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