Bioautomation, 2005, 2, 1-7 ISSN 1312-451X

Application of a Fuzzy Neural Network for Modeling of the Mass-Transfer Coefficient in a Stirred Tank Bioreactor

Mitko Petrov[*1], Tatiana Ilkova[1], Stoyan Tzonkov[1], Uldis Viesturs[2]

[1]*Centre of Biomedical Engineering "Prof. Ivan Daskalov" - Bulgarian Academy of Sciences, 105, Acad. George Bonchev Str., 1113 Sofia, Bulgaria*
E-mail: mpetrov@clbme.bas.bg

[2]*Latvian State Institute of Wood Chemistry, 27 Dzerbenes Str., LV-1006 Riga, Latvia*
E-mail: koks@edi.lv
[*]Corresponding author

Received: December 14, 2004 **Accepted: April 19, 2005**

Published: April 28, 2005

Abstract: *A type of a fuzzy neural network for mathematical modeling of the volumetric mass-transfer coefficient is presented in the paper. Performed investigations show that the presented fuzzy neural network can be successfully used for modeling of such a complex process, like mass-transfer.*

Keywords: *Artificial neural networks, Modeling, Fuzzy neural network, Volumetric mass-transfer coefficient*

Introduction

The volumetric oxygen mass-transfer coefficient (K_La) defines the bioreactor effectiveness for aerobic biotechnological processes. The K_La magnitude depends on a considerable number of constructive and regime parameters, as well on physics-chemical parameters of culture medium. The increase of K_La value is a basic problem for the bioreactors design.

Recently, an increasing number of publications concerned with artificial neural networks (ANN) and fuzziness have appeared [6, 9, 10]. Interesting and promising algorithms for training ANN were proposed by using paradigms of fuzzy sets theory [7, 11].

The main advantage of ANN, known as a "flexible" model, is that they allow modeling of complex and ill-defined objects. However, usually used learning algorithms (backpropagation, reinforcement learning etc.) are a lot of time consuming [4, 8, 12].

A simplified type of ANN, that consists of two layers, is considered in the paper. Transfer functions (somatic mapping) of every neuron from the second layer are considered to be piece-wise linear.

The weights of the neurons the first layer are random chosen by between -1 and +1. The consideration of the transfer function as a crisp value is an idealization. A powerful tool for more "flexible" description, which can be considered as more appropriate and closely to the biological nature of the neurons action, are fuzzy relations [6].

We use fuzzy relation in order to achieve more adequate somatic mapping. Therefore, the training task is a fuzzy optimization problem. Applying new results in this field [1, 2] and their possibilities for neural networks learning [3], a non-iterative algorithm for training of mentioned above type of ANN is proposed in the paper. Using a fuzzy neural network (FNN), which input signals are the constructive and regime bioreactor parameters, is an alternative approach for modeling and investigation their influence under the K_La.

The aim of this paper is to be synthesized of a model of the volumetric mass-transfer coefficient using a fuzzy neural network.

Structure of proposed FNN

The structure of proposed FNN is shown on Fig. 1.

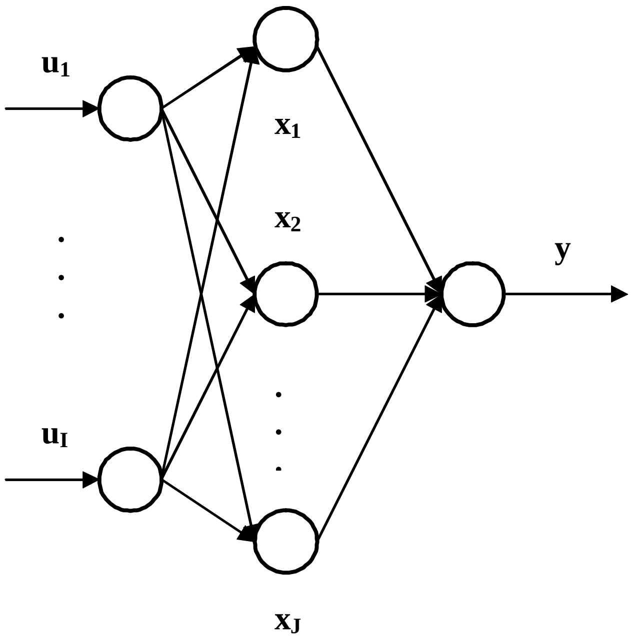

Fig. 1 Type of the FNN

The transfer function at the first layer is sigmoidal:

$$x_j \cong \left[1 + exp\left(-\sum_{i=1}^{I} a_{i,j}\, u_i \right) \right]^{-1}, \qquad (1)$$

where: x_j-signal in *j-th* neuron in the hidden layer; "$\cong$"-fuzzy relation represented by its membership function; u_i-input signal; I-number of input signals; $a_{i,j}$-weights of the connections *i-th* neuron in the first layer to *j-th* neuron in hidden layer, $a_{i,j} \in [-1,1]$.

The somatic mapping at the second layer is represented as a piece-wise linear function on the basis of the fuzzy equation:

$$y_j \cong \sum_{j=1}^{J} w_j\, x_j\ , \qquad (2)$$

where: y_j-output signals; J-number of hidden signals; w_j-weights of the neurons.

The membership function of (1) is as follows:

$$\mu = \left[1 - \left(y - \sum_{j=1}^{J} w_j\, x_j \right) \right]^{-2} \tag{3}$$

Training of the proposed type of FNN

The training task includes a determination of the weights which minimizes the total error:

$$E = \sum_{r=1}^{R} \left(y^r - Y^r \right)^2 \quad \rightarrow \quad m\tilde{i}n\,, \tag{4}$$

where: R-size of the training set, y-vector of the experimental outputs (from the training set), $m\tilde{i}n$ -denotes fuzzy minimization.

In general, the training task is presented as follows:

$$E \rightarrow m\tilde{i}n \tag{5}$$

$$y^r \cong \sum_{j=1}^{J} \frac{w_j}{1 + exp\left(\sum_{i=1}^{I} - a_{i,j}\, u_i^r \right)} \tag{6}$$

This problem belongs to class of fuzzy mathematical programming problems and a theorem [1, 2] introduced recently can be here applied. As a result, the best possible weights could be found as a solution of the following linear equations [1, 2]:

$$\mathbf{M}\ \mathbf{w} = \mathbf{B}, \mathbf{M} \in R^{JxJ}, \mathbf{B} \in R^{Jx1}, \tag{7}$$

The elements of the matrixes **M** and **B** are determined by the following relations:

$$\mathbf{M} = \begin{vmatrix} m_{2,1} & m_{2,2} & \dots & m_{2,J} \\ m_{3,1} & m_{3,2} & \dots & m_{3,J} \\ \dots & \dots & \dots & \dots \\ m_{R,1} & m_{R,2} & \dots & m_{R,J} \end{vmatrix}; \quad \mathbf{B} = \begin{vmatrix} b_1 \\ b_2 \\ \dots \\ b_J \end{vmatrix}, \tag{8}$$

where:

$$m_{r,j} = \frac{1}{1 + exp\left(- \sum_{i=1}^{I} a_{i,j}\, u_i^r a_{i,j}\, u_i^{r-1} \right)} + \frac{1}{1 + exp\left(- \sum_{i=1}^{I} a_{i,j}\, u_i^r \right)}$$

$$b_r = y^{(r-1)} - y^r\,, j = 1,\dots,J\,; r = 2,\dots,R$$

The best possible weights of the neurons in the second layer are obtained, received after the solving equation (7). As far as the number of neurons in the first layer is known (it is equal to the number of input signals), then the number of neurons has to be determined. It will determined simultaneously with the training of the neural network.

A simple non-iterative algorithm for training this FNN is developed by authors.

Training algorithm

1. The initial data (u^r_i, y^r, I, J, R) is inputted. The coefficients $a_{i,j} \in [-1, 1]$, $R=J+1$ are determined by randomization;
2. The elements of the matrixes **M** and **B** are calculated;
3. The matrix **M** is inverted ($\mathbf{M}^{-1}$);
4. The weights vector is calculated from $\mathbf{w}=\mathbf{M}^{-1}\mathbf{B}$;
5. The simulation of FNN is realized (y^r are printed);
6. Stop.

On the basis of the propose algorithm a program on FORTRAN 77 v. 5.0 is developed.

The proposed FNN will be used for modeling of the K_La in dependence on some constructive and regime parameters of the bioreactor. On the basis of a preliminary analysis of the factors and assessment of the conditions for realization of the experiment, (in this paper) the following constructive and regime parameters of the bioreactor are considered:

Name of the parameter	Symbol	Min. value	Max. value
Eccentricity of impeller toward its rotation axis	u_1	0.0 mm	1.5 *mm*;
Width of baffles	u_2	10.0 mm	14.0 *mm*;
Slope angle of stirrer’s blades	u_3	45^0	90^0;
Number of impeller	u_4	1	3
Impeller speed	u_5	2 s^{-1}	20 s^{-1};
Gas flow rate	u_6	50 *l/h*	300 *l/h*.

They are coded in the interval [-1, +1]. The coding is performed based on the equation:

$$u_i = \left(\bar{u}_i - u_{i,0}\right) / \left(u_{i,max} - u_{i,0}\right),$$

where: $u_{i,0} = 0.5\left(u_{i,min} + u_{i,max}\right)$, $\bar{u}_i$, $u_{i,min}$, $u_{i,max}$, $u_{i,0}$ and u_i are respectively the current, maximum, minimum and mean real values of the examined parameters.

The chosen constructive and regime parameters of the bioreactor $u_i=u[u_1,\ldots,u_I]$, $I=6$ are the input signals of the FNN. The output signal from the FNN is $y=K_La$ (Fig. 1).

Experimental investigations

The experiments are carried out in a laboratory bioreactor 2L-M with a magnetic coupling with maximal volume 2 L. The bioreactor is included in an automatic control system (ACS). The ACS has been developed by a scientific team from Centre of Biomedical Engineering. It gives a possibility for control of two bioreactors. The scheme of the experimental is presented in [5].

In order to compare the results, all experiments are performed at constant conditions (Table 1). The measurement of the K_La is realized based on the method of degasation in pattern medium – distilled water [5].

Table 1. Basic measurement and conditions for experiment investigations

Basic measurement and conditions for experiment investigations	Value
Vessels diameter, D	120.0 mm
Impeller diameter, d	58.0 mm
Width of paddle impeller, b	14.0 mm
High of paddle impeller, h	12.0 mm
Distance between vessel bottom and impeller, h_1	58.0 mm
Distance between two impellers, h_2	58.0 mm
Diameter of aerator, D_a	50.0 mm
Number of baffle assembly	3
Number of perforation of aeration	120
Height of liquid in the bioreactor, L	120.0 mm
Volume of liquid in the bioreactor, V	1.2 *l*
Temperature, T	25^0C

The obtained experimental results are shown in Table 2.

Table 2. Experimental investigations

N^0	u_1	u_2	u_3	u_4	u_5	u_6	K_La, h^{-1}	N^0	u_1	u_2	u_3	u_4	u_5	u_6	K_La, h^{-1}
1	-1	-1	-1	-1	-1	-1	103.0	24	1	1	1	-1	1	-1	104.0
2	1	-1	-1	-1	-1	1	121.6	25	-1	-1	-1	1	1	-1	101.0
3	-1	1	-1	-1	-1	1	113.1	26	1	-1	-1	1	1	1	114.1
4	1	1	-1	-1	-1	-1	94.8	27	-1	1	-1	1	1	1	131.5
5	-1	-1	1	-1	-1	1	83.7	28	1	1	-1	1	1	-1	139.1
6	1	-1	1	-1	-1	-1	91.0	29	-1	-1	1	1	1	1	140.9
7	-1	1	1	-1	-1	-1	103.4	30	1	-1	1	1	1	-1	142.5
8	1	1	1	-1	-1	1	107.1	31	-1	1	1	1	1	1	137.2
9	-1	-1	-1	1	-1	-1	110.1	32	1	1	1	1	1	1	121.5
10	1	-1	-1	1	-1	-1	120.1	33	-1	0	0	0	0	0	117.7
11	-1	1	-1	1	-1	-1	123.7	34	1	0	0	0	0	0	139.3
12	1	1	-1	1	-1	1	110.0	35	0	-1	0	0	0	0	139.5
13	-1	-1	1	1	-1	-1	100.1	36	0	1	0	0	0	0	98.6
14	1	-1	1	1	-1	1	112.0	37	0	0	-1	0	0	0	105.0
15	-1	1	1	1	-1	1	117.6	38	0	0	1	0	0	0	107.0
16	1	1	1	1	-1	-1	92.5	39	0	0	0	-1	0	0	147.5
17	-1	-1	-1	-1	1	1	69.6	40	0	0	0	1	0	0	148.2
18	1	-1	-1	-1	1	-1	81.1	41	0	0	0	0	-1	0	171.9
19	-1	1	-1	-1	1	-1	100.0	42	0	0	0	0	1	0	44.8
20	1	1	-1	-1	1	1	96.0	43	0	0	0	0	0	-1	172.4
21	-1	-1	1	-1	1	-1	87.6	44	0	0	0	0	0	1	109.6
22	1	-1	1	-1	1	1	96.4	45	1	1	1	1	1	1	229.6
23	-1	1	1	-1	1	1	107.4	-	-	-	-	-	-	-	-

Training of FNN and analysis of results

The training of FNN is realized on the basis of the developed algorithm and program. After the training of the network, the following values for the number of the neurons in the second layer and their weights are obtained:

$J=8; w_1=11.97,\ w_2=-2.94,\ w_3=3.53,\ w_4=-10.77,\ w_5=-14.76,\ w_6=12.84,\ w_7=-0.49,\ w_8=1.06,$

i.o. for only the first eight experiments, listed in Table 2, are used for training of FNN.

The experimental results and the prediction after the training of the FNN are shown on Fig. 2.

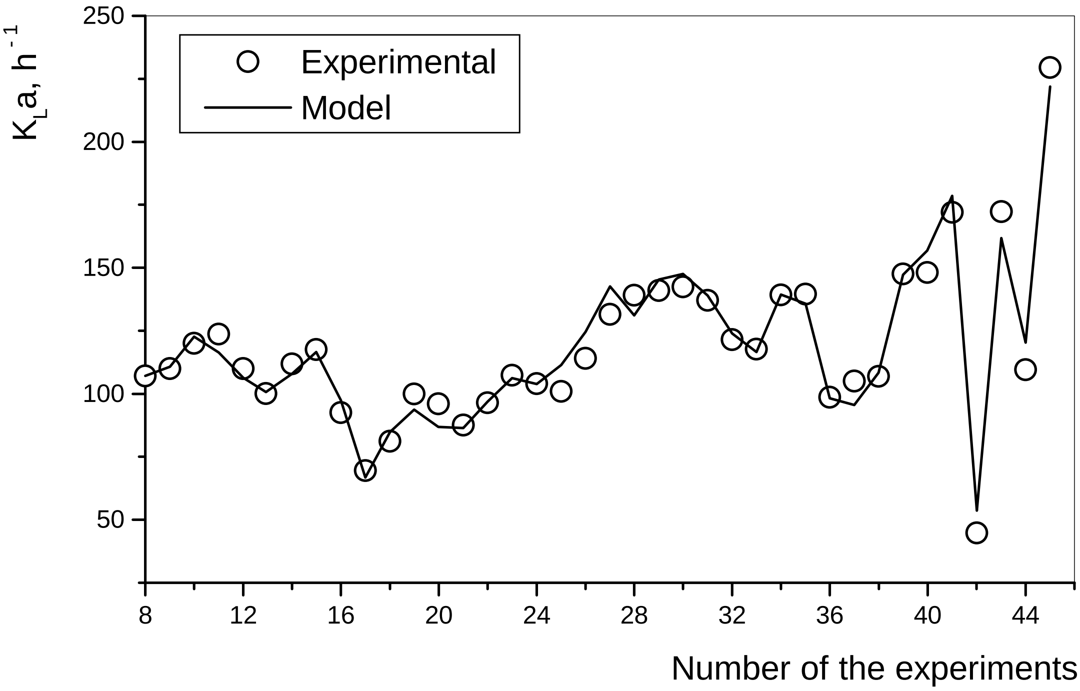

Fig. 2 Experimental data and obtained results by ANN

A statistical analysis of the obtained results is performed. It gave the following results: an experimental correlation coefficient $R^2=0.983$, a theoretical correlation coefficient $R^2_T=0.325$ at degree of freedom $\nu=35$ and a level of notability $\beta=\pm5\%$. The experimental and the theoretical Fisher quotients are: $F_E=1.01$ and $F_T=2.11$.

Fig. 2 and obtained results shows that FNN describes very well the experimental data. The model is adequate and this network can be used for modeling of the volumetric oxygen mass-transfer coefficient.

Conclusions

1. The performed investigations show that the proposed type FNN can be successfully used for modeling of the volumetric oxygen mass-transfer coefficient in dependence on the constructive and regime parameters of the bioreactor.

2. Using of neural network is the advisable for description of such a complex process like mass-transfer. Therefore the necessity of solving of complex nonlinear differential equations and further parameter identification, that needs more experimental data in comparison with the training of the neural network, drops off.

Acknowledgments

The investigations are partially supported by National Fund for Scientific Investigations by grant TH-1314/2003.

References

1. Angelov P. (1993). An Analytical Approach for FMP Solving and its Application to Neural Network Learning, 1st European Congress on Fuzzy and Intelligent Technologies - EUFIT'93, Aachen, Sepember, 3, 1255-1264.
2. Angelov P. (1994). A generalized Approach to Fuzzy Optimization, International Journal of Intelligent Systems, 9, 261-268.
3. Angelov P., L. Kuncheva (1993). Analitycal Solving Fuzzy Optimization Problems, International Conference MMSC'93, Sozopol, Bulgaria, 109-112.
4. Berenji H. (1992). A Reinforcement Learning-Based Architecture for Fuzzy Logic Control, International Journal of Approximate Reasonings, 6, 267-271.
5. Georgiev A., R. Nenov, M. Petrov (1992). Influence of Basic Constructive Parameters on the Mass Transfer of Laboratory Fermenters, Bioautomation, 12, 56-62.
6. Gupta M. (1992). Fuzzy Logic and Neural Networks, 2nd International Conference on Fuzzy Logic & Neural Networks, Iizuka, Japan, June, 157-160.
7. Keler J. C. Zhihong (1992). Learning in Fuzzy Networks Utilizing Additive Hybrid Operators, 2nd International Conference on Fuzzy Logic & Neural Networks, Tizuka Japan, May, 132-140
8. Keler J., J. Thibault., V. Van Berusegen V., A. Cheruy (1990). On-line Prediction of Fermentation Variables Using Neural Networks, Biotechnology & Bioinstrumentation, 36, 1041-1050.
9. Kosko B. (1992). Neural Networks and Fuzzy Systems, Prentice-Hall, Cl. Englewood Cliffs.
10. McClelland J. D. Rumelhard (1988). Parallel Distributed Processing, Explorations in the MIT Press, Cambridge, II Ed.
11. Nauck D., F. Klawoon, R. Kruse (1993). Combining Neural Networks and Fuzzy Controllers, Lecture Notes in Computer Science, 35-46.
12. Puyin Liu, Hongxing Li (2004). Fuzzy Neural Network Theory and Application, World Scientific Publication, http://www.worldscientific.com.