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Application of Artificial Neural Networks to Predict Fructose Concentration

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Abstract. Analysis of fructose concentration in a glucose isomerisation process using commercial Immmobilised glucose Isomerase (IGI), is typically performed by HPLC. Presently, analysis of fructose was carried out by HPLC with UV detector at 195 nm. This study focused on the prediction of fructose concentration based on the experimental data using artificial neural network (ANN) technique, with five inputs, one output, and twelve neurons in a hidden layers that utilized sigmoid as a transfer function. The Input consisted of current temperature, T_k, previous temperature, T_{k-1}, initial glucose concentration, [G], pH, and previous pH, pH_{k-1}. The output layer was composed of fructose concentration. The data for the prediction was taken from experimental works using 12g rehydrated of IGI in a 2L batch reactor. The temperature and pH range under study was from 55^0C to 70^0C and pH 5 to 9 respectively. It was found that temperature and pH effect were related to fructose concentration of the chemical analysis ($R^2 > 0.95$). From the results, ANN and ANN2 demonstrate its potential as an alternative and rapid technique rather than a conventional method for prediction of fructose concentration.

Keywords: Artificial neural network; Batch reactor, Conventional method; Glucose Isomerisation; Prediction

1. Introduction

Isomerisation of glucose to fructose by immobilized glucose isomerase enzyme is an example of a solid catalyzed bioreaction. Such reaction is industrially important and is a reversible reaction with an equilibrium conversion of 50% at 65ºC (Salehi et al., 2004). Comparable to the sucrose syrup, fructose has more desirable functional properties such as high osmotic pressure, high solubility, and a source of instant energy as well as preventing crystallization of sugar in food products (Kurup.et al., 2005).

In this research, an artificial neural network (ANN) is used to predict the results and compare thereafter with experimental outcomes. Artificial neural networks (ANN) could be defined as structures comprised of densely interconnected adaptive simple processing elements similar to the biological neurons, also called neurons or nodes that are capable of performing massively parallel computations for data processing and knowledge representation (Serra et al., 2003; Molga. and Cherbanski., 2003; Chen et al., 2004, Basheer, 2000). According to Linko et al(1999), Bhat and McAvoy (1990) were the first to use backpropogation neural networks in the dynamic modeling of a continuous stirred-tank reactor. Other researchers successfully applied artificial neural network in modeling of biological system (Bas, 2007a, 2006, Geeraerd, 1998, Hajmeer, 1997, Lou, 2001, Sun, 2003, Torrecilla, 2004). According to Jain et al (1996), the attractiveness of ANNs comes from the remarkable information processing characteristics of the biological system such as no linearity, high parallelism, robustness, fault and failure tolerance, learning, ability to handle imprecise and

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fuzzy information and their capability to generalize. This study was different from Baş (2007(a, b) in terms of parameters and type of reactor used. Enzyme-based processes are more favourable since they are operated at lower temperatures while as generating less toxic and pollutant waste, fewer emissions and by products compared to conventional chemical processes (Bhosale et al, 1994; Tomotani and Vitolo, 2007). Two main variables under study were temperature and pH of the system and glucose concentrations were kept constant (1.8% w/v), whereby in Baş (2007 a, b) assumed those variables to be constant.

To explore an alternative method for estimation of fructose concentration without using an analyzer such as HPLC system is the key interest of this research work. The previous research using HPLC system with UV detection was made at 195 nm with column temperature of 30^0C. The flow rate was set to 0.6mL/min and injections of 20μL were made. The column used was Kromasil NH_2 column (250mm x 4.5mm, 5 μm, Supelco). The ratio of acetonitrile and the deionised water used was 80% to 20%. The guard column attached to the column was used in order to prevent clogging of the column. These alternative methods have the following features: (i) does not require experimental work, (ii) applicable for all type of reactor effectively (iii) does not require any assumptions about kinetic study. In this study, artificial neural networks (ANN) were used for the estimation of fructose concentration instead of chemical analysis.

2. Materials and Method

2.1. Materials

The materials for this study were D-glucose (G), D+fructose (F) and $MgSO_4.7H_2O$ (R&M Chemical, UK). 12g of Immmobilised Glucose Isomerase (IGI) was obtained from *S. murinus*, brown cylindrical shape granules, diameter 0.3 to 1.0 mm, length of 1.0 to 1.5 mm with activity of 350 IGIU/g (Sweetzyme, Novozymes, Denmark). For HPLC analysis, deionised water and acetonitrile (ACN) (HPLC grade) are used. Different series concentrations of glucose from 1.8 to 30% w/v were prepared. All analytical samples were diluted with distilled water and filtered through 0.45μm Nylon filters prior to HPLC-analysis.

2.2. Method

As shown in Figure 1, the reactor system consists of a 2 litre double –jacketed batch reactor, made from Borosillicate glass 3.3 DN 120 043943. The reactor was connected to a waterbath (Huber, Germany) and is equipped with propeller type impeller driven by a motor (Heildoph with RZR323 control). The function of the waterbath was to control the jacketed bioreactor at the required temperature. The feed consisted of 1 Litre of solution containing 18g glucose and 1g of $MgSO_4.7H_2O$ (i.e. 0.1M glucose and 1g/L $MgSO_4.7H_2O$ in a distill water. All the experiments were conducted at a constant agitation speed of 150 rpm. The enzyme was rehydrated with distilled water for 24 hours at a cold room before being added to the reactor. The reactions were carried out at different temperatures (55^0C, 60^0C, 65^0C and 70^0C) and pH (3 to 10) in a non buffer solution. Samples were withdrawn every 10 minutes for analysis.

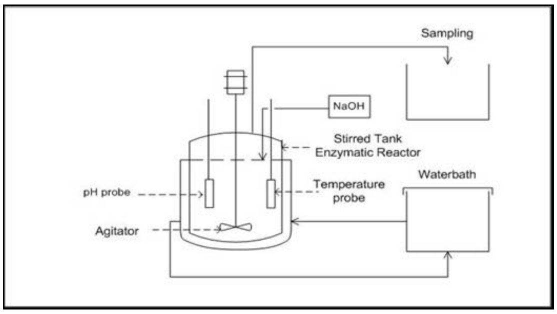

Fig. 1: Schematic diagram for Batch Reactor.

2.3. Artificial Neural Networks (ANN) Training

The Artificial Neural Networks (ANN) programming was carried out using the Neuralware product and Predict software (Neuralware Carnegie, USA, Product release 3.2). For the batch reactor, the Artificial Neural Network (ANN) consisted of five neurons in the input layer, one output neuron in the output layer with linear transfer function, and twelve neurons in the hidden layers and used sigmoid as the transfer function for the hidden layer. The inputs of the neural network were temperature, T_k, previous temperature,

T_{k-1} , initial glucose concentration, [G], current pH, and previous pH, pH_{k-1}. These were the variables having significant effect on the fructose concentration. The output of the system was the fructose concentration, [Fr]. The proposed ANN Model is given in Fig. 2

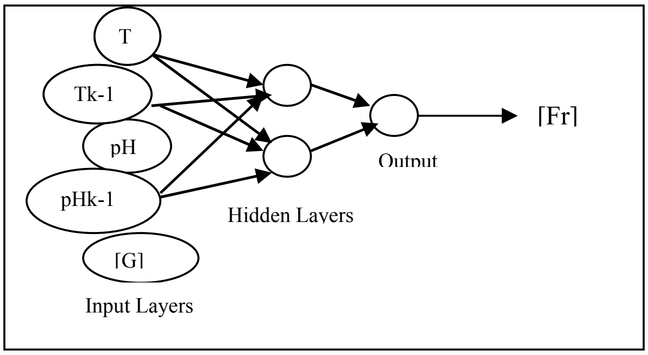

Fig. 2: The architecture of proposed ANN model (Batch Reactor)

A comparative analysis between the experimental works and the application of Artificial Neural Network (ANN) was done in order to determine the correlation between their results. The performance of ANN was observed based on the average absolute error, AAE and R^2 (Togun and Baysec, 2010) for both training and testing of the ANN. The equation for the average absolute error (AAE) of the samples is given by (Baş et al. 2007b),

$$AAE = \left\{ \left[\sum_{i=1}^{n} \frac{\left| x_{i,exp} - x_{i,,cal} \right|}{x_{i,exp}} \right] / n \right\} * 100 \tag{1}$$

Where $x_{i,exp}$ is the experimental values, $x_{i,cal}$ is the calculated values using the ANN and n is the total number of the estimated or calculated values.

2.4. Improvement of Artificial Neural Network (ANN) For Prediction of Fructose Formation in the Batch Reactor

In this section, the application of Artificial Neural Network (ANN) for prediction of fructose formation was further investigated in a batch reactor in order to improve the performance of ANN, known as ANN2 as a software sensor. The performance of ANN was observed based on the average absolute error, AAE (Baş et al. 2007b) and R^2(Togun and Baysec, 2010) for both training and testing of ANN2. The proposed ANN2 Model is similar to Fig. 2. The main difference in this section was that the data for fructose prediction was gathered from experimental data and the proposed model, MM3 which has been seen to be in agreement with the experimental works.

$$r = \frac{[v_0 e^{-\frac{E_a}{RT}}][e^{-[k_{d0} e^{-\frac{E}{RT}}]t}]S*[H^+]}{k_m + S*[H^+]} \tag{2}$$

Eqn. (2) is known as MM3 with a function of temperature, pH and bulk substrate concentration. The input and output of ANN2 is similar as in section of Artificial Neural Networks (ANN) Training.

2.5. Results and Discussion

For batch reactor, data obtained from 47 runs were used for the training of the ANN and another 21 runs were used for testing the trained network. The output of the ANN was compared with the experimental data in Table 1 and Table 2 respectively.

Table 1: The statistical analysis for temperature under study (Batch Reactor, pH=8, Testing data)

Temperature	55°C	60°C	65°C	70°C
AAE	0.006	0.202	0.168	0.002
R^2	0.997	0.973	0.948	0.981

Table 2: The statistical analysis for pH under study (Batch Reactor, T=60oC, testing data)

pH	3	4	5	6	7	8	9	10
AAE	0.654	0.349	0.216	0.096	0.451	0.172	0.072	0.122
R^2	0.985	0.975	0.986	0.995	0.982	0.955	0.996	0.933

This finding shows that ANN would be able to predict the fructose formation based on the data provided by the experimental works which were clearly shown by the accurancy of the testing works. Another advantage of using ANN was that it was faster compared to the mathematical model . Beside that more data used in training and testing would influence the end-product. From the data provided which included the effect of temperature and pH , the ANN easily predicted the fructose formation. Another factor to be considered using this technique was that, even though the kinetic parameters and enzyme activity were unknown to the ANN, it still could predict the values of the product. This was the most interesting facts when using this artificl intelligence technique. It is obvious that well trained network will have high performance. From the results, it shows that pH has higher effect to the process in terms of more fructose produced and the difference between the experimental and estimated values was less compared to temperature effect.

In section Artificial Neural Networks (ANN) Training, the results for the batch reactor (AAE and R^2) show that the AAE was high, 0.927 and the R^2 was 0.955. Figure 3 to 4 shows a comparison study for temperature and pH effects between proposed ANN, ANN2, (TANN2, pHANN2) based on the testing data and MM3 data (TMM3, pHMM3). The error bars in the figures refer to 0.5% of the error amount. Fructose production in the batch reactor is shown in Figure 3. It represents the relationship between the fructose concentration and temperature including both the proposed model data, MM3 and the proposed ANN, ANN2.

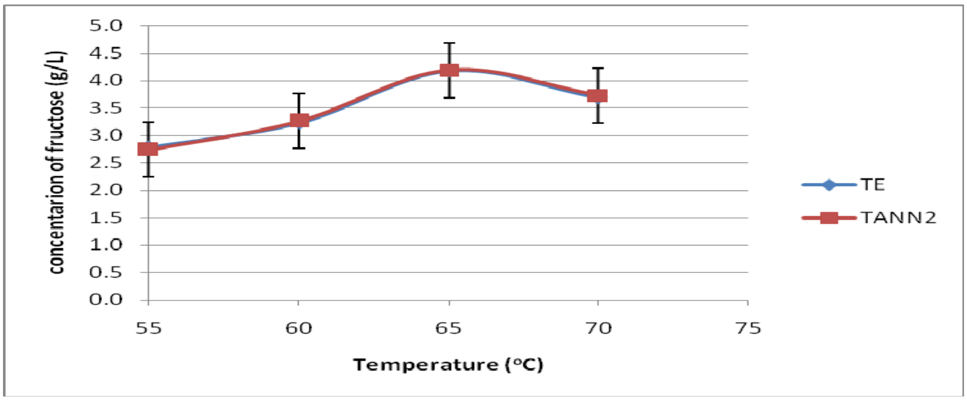

Fig. 3: Effect of temperature on the fructose formation with various models (pH8, Testing data)

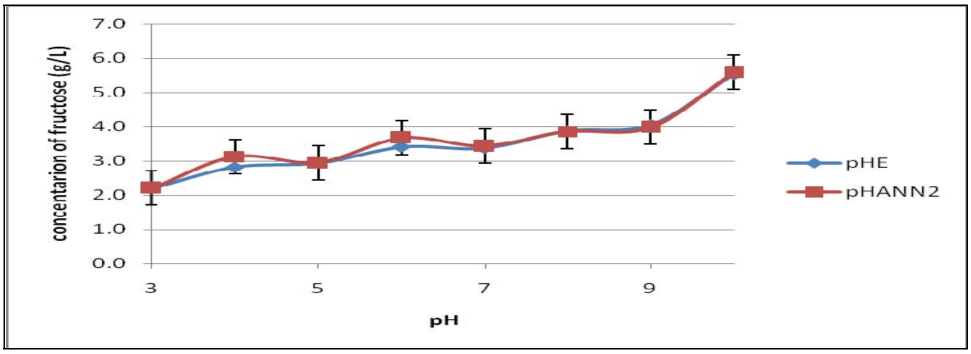

Fig. 4: Effect of pH on the fructose formation with various models (T=60°C, Testing data)

It is shown in Fig.3 that fructose production varied from 55°C to 70°C. Increasing temperature increased the fructose production until at 65°C for both models, MM3 and ANN2. The highest fructose concentration was observed at 65°C (4.0 g/L). Variation in fructose production during glucose isomerisation could be due to changes in the enzyme activity and other environmental factors which influence the activation energy of the process (Santos et al., 2007).

Figure 4 represents the pH profiles, which were dynamically measured at different models, MM3 and ANN2. The maximum concentration of fructose reached a pH of 10 but it was not acceptable industrially due to its alkaline in nature (Linko et al, 1977). The difference between experimental and modeling, MM3 and ANN2 occurred due to some assumptions in modeling such as the pH values were included in the substrate concentrations.

From Figure 3 and 4, it shows that an improvement of the results occurred for both effects of temperature and pH with ANN2. For each temperature and pH under study, there were a very good agreement between proposed model data, MM3 and ANN2. The performance of ANN2 was improving in terms of R^2 where a good correlation between training and testing (R^2 > 0.95). This shows that with more accurate data the performance of ANN is closely in agreement with experimental data.

Table 3: Comparison study between ANN and ANN2 (Batch Reactor, testing data)

		ANN	ANN2
Temperature			
°C	AAE	0.927	0.885
	R^2	0.955	0.994
pH	AAE	1.590	0.897
	R^2	0.993	0.994

Table 3 summarised a comparison study between ANN and ANN2 for the batch reactor. As the overall AAE values are less than one (0.885 for the effect of temperature; 0.897, for the effect of pH) and high values of R^2 (0.994, effect of temperature and pH), proved that ANN2 was sufficient to predict the effects of isomerisation temperature and pH within the limits of this study (55°C-70°C, pH of 3 – pH of 10) as shown in Table 7.

2.6. Conclusions

The results of the research work shows that for estimation of fructose concentration, the developed program has a higher performance and requires less time for the prediction. The validation of the models with experimental data was analysed in terms of AAE and R2. The values of coefficient, R2 (> 0.95) indicates that the proposed ANN was well fitted to the experimental data. The proposed ANN successfully predicts the effects of isomerisation temperature and pH within the limits of this study (55oC-70oC, pH of 3 – pH of 10) while the ANN2 (more data added from simulation results) was sufficient to predict the effects of isomerisation temperature and pH within the limits of this study (55oC-70oC, pH of 3 – pH of 10) for the batch reactor.

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