanol) were measured. The responses concerned in this study (biomass, substrate and alcohol) were determined by gravimetric and refractometric methods and refractometric method after a distillation, respectively (Thonart, 2001). For the purpose of this study, 28 batches were performed.

Neural Network Creating and Training:

The neural network that computes the value of the kinetic relationship is Multi Layer Perceptron with one hidden layer. The activation function employed in the hidden layer is sigmoid (tanh) function while for outer layer linear function was used. The number of the hidden neuron was firstly varied from 1 to 10. Backpropagation technique was used to train the net and weights and biases were determined using Levenberg-Marquardt algorithm.

The neural network in the hybrid model computes parameters kinetics (i.e. μ_s, μ_x and μ_p) that is estimated from derivatives of substrate and product profiles during the process. These profiles were built from experimental data using spline interpolating function. The input variables concerned biomass, ethanol, substrate concentration and fermentation time while the output variables were μ_s, μ_x and μ_p, respectively substrate consumption rate, the biomass and ethanol production yields.

About 361 pairs of input/output data were computed. This data set was subdivided in 3 subsets training, validation and test (Assidjo *et al.*, 2006). Before training process, data were all normalized in order that their values were in (-1, +1) range.

The optimal artificial neural network is that for which the lowest prediction error of the hybrid model was obtained. The prediction error being the mean square error (MSE) defined as follows:

$$mse = \frac{\sum (y_c - y_o)^2}{n} \tag{1}$$

with y_c and y_o the calculated and observed responses, n the number of data.

Calculations for artificial neural network were implemented in Matlab R2007b (MathWorks Inc., Massachussets, USA).

Differential Equations:

As intensively studied elsewhere, batch fermentation occurs when yeast are in a sugar- rich medium (Moore *et al.*, 2001; James et al., 2002; Nandasana and Kumar, 2008). During this process, yeasts consuming simple sugars (i.e. glucose) produce ethanol and CO_2. The kinetics of this phenomenon is summarized by following equations:

$$\frac{dX}{dt} = \mu_x \cdot X \tag{2}$$

$$\frac{dP}{dt} = \mu_p \cdot X \tag{3}$$

$$\frac{dS}{dt} = -\mu_s \cdot X \tag{4}$$

In this work, the equations 2 to 4 were integrated using fourth-order Runge- Kutta formula in Matlab R2007b (MathWorks Inc., Massachussets, USA).

RESULTS AND DISCUSSION

Fermentation Process:

During the batch fermentation, sugar, biomass, alcohol and CO_2 were determined each hour. The results are plotted in figures 1 to 4.

It appears, analyzing these figures that sugar concentration decreases from 14 g/L to about 6 g/L. Indeed, yeasts by mean of enzymes produced use substrate for growth and maintenance. This fact is also pointed out by the increase of biomass till an optimum (figure 2). After this optimum, a slight decrease is observed due to death of microorganisms caused by lack of energy source (sugar) and inhibition of alcohol presence.

The figure 4 presenting the evolution of alcohol concentration in the medium, shows that from 0 to 5 hours, the increase of alcohol concentration is low. After this time to 14 hours, this increase is exponential. The alcohol concentration is somewhat constant at about 5.0 %, from 14 hours till at the end of fermentation, concomitantly to yeast death (figure 2).

The different steps observed herein were already been pointed out by many authors (Moore *et al.*, 2001; James et al., 2002; Pramanik, 2004; Nandasana and Kumar, 2008), and results are concordant.

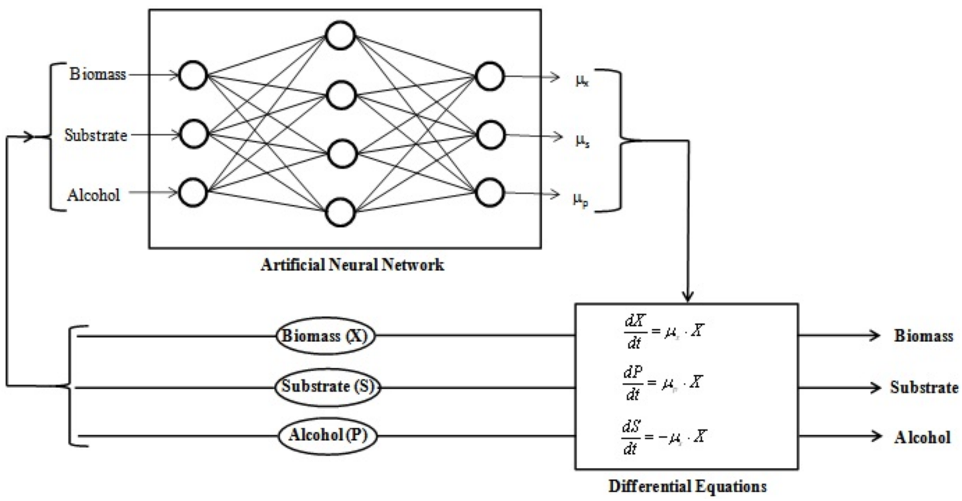

Fig. 1: Hydrid Neural Network flowchart

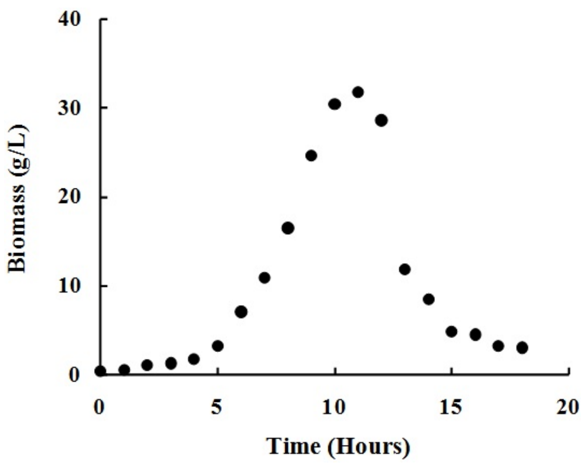

Fig. 2: Biomass according to time

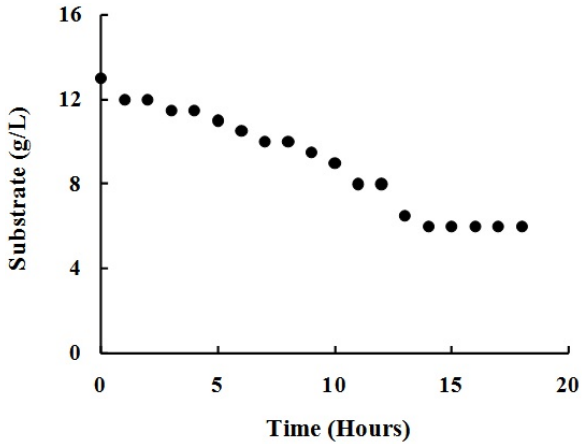

Fig. 3: Substrate evoluion

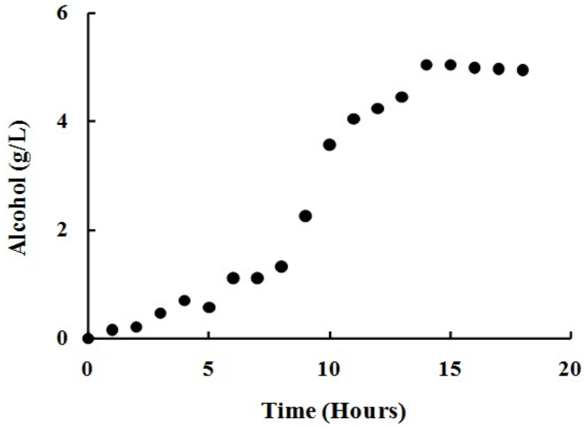

Fig. 4: Alcohol evolution during fermentation

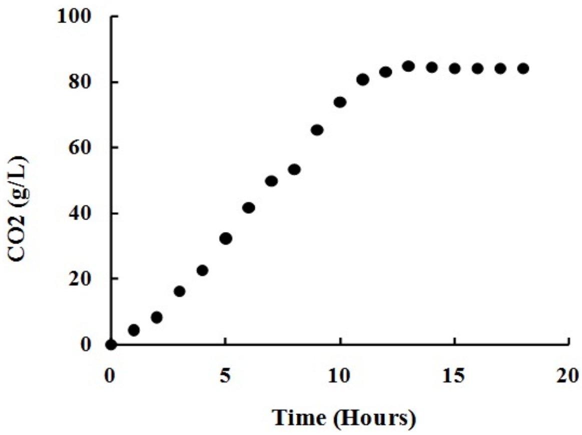

Fig. 5: Carbon Dioxide according to time

Simulation by Hybrid Neural Network:

The prediction capability of artificial neural network depends also on its topology. In this work, a multilayer perceptron was used with one hidden layer. If it is easier to find out the number of neurons in the input and output layers, it is not the case for hidden layer (Assidjo *et al.*, 2006). Indeed, while input layer neuron number is equal to predictive variables (factors), that of outer layer depends on responses number.

Unfortunately, there is no rule to determine the number of hidden neurons. Many methods where proposed (Le cun *et al.*, 1989). But here, we have varied arbitrarily this number from 1 to 10. The predictive error (MSE) of each architecture was determined. The results obtained are presented in table 1.

Table 1: ANN performance for training and test subsets

	Training			Test			
Neurons	Biomass	Substrate	Alcohol	Biomass	Substrate	Alcohol	MSE
5	0.9981	0.7801	0.8220	0.9982	0.7804	0.8260	0.0410
6	0.9986	0.8595	0.9763	0.9988	0.8607	0.9780	0.0000
7	0.9988	0.9856	0.9851	0.9988	0.9872	0.9867	0.0300
8	0.9994	0.9829	0.9811	0.9994	0.9849	0.9839	0.0360
9	0.9987	0.9983	0.9935	0.9987	0.9983	0.9936	0.0190
10	0.9985	0.9988	0.9964	0.9985	0.9988	0.9965	0.0001

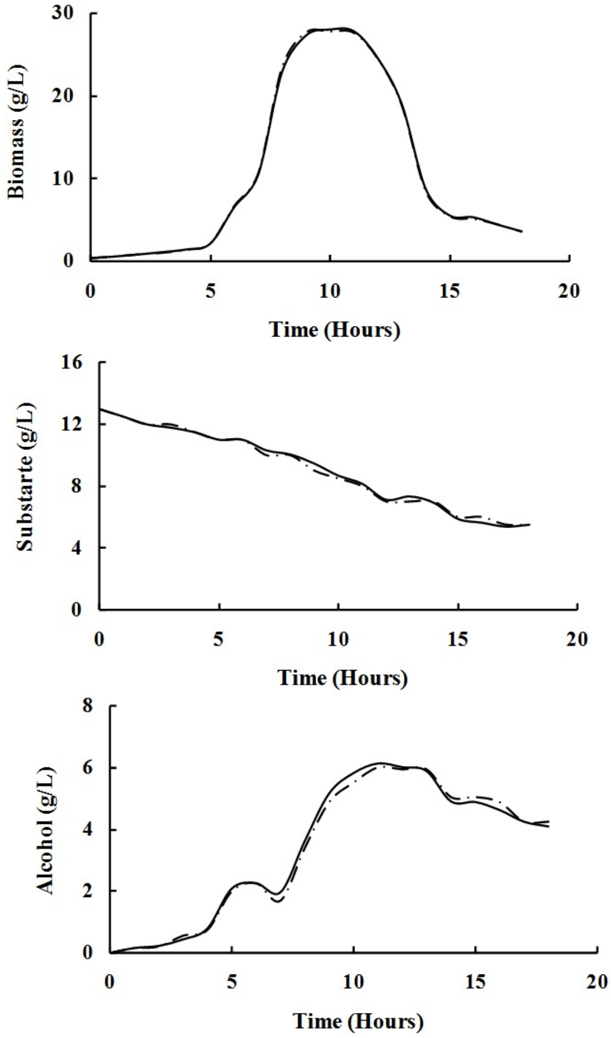

Fig. 6: Comparison of experimental and predicted evolution of biomass, subtrate and alcohol.

The MSE values are low and range from 0.001 to 0.041. The lowest value obtained (0.001) is for ANN topology 3-10-3.

R values, also presented in table 1 and denoting the discrepancy between observed and predictive values, vary from 0.7801 to 0.9994. More higher is R value, more adequate is the network. Thus, we noticed that the best value is reached when the architecture 3-8-3 is considered, about for biomass. But the best compromise between lower MSE and higher R is achieved, considering all responses (i.e. biomass, substrate and alcohol), when there is 7 hidden neurons on the network. Therefore, the hybrid neural network model for simulating this batch fermentation is composed of a 4 differential equation system and the Neural Network retained earlier (3-7-3).

The prediction capability of the hybrid model obtained is 0.0282. This value is slightly different from that of the ANN used alone (0.030). Graphs in figure 6 (A, B and C) compare the experimental values of sugar, biomass and alcohol not used for training to those computed by the hybrid neural network. It clearly appears that the hybrid neural network derived in this work is very suitable to simulate the batch fermentation studied with residuals whose values are inferior to 5 per cent in absolute value (figure 7).

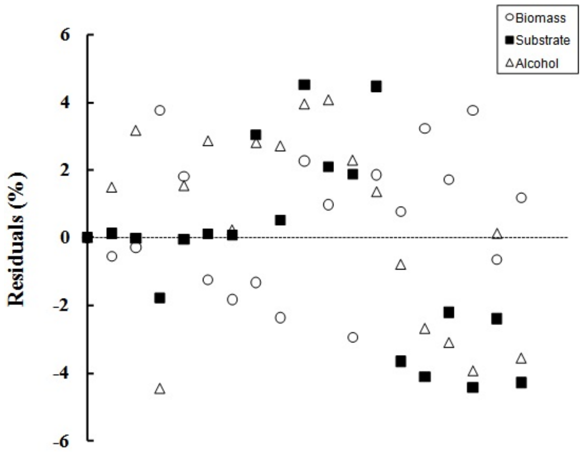

Fig. 7: Biomass, substrate and alcohol residuals

Conclusion:

The complexity of the fermentation process does not enable easy description of the phenomenon through simple mathematical equations. But without an expression for the kinetics parameters, the mathematical models cannot be solved.

However, a properly designed hybrid neural network (containing 3-7-3 neural network structure and 3 differential equations of the process) has shown ability to simulate accurately the batch fermentation studied.

REFERENCES

Andrés-toro, B., J.M. Girón-Sierra, P. Fernández-Blanco, J.A. López-Orozco and E. Besada-Portas, 2004. Multiobjective optimization and multivariable control of the beer fermentation process with the use of evolutionary algorithms. J. Zhejiang Univ. SCI., 5: 378-389.

Assidjo, E., B. Yao, D. Amane, G. Ado, C. Azzaro-Pantel and A. Davin, 2006: Industrial Brewery Modelling by Using Neural Network. J. Appl. Sci., 6: 1858-1862.

Bazaei, A. and V.J. Majd, 2003. Feedback linearization of discrete-time nonlinear uncertain plants via first-principles-based serial neuro-gray-box models. J. Proc. Control, 13: 819-830.

Coleman, M.C. and D.E. Block, 2006. Retrospective optimization of time-dependent fermentation control strategies using time-independent historical data. Biotechnol. Bioeng., 95: 412-423.

Haykin, S., 1994. Neural Networks, A Comprehensive Foundation, Macmillan College Publishing Company Inc., New York.

James, S., R. Legge and H. Budman, 2002. Comparative study of black-box and hybrid estimation methods in fed-batch fermentation. J. Proc. Control, 12: 113-121.

Laursen, S.Ö., D. Webb and W.F. Ramirez, 2007. Dynamic hybrid neural network model of an industrial fed-batch fermentation process to produce foreign protein. Comp. Chem. Eng., 31: 163-170.

Le Cun, Y., J.S. Denker, and S.A. Solla, 1989. Optimal brain damage. Adv. Neur. Inform., 2: 1-12.

Lee, D.S., C.O. Jeon, J.M. Park and K.S. Chang, 2002. Hybrid neural network modeling of a full-scale industrial wastewater treatment process. Biotechnol. Bioeng., 78: 670-682.

Linko, S., 1998. Expert systems- What they can do for food industry? Trends Food Sci. Technol., 9: 3-12.

Marin, M.R., 1999. Alcoholic fermentation modelling: current state and perspectives. Am. J. Enol. Vitic., 50: 166-178.

Moore, C.F., N. Kaistha and M.S. Johnson, 2001. Monitoring and analysis of batch profiles. J. Process Anal. Chem., 2: 65-80.

Nandasana, A.D. and S. Kumar, 2008. Kinetic modelling of lactic acid production from molasses using *Enterococcus faecalis RKY1.* Biochem. Eng. J., 38: 277-284.

Pramanik, K., 2004. Use of artificial neural networks for prediction of cell mass and ethanol concentration in batch fermentation using *saccharomyces cerevisiae* yeast, IE (I) J. CH, 85: 31-35.

Psichogios, D.C. and L.H. Ungar, 1992. A hybrid neural network-first principles approach to process modeling. AIChE J., 38: 1499-1511.

Rivera, E.C., I. Mantovaneli, A.C. da Costa and M.R. Filho, 2006. Hybrid modeling for continuous production of bioethanol. Comp. Aid. Chem. Eng., 21: 613-618.

Savkovic-Stevenovic, J., 1994. Neural networks for process analysis and optimization: modelling and applications, Comp. Chem. Eng., 18: 1149-1158.

Sinha, S., P. Bose, M. Jawed, S. John and V. Tare, 2002. Application of neural network for simulation of upflow anaerobic sludge blanket (UASB) reactor performance. Biotechnol. Bioeng., 77: 806-814.

Thonart, P., 2001. Industries d’extraction et de fermentation: 1ère partie, Centre Wallon de Biologie Industrielle, Gembloux, Belgique.

Werbos, P.J., 1990. Backpropagation through time: What it does and how to do it?. Proc. of the IEEE., 78: 1550-1560.