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Application of neural networks for controlling and predicting quality parameters in beer fermentation

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The biochemical pathways involved in the production of ethyl caproate, a secondary product of the beer fermentation process, are not well established. Hence, there are no phenomenological models available to control and predict the production of this particular compound as with other related products. In this work, neural networks have been used to fit experimental results with constant and variable pH, giving a good fit of laboratory and industrial scale data. The results at constant pH were also used to predict results at variable pH. Finally, the application of neural networks obtained from laboratory experiments gave excellent predictions of results in industrial breweries and so could be used in the control of industrial operations. The input pattern to the neural network included the accumulated fermentation time, cell dry weight, consumption of sugars and aminoacids and, in some cases, the pH. The output from the neural network was an estimation of quantity of the ethyl caproate ester.

Keywords: neural networks; predictive control; beer fermentation; ethyl caproate

Introduction

In order to obtain satisfactory industrial process performance, the maintenance of operating conditions at designed values is required. Because of unpredictable disturbances which invariably enter a process and also as a result of chemical changes within the process, control action is usually required if the specified conditions are to be maintained. Sometimes it is possible to improve bioreactor performances by varying process conditions such as temperature or pH in a predetermined manner while the reaction is taking place.

Two approaches to a fermentation control system can be considered: one mechanistically based, where the metabolism of the product needs to be known perfectly, and the other that implies treatment of the data in a statistical way. In our case, the latter has been the one considered although some available biochemical information was also considered. From another point of view, two different major types of control, static and dynamic, are usually considered [15] and among the latter, two new types can be considered: predictive and on-line dynamic. The predictive type needs some initial data in order to predict the evolution of the process. The on-line dynamic model requires continuous measurement of some of the properties of the process in order to be related to a controllable magnitude. This type of control means that the process can be studied continuously and therefore can be modified at any time. In our case, the pH could be the data to be monitored continuously.

Neural networks theory developed in the 1950s and is now one of the most active fields within the domain of artificial intelligence. Neural networks have a number of applications such as control of processes [7,11], interpretation of sensors, dynamic models and robotics. There are some examples of the application of neural networks technology to the modelling of the dynamics of biological process and of the evolution of fermentation variables [16–18]. In this sense, Thibault *et al* [17] studied the biomass and substrate evolution in a fermentation tank as did Zhang *et al* [18], while Simutis *et al* [16] applied the neural network to another specific example: alcohol production during industrial beer production. Lately, Glassey *et al* presented their results working with an industrial recombinant fermentation [6].

In a previous work [3], we successfully predicted the production of certain esters in industrial beer fermentation by *Saccharomyces carlsbergensis*. Ester production was analysed using knowledge of the metabolic pathway to establish a kinetic model at different constant temperature and pH values, and to predict results in an experiment with freely changing pH. However, in the case of ethyl caproate, which is produced in small amounts but of interest because of its flavour in the beverage [1], no kinetic equation was obtained because the metabolic pathway is not well known, and prediction was not possible. The advantage of employing neural networks lies in the fact that, without having exhaustive knowledge of the processes involved, the network can learn from previous experiences in order to predict the system behaviour when some variables are modified.

In this work, the essential characteristics of neural networks will be introduced, to go on to build up the network with the adequate structure for analysing ethyl caproate production during the beer fermentation process at laboratory scale. A similar study was later carried out for experiments at variable pH, this being included as an input parameter of the network and predictions for the constant pH networks are compared with the variable pH experiments.

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Finally, the neural network fitted with laboratory scale experiments at variable pHs was applied to the prediction of industrial brewery fermentations and compared with the brewery results. It is worth pointing out the necessity of developing evaluation processes, such as these neural networks, for their application in control systems and industrial predictions. The design of a neural network for controlling and predicting the evolution of the desired products is a valid option in the elaboration of a model for the microbiological process which can be applied at an industrial level.

Control considerations

i) The problem statement

Beer fermentation is a process in which a great number of secondary products are obtained. Among these, diacetyl, fusel alcohols and esters are of great importance, decisively influencing the final flavour of the beer. The main factors affecting beer fermentation are the strain of yeast employed and the wort characteristics (mainly fermentable sugars and aminoacids). Such parameters as pH, temperature and even agitation must also be considered, because, depending on their initial values and evolution, the final concentration of these compounds will be quite different.

If the metabolic pathways of these compounds are known, it is possible, in conjunction with the experimental data on nutrient consumption and product formation, to obtain kinetic models at different constant temperature and pH values that allow us to control and to predict their behaviour during the beer fermentation process. This has been previously done at laboratory and industrial scales [3–5]. However, when the metabolic pathway of production for a compound is not well known, it is not possible to work in this way. This is exactly the case for ethyl caproate, and so neural networks technology offers a way of working out its control and predicting its production.

ii) Description and elaboration of a neural network

A neural network is formed by a number of layers of interconnected units: the neurons. The first layer is made up of as many input variables as exist in the process to be simulated, adding an additional neuron with a constant input, the usually denominated bias [12]. If we indicate the input in the k^{th} neuron of the first layer as i^1_k, the data are transferred, by linear connections with weights w_{jk}, to the next layer of neurons, so that the input to the j^{th} of the second layer will be: $i^2_j = \sum_k w_{jk} i^1_k$.

In this work, neural networks of three layers are considered, which is usual for this type of application [6,16–17]. The second layer being known as the hidden layer and the third corresponding to the variable outputs. The inputs to the second and the third layers are processed by a sigmoidal function type, so the outputs of the second layer will be written as: $o^2_j = 1/[1 + \exp(-i^2_j)]$. These outputs are once more linearly combined with weights $\bar{w}_{ij}$ and are finally processed by the last layer, thus obtaining the values of the output variables generated by the net, o^3_i. These values will depend on the weights assigned to the connections.

The selection of the input and output variables will depend on the process to be simulated; the first to be considered being data which are known and easily controlled, and the second, data whose prediction is of interest. Of course, the fundamental thing is to try to reproduce a real process. Therefore, the aim is to obtain, from experimental data of the input and output variables achieved in a set of experiences, the values of the weights that minimise the average quadratic error between the experimental values of the output variables, o_i, and those generated by the network from the experimental data of the corresponding input variables, o^3_i. This error will take a value of $\sum_i (o_i - o^3_i)^2$ for each group of data, it being necessary to add the errors achieved in all the experiences made.

Usually, the minimisation is carried out by employing the generalised delta rule [6,9–13]. This method consists of the modification of the initially random chosen weights by means of a mechanism of retropropagation, using a descent gradient method. This technique has been used for chemical engineering [7] and for fermentation [17] processes. In our case, the method of the conjugate gradient [2] was chosen, because it proves much more efficient [10] when working with conventional computers. This technique also offers a quicker and safer convergence towards the minimum values of the quadratic error.

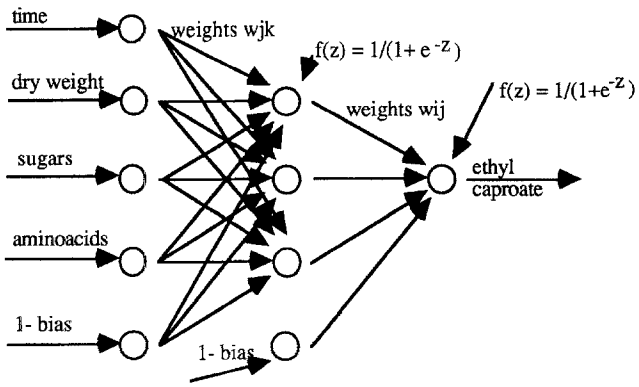
As can be seen, this neural network offers a black box technique for data fitting: if the weights that minimise the error are chosen, afterwards it is possible to make predictions with these weights about the behaviour of the process when the input data are changed, which is a very interesting alternative. The experience with neural networks shows that the network is able to learn very complicated mechanisms in a natural way without requiring knowledge of the structure of the model.

Initially, ethyl caproate production was studied in a laboratory fermenter at a constant pH. Experiments were carried out at pH 3.56, 4.00 and 5.02; the following parameters being considered as input variables: time, dry weight, sugar and aminoacids concentration, while the output variable was the concentration of ethyl caproate. A neural network was designed for each pH and our networks were formed of three layers with five neurones in the first layer, corresponding to the inputs and to the bias, four neurones in the second layer, one of them with a constant input (bias), and only one neurone in the third layer, corresponding to the ethyl caproate concentration. The resulting neural network is shown in Figure 1.

As there is no clear description in the literature as to how many neurones the second layer should contain, after some initial trials the most suitable alternative in terms of rapidity and effectiveness was chosen. In a second stage in the design of a neural network, the pH was included as an input variable, the same procedure being followed, except that this network has an additional neurone in the first layer, corresponding to the pH.

Material and methods

The microorganism was a lager production strain of *Saccharomyces cerevisiae* provided by the former brewery 'El



f(z) = Activation function

Figure 1 Neural networks for the beer fermentation process at a constant pH

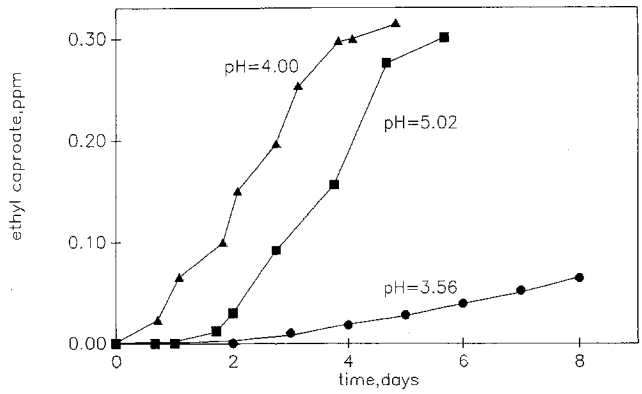


Figure 2 Ethyl caproate production at three different pHs (●,■,▲), and their respective fittings without including the pH as an input variable (continuous line)

Aguila Negra' in Spain. The yeast cells were cultured in a natural wort medium at 12° C (initial conditions; pH = 5.1; °B = 11.8). The culture procedures at both laboratory and industrial scale were described previously [3–5]. The method employed for obtaining the experimental data relative to the pH, the microorganism dry weights and the sugars and aminoacids content of the wort, at both scales, have also been described [3–5].

The culture at a laboratory level was carried out in a 5-L laboratory fermenter (New Brunswick Scientific Co, Inc, BIOFLO III) with external agitation (150 rpm). The pH was kept constant, if required, by automatic addition of 0.01 mM NaOH. The medium was initially saturated with oxygen (9 ppm). Cultures were also carried out in a 2×10^5-L (3.5 m in diameter and 18 m in height), industrial, non-externally agitated, cylindro-conical fermenter. In this case the inoculum was added to the fermenter in several loads at the same time as the wort. The temperature of fermentation was in all cases 12° C.

Ethyl caproate was determined by gas chromatography (Perkin-Elmer 8600) equipped with a flame ionisation detector as follows: 100-ml samples, previously degassed, with an internal standard of *n*-butanol were kept at 40° C for 1 h. A volume of 3 ml of head space was directly injected into a Carbowax 1540, 8% chromosorb W-AW-HMDS-98-100 column 4 m long and 2 mm in diameter. The column temperature was initially 50° C and was then raised 4° C min^{-1} to 120° C. The results presented are always the mean of at least three assays.

The neural network calculations were carried out with a PC 486, at 66 MHz. The programs were written in FORTRAN and optimization routines based in the conjugate gradient method [2,8–14] were used to minimize the error function. The convergence to the minimum values of the quadratic error was quick and safe in all the cases.

Results and discussion

a) Neural networks application in fermentation at laboratory scale

When fermentations were carried out in 5-L stirred tanks, ethyl caproate was produced from the beginning of the fermentation, accompanying the production of ethanol (data not shown), giving a concentration of 0.043 ppm in one day and a half, and reaching values of 0.314 ppm at the end of this primary fermentation. This pattern of production is equal to that offered by the other esters usually produced in beer fermentation, increasing in parallel to the decrease observed in the consumption of fermentable sugars and aminoacids, the main sources of carbon and nitrogen, respectively.

a.1) Fitting at constant pH without pH inclusion: The first step was to initiate the connections with random weights and to look for the minimum of the error function by employing the method of the conjugate gradient. For distinct initial weights, a convergence is obtained at different local minima. We keep the local minima which produce a nearly perfect fitting to the experimental data, Figure 2, and discard those which give big errors. The chosen minima will be used later in the prediction (section *b.2* below).

As an example, the weights for pH 4.00 that minimise the error are presented in Table 1. In Formula 1, the weights for the connections between the first and the second layer appears as a matrix, while Formula 2 indicates the corresponding weights between the second and the third layer.

a.2) Fitting at constant pH including this as an input: The design of a neural network, incorporating the pH as an input variable, was also carried out. This network includes an additional neuron in the first layer and an attempt was made to fit all the data obtained at the constant pHs of 3.56, 4.00 and 5.02. To summarize, we train this neural network with all the data obtained at the different constant pHs. The fitting achieved was not as good as that

Table 1 Weights for pH 4.00 that minimise the error

Formula 1.	w_{jk}			
−0.9939	−0.1072	−0.0048	2.2923	1.4450
−0.4378	0.3291	−1.2872	−0.2584	−0.0034
3.2847	1.1856	−0.1010	2.5868	1.5846
Formula 2.	$\bar{w}_{ij}$			
−1.8120	−0.0042	4.8955	−5.6030	

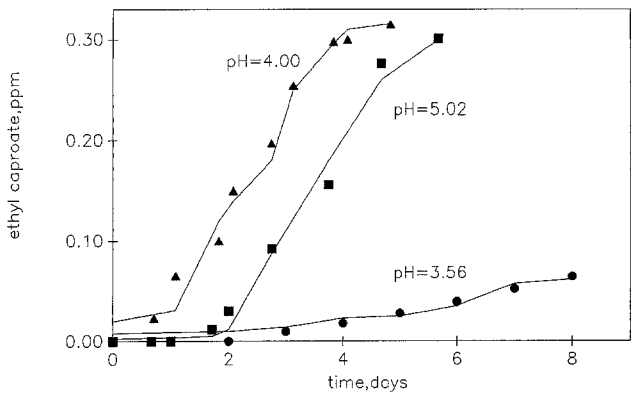


Figure 3 Ethyl caproate production at three different pHs (●,■,▲) and their respective fittings including the pH as an input variable (continuous line)

obtained in *a.1*, when a single network is considered for each pH, since all the data now have to be reproduced by a single network. In this case, 22 connections among neurons were achieved instead of the 19 previously obtained. The fitting of the data obtained with this neural network is presented in Figure 3.

b) Predictions of laboratory experiments at variable pH

It must be taken in account that when the pH is allowed to evolve freely, some physiological changes will appear which will add major complications to the predictions. Nevertheless, experiments at a variable pH had been previously carried out [3–5] and the results obtained have now been used in this work for testing the possible application to the prediction of a beer laboratory fermentation at a variable pH.

b.1) Prediction using the neural network including pH as an input: The experimental pH values were introduced in the neural network obtained in *a.2* and this was then used to simulate ethyl caproate evolution. The single neural network was built by taking all the experimental laboratory data at the three different pHs assayed and afterwards, in order to make the prediction, all the data at variable pHs were introduced to the neural network. In Figure 4, pH evolution is shown together with the predicted and experimental laboratory data for ethyl caproate; a reasonably good fit was obtained.

When trying to predict experimental results, the problem arises that different local minima give rise to a similar fitting with very similar errors, producing different predictions at variable pHs. Some predictions, such as those presented in Figure 4, are quite good, while others are not as good. Thus, many data are needed for training the network and selecting *a priori* the most adequate weights in order to make the prediction. This last simulation presented was accomplished by introducing different pH values at each time, but less information will be needed if an acceptable prediction could be achieved using a neural network with constant pH, as indicated in the next section.

b.2) Prediction at variable pH using the networks at constant pH: An attempt was made to reproduce the results obtained at a variable pH using the networks designed for constant pHs. The prediction of experimental results, changing the operation conditions used in the fitted networks, is not the usual application of the neural networks. With this in mind, experiments at a variable pH were also carried out [3–5] and the results of section *a.1* were used to test the possible application of constant pH experiments for the prediction of a beer laboratory fermentation at a variable pH. The experimental results of ethyl caproate evolution in laboratory fermenters when the pH was not fixed and the predictions achieved using the neural networks of the different fermentations at the distinct constant pHs are shown in Figure 5.

Taking into account changes in pH with time, predictions at a constant pH of 5.02 are compared with the data for ethyl caproate obtained at the beginning of the process and predictions at pH 3.56 with the data at the end. Predictions achieved at pH 4.00 are presented all through the process. The excellent agreement achieved between the predictions obtained with the neuronal network at pH 4.00 and the experimental data at a variable pH is noteworthy, particularly at the end of the process and, globally, follows the tendency of ethyl caproate evolution, even though a considerable error is obtained at intermediate times. This accord is common with different weights that provide very similar local minima.

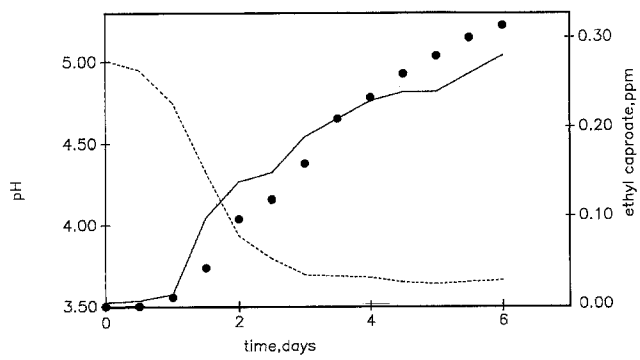


Figure 4 Ethyl caproate production (●) at variable pH, and the corresponding prediction from the neural network considering the pH as an input variable (continuous line). pH evolution is also shown (discontinuous line)

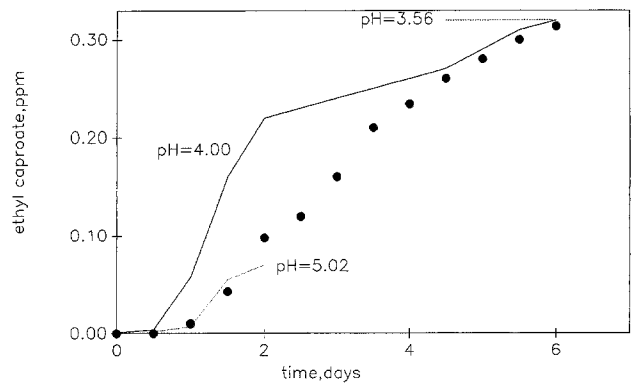


Figure 5 The production of ethyl caproate (●) at variable pH, and the three corresponding predictions from the neural networks considering three different constant pHs

c) Analysis for the control at industrial scale

It is important to evaluate the possibility of using the experimental data obtained in fermentations at a laboratory level for the elaboration of neural networks able to predict adequately the results obtained in industrial breweries. In order to do this, industrial fermentations have been carried out and the results analysed. The shape of the curve that can be plotted from the experimental results (Figure 6) is quite similar to that obtained in previous laboratory experiments, although a delay of two days was found in the industrial bioreactor. Thus, the final values of 0.300 ppm of ethyl caproate were reached on the 8th day of the fermentation instead of on the 6th as happened with the laboratory conditions. This delay has been attributed mainly to loading strategies in the industrial plant and to the absence of agitation that happens in the industrial fermenter at the beginning of the process [3–5].

c.1) Fitting at industrial scale: The design of a neural network, incorporating pH as an input variable, in the same way as described previously for the laboratory scale, has been carried out for ethyl caproate during a fermentation process in a 2×10^5-L industrial bioreactor. The same initial conditions as in previous laboratory experiments were employed, and the pH value was of course not fixed. The fitting of the data obtained at an industrial scale to this new neural network is also presented in Figure 6; an excellent fit was achieved.

c.2) Prediction using the networks at laboratory scale: The prediction of this beer fermentation process at an industrial scale from data obtained at a laboratory scale and at variable pH is of great interest. The prediction initially obtained for the evolution of ethyl caproate carried out in this way using the experimental laboratory data, was not satisfactory at all because the existing delay observed between both fermentations had not been taken into account. Therefore, two days were added to the laboratory data in order to carry out the prediction. The resulting prediction achieved is presented in Figure 6, and the fit was very good for most of the process. The results presented here are encouraging since they allow us to make consistent predictions based on previously-designed neural networks.

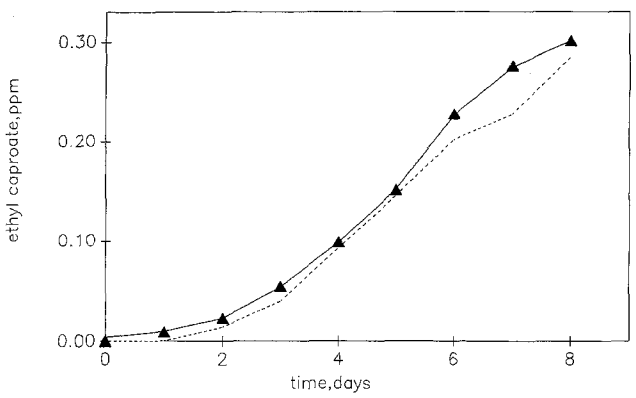


Figure 6 Ethyl caproate production at an industrial level (▲) at variable pH, and the corresponding specific neural network fitting (solid line). The discontinuous line corresponds to the prediction based on the neural network elaborated from the laboratory experimental data at variable pH

Final remarks

In this work, we have dealt with the application of the neural networks technique to the control and prediction of a fermentation process such as beer production for which a detailed mechanistic mathematical model was not available due to the complexity of the reactions involved. Neural networks have proved to be a good substitute for the phenomenological models when fitting the evolution of ethyl caproate to the experimental results obtained during the beer fermentation process, at both laboratory and industrial scales, and therefore may be applied in the control process, both at constant and at variable pH, with or without pH as an input parameter.

When experimental data, obtained at laboratory level and at variable pH, were used to predict these data using the networks at constant pH, the results achieved were quite good. The difficulty that appears when using this approach must be taken in account, which is mainly due to physiological changes that the yeast cells will undergo when incubated at constant or varying pH. This will affect the predictions of the experimental results obtained at variable pH when the neural networks were designed using experiments at constant pH.

Finally, free pH experimental data obtained at a laboratory level (5-L stirred tank) were used to achieve suitable neural networks to be employed in the control of industrial fermentations (2×10^5-L tank). In this case, and due to the two-day step-by-step way of loading of these industrial fermenters which means a low initial level of agitation, a delay time must be introduced with respect to the laboratory process. When this delay time is considered, an even better prediction for the industrial process than that previously obtained at the laboratory level is achieved, although in that case the prediction was made based on neural networks built using constant pHs.

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