Software Sensor to Enhance Production of Fructose

Norliza Abd. Rahman¹, Mohd. Azlan Hussain², Jamaliah Md. Jahim¹ & Siti Rozaimah Sheikh Abdullah²

¹ Department of Chemical Engineering & Process, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, Malaysia
² Department of Chemical Engineering, Faculty of Engineering, University Malaya, Malaysia

Correspondence: Norliza Abd. Rahman, Department of Chemical Engineering & Process, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600 Bangi, Malaysia. Tel: 60-389-216-115. E-mail: liza@eng.ukm.my

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Abstract

Present studies describe the on-line prediction of fructose concentration by using Artificial Neural Network (ANN) that employed as software sensor in the batch reactor for the biosynthesis of fructose by Immobilised Glucose Isomerase (IGI) of S.murinus. The process of fermentation was carried out in a 2-L batch bioreactor (New Brunswick Scientific, USA) with a working volume of 1.5 L reactor. All of the parameters were automatically controlled with the help of attached software. The optimum pH and temperature, for the production of fructose by Immobilised Glucose Isomerase (IGI) of S.murinus were found to be 8 and 60 °C, respectively. Accuracy of the proposed soft sensor was calculated by the correlation coefficient ($R^2$) and mean square error (MSE). In this study, value $R^2$ were greater than 0.95 and the values of MSE were less than 0.2, indicating a good fit of the ANN-soft sensor to the experimental data, accurate up to 95.7% for training and 100% for testing. Thus, the proposed ANN-soft sensor was the most precise in predicting fructose concentration.

Keywords: fructose, on-line prediction, batch bioreactor, mean square error

1. Introduction

Artificial Neural Networks (ANN) is defined as structures comprised of densely interconnected adaptive simple processing elements similar to the biological neurons that are capable of performing massively parallel computations for data processing and knowledge representation (Serra et al., 2003; Molga & Cherbanski, 2003; Chen et al., 2004; Basheer & Hajmeer, 2000). Researcher successfully applied using artificial neural network in modeling of biological system (Boyaci, 2005; Geeraerd et al., 1998; Hajmeer et al., 1997; Lou, 2001; Sun, 2003; Torrecilla et al., 2004). According to Jain et al. (1996), the attractiveness of ANNs comes from the remarkable information processing characteristics of the biological system such as non-linearity, high parallelism, robustness, fault and failure tolerance, learning, ability to handle imprecise and fuzzy information and their capability to generalize.

The analogy between biology neuron and artificial neuron is; the connections between nodes represent the axons and dendrites, the connections weights represent the synapses and the threshold approximates the activity in soma. Figure 1 illustrates n biological neurons with various signals of intensity $x$ and synaptic strength $w$ feeding into the neuron with the threshold of $b$ and the equivalent artificial neurons system.
Generally the applications of ANNs fall into seven categories known as pattern classification, clustering, function approximation, forecasting, optimization, association and control. In this study the application of ANNs is under the function approximation. Function approximation (modeling) involves training ANN on input–output data so as to approximate the underlying rules relating the inputs to the outputs. Function approximation is applied to problems (i) where no theoretical model is available, i.e., data obtained from experiments or observations are utilized, or (ii) to substitute theoretical models that are hard to compute analytically by utilizing data obtained from such models.

Bioprocess and chemical process systems are instrumented with a large number of sensors and require precious instrumental analysis or statistical analysis with a large amount of experimental data (Chung et al., 2010). According to previous researcher (Mithra, 2011; Norliza et al., 2011; Yu et al., 2011; Ferreira et al., 2003; Crabb & Shetty, 1999; Luong et al., 1997; Lammers & Schep, 1997; Crabb & Mitchinson, 1997) application of soft sensors is still relatively inadequate for enzymatic reaction due to numerous factors such as need for regular calibration and maintenance, high cost, short operational life, unreliable supervisory systems for on-line fault detection and correction.

According to (Kadlec et al., 2009), soft sensors are predictive model and the term soft refers to “software” whereas sensors are delivering similar information as their hardware counterparts. In general, there are two different types of soft sensors, namely model-driven and data-driven.

First Principle Models (FPM) is commonly used in model-driven soft sensors but their drawback is an assumption of steady-states of the processes. As a result, data-driven soft sensors gained increasing popularity in the process industry as shown by previous researcher (Yuan et al., 2000; Yang et al., 1998; Chen & He, 1997; Latrille, 1997; Rouzic & Le, 1997; Acuna et al., 1995; Thibault et al., 1990; Pfaff, 1995; Oh, 1995). Therefore in this work, data-driven soft sensors are used since they are based on the data measured within the processing plants, and thus describe the real process conditions. The applications of soft sensors are mostly for on-line prediction, process fault detection, process monitoring and sensor fault detection.

In this proposed study, we apply neural network data-driven soft sensor is applied in a batch process to estimate fructose concentration for on-line prediction. This is due to the dynamic behaviour during the process where there is no steady state operating point and wide operating ranges may be encountered due to frequent start-up and shutdown (Seborg et al., 2004).

The research conducted will then be described, starting with the research procedures (Section 2), some results and discussion (Section 3) and the conclusion.
2. Materials and Methods

This section describes close-loop studies, batch systems and computer accessories firstly for conventional control followed by development of a software sensor which acts as an estimator or prediction.

2.1 Close-loop Studies and Batch Systems

Preliminary experiment for glucose isomerisation was conducted in a 2 liter stirred double-jacketed bioreactor made of Boroslicate glass 3.3 DN 120 043943 with 3 blades of propeller agitator. Figure 2 and Table 1 give the dimension of the batch bioreactor used in this study. The speed of the agitator in the experiment was set in the range of 100 to 200 rpm. The heater was installed to control the temperature and a dosing pump was added of pH by addition of NaOH. For temperature control, the usage of heater of 21 cm in length (only 8 cm for heating zone) with diameter of 1.3 cm was implemented inside the reactor. The function of the waterbath was to maintain the reactor temperature.

![Figure 2. Dimension of a batch reactor](image)

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter of impeller, D_i</td>
<td>5 cm</td>
</tr>
<tr>
<td>Diameter of reactor, D_t</td>
<td>11.5 cm</td>
</tr>
<tr>
<td>Height of impeller blade, W</td>
<td>0.5 cm</td>
</tr>
<tr>
<td>Height of reactor, H_t</td>
<td>20.9 cm</td>
</tr>
<tr>
<td>Height of liquid in the reactor, H_L</td>
<td>8.5 cm</td>
</tr>
</tbody>
</table>

The objective of this experiment was to determine the optimum values for the reaction conditions such as temperature, pH, enzyme activity, and kinetic parameters for the reaction. 0.1 M of glucose solution and 12 g of rehydrated IGI were added to give one liter of solution A in the reactor and heated up to the reaction temperature of 55 °C, 60 °C, 65 °C and 70 °C and pH of 3, 4, 5, 6, 7, 8, 9 and 10. The glucose-IGI mixture was agitated for 2 hours at 150 rpm. Once the experiment was completed, the samples were deactivated and analysed for the fructose content.

2.2 Computer and Accessories

The main purpose in the closed-loop system was to control the temperature and pH of the reaction at the desired set point. Figure 3 shows the schematic diagram for wiring of both the temperature and pH control, where the interface card of RS232 type was used to connect the reactor with the computer. The PC used in this work operated with Intel Celeron 667/800 MHz, with more than 1 GB. For proper installation and execution, the following software specifications were installed as shown in Table 2.
Figure 3. The schematic diagram of wiring for both temperature and pH control

Table 2. Software specifications

<table>
<thead>
<tr>
<th>Software</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating system</td>
<td>Window XP</td>
</tr>
<tr>
<td>C Compiler</td>
<td>Microsoft Visual Basic</td>
</tr>
<tr>
<td>FULDEK</td>
<td>Version 1.0</td>
</tr>
<tr>
<td>MATLAB/Simulink</td>
<td>Version 12a</td>
</tr>
</tbody>
</table>

The control hardware consists of the following items below:

- **Sensors**: Mattec-T PT100, thermocouple, temperature sensor (from 0 °C to 100 °C) with 4mm diameter and 150 mm in length and pH probe (Amphel) (pH from 3 to 10).
- **Transmitter**: Temperature transmitter; (FlexTop 2202, Baumer, 4 to 20 mA signal, 3 wire sensors, accuracy better than 0.25 °C), pH transmitter; (FlexTop 2202, Baumer, 4 to 20 mA signal, 3 wire sensors, accuracy better than 0.1).
- **Converter**: SSR and RS232 for Heater converter.
- **Analog-digital interface card**: AIO-3310/1/2 (JS Automation Corp., Taipei, Taiwan); PCI plug and
play function with 16 identical cards. Analog function: for software selectable input range; -10 V~+10 V. For Digital I/O function; 232 bit multifunction up to 33 MHz.

2.3 Software Sensor for Estimation of Fructose Concentration

The experimental work so far in this study used analytical method for determination of fructose concentration. Time consuming and high maintenance cost for the analysis of fructose concentration using analytical method trigger the development of a software sensor which acts as an estimator or prediction. The application of ANN has been widely used as a prediction for the fructose formation in the glucose isomerisation. The proposed sensor was introduced into the batch reactor due to the dynamic and variation of the process. Figure 4 shows the schematic diagram of batch reactor with the software sensor.

![Figure 4. Schematic diagram of batch reactor for glucose isomerisation process with software sensor](image)

Based on the initial data of closed-loop experiment for temperature and pH effect (inputs for the software sensor) the software sensor was introduced to estimate the fructose concentration (output). The procedure and control hardware to perform this experiment is similar with the closed loop experiment.

3. Results and Discussion

Analytical methods for the determination of simple sugar are generally based on the HPLC column using RI detector such as by (Gram & Bang, 1990) followed by several researchers (Bhosale et al., 1996; Crabb & Shetty, 1999; Salehi et al., 2004; Lee & Hong, 2000). Rački et al. (1991) reported a Dische-Borenfreund method for the determination of fructose concentration. This method is time consuming and costly for material in handling the HPLC as well as maintenance of it. For this purpose, Artificial Neural Networks was used in this study for the estimation of fructose concentration instead of chemical analysis.

According to (Anantachar et al., 2010), there are two main advantages for the application of Artificial Neural Networks. The primary advantage is that, it does not require a user-specified problem solving algorithm, instead it ‘learns’ from examples, much like human being. Moreover, it has inherent generalization ability. The alternative method has the following properties: (i) it is applicable for all type of reactors without any limitations (ii) it does not require any assumptions about kinetic study.

The Artificial Neural Networks was carried out using the Neuralware Product and Predict Software (Neuralware Carnegie, USA, product release 3.2, February, 2007). By using data of experiment for batch reactor, Stirred Tank Reactor (STR), the ANN was developed. For the STR, the ANN was built up which consists of five inputs, one output with linear transfer function, and ten hidden layers, using sigmoid as a transfer function in the hidden layers. The inputs of the neural network were temperature, ($T_k$), previous temperature, ($T_{k-1}$), glucose concentration, $[G]$, pH$_k$ and previous pH, (pH$_{k-1}$). The output of the system was the fructose concentration, $[Fr]$. 


3.1 On-Line Prediction

The application of soft sensor in this study is for on-line prediction of fructose concentration which is the most common application (Kadlec et al., 2009). These ANN-based software sensors are used coupled with the primary on-line sensors, which capture large volumes of real-time isomerisation data (Rivera et al., 2010). Accuracy of the proposed soft sensor was calculated by the correlation coefficient ($R^2$) and mean square error (MSE) (Rivera et al., 2010).

The performances of the ANN-soft sensor for the effect of temperature and pH in the batch reactor are shown in Figure 5 and Figure 6. Table 3 and 4 summarized the values of $R^2$ and MSE.

Figure 5 shows the proposed soft sensors predicting (named PT55, PT60, PT65 and PT70) accuracy of fructose concentration from easily measurable input variables at each temperature. The experimental results refer to the off-line analysis of fructose concentration using HPLC (named ExT55, ExT60, ExT65 and ExT70). The results were further emphasized in terms of $R^2$ and MSE.

![Figure 5](image5.png)

Figure 5. Experimental (filled shapes) and performance of the ANN-soft sensor for the fructose concentration (lines) in the Batch Reactor (change of temperature)

The accuracy of ANN-soft sensor with the effect of pH is shown in Figure 6. From Figure 6, throughout the reaction time for each pH under study, the ANN-soft sensor prediction of fructose concentration function almost as accurately as the experimental works (refer to off-line analysis by HPLC method). The performance of the soft sensor was indicated by the values of $R^2$ and MSE.

![Figure 6](image6.png)

Figure 6. Experimental (filled circles) and performance of the ANN-soft sensor for the fructose concentration (lines) in the Batch Reactor (change of pH)
Table 3. Performance of Soft sensor in the Batch reactor with temperature effect

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$R^2$</th>
<th>MSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>55</td>
<td>0.993</td>
<td>0.056</td>
</tr>
<tr>
<td>60</td>
<td>0.987</td>
<td>0.165</td>
</tr>
<tr>
<td>65</td>
<td>0.993</td>
<td>0.107</td>
</tr>
<tr>
<td>70</td>
<td>0.991</td>
<td>0.116</td>
</tr>
</tbody>
</table>

Table 4. Performance of Soft sensor in the Batch reactor with pH effect

<table>
<thead>
<tr>
<th>pH</th>
<th>$R^2$</th>
<th>MSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.993</td>
<td>0.122</td>
</tr>
<tr>
<td>6</td>
<td>0.996</td>
<td>0.069</td>
</tr>
<tr>
<td>7</td>
<td>0.984</td>
<td>0.137</td>
</tr>
<tr>
<td>8</td>
<td>0.998</td>
<td>0.077</td>
</tr>
<tr>
<td>9</td>
<td>0.998</td>
<td>0.043</td>
</tr>
<tr>
<td>10</td>
<td>0.996</td>
<td>0.110</td>
</tr>
</tbody>
</table>

From Table 3 and 4, $R^2$ were greater than 0.95 and the values of MSE were less than 0.2, indicating a good fit of the ANN-soft sensor to the experimental data, accurate up to 95.7% for training and 100% for testing. From these criteria, it was concluded that the proposed ANN-soft sensor was the most precise in predicting fructose concentration.

4. Conclusion

ANN soft sensor was the most precise in predicting fructose concentration with $R^2$ were greater than 0.95 and the values of MSE were less than 0.2, indicating a good fit of the ANN-soft sensor to the experimental data. From these criteria, it concludes that the proposed ANN-soft sensor for on-line prediction is capable of achieving a satisfactory prediction performance. Based on the results of this study, artificial intelligence techniques of other different process are proposed using other types of reactor such as fluidized reactor for higher values of product and lower cost of operating should be studied. Beside that implementation of other control strategies such as model predictive control to the batch and continuous system should be introduced.

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References


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