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Mathematical Models for Prediction of Glucose Concentration by Neural Network

Raghvendra Singh[1], Archana Shukla[2], Pushpendra Kumar[3*], Rajendra Kumar Tripathi[4]

[1]School of Sciences, UP Rajarshi Tandon Open University, Prayagraj

[2]Department of Mathematics, Nehru Gram Bharati (deemed to be) university, Prayagraj

[3]Department of Mathematics, Shri Khushal Das University, Pilibangan, Hanumangarh

[4]Applied science and Humanities (Mathematics), Faculty of Engineering and Technology, Khwaja Moinuddin Chishti Language University, Lucknow

Email: 10singh.raghvendra@gmail.com; archanashuklaald@gmail.com; pushpendrasaini22@gmail.com; drrktripathi_fgiet@rediffmail.com

Corresponding author*

Abstract:

A study on Mathematical Models an Artificial Neural Networks (ANN) for Prediction of Cellulose hydrolysis is a complicated process due to the numerous inhibitory and enzyme inactivation processes that take place during the course of hydrolysis. When it involves building predictive fashions for tactics containing complex response kinetics that might in any other case be not possible to simulate the usage of extra widespread deterministic approaches, Artificial Neural Networks (ANNs) are extraordinarily effective. The present day research turned into done so as to research the software of ANN as a device for predicting glucose manufacturing with the aid of using enzymatic hydrolysis of natural cellulose, in addition to the contrast of the anticipated glucose manufacturing with mathematical fashions and experimental findings. In order to forecast glucose manufacturing, a feed ahead neural community with one hidden layer turned into educated and utilised to make predictions.

Keywords: Artificial Neural Network, Cellulose, Enzymatic hydrolysis, Modelling, Cellulose.

1. Introduction:

Enzymatic hydrolysis of cellulose to supply lowering sugars has lengthy been pursued due to its capability significance in bioethanol manufacturing. Bioethanol may be a sustainable replacement for petroleum-derived merchandise of the blessings of enzymatic hydrolysis of cellulose over different hydrolysis techniques inclusive of acid hydrolysis are decrease utility (cooling water, gas, electricity) and disposal charges and no corrosion troubles for the equipment's [1-2]. The enzyme gadget for conversion of cellulose to glucose contain endo-β-glucanase, cellobiohydrolase and β-glucosidase (additionally known as cellobiase), which act sequentially and cooperatively to degrade crystalline cellulose to glucose [3-4]. In drawing close the technique layout for the enzymatic hydrolysis of celluloses, it's far vital with the intention to expect processing outputs in reaction to exclusive enter variables, inclusive of substrate

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preliminary awareness, enzyme pastime and hydrolysis time. The technique of the enzymatic hydrolysis is especially complex, rendering it tough to set a version for assured prediction. Enzymatic hydrolysis kinetics of cellulose were studied for decades however the improvement of correct mathematical fashions for this response continues to be a important challenge. An opportunity method to gain a version of the response could be the usage of Artificial Neural Networks (ANNs).

2. Literature Survey:

ANNs can manage incomplete records and cope with nonlinear problems. It also can carry out prediction and generalization at once after the schooling technique. Artificial NNs appear to be a possible opportunity in numerous instances, and their utility for biotechnological techniques is constantly growing [5-6]. With admire to biotechnological techniques in particular, numerous research may be determined in literature, inclusive of the outline of the α-amilase inactivation, the prediction of the very last awareness of ethanol in a batch fermentation technique and as a gentle-sensor. ANN fashions are normally used for prediction, characteristic approximation, classification, and clustering [7-10]. However, few papers have been pronounced approximately ANN-primarily based totally version for enzymatic hydrolysis and gentle computing strategies and deliver chain management. A new method for fixing trouble associated with optimization is mentioned by (23-55), that's associated with gentle computing and management. The intention of the existing examine is to test the validity of ANN to expect the glucose manufacturing below numerous enzymatic hydrolysis situations with to be had experimental records and examine ANN outcomes with kinetic version outcomes.

3. Theoretical Mathematical Model:

A have a look at modelling of the enzymatic hydrolysis of cellulose has been studied in severa posted works. The mathematical fashions hired on this paintings for the enzymatic hydrolysis had been tailored from [11-12]. The conversion of microcrystalline cellulose (Merck, Germany) and microcrystalline cellulose (Sigmacell, Sigma, Deisenhofen, Germany) to glucose had been investigated, respectively.

This proposed model includes the hydrolysis kinetic for microcrystalline: definition of an powerful substrate awareness [Eq. (1)], relation of substrate hydrolysis to product formation [Eq. (2)], and the powerful substrate awareness in presence of cellobiose [Eq. (3)].

$$S_{eff} = aS_{eff,o}\exp\left(-k_{1,max}\frac{E}{(K_1+E}t\right) + (1-a)S_{eff,o}\exp(-k_{2,max}\frac{E}{(K_2+E)}t) \ \ldots \quad (1)$$

$$S_{eff,o} - S_{eff} = G \ \ldots \quad (2)$$

$$S_{eff,o} = S_0\frac{K_{eff}E_\beta^n}{(S_0+K_{eff}E_\beta^n)} \ \ldots \quad (3)$$

As bear in mind the generally left out particle length discount in the course of the hydrolysis, they assumed that those debris decrease. In some other word, the particle length reduces even as

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the particle form stays constant. This assumption allowed them to simplify a completely complex 3 dimensional version to a far less difficult one dimensional version. Their foremost assumptions can be indexed as below:

1. A fraction of the cellulose enzymes is absorbed immediately at the particle floor.
2. Some components of the debris that are occupied with the aid of using non-cellulosic substances are completely inert to the hydrolysis reaction.

3. The range of web sites to be had for enzymes is proportional to the powerful outside floor of the debris.
4. Transfer of enzymes from the answer to the particle floor may be very fast in order that it does now no longer have an effect on the hydrolysis price.

5. Product inhibition negatively influences the price of hydrolysis and enzyme activity.

6. Particles decrease in the course of the hydrolysis reaction. This mathematical version offers distinctive equations for 2 ranges of the technique. In the primary level of the technique the debris decrease with none huge enzyme desorption (go back of absorbed enzymes to the answer), even as within the 2nd level part of the absorbed enzymes go back to the answer and the equations could be distinctive. The equation is derived for the first stage:

$$(1-y)+\left(\alpha\theta_0+\frac{1}{K_{eq}}\right)\ln\left(\frac{\alpha\theta_0+y-1}{\alpha\theta_0}\right)=\left(\frac{-K_d}{K_{ed}}\right)t \qquad (4)$$

Where t is time, y is the ratio of substrate concentration to the initial substrate concentration θ_0, K_d and K_{ed} are model parameters.

The following equation is developed for the second stage of the model:

$$\left(\frac{K_d}{3}\right)(t-t_1)=K'_{ed}\left[\left(-\frac{1}{3}\right)(Z_1^3-Z^3)+\left(\frac{\alpha}{2}\right)(Z_1^2-Z^2)-\alpha(Z_1-Z)\right]+(\alpha^3K'_{ed}+1)I_2+\alpha K'_{ed}I_1-\alpha^2K'_{ed}I_0 \quad (5)$$

Where $\frac{Z}{3}=y^{1/3}$ and $I_0, I_1\ and\ I_2$ are expressions which have different definition in different condition.

3.1 Neural Network Model:

ANN is a mathematical tool, which attempts to symbolize low-stage intelligence in herbal organisms and it's miles a bendy structure, able to creating a non-linear mapping among enter and output areas as programs of ANN fashions encompass fermentation, extrusion approaches, filtration, drying process, etc [13-16]. ANN were efficaciously carried out to modeling of diverse organic approaches in current years. They are one of the maximum famous synthetic studying gear in biotechnology, with programs starting from sample popularity in chromatographic spectra and expression profiles, to practical analyses of genomic and proteomic sequences. All neural networks encompass 3 important layers (enter, hidden) [17-19] and many straightforward computational elements, known as nodes or neurons, organized in layers and working in parallel. The ANN weights, which outline the energy of the relationship among the nodes, are envisioned

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from empirical information. There are numerous sorts of Artificial Neural Network. The maximum not unusual place kind of ANN in chemical engineering utility is multilayer perceptron (MLP). In this observe multi-layer feed ahead neural network primarily based totally on returned propagation studying rule changed into used to expect glucose manufacturing of natural cellulose.

3.2 Verification of predicted data:

In the existing work, to check the prediction competencies of the fashions, the anticipated values acquired from mathematical fashions and ANN had been as compared with the experimental values. The coefficient of determination (R2), suggest rectangular error (MSE), and common relative deviation (ARD) had been decided and used to evaluate ANN and mathematical version. The R2, MSE, and ARD had been calculated with the aid of using following Eq. (6), (7) and (9) respectively:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(X_{pre,i} - X_{exp,i}\right)^2}{\sum_{i=1}^{n}\left(X_{pre,i} - \bar{X}\right)^2} \ldots. \qquad (6)$$

$$\mathrm{MSE} = \frac{\sum_{i=1}^{n}\left(X_{pre,i} - X_{exp,i}\right)^2}{n} \ldots \qquad (7)$$

$$ARD = \frac{100}{n} \times \sum_{i=1}^{n} \left|\frac{X_{exp,i} - X_{pre,i}}{X_{exp,i}}\right| \ldots \qquad (8)$$

Where $X_{pre,i}$ is the predicted output from observation (i), $X_{exp,i}$ is the experimental output from observation i, X is the average value of experimental output and n is the total number of data. R^2 be closed to 1, the MSE and the ARD between the predicted and experimental data must be as small as possible.

3.3 Identification of the Effects of Different Parameters on the Enzymatic Hydrolysis Process: Based at the case observe, there are 3 parameters which perceive the contribution at the manufacturing of glucose of hydrolysis process. The parameters concerned are the interest of brought cellulose (FPU), substrate preliminary concentration (g.L-1) and working time(t). The predictive version changed into advanced with the aid of using the use of ANN primarily based totally the experimental information supplied from literature of preceding observe.

3.4 The Development and Validation of the Model:

The prediction version became advanced primarily based totally at the real values extracted from literature. The version is administered the use of ANN. The form of ANN used on this observe is a multilayer perceptron (MLP) including multi-layer feed ahead neural community primarily based totally on lower back propagation mastering rule to are expecting the manufacturing of glucose from the enzymatic hydrolysis of rice straw. There are some concerns required to expand an ANN-primarily based totally version, such version structure (architecture) and ANN version schooling. The MLP with one hidden layer of sigmoidal neurons and a layer of linear output neurons became hired on this observe. The MLP especially includes 3 layers; an enter layer, an

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output layer and one or greater hidden layers, whose numbers of neurons for every layer represented with the aid of using N, M and K respectively.

The go validation method is used to discover genuine range of neurons in hidden layers and additionally to keep away from the version from over-becoming at the same time as accomplish correct generalisation from the schooling records set. These experimental records or records samples had been required to break up into schooling records set and a validation dataset. Then neural networks with one-of-a-kind range of hidden nodes are skilled with the schooling dataset. The overall performance of the version became evaluated at the cap potential to are expecting of the validation dataset with the aid of using calculating imply rectangular error (MSE) as specific in equation (2).

Where g_k represents the prediction of the neural networks and d_k is the preferred output, which which on this observe glucose attention $Y(g.L-1)$ illustrates the general framework of the model based approach proposed in this work. The inputs of the MLP neural network model are the activity of added cellulose X_1(FPU), substrate concentration, $X_2(g.L-1)$ and the hydrolysis time,$X_3(h)$ while the model output was glucose concentration, $Y(g.L-1)$. The systematic method advanced may be used to construct fashions with greater than inputs such on this case; enzyme attention varies from $(X_1, X_2, X_3 \ldots \quad X_n)$.

4. The Performance of the Predicted Data:

The expected facts received from the ANN version changed into in comparison with the experimental values and RSM values. The comparative step is completed to check the competencies of the version developed. Experimental facts are received from literature had been used to train, validate and check synthetic neural networks (MLP) for prediction of glucose awareness throughout enzymatic hydrolysis. The variety of test facts used.

Result and Discussion: The information about process conditions of the enzymatic hydrolysis can be found in Table.

Table: Process conditions in the enzymatic hydrolysis

Process Parameter	**Value**
Temperature (℃)	50
Initial Solid Concentration$(g.L-1)$	40-80-120-160
Enzyme loading	
Celluclast $\left(CCN\frac{3000}{85}-4\right)FPU/g$	6.25-8.33-12.5-25
Novozym188$\left(DCN\frac{003}{87}-11\right)IU/g$	6.25-8.23-12.5-25
Operating time(h)	200
Ph	4.8

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Temperature (℃)	50
Initial Solid Concentration$(g.L-1)$	10-20-50
Enzyme loading	
Celluclast $\left(CCN\frac{3000}{85}-4\right)FPU/g$	3.7-9.25-18.5
Novozym188$\left(DCN\frac{003}{87}-11\right)IU/g$	
Operating time(h)	24
pH	5

Note: FPU=filter paper unit; IU= International unit of enzyme activity.

Two mathematical version for enzymatic hydrolysis had been used on this work [11- 12]. In the version conceived via way of means of so that it will describe the hydrolysis of microcrystalline cellulose, an powerful substrate awareness changed into described which deviates from bulk awareness of cellulose. They taken into consideration following assumptions of their version: fractions of substrate, the enzyme-to-substrate ratio, and the powerful substrate awareness. The consequences confirmed that the version predictions matched the experimental hydrolysis facts thoroughly over a huge variety of substrate and enzyme concentrations. Based on a assessment of the R2 (coefficient of determination), MSE (suggest rectangular mistakess), and ARD (common relative deviation) values among the neural community and mathematical models, it changed into decided that the neural community version is greater correct than the mathematical models. The received consequences show that the synthetic neural community (ANN) may be a precious device for the layout of enzymatic hydrolysis, the usage of an synthetic neural community (ANN), the authors wish to count on the manufacturing of glucose withinside the hydrolysis process, after which examine their predictions to the experimental consequences received. The ANN consists of 3 layers: the enter layer, the hidden layer, and the output layer. A layer of enter variables is represented via way of means of the interest of extra cellulose in addition to substrate preliminary awareness and hydrolysis time on glucose manufacturing withinside the case study, while the layer of an output variable is represented via way of means of a layer of glucose awareness withinside the case study [21-22]. The coefficient of determination, suggest rectangular mistakess, and common relative deviation had been all used to assess the version's performance, along side different metrics. The coefficient of determination, 0.8361, attained with a tiny suggest rectangular mistakess of 0.1947 and a mean relative deviation of 5.644, demonstrates a promising final results for the prediction version. It virtually demonstrates that the ANN is able to making correct predictions approximately the enzymatic hydrolysis required for the introduction of glucose.

Conclusion: According to the findings of this study, neural networks provide excellent fits to experimental data. Using experimental data from the enzymatic hydrolysis of cellulose, the researchers discovered that training an artificial neural network with this data has shown to be highly successful. In a heterogeneous system, the ANN was able to precisely simulate an enzyme

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reaction without any errors. In addition, when compared to the RSM model, the ANN model is clearly more accurate. Because the estimation is realised by simple arithmetic operations, the neural network model is not overly complicated. It is declared that synthetic neural networks (ANNs) can function a hyperlink among remoted experimental facts and bring about a synergy among the impartial investigations. The packages of synthetic neural networks may be hired efficiently for the online country estimation and manage of enzymatic hydrolysis processes, as proven on this paper.

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