AN INVERSE ARTIFICIAL NEURAL NETWORK BASED MODELLING APPROACH FOR CONTROLLING HFCS ISOMERIZATION PROCESS

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Abstract: Isomerization of the glucose content of high fructose corn syrup (HFCS) into fructose needs to be strictly controlled in order to obtain a balanced product for sweetness and solubility, creating a non-trival problem. This work presents an approach to modelling of a real industrial isomerization reactor by artificial neural networks (ANN) pre-processed with principal component analysis (PCA). The initial model considered the exit fructose concentration as the output variable while the substrate flow rate to the reactor as the principal input (manipulated) variable. Then the neural network model was restructured and inversely trained by assuming the exit fructose concentration as the input variable and the feed flow rate as the output variable. Results indicate good performance by application of the developed strategy to an extensive industrial data set.
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1. INTRODUCTION

Glucose syrups and blends are used as an alternative to sugar or sucrose in many applications such as food, chiefly confectionery but also bakery and soft drinks. High Fructose Corn Syrup (HFCS) is a nutritive sweetener with high commercial potential. Most of HFCS is produced by the hydrolysis of starch into glucose. Glucose has only about 70 % of the sweetness of sucrose and is less soluble. At high concentrations, glucose syrup must be kept warm to avoid crystallization. On the other hand, fructose is 30 % sweeter than sucrose and twice as soluble as glucose at low temperatures (Asif and Abaseed, 1998). Using enzyme technology, the conversion of glucose to fructose by at least 50 % overcomes both problems giving a stable high-fructose corn syrup (HFCS) that is as sweet as a sucrose solution. Therefore, large percentage of the glucose derived from starch hydrolysis is converted into its sweeter-tasting isomer fructose, by the use of enzymes. The crystal clear syrup performs many of the same functions as sugar, but sold at a price considerably below sugar. Thus, HFCS is finding an increased use in soft drinks manufactured in the advanced countries. Presently, two normal grades i.e. 42 wt % HFCS and 55 wt % HFCS and an enriched grade 90 wt. % HFCS are commercially available.

In HFCS production it is important that the concentration of the product from isomerisation reactor maintains a constant value for consumer satisfaction. The process is complicated because of the interrelated influences arising from the enzyme activity, inflow concentrations, temperature and dry substrate. In practice, this control problem is generally solved by relying on the past experience of the operators with help from current daily process measurements. Therefore the industry is eager for sophisticated techniques that will allow them to control the process strictly and with ease. This in turn requires that a representative model of the isomerisation reactor be identified.

On the other hand, in cases where abundant data (i.e. process measurements) is available, one of the major developments in model building and control has been in the field of artificial neural networks (ANNs). During the last decade ANNs evolved from only a research tool into a tool that is applied to many real world engineering problems, statistics, even medical and biological fields. The number of European patents obtained in the last decade corroborates the trend of increased applications of ANNs (Kappen, 1996).

The fact that glucose content of HFCS is sweeter but less soluble than its fructose content dictates that the conversion of glucose to fructose is required, but at a certain level. Thus, this izomerization process needs to be strictly controlled in order to obtain a balanced product, creating a non-trival problem due to the complexities in the enzyme technology and interrelation of variables involved. The industry

tends to rely on data based techniques that would be representative of their past experience.

In this paper, we have investigated the modeling and control of the production of high-fructose corn syrup in an industrial isomerisation process by artificial neural networks with pre-processing with principal component analysis. An inverted control-oriented model was developed to regulate the fructose concentration in the reactor by manipulating the substrate flow rate. The back-propagation algorithm was applied to training and testing the network. The compliance of the prediction of the regular model to the real industrial data, and the possible use of the inverted control model is presented and discussed here.

2. PROCESS DESCRIPTION

The first step in the manufacture of HFCS is the production of aqueous starch slurry. For HFCS processing, corn is cleaned, and soaked in hot water containing a preservative such as dissolved SO_2. Determination and consequent removal of oil bearing germs is achieved through partial grading of corn. The oil-bearing germs are separated, dried and expelled to extract the oil, which is a by-product with high market value. Oil bearing genus free corn grains are ground and processed to remove fibrous materials, and proteins. The refined starch slurry is sent to a jet-cooking unit wherein an appropriate dose of enzyme alfa-amylase catalyses its conversion into meltodextrins which is a low dextrose equivalents (DE) oligosaccharide. The next step is saccharification, where the low DE syrup is further converted to dextrose by the action of glucoamylase enzyme. Most modern plants use continuous saccharifications process. It takes 65-75 hrs to obtain a 94-96% dextrose hydrolysate, which is then sent for isomerisation after proper refining. This dextrose syrup (94-96 % DS, dry substrate) is passed over columns (reactors) packed with immobilized isomerase enzyme to obtain 42 weight % HFCS. The degree of isomerisation can be controlled by the flow of the substrate. This part of the process, which is the subject of this study, is crucial in the sense that the concentration of the fructose in the reactor exit determines the final product specification, and thus needs to be strictly regulated. The enriched grade i.e. 90 % HFCS is obtained form the 42 % HFCS by chromatographic separation technique. 55 % HFCS is produced by blending 42 % HFCS with the enriched HFCS. Figure 1 depicts the input and output variables on a block representation of the isomerisation reactor.

3. ARTIFICIAL NEURAL NETWORK MODELLING WITH PCA PREPROCESSING

An Artificial Neural Network (ANN) is an information processing system that roughly replicates the behaviour of a human brain by emulating the operations and connectivity of biological neurons. It performs a human-like reasoning, learns the attitude and stores the relationship of the processes on the basis of a representative data set that already exists. In general, the neural networks do not need much of a detailed description or formulation of the underlying process, and thus appeal to practicing engineers who tend to mostly rely on their own data.

Depending on the structure of the network, usually a series of connecting neuron *weights* are adjusted in order to fit a series of inputs to another series of known outputs. When the weight of a particular neuron is updated it is said that the neuron is *learning*. The training is the process that neural network learns. Once the training is performed the verification is very fast. Since the connecting weights are not related to some physical identities, the approach is considered as a black-box model. The adaptability, reliability and robustness of an ANN depend upon the source, range, quantity and quality of the data set.

The feedforward neural networks consist of three or more layers of nodes: one input layer, one output layer and one or more hidden layers. The input vector passed to the network is directly passed to the node activation output of input layer without any computation. One or more hidden layers of nodes between input and output layers provide additional computations. Then the output layer generates the mapping output vector. Each of the hidden and output layers has a set of connections, with a corresponding strength-weight, between itself and each node of preceding layer. Such structure of a network is called a *Multi-Layer Perceptron* (MLP).

Neural network training can be made more efficient if certain preprocessing steps are performed on the network inputs and targets. Particularly in some situations where the dimension of the input vector is large and the components of the vectors are highly correlated, it is useful to reduce the dimension of the input vectors. An effective procedure for performing this operation is principal component analysis (PCA). This technique has three effects: it orthogonalizes the components of the input vectors (so that they are uncorrelated with each other); it orders the resulting orthogonal components (principal components) so that those with the largest variation come first; and it eliminates those components that contribute the least to the variation in the data set. The input vectors are multiplied by a matrix whose rows consist of the eigenvectors of the input covariance matrix. This produces transformed input vectors whose components are uncorrelated and ordered according to the magnitude of their variance.

A feed-forward back-propagation artificial neural network (BPNN) is chosen in the present study since it is the most prevalent and generalized neural network currently in use, and straightforward to implement. Figure 2 illustrates the basic

configuration of the network, particularly for the case of control-oriented inverted model. Each interconnection in the model has a scalar weight associated with it, which modifies the strength of the signal. The function of the neuron is to sum the weighted inputs to the neuron and pass the summation through a non-linear transfer function. In addition, a bias can also be used, which is another neuron parameter that is summed with the neuron's weighted inputs. Back-propagation refers to the way the training is implemented and involves using a generalized delta rule. A 'learning' rate parameter influences the rate of weight and bias adjustment, and is the basis of the back-propagation algorithm. The set of input data is propagated through the network to give a prediction of the output. The error in the prediction is used to systematically update the weights based upon gradient information. The network is trained by altering the weights until the error between the training data outputs and the network predicted outputs is small enough. There are many back-propagation training algorithms available. The choice of algorithm depends on the type of problem and may require experimentation of different algorithms. The algorithms have different computation and storage requirements, and train data at different speeds. The goal of selection is to efficiently and accurately train the network while keeping the speed of training relatively fast. In this work the Levenberg–Marquardt algorithm was used.

After generating sets of training patterns, appropriate NN architecture and associated parameters must be chosen for the particular application. The main design parameters are the number of hidden layers, number of neurons in each layer, and the neuron processing functions. The choice of these parameters will depend on the complexity of the system being modelled and they will affect the accuracy of the model. There is no exact guide for the choice of the numbers. The architecture of most ANN model is designed by trial and error.

In this work, a three-layer feed-forward network was created. The first layer has six hyperbolic tangent sigmoid neurons, the second layer has twenty logarithmic sigmoid neurons and last layer has one linear neuron. The performance function was calculated by using mean squared error. The network was trained for 2000 epochs.

4. RESULTS AND DISCUSSION

In this study the HFCS isomerisation process is modelled with ANN, and ANN with preprocessing PCA. The first regular model was created by considering the fructose concentration in the isomerization reactor as the output variable, such as illustrated in the process input-output diagram in Figure 1. Then the model was inverted such that the substrate flow rate was regarded as the output, so that a simple control strategy can be created to regulate the fructose concentration at a certain level by

changing the input flow rate. The inverted model is depicted in Figure 2 where the network structure is also identified. Comparison of Figures 1 and 2 reveals the interchange of the substrate flow rate and the fructose concentration between the regular model and inverted model.
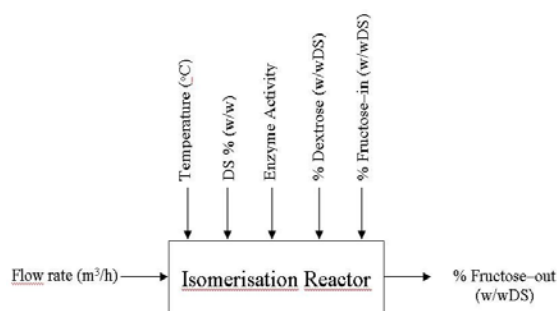

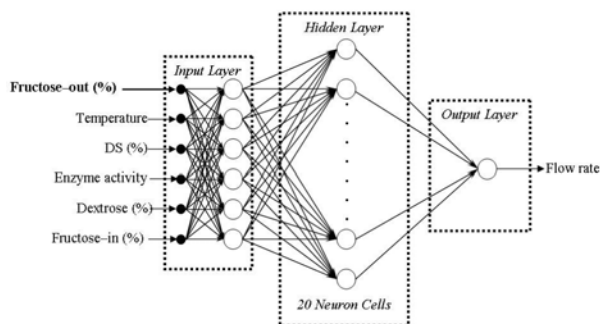Fig. 1. Process block diagram represented by the regular model

Fig. 2. Selected neural network structure depicting the form of inverted model

For development of neural network models the Neural Network Toolbox 4 and MATLAB 6.5 (The Mathworks Inc.) were used. A MATLAB script was written, which loaded the data file, trained and validated the network and saved the model architecture. The input and output data were normalised and de-normalised before and after the actual application in the network. A personal computer with Pentium-4 1.2 GHz processor and 512 Mb internal memory was used for processing neural network models.

The training and testing data was provided by Cargill Inc. from their Orhangazi–Turkey plant. Each data represents the measurements of one day, and the whole set is a mixture of data recorded from different reactors. Prior to conducting the network training operation using the back propagation algorithm, the industrial data set (1200 data altogether) was divided into two sections; a training set, which consisted of 1000 data, and a testing set that was formed by remaining 200 data. Dividing of training and testing sections was made by random selection.

The ANN model used first for regular representation of the reactor consists of six input nodes corresponding to (a) flow rate (manipulated variable for control) (m3/h), (b) temperature (^{o}C), (c) dry substrate DS (w/w %), (d) cumulative flow rate as

enzyme activity, (e) dextrose concentration in the input stream to the reactor (w/wDS %), (f) fructose concentration in the input stream to the reactor (w/wDS %). The single output was the fructose concentration in the reactor (w/wDS %). Thus a three layer feed-forward neural network was chosen for modeling purposes. In the hidden layer, twenty hidden neurons were used. For training, the classical back-propagation algorithm was used. Activation functions used were logarithmic sigmoid and tangent sigmoid. The selected 'control-oriented' network structure is shown in Figure 2 where the substrate flow rate and the fructose concentrations are interchanged to form the inverted model. MLP network structure and ANN parameters are shown in Table 1.

Table 1. ANN parameters

Parameter	ANN	ANN+PCA	Invers ANN+PCA
Learning rate	0.1	0.1	0.1
Epochs	2000	2000	2000
No. MLP layers	3	3	3
Input nodes	6	6	6
Hidden nodes	20	20	20
Output nodes	1	1	1
Training accuracy	86.6	99.47	92.8
Test accuracy	85	98.1	91.4

The model was first trained for the regular input-output behavior of the isomerisation reactor, whose results are shown in Figure 3 in parity plot form. The behaviour of the network for the test data is reflected in the following Figure 4. As can be detected from Figure 4, the network model captures the general trend in the output but obviously does not give very close prediction.
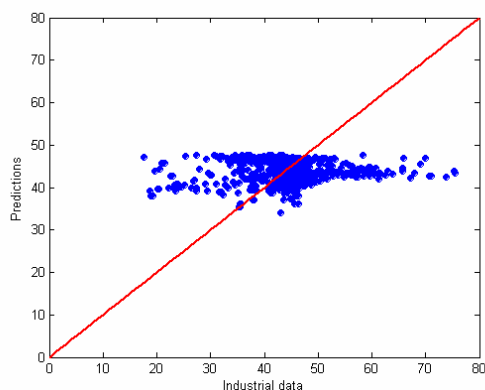

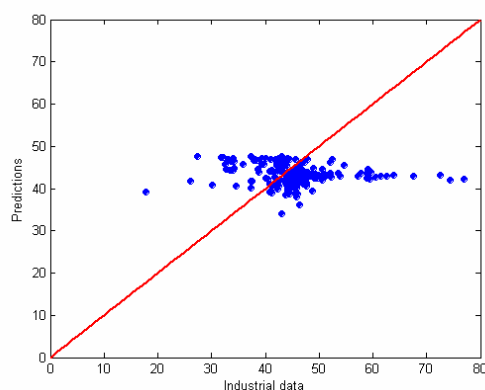Figure 3. ANN model for learning data (% fructose in reactor)

Figure 4. ANN model for test data (% fructose in reactor)

Therefore, preprocesssing with PCA technique was applied, whose results are depicted only for the test data in Figure 5 for predicting the fructose concentration. We have conservatively retained those principal components which account for 99.8 % of the variation in the data set. There was apparently redundancy in the data set, since the principal component analysis has reduced the size of the input vectors from 6 to 5.

When figures 4 and 5 are compared, it becomes evident that the pre-processing improves the prediction capability of the model tremendously.
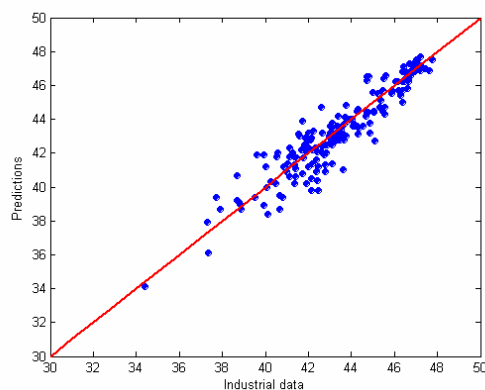

Figure 5. ANN model with PCA preprocessing for test data (% fructose in reactor)

Satisfied with the results obtained from pre-processed ANN model, the structure of model was then inverted to form the ANN model shown in Figure 2 with interchanged substrate input flow rate and fructose concentration in the reactor. Figure 6 shows the learning results of the network for predicting the flow rate of the substrate to the reactor. The inverted model was then validated with the test data revealing the results shown in Figure 7, which demonstrates close agreement of the model predictions with the industrial data.
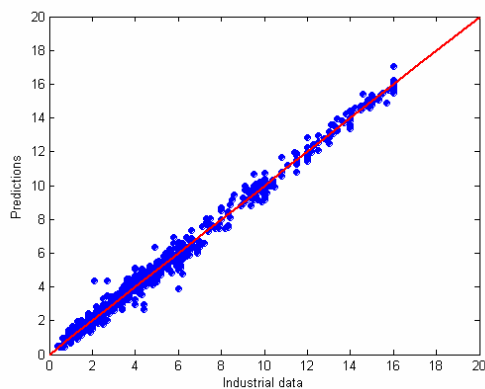
Figure 6. Inverted ANN model with PCA
preprocessing for learning data
(substrate input flow rate to the reactor, m^3/h)
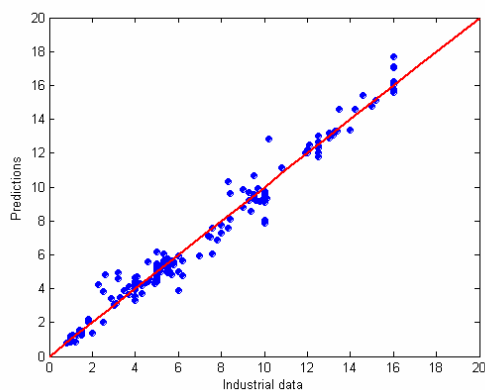

Figure 7. Inverted ANN model with PCA
preprocessing for test data
(substrate input flow rate to the reactor, m^3/h)

Overall evaluation of these results demonstrate that the ANN model preprocessed with PCA accurately predicts the behaviour of HFCS isomerisation reactor, and therefore holds promise for application in real industrial world.

5. CONCLUSIONS AND FUTURE WORK

An artificial neural network model with pre-processing with PCA was developed in this work to predict the substrate feeding rate to the isomerisation reactor in HFCS processing for control purposes. Since the sampling rate is inherently slow in the process, the results allow the interpretation that by implementation of the suggested model it will be possible to regulate the fructose concentration of the exit stream at the desired level.

With the promising results obtained from this work, our current efforts are directed towards two directions:

(a) Developing a graphical user interface (GUI) to implement the suggested strategy for controlling the fructose concentration in the HFCS

isomerisation reactor. The suggested method, with the help of this GUI, will allow operators to decide what flow rate of input substrate is to be used for maintaining the fructose level at the output, based on daily measurements of other process variables.

(b) We are also considering a model-based control strategy with the ANN model. Although the sampling rate in practice is very slow to merit such a technique, it would be interesting to see the performance of a model predictive neural network controller for such real industrial data.

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