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ARTIFICIAL NEURAL NETWORKS USED FOR THE SIMULATION OF THE BATCH FERMENTATION BIOREACTOR

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ABSTRACT. The paper presents the modelling results of the batch alcoholic fermentation bioreactor using both the first principle and the Artificial Neural Networks (ANN) approach. For the nonlinear fermentation process the first principle model validated with experimental data considers for the biomass the Monod and for substrate the Bovée and Strehaiano models, including the temperature influence. It has been used for the ANN model development. A design and training methodology is proposed for statistical modelling based on artificial neural networks. Comparison between the two models is performed revealing the incentives of the ANN modelling method for reducing the computational time and sparing the computer resources.

Keywords: alcoholic fermentation, Artificial Neural Networks, modelling

INTRODUCTION

Winemaking technology is a complex process implying a succession of operations affected by the large variety of must and microbiota. The grape juice transformation into wine is substantially influenced by the wine makers' tradition and processing techniques are usually emerged from their experience [1]. Investigation of the mechanisms and phenomena lying behind the alcoholic fermentation is difficult as the stoichiometry and kinetics of the biochemical processes are only possible by lumping the numerous involved components and due to the need for simplifying the biomass characterization [2]. The oenologists claim that organoleptic properties of the wine are also dependent on the alcoholic fermentation in a very complex relationship [3, 4].

The alcoholic fermentation of wine is a biochemical process of transforming the sugar into alcohol and CO_2. Metabolites are the result of enzymatic reactions for the different metabolic paths [5]. Kinetics of the enzymatic reactions, as well as of the chemical reactions, is influenced by a set of factors. The most important of them are: composition of the culture medium, concentration of the limiting substrate, temperature, pH, concentration of the dissolved oxygen and stirring intensity. Setting optimal conditions for the

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development of the fermentative process is directly related to the knowledge of the way of influencing the enzymatic reactions. Interaction between variables is strong as the change of a single parameter may affect the all the others [6].

Due to all these aspects the need for building reliable models is obvious and is highly appreciated as they may serve for better understanding the intrinsic processes and consequently, for optimizing the wine production according to the desired criteria [7, 8]. The first principle modelling allows logical description and interpretation of the involved phenomena, on the expense of a substantial modelling effort and with possible errors. Development of the analytical models is complex and time consuming as they imply a good knowledge of the phenomena and processes taking place inside the modelled system. Statistical mathematical models (such as the Artificial Neural Networks models) are based on observation data and measurements originating from the process. The statistical models require less effort and may reduce the modelling errors if an appropriate set of data is available [9-11].

In this paper a new statistical model based on Artificial Neural Networks (ANN) is proposed as an alternative to the first principle modelling of the alcoholic fermentation process performed in a batch bioreactor. Comparison between the first principle and ANN modelling results is performed, showing the benefits of the proposed ANN approach.

RESULTS AND DISCUSSION

A previously developed first principle model was available and used to generate the sets of input-target data further employed for training the ANN. The detailed analytical model used in the present work is described in [12]. This model has been validated with experimental data. Each of the biomass latent, exponential growing and decline phase has been described. Consequently, specific kinetic models of the biomass, substrate and alcohol have been considered. For substrate consumption the Bovée and Strehaiano model has been used [13]. Heat balances for the bioreactor vessel and jacket have been also accounted for.

This ANN based modelling approach has been considered as the first step for investigating the capability of designing and training an ANN model of the fermentation bioreactor. The developed ANN model design and training procedure may be considered as a prerequisite for the future step consisting in building the ANN dynamic simulator based on pure experimental data.

As the aim of the study bas been the development of a dynamic simulator of the alcoholic fermentation process, the following main process variables have been selected to demonstrate the time evolution of the process: substrate (glucose) concentration, biomass (Saccharomyces cerevisiae) concentration, alcohol concentration, reactor temperature and jacketed reactor cooling agent temperature. The ANNs based models have been designed and trained for revealing the dynamics of the five previously mentioned process variables, as a result of starting from different initial conditions of the batch fermentation

process. These initial conditions are specified by the subsequent variables: reactor inventory initial temperature, substrate initial concentration and biomass initial concentration. A sampling time of 3 hours has been considered for all process variables. One distinct ANN has been developed for each of the five process variables. Each of these ANNs has 3 inputs (the initial conditions) and 68 outputs. The outputs are the values of the respective process variable at the 68 moments of time multiples of the sampling time (starting with moment 0 h and finishing with moment 201 h). Two hidden layers with 3 and 4 neurons were used.

The set of training and testing data consists in 546 *input-desired output* pairs of data. The main part (75%) of the available set of data has been used for the training and validation step of the ANN model building. A quarter (25%) of the set of data has been used for testing the already trained ANN. Training and validation subset of data has been further divided: 75% of data was used for training and the rest for validation [14].

Following the training and validation step, the first testing step has been performed in order to assess the quality of the trained ANN. This testing step has been carried out on the set of input-desired output pairs of testing data not involved in the first training and validation step. Results obtained by the trained ANN on the set of testing data show a good quality of the training phase, as the correlation coefficients (R-value) for the set of ANN simulated and desired output (targets) sets of data are close to unity. They are not presented in the paper due to space saving reasons and to the next more comprehensive test.

The second testing step and more ample assessment of the prediction ability of the trained ANN have been performed for a new set of input data not yet used during the previous training-validation-testing steps and comparison with the analytical simulation results has been accomplished. These comparative first principle and ANN model simulations used random chosen initial conditions consisting in the following particular values: reactor inventory initial temperature $T_0=299\ K$, substrate initial concentration $S_0=190\ g/l$ and biomass initial concentration $X_0=0.75\ g/l$.

The comparative results between the analytical simulation and ANN simulation results, obtained for the five investigated process variables, are presented in Figures 1 to 5.

The simulation results reveal a good training procedure of the ANN, demonstrated by very close values of the bioreactor main process variables obtained with the first principle and the ANN models. For the substrate concentration, alcohol concentration and reactor inventory temperature the simulated evolutions of the variables are almost identical. For the biomass concentration and cooling agent temperature variables almost identical values have been also obtained for the periods of time when the change of these variables is reduced. For the time interval when the two previously mentioned variables have large changes in time, such as the time interval between 30h and 45 h, some differences may be noticed. But these differences, featuring in fact reduced relative errors, are mainly caused by the use of a relative large

sampling time compared to the time interval when the involved variables show large changes in time. It is expected that by reducing the sampling time these not essential differences to become smaller. According to the obtained results it may be appreciated the good fit between the ANN model and first principle model behaviour.

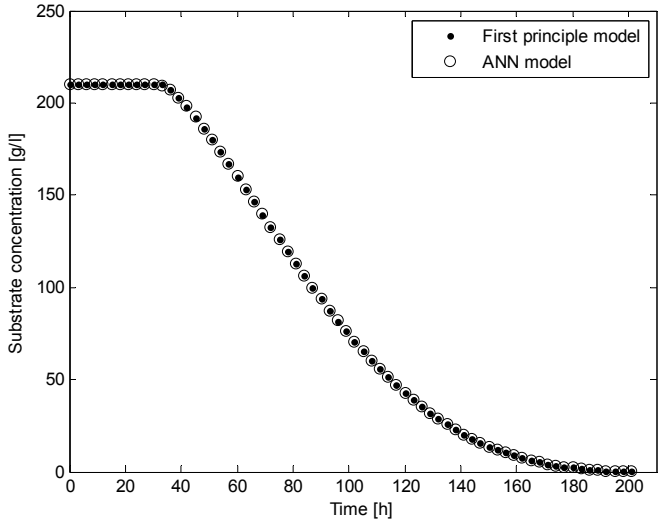

Figure 1. Comparative simulation results obtained by the first principle model and the ANN model, for the substrate concentration variable

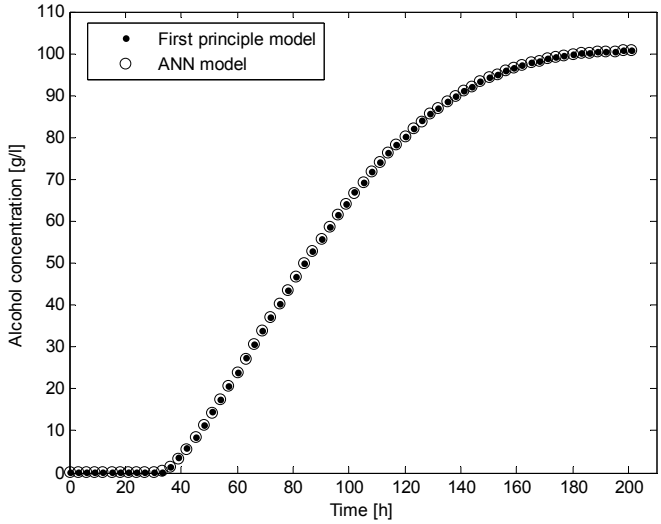

Figure 2. Comparative simulation results obtained by the first principle model and the ANN model, for the alcohol concentration variable

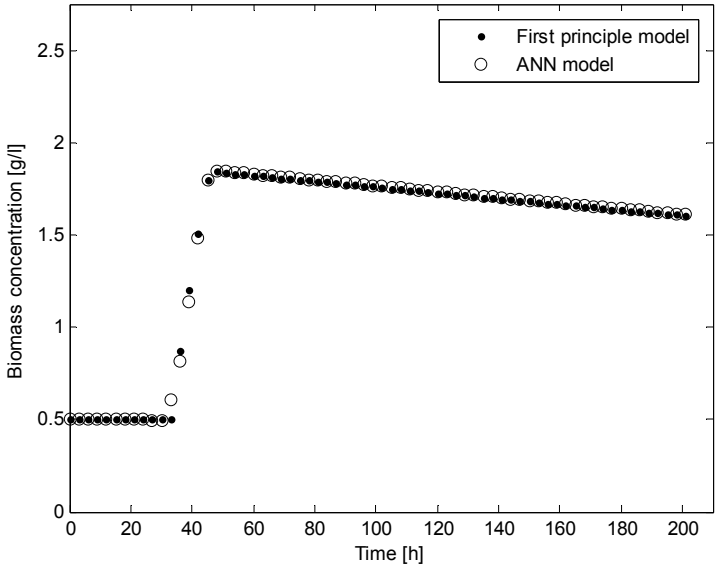

Figure 3. Comparative simulation results obtained by the first principle model and the ANN model, for the biomass concentration variable

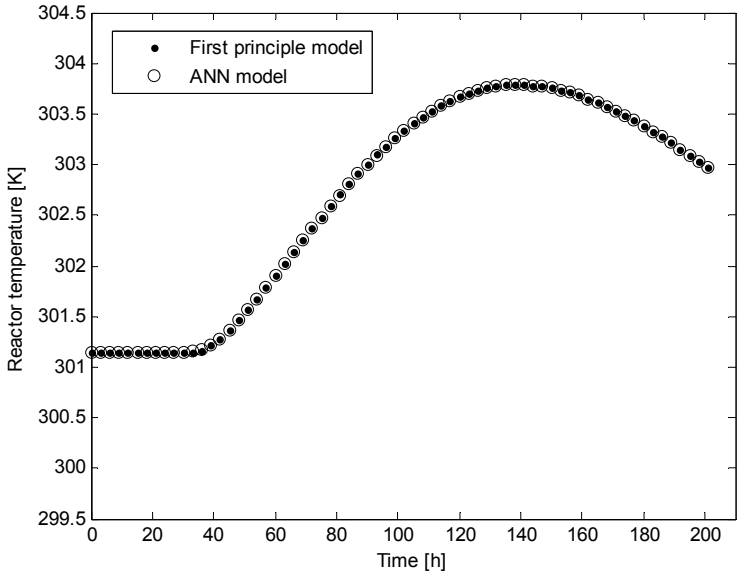

Figure 4. Comparative simulation results obtained by the first principle model and the ANN model, for the reactor temperature variable

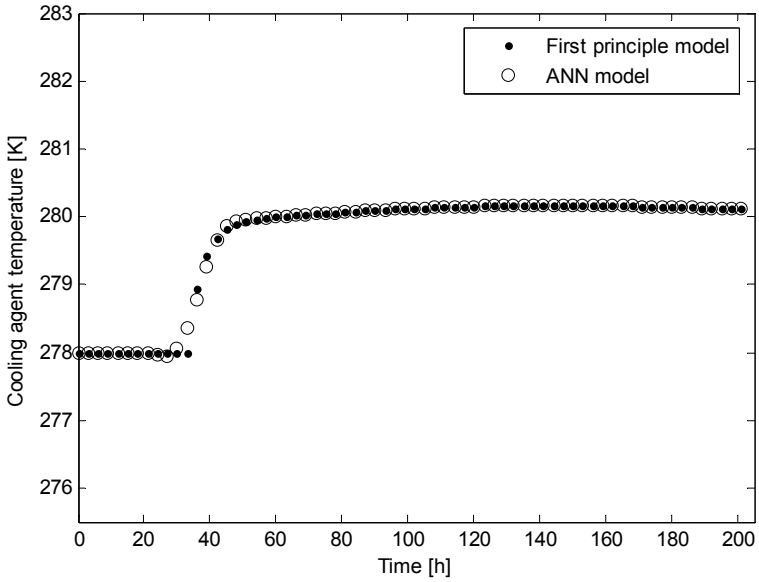

Figure 5. Comparative simulation results obtained by the first principle model and the ANN model, for the reactor cooling agent temperature variable

CONCLUSIONS

The paper presents the simulation results of successfully using Artificial Neural Networks for modelling the dynamic behaviour of the alcoholic fermentation bioreactor main process variables. The way the ANN has been designed and subsequently trained proved to be efficient for obtaining a useful dynamic simulator. The reduced relative errors proved by the good fit between the desired process outputs and the ANN simulated outputs are proofs of the ANN performance. Incentives of the ANN based model consist in the development of an efficient methodology of building the ANN model of the complex alcoholic fermentation bioreactor associated to the reduced modelling effort. The ANN model may exclusively rely on experimental data and implicitly does not imply comprehensive knowledge of the detailed physical, chemical and biological first principle description.

Another main advantage of the ANN based modelling consists in the important reduction of the simulation time (exceeding one order of magnitude), hence resulting in an efficient management of the computing resources. This incentive may become much appreciated for its potential use in bioreactor real time control applications based on mathematical models where implementation feasibility is very challenging.

EXPERIMENTAL SECTION

The ANN architecture for the batch alcoholic fermentation process consists in a feedforward ANN having four layers (one input, two hidden and one output layers), for which the weights and biases have been trained according to the backpropagation training algorithm [15]. The number of neurons in the hidden layers (4 and 3) has been set on the basis of a heuristic procedure, as a consequence of the errors analysis performed during the repeated training steps. The neurons transfer function in the hidden layers has been selected to be *tansig* (hyperbolic tangent sigmoid) and for the output layer *purelin* (linear). The quasi-Newton type Levenberg-Marquardt algorithm has been used for training the ANN. Overfitting has been avoided by early stopping, improving the generalization capability of the ANN.

During the repeated training sequences, random initial values have been used for the ANN weights and biases in order to prevent convergence to local minima. The input and desired output sets of data have been scaled (based on minimum and maximum values) and principal component analysis has been used for improving the computation precision and training performance.

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