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A COMPARISON OF FIRST PRINCIPLE AND NEURAL NETWORK MODELLING FOR A NOVEL DEPOLLUTION PROCESS

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***Abstract*— The capability of first principles models and neural networks for predicting the main state variables (biomass and substrate concentrations) in a novel depollution bioprocess has been tested. Experimental data recorded from batch sequential cultures of anaerobic bacteria and yeast to transform organic nitrogen and carbonaceous substrates into useful feed material were used to train the net and validate the first principle model. Both modeling approaches were tested for a number of experiments carried out under different conditions (maximum growth rate cultures, high pH conditions and starving nutrient conditions). The results indicate that the performance of a simple well-trained neural network model was equivalent or better than the first principles model but showed some limitations for providing insight into the mechanism governing the bioprocess. Limitations of both modeling approaches are finally discussed.**

***Keywords*— Mathematical models, first principles, artificial neural networks, depollution process.**

I. INTRODUCTION

Mathematical modeling provides useful tools in simulation, experimental design, optimization and control of bioprocesses (Bastin and Dochain, 1990). Bioprocesses are very complex systems that in order to fully understand all the network of independent reactions, a detailed and rigorous structure is necessary. Many mathematical models at the cell level have been developed and used to predict substrate consumption, cell growth and cell composition, product formation, etc. The progress in understanding of cellular metabolic processes and the regulation system structure for specific pathways have made it possible to establish mechanistic, structured models including many of the fundamental processes involved in cellular metabolism of complex biochemical processes. Prediction capabilities of such models may be reduced if the parameters are unknown or inaccurate, even if an accurate model structure has been established. For this reason, efforts by many researchers have been made for the evaluation of the state variables and estimation of the bioprocess parameters (Chen and Rollins, 2000).

Recent developments in the field of artificial intelligence such as artificial neural networks (ANN) have complemented those rigorous modeling, allowing complex system to be modeled relatively easily and permitting loosely related observations to be linked in a more meaningful fashion. The ANN approach is an exciting technology which can also be used for estimation and prediction (Narendra and Parthasarathy, 1990; Baughman and Liu, 1995).

In this contribution, the authors derived a neural network model of a depollution process and demonstrated that simple well trained neural networks can be employed to overcome the modeling problems without detailed prior knowledge of the relationships of process variables under investigation. In this second paper, the authors compare the performance of the neural network (ANN) modeling approach to a first principle (FP) modeling approach. Both modeling approaches focus on the prediction of the kinetic behavior of *C. utilis* on butyric acid and ammonium-nitrogen for carbon and nitrogen removal purposes and use the initial conditions of pH, ammonium-nitrogen, biomass and butyric acid to predict the dynamic behavior of the bioprocess. We show that both approaches provide useful information of the depollution process under specific conditions and that they can be used to develop a rational scale-up procedure and to control the given depollution process.

II. PROCESS DESCRIPTION

The depollution processes considered in this paper offers the interesting possibility of purification and biorecovery of nitrogen and carbon in the form of single cell protein in two bioreactors. It uses anaerobic bacteria to transform the organic nitrogen and the carbonaceous substrates into ammonium-nitrogen (NH_4^+-N) and volatile fatty acids (VFA). Then, yeasts assimilate and convert these nutrients into single cell protein in a sequential bioreactor. A detailed description of the process is given by Bories *et al.* (1992).

III. FIRST PRINCIPLE MODEL

A mathematical model describing the yeast batch reactor was derived from the mass balances applied to each component under aerobic conditions without oxygen transfer limitations. This model is given by the following system of differential equations:

$$\begin{aligned} \frac{dX}{dt} &= \mu X \\ \frac{dS_1}{dt} &= -\frac{\mu X}{Y_{X/S_1}} \\ \frac{dS_2}{dt} &= -\frac{\mu X}{Y_{X/S_2}} \end{aligned} \tag{1}$$

where X, S_1 and S_2 are the concentrations of biomass, butyric acid and ammonia, respectively, while $Y_{X/S1}$ and

$Y_{X/S2}$ are yield coefficients of biomass to butyric acid and ammonia, respectively. The specific growth rate expression, μ, is described by two inhibitions functions in which the unionized butyric acid acts as both the rate limiting and rate inhibiting substrate. The expression also accounts for free ammonia inhibition and ammonium-nitrogen limitations, and is given by

$$\mu = \mu\max_1 \frac{[HBA]}{K_{HBA}+[HBA]}\left(1-\frac{[HBA]}{[HBA]_{\max}}\right)^{\alpha} * \left\{1+\frac{\mu\max_2}{\mu\max_1}\frac{[NH_3]}{K_{NH3}+[NH_3]+\frac{[NH_3]^2}{Ki_{NH3}}}\right\} \quad (2)$$

The first part of the equation dominates at low NH^+_4-N concentrations whereas the second one account for both observed undissociated butyric acid and free ammonia inhibitions. Here, *HBA* and NH_3 are the concentrations of undissociated butyric acid and ammonia, respectively. The affinity constants for NH_3 and *HBA* are denoted by K_{NH3} and K_{HBA}, respectively, while Ki_{NH3} is the inhibition constant for free ammonia. Finally, μ_{max} is the maximum specific growth rate.

IV. ARTIFICIAL NEURAL NETWORKS

The main attraction of neural networks over other forms of process representations is their versatility in mimicking non-linearities in the process. This is done to a far greater accuracy than most other forms of models. Although the individual components of the network are simple, it is the aggregation of these simple components which renders the methodology very powerful.

The basic element of an artificial neural network (ANN) –the neuron-is shown in Fig. 1. It is made up of a number of nodes and interconnections. The nodes represent "neuron-like" processing elements, and use a variety of nonlinear activation functions. In this work we use the sigmoid function:

$$f(z) = \frac{1}{1+\exp(-\lambda_j z)} \quad (3)$$

where λ_j is the learning gain of the sigmoid function.

The training algorithm is based on a neural network estimator and is given by (Karim and Rivera, 1992):

a) Determine available measurements (on-line or infrequent off-line) to be used by the model. This will define the number of inputs, *N*.
b) Determine which process variables should be estimated and /or predicted. This will define the number of outputs, *L*.
c) Define a training set consisting of *P* pairs of inputs/outputs vectors.
d) Select a network configuration of *N* inputs and *L* outputs.
e) Train the network off-line using a training set.
f) Test the network by presenting a set of inputs and observing predicted outputs.
g) Calculate error difference between predicted outputs and real outputs. Obtain mean square error as a performance index for the network.

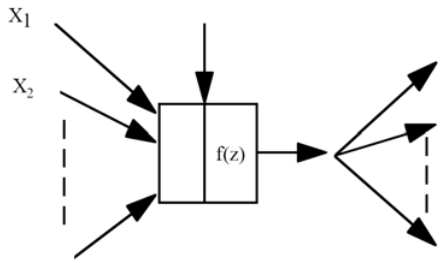

Figure 1. A simplified representation of an artificial network.

h) If mean square error is acceptable, continue. Otherwise, use a different configuration by repeating the algorithm from point 4.
i) Use the already trained network on-line and generate the desired variable predictions.

In this investigation the Levenberg-Marquardt method (More *et al.*, 1980) was used to calculate the weights in the network which minimize the squared errors between predicted and the actual network outputs. Nevertheless, many other architectures can be used according to the application sought (see for example Patnaik, 1999; or Lin, 1994).

V. MATERIALS AND METHODS

Strain. The yeast strain used was *Candida utilis* ATCC 9950.

Culture conditions. The growth medium was that used by Henry *et al.* (1983).

Inoculum. Inocula were prepared in 250 ml Erlenmeyer flasks, containing 100 ml of growth medium and placed on an orbital shaker (160 rpm) in a thermostated room (30 °C). The carbon and nitrogen sources were, respectively, glucose 10 g $liter^{-1}$ and $(NH_4)_2SO_4$ 0.5 g $litre^{-1}$. The pH was adjusted to 6 with 2 N NaOH before sterilization. Each inoculum was standardized by measurement of the optical density.

Culture apparatus. The cultures were grown in a 2 l LSL Biolafitte fermentor containing 1.5 l of Henry's medium aerated at a constant air flow of 1 vv^{-1} min^{-1} and mixed at 800 rpm. Temperature was controlled at 30°C and pH as required with 6 N HCl with a proportional regulator. The substrates used were butyric acid and ammonium sulphate at concentrations chosen as required. Inoculation was carried out using 75ml (5%vv^{-1}) of the precultures. Foaming was avoided by adding, initially, 1-2 ml of 5% (vv^{-1}) Sigma silicon emulsion.

Analytical methods. 5 ml samples were taken periodically and centrifuged at 15000 rpm for 15 min at 4°C and immediately deep frozen until required for analysis. Optical density (OD) was also measured immediately at 600 rpm with a Varian spectrophotometer. Non-inoculated culture medium was used as blank. To determine the dry weight of the microorganisms, 50 ml volumes from end exponential phase cultures were filtered through 0.5 λm Millipore membrane previously weighed, washed twice with distilled water and dried to a constant weight at 105 °C. Dilutions of the precultures were also made and the OD was measured. The calibration curve, permitting the correlations between the OD

with dry cell weight, gave a straight line. The OD was found to be linear from 0.1 to 0.8. If an OD reading was higher than 0.7, the sample was then diluted using distilled water. Butyric acid concentrations were measured by gas chromatography using a Chrompack CP 900 (flame ionization detector) with a semicapillary column (Shimadzu CR 3A). The injector and detector temperatures were 250 and 275 °C, respectively, the oven temperature was preprogrammed from 80 to 120°C at a rate of 10°C min^{-1} . Ethyl 2-butyric acid was used as an internal standard. The total time for gas chromatography separation and the integration using a nitrogen carrier at a flow rate of 335 kPa was 12 min for each sample. The ammonium-nitrogen concentration was determined using a Buchi 320 apparatus.

Determination of ammonia. Additional experiments were conducted to determine the NH_3 desorbed. The quantification of the NH_3 volatilized from the reactor was performed in the absence of microorganisms. During the experiments, the experimental conditions were identical to those used in inoculated cultures. The air leaving the reactor was recovered in a sulfuric acid trapping solution (2N) and ammonium-nitrogen was then determined in order to evaluate the N H_3 desorbed.

VI. RESULTS

Solution to the first principles model. The FP model simulations were carried out using the MATLAB program package (MathWorks, 2003). This model was solved by a numerical integration method (e.g. fourth order Runge Kutta) to determine concentrations of biomass, butyric acid and ammonium-nitrogen during cultures. To define the mathematical relationships between μ and component concentrations, data were fitted to the model using Bio-ASPRO, a software tool designed in our laboratory as an aid for bioprocess modeling and control. The resulting physicochemical parameters are listed in Table 1.

The ANN model structure. As in the previous modeling approach, the MATLAB program package (MathWorks, 2003) was used for carrying out the neural network model validation. The general structure of ANN used in this work was detailed outlined (Steyer *et al.*, 2000) and is shown in Fig. 2. The ANN employs four input nodes given by the operating conditions, pH and initial concentrations of biomass, ammonium-nitrogen and butyric acid, and three output nodes corresponding to the biomass, ammonium-nitrogen and butyric acid concentrations. The number of nodes in the hidden layer was selected by using a trial and error method that consists of selecting an over dimensioned number of hidden nodes and studying the evolution of some performance index as the number of nodes is decreased. The process of selection finishes when a topology is reached that gives a minimum value of the performance index. The criterion used consists of selecting the number of nodes which gives the minimum square identification error in a minimal number of iterations during the off-line training of the ANN.

Training of the neural network. Various batch experimental runs were conducted to provide information of the process behavior and to train the network. These runs were carried out at various pH values (6.5, 7.5, 8, and 8.4) and by using several initial butyric acid concentrations (2.5, 4.8, and 10.2 g $liter^{-1}$) and initial ammonia concentrations (0.08, 0.22, 0.52, and 0.6 g $liter^{-1}$). The ANN modeling results for the training data set are not shown in this work.

Performance evaluation of first principles and neural network modeling approaches. In the following sections, we have evaluated and compared the performance of the FP and ANN modeling approaches. Three study cases were chosen for such a purpose: I) a culture conducted under favorable operating conditions where maximum growth rate is achieved; II) a culture carried out at a high pH and III) a culture performed under starving nitrogen conditions.

Table 1. List of kinetic parameters for first principle model.

Parameter		Units
μ_{max1}	0.10	h^{-1}
μ_{max2}	0.07	h^{-1}
$Y_{X/S1}$	0.58	gg^{-1}
$Y_{X/S2}$	20	gg^{-1}
K_{HBA}	0.007	g $liter^{-1}$
K_{NH3}	0.0001	g $liter^{-1}$
Ki_{NH3}	0.05	g $liter^{-1}$
HBA_{max}	0.81	g $liter^{-1}$
α	0.2	
K_{TBA}	1.484×10^{-5}	

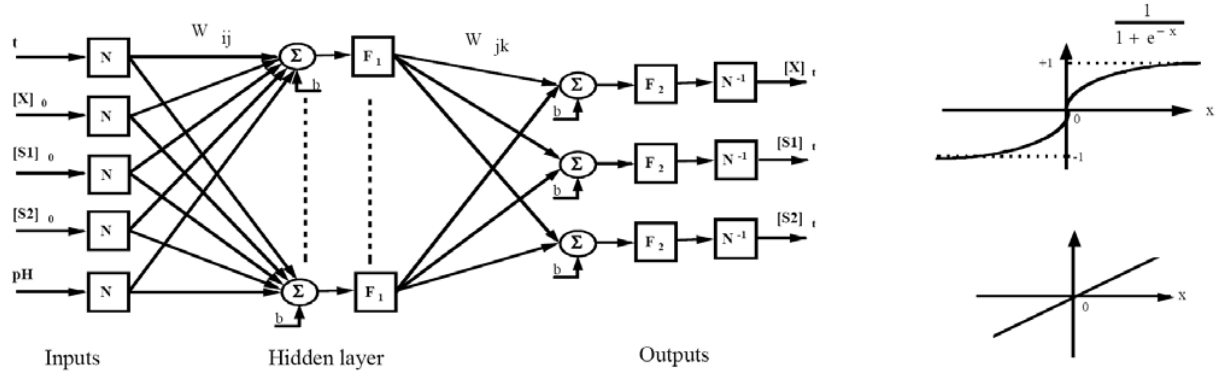

Figure 2. Structure of the artificial neural network for 1 hidden layer and 9 neurons, used to model the growth of *Candida utilis* in the new depollution process.

Case 1. Maximum growth rate culture. This case is illustrated by experiments conducted at moderate pH´s (6) where inhibition by TBA and/or NH3 is unlikely to occur (Pelayo-Ortiz *et al.*, 1997). Modeling and experimental results for butyric acid, ammonia and biomass concentrations are confronted in Fig. 3. It is evident that both modeling approaches were able to provide good estimates of the three output variables.

Case II. Culture at high pH values. This case corrsponds to an experiment carried out at pH 8, with an initial butyric acid concentration of 14.6 g liter^{-1} and an initial ammonia concentration of 0.35 g liter^{-1}. The estimated and experimental results for both modeling approaches are depicted in Fig. 4.

It can be seen that the ANN estimate is representative of the underlying bioprocess behavior. The figure also shows the network ability to recognize patterns for

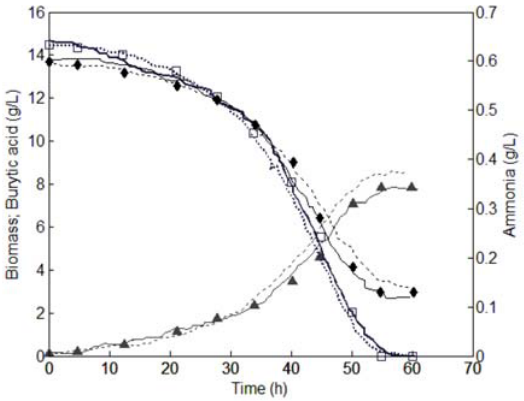

Figure 3. First principle and ANN simulations of *C. utilis* growth on butyric acid and ammonium-nitrogen in a batch reactor under favorable environmental conditions. The dashed curves represent values calculated using the first principle model, the solid curves represent values calculated using the trained ANN model and the symbols represent experimental data (biobiomass (▲), butyric acid (□), NH_4^+-N (♦)). Initial conditions: [TBA] = 14.5 g liter^{-1}, [NH_4^+-N] = 0.6 g liter^{-1}.

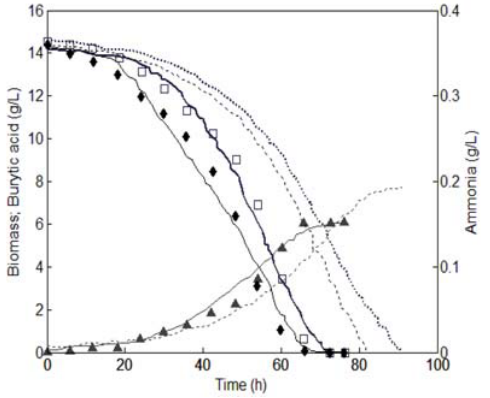

Figure 4. Simulations of C. utilis growth on butyric acid and ammonium-nitrogen in a batch reactor without considering loss of ammonia by stripping. The dashed curves represent values calculated using the first principle model, the solid curves represent values calculated using the trained ANN model and the symbols denote experimental data (biobiomass (▲), butyric acid (□), NH_4^+-N (♦)).

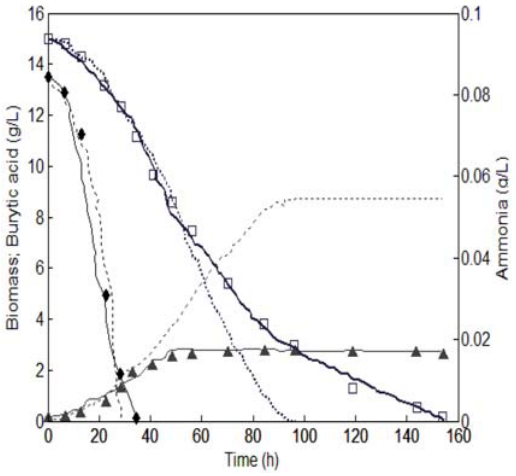

Figure 5. Comparison of experimental data of a nitrogen limited *C. utilis* culture with calculated values from the models. The dashed curves represent values calculated using the first principle model, the solid curves represent values calculated using the trained ANN model and the symbols represent experimental data (biobiomass (▲), butyric acid (□), NH_4^+-N (♦)).

which it was not trained for. On the other hand, one can see that the FP modeling approach was no longer applicable to the system. Note also that the dynamic response of the model for the biomass concentrations was satisfactory only at the early stages of the culture but it deteriorated as the same one progressed. The main reason why the FP simulation curves did not give a better agreement is the effect of pH on the culture was not accounted for in the model. In a previous study, Pelayo-Ortiz *et al.* (1997) showed that an increase of pH results in a decrease in the concentration of NH_4^+-N. Therefore, it is reasonable to expect a transition of NH_4^+-N to NH_3 and then the liberation of this gas from the culture. For the first principles model to be success fully applied, one must incorporate in the mass balance equation for NH_4^+-N, a term reliant the rate of NH_3 transfer in the liquid and gas phases which demands knowledge of the mass transfer coefficient, k_La.

Case III. Experiment under nitrogen-limiting conditions. This culture was conducted at pH 7.5 with initial butyric acid and ammonia concentrations, 15 and 0.08 g liter^{-1}, Fig. 5 illustrate the performance comparison of both modeling approaches.

The ANN, on the one hand, yielded perfect results and showed excellent recognition properties of complex *C. utilis* culture patterns. In contrast, the FP model was not able to predict the dynamic behavior of biomass and butyric acid concentrations under nutrient starvation conditions. It is clear that this operating condition produced a shift in the yeast metabolism which may have induced the accumulation of storage lipids or reserve polymers (Yamauchi *et al.*, 1983; Anderson and Dawes, 1990). In order to have better estimate for this complex culture, it is necessary to conduct supplementary studies to identify the synthetic products formed and to include their mass balances in the FP model.

VII. DISCUSSION

First principle and artificial neural network modeling approaches have the same final goal: they provide useful tools in simulation, experimental design, optimization and control of biotechnology processes. However, the construction of a model from FP or by using a particular ANN methodology constitutes two different tasks. On the one hand, FP modeling of bioprocesses demands thrust knowledge of physical and biochemical mechanisms of the process. FP models, like the model presented in this work, are of particular interest to biochemists and microbiologists since the kinetic parameter involved in the model may have physical meaning (specific growth rate, inhibition constants, conversion yields of the substrates, etc.). FP make it possible to model various types of mode reactor (fed-batch or continuous) without changing the structure of the model. Nevertheless, these models require knowledge of such parameters which sometimes are difficult to identify and estimate, particularly if these parameters are uncertain or time-varying.

On the other hand, modeling of bioprocesses by using ANN involves features which make it easily implemented in practice once the network structure selected (number and type of neurons, number of hidden layers, number of iterations, etc) has been adapted to the proposed problem. This approach, however, has some limitations. The parameters involved in the resulting model do not have any biological or physical meaning and hence, they do not give any insight into the mechanisms governing the process. Furthermore, these models are trained with a specific experimental data and therefore, they are not able to predict the dynamic behavior of the bioprocess in a different process configuration.

VIII. CONCLUSIONS

In this comparison study we showed that eventhough, the first principle and artificial neural network modeling approaches have some limitations, they are complementary. From the results presented here, it is clear that the first principle modeling approach must be selected when the process is well understood while the artificial neural network approach should be applied in cases where a detailed knowledge of the process mechanistic relationships are not available. At present, we are developing a hybrid approach (introducing artificial neural networks into the mechanistic model) to enhance modeling predictions and to solve the difficult modeling problem of the proposed depollution problem.

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