STEADY STATE MODELLING OF CHEMICAL SYSTEMS BY USING NEURAL NETWORKS

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Abstract:

This paper presents the development of artificial neural network (ANN) models for two steady state chemical engineering systems, which are, 1) physical properties of palm oil components, and 2) pore size determination for membrane categorization by using ANN. Even though studies on ANN applications in chemical engineering in the literature are more concentrated on utilising dynamic models, there has been a rapidly increasing trend for diverse application of ANN to model steady state systems. For the crude oil distillation column standard radial basis function (RBF) gave sufficiently accurate predictions. For the physical properties of palm oil components, a multi layer perceptron (MLP) network model was able to give a much better prediction of the density of trilaurin than a thermodynamic correlation that is based on group contribution method. For pore size determination of an asymmetric membrane, stacked network gave slightly better prediction than the more commonly used single MLP network. On the whole, this study shows that there is high potential for various applications of ANN models in chemical engineering.

I. Introduction

Artificial neural networks (ANN) have been designed on the premises of mimicking the complexities of the brain functions in an effort to capture (or at least partially capture) the amazing learning capabilities of the brain. ANN is a sort of parallel computer/processor designed to imitate the way the brain accomplishes a certain task [Willis, et al, 1991]. The smallest processing element of ANN is a neuron (also called node), which performs simple calculations. Using the nodes collectively with massive connections among them results in a network that is able to process and store information for mapping the network inputs to its outputs. With this capability, there are widespread interests due to on-going and potential applications in solving complex problems particularly in the fields of pattern recognition (especially in speech and image processing), classification, control, forecasting, systems identification and optimization.

ANN had generated much interest in the chemical engineering community since the late eighties. While there have been numerous successful applications of neural networks in the chemical industry there are also those who claim neural networks to be nothing more than a class of nonlinear parameter estimation techniques. While the criticisms were sometimes well founded, there is a need to remember that drawbacks, extreme expectations and negative reactions are the norm in the exploration of an emerging field. Hence, there is a need to find suitable roles that can best exploit the capabilities of neural networks in the chemical engineering field.

Currently, research in chemical engineering on ANN is mostly in process fault diagnosis, dynamic process modeling and process control. Compared to the large number of literature found on dynamic modeling, there are fewer papers on steady-state ANN process models. Nevertheless, there has been lately an increasing trend for diverse application of ANN to model steady-state processes.

II. Crude oil distillation column

A. Background

The ANN models developed for the industrial crude oil distillation column is for use in real-time optimisation (RTO). RTO, which is the continuous evaluation and adjustment of a process operating conditions to optimise the economic productivity subject to constraints, traditionally uses steady state first principles (FP) models. Developing FP models require in-depth knowledge of material, energy and momentum conservation, as well as thermodynamics and kinetics, of the processes. As a result, the model is complex and requires a high level of expertise to develop and maintain. Model development is also time-consuming and expensive. The crude tower is a practical candidate for RTO due to variations in operating conditions and its complex, multivariable nature.

The ANN models developed are steady-state, multivariable models for the complete process. This is different than ANN models developed for process control or other off-line applications, which are dynamic models used to predict one or two variables. RTO requires steady-state models that can yield all output variables required by the optimiser. For large, multivariable processes, there can be more than 100 input and output variables. In addition, since the application is on-line, the models must also have short computation times.

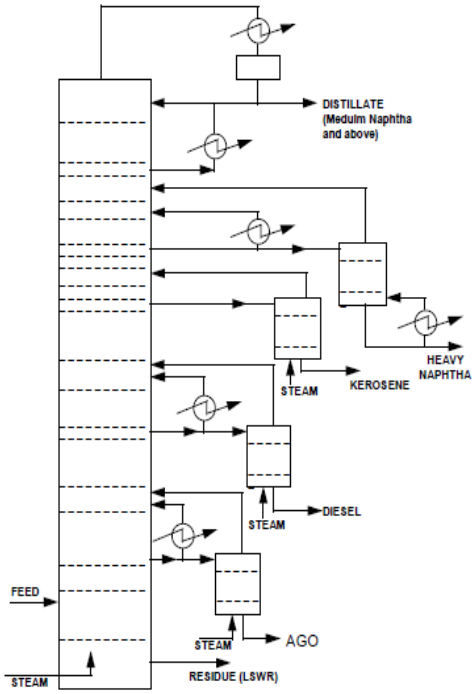

Fig.01 Schematic diagram of the crude oil distillation column.

Figure 01 shows a schematic diagram of the crude distillation column. The column has four pump rounds (p/a), four side strippers and six product streams, which are the distillate, heavy naphtha, kerosene, diesel, atmospheric gas oil (AGO) and low sulphur waxy residue (LSWR) streams. In actual operation, the product draw-off flow rates are adjusted to ensure on-specification products and to achieve the targeted production rate. The feed flow rate is adjusted according to the production target. Feed going into the column consists of a mixture of two different feed streams: a condensate stream, of which the light components were first flashed off, and a sweet crude oil stream. The feed composition depends on the mixture of the oil being fed to the column.

B. Model Development

The model for the crude tower is divided into the following sections: 1) top (T), 2) heavy naphtha stripper (HN), 3) kerosene stripper (K), 4) diesel stripper (D), 5) AGO stripper (AG), and 6) bottom (B). Only variables associated with the particular section are included in the network model. Product from the side draws must meet certain specifications. Operators obtain these specifications from the production planning section and adjust the tower operating conditions (ie. set points) to ensure on-spec products. Therefore, the ability to predict these cold properties would be an added advantage. Table 1 lists the specifications and the corresponding products and manipulated variables. Since the results of the different sections are similar, only the results obtained on the top and heavy naphtha (HN) stripper are shown in this paper.

	Specifications/ Properties	Manipulated Variables
Heavy	IBP	Top Temperature or Q
Naphtha	FBP	HN draw
Kerosene	Flash point/IBP Freeze point/FBP	HN draw SS Kerosene draw
Diesel	Pour Point / Colour IBP FBP	Diesel draw Kerosene draw Diesel draw
AGO	Pour Point / Colour IBP FBP	AGO draw Diesel draw AGO draw
LSWR	Pour point	AGO draw

Table: Product specifications and manipulated variables.

Note: IBP is initial boiling point
FBP is final boiling point
Q is re -boiler duty
SS is stripping steam rate

III. PHYSICAL PROPERTIES OF PALM OIL COMPONENTS

A. Background

Physical properties are essential in the design of chemical processes. The design of processes in the palm oil industry is of no exception. Since palm oil is very significant in the Malaysian economy, determination of its properties is important. Palm oil, like other vegetable oils, are made up of mostly glyceridic components with some non-glyceridic components in small or trace quantities. The chemical composition determines the chemical and physical characteristics of palm oil.

Triglycerides, which are esters formed from glycerol and fatty acids, are the major component of the glyceridic material in palm oil. The chain lengths of the fatty acids present in the triglycerides fall within a range from twelve to twenty carbons. Palm oil triglycerides consist of myristic acid, stearic acid, linoleic acid, palmitic acid and oleic acid .The design and optimisation of processes can only be achieved with the availability of physical properties. Examples of these physical properties are density, viscosity, specific heat and vapour pressure. These properties are not constants, but vary with temperature.

The determination of physical properties of chemical components is found through experiments. However, it is expensive and impossible to perform experiments for all variations of the independent variable. The common practice is to fit these experimental data to suitable thermodynamic correlations. For palm oil, there is a lack physical properties data and inadequate correlation methods for proper prediction [Morad 1995], which is definitely a setback in the development of local technology.

In this research, instead of using the traditional thermodynamic correlations, ANN models were developed to calculate the values of the physical properties of palm oil components. Models were developed for physical properties like density, specific heat and viscosity for several palm oil components. This section describes the development of an ANN model for predicting the density of trilaurin.

B. Model Development

Experimental data of trilaurin for training and testing the network model were obtained from [Morad 1995]. There are a total of 14 data points (ranging from 60^oC to 190^oC), of which 8 were used for training and 6 for testing. These data were scaled between 0 to 1 to give better results. The ANN model chosen was the multi-layer perceptron (MLP) feed forward network that was trained using the Levenberg-Marquadt algorithm. The network model has one hidden layer with five nodes and sigmoid activation function. Similar to the crude tower models, the RMSE of the network prediction was calculated to find the best model. The density of trilaurin was also calculated using a group contribution method for calculating density, GCVOL [Morad 1995], for the purpose of comparison with the ANN model.

IV. Artificial Neural Networks

A. Prologue to Neural Networks

Neural networks, or more specifically, artificial neural networks are mathematical models inspired from our understanding of biological nervous systems. They are attractive as computation devices that can accept a large number of inputs and learn solely from training samples. As mathematical model for biological nervous systems, artificial networks are useful in establishing relationships between inputs and outputs of any kind of system. Roughly speaking, a neural network is a collection of artificial neuron. An artificial neuron is a mathematical model of a biological neuron in its simplest form. From our understanding, biological neurons are viewed as elementary units for information processing in any nervous system. Without claiming its neurobiological validity, the mathematical model of an artificial neuron is based on following points

1. Neurons are the elementary unit in a nervous system at which information processing occurs.
2. Incoming information is in the form of signals that are passed between neurons through connection links.
3. Each connection link has a proper weight that multiplies the signal transmitted.
4. Each neuron has an internal action, depending on a bias or firing threshold resulting in an activation function being applied to the weighted sum of the input signal to produce an output signal.

The sensitivity analysis feature in Aspen Plus was used to generate training and testing data for the crude tower. Input variables for the ANN models include the feed flow rates for the two feed streams, and the specified variables of a particular section for the tower operation. The output variables are the dependant variables that were needed by the optimiser and were calculated due to changes in the input variables. Ranges for the variables were within the operating region of the column. Within this region, the variables in each section of the column have negligible influence on other sections in the column, except the sections that are immediately above and below it. This allowed data to be generated one section at a time.

In this work, all ANN models were developed in MATLAB environment and utilizes MATLAB neural network toolbox. The type of ANN chosen was the radial basis function networks (RBFN), a feed forward network that has a single hidden layer of nodes with Gaussian density function. MATLAB uses the orthogonal least squares (OLS) algorithm by Chen et al. [1991] to solve for the RBF centers and weights for the connections between the nodes in the hidden and output layers. To develop the RBFN models, other than specifying an error goal, the spread constant (σ), which determines the width of the receptive fields must also be specified. 'σ' should be large enough for the receptive fields to overlap one another to amply cover the whole input range. Nevertheless, it should not be too large that there is no distinction between the output of different nodes in the same area of the input space. For the RBFN models, the OLS algorithm calculated the number of hidden nodes.

Evaluations of the models are based on root mean squared (RMS) error from each model prediction. Error is defined as the difference between desired (or actual value provided by the testing data) output value and the predicted output value. Training time was also taken into consideration, mainly because of the convenience in developing models with short training times. Nevertheless, this is not as important as RMS error because once a connectionist model is trained; the execution of the model is very fast. The training time will only be a major concern when the model is periodically updated on-line. For all the models, the results presented in this paper are the best ones obtained after numerous trials of different training error tolerance and spread constant.

The crude tower model was not developed as a single lumped system. Since changes within the operating range for a section in the crude distillation tower affects only the sections that are immediately above and below the section, this allows the crude tower model to be divided into sections where the variables that are related are grouped together, and thus make the model more manageable.

B. Implementation of Neural Networks

The implementation of Neural Networks for finding best iterative process the experimental results has been simulated in the Matlab environment. For running the Matlab program the experimental results has been taken as input to the neural network.

The number of inputs to the neural network is 6 numbers, and the number of hidden layers is 100 and the ANN output is 6

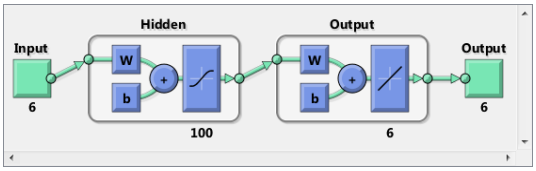

Fig 02 Neural network model of the simulated model

The simulink models of the ANN networks is shown in the below

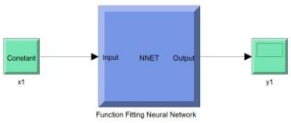

Fig 03 Simulink model of the Neural Network model

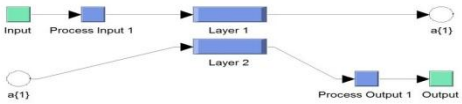

Fig 04 Representation of the inner block Function fitting Neural network

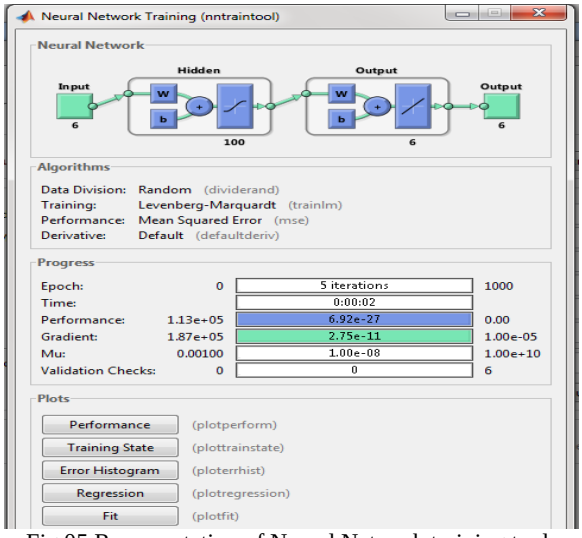

Fig 05 Representation of Neural Network training tool

By running the experimental results with the matlab environment there should a definite improvement as compared with the experimental results the below shown fig 06 show the simulated results of the ANN Model

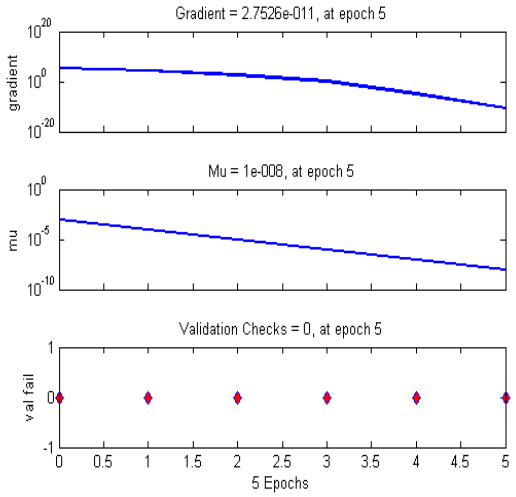

Fig 06 Comparison of ANN model prediction and with experimental data used for testing.

The results has been show in the Tabulated form in the below table 02

S.No	Temp	Experimental data		ANN Model	
	deg	Scaled	g/ml	Scaled	g/ml
1	70	0.7093	0.877888	0.718	0.87978
2	90	0.6132	0.869034	0.6168	0.8694
3	110	0.483	0.855675	0.4809	0.85546
4	130	0.3055	0.837469	0.3126	0.83819
5	150	0.1574	0.822282	0.168	0.82337
6	170	0	0.806132	0.0021	0

The graphical results of the performance of an experimental results when it has been trained in the ANN program is shown in the below figure 07

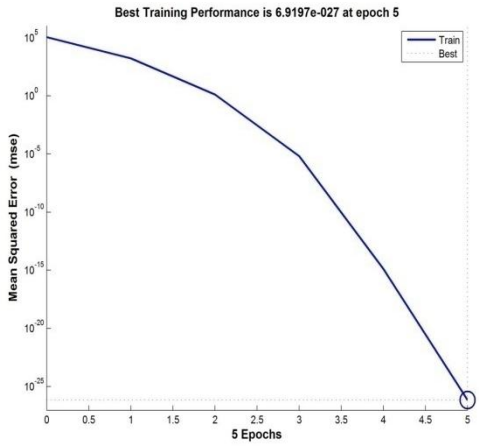

Fig 07 Best Training performance of the experimental data by using the ANN Model

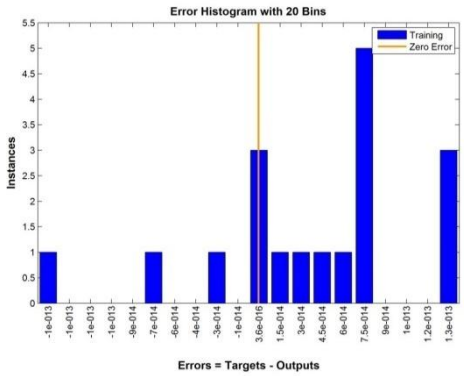

Fig 08 Representation of Error data when the experimental data is ran in ANN Model in Matlab environment.

V. Conclusion

Research done on the three cases described revealed further potential for the use of ANN in chemical engineering. From the results obtained, the ANN models were found to give at least satisfactory, if not excellent predictions. Although there are undoubtedly problems and setbacks to be overcome, they only serve as challenges and motivating factors that fuels further interest in the area.

VI. References

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