Development of Artificial Neural Network Model for Pale Crepe Rubber Processing

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บทคัดย่อ

ยางเครพขาวเป็นยางธรรมชาติสีจางที่ผลิตจากน้ำยางสดพันธุ์ RRIM600 ทำให้ได้ยางคุณภาพสูงซึ่งมีสมบัติพิเศษ คือ มีสีอ่อน เหมาะสำหรับอุตสาหกรรมผลิตผลิตภัณฑ์ยางสีต่างๆ เช่น ผลิตยางขอบรองเท้า พลาสเตอร์ยา อุปกรณ์กีฬา และอุปกรณ์การแพทย์ เป็นต้น ส่งผลให้ราคายางเครพขาวสูงกว่ายางแผ่นรมควันชั้น 1 อย่างไรก็ตาม พบว่า การผลิตยางเครพขาวยังไม่เป็นที่นิยมในประเทศไทยเนื่องจากสารฟอกสีมีราคาสูง เพื่อแก้ปัญหาดังกล่าว งานวิจัยนี้จึงศึกษาการผลิตยางเครพขาวด้วยวิธีการจับตัวบางส่วนเพื่อแทนที่ขั้นตอนการฟอกสียาง โดยมีวัตถุประสงค์เพื่อสร้างแบบจำลองโครงข่ายประสาทเทียม (ANN) สำหรับกระบวนการผลิตยางเครพขาวด้วยวิธีการจับตัวบางส่วน และเพื่อหาสภาวะดำเนินการที่ดีที่สุดบนพื้นฐานของแบบจำลอง ANN ที่ได้โดยการวิเคราะห์พื้นผิวตอบสนอง

การศึกษาในครั้งนี้แบ่งเป็น 3 ส่วน คือ การทดลอง การออกแบบโครงข่ายประสาทเทียมสำหรับกระบวนการผลิตยางเครพขาว และการหาสภาวะดำเนินการที่ดีที่สุดบนพื้นฐานของแบบจำลอง ANN ที่ได้ ในส่วนของการทดลองได้ศึกษาการผลิตยางเครพขาวด้วยการจับตัวบางส่วนโดยใช้กรดอะซิติกเข้มข้น 1% โดยน้ำหนักเพื่อจับตัวเนื้อยางบางส่วน ในส่วนนี้ได้ศึกษาผลของปริมาณกรดอะซิติกและเวลาที่ใช้ในการจับตัวบางส่วนต่อสมบัติของยางเครพขาว คือ ค่าสี (Lovibond color), ค่าความหนืดมูนี่ (MV), ค่าความอ่อนตัวเริ่มต้น (P_0) และดัชนีความอ่อนตัว (PRI) ผลการทดลองพบว่าที่ปริมาณกรดอะซิติก 0.15% โดยปริมาตรต่อน้ำหนักเนื้อยางแห้ง และเวลาที่ใช้ในการจับตัว 2 ชั่วโมงทำให้ได้สมบัติของยางเครพขาวผ่านเกณฑ์มาตรฐาน นั่นคือ ค่าสีน้อย $\leq$ 3, ค่าความหนืดมูนี่ > 60, ค่าความอ่อนตัวเริ่มต้น > 35 และดัชนีความอ่อนตัว > 60

ในส่วนที่สอง ได้ออกแบบโครงข่ายประสาทเทียมโดยศึกษาจำนวนชั้นซ่อน 1-2 ชั้นและผลของจำนวนโหนดในแต่ละชั้นซ่อน (1-10 โหนด) โครงข่ายประสาทเทียมเป็นแบบป้อนไปข้างหน้า โดยมีข้อมูลอินพุต 4 ข้อมูลคือ (1) ปริมาณกรดอะซิติก (2) เวลาที่ใช้ในการจับตัว (3) เปอร์เซนต์เนื้อยางแห้ง (%DRC) และ (4) เปอร์เซนต์ปริมาณของแข็งในน้ำยาง (%TSC) ข้อมูลเอาต์พุตรวม 4 ข้อมูล คือ (1) ค่าสี (2) ค่าความหนืดมูนี่ (3) ค่าความอ่อนตัวเริ่มต้น และ (4) ค่าดัชนีความอ่อนตัว สำหรับชั้นของเอาต์พุตใช้ฟังก์ชันกระตุ้น (PURELIN) และเทรนด้วยอัลกอริทึม Levenberg-Marquardt ข้อมูลที่ใช้ในการออกแบบโครงข่ายประสาทเทียมประกอบด้วย 30 ชุดข้อมูล โดยแบ่งออกเป็น 80% ของชุดข้อมูลสำหรับการเรียนรู้ และ 20% ของชุดข้อมูลสำหรับการทดสอบ ในส่วนนี้ได้ศึกษาผลของจำนวนชั้นซ่อน, ฟังก์ชันกระตุ้น และการเลือกตัวแปรอินพุต ต่อประสิทธิภาพการทำนายของโครงข่ายประสาทเทียม

กรณีออกแบบโครงข่ายประสาทเทียมที่มี 1 ชั้นซ่อน ได้ศึกษาผลของฟังก์ชันกระตุ้น 7 ฟังก์ชัน ซึ่งได้แก่ TANSIG, LOGSIG, HARDLIM, HARDLIMS, SATLINS, POSLIN และ RADBAS เพื่อใช้ทำนายสมบัติของยางเครพขาว จากผลการจำลองพบว่า โครงข่ายประสาทเทียมที่เหมาะสมที่สุดมีจำนวนโหนดเท่ากับ 6 และใช้ฟังก์ชัน TANSIG ซึ่งให้ค่า MSE และ IAE ของการทำนายรวมต่ำที่สุด MSE/IAE = 0.029/3.109 สำหรับผลของการออกแบบโครงข่ายประสาทเทียมที่มี 2 ชั้นซ่อน (TANSIG) พบว่าโครงข่ายประสาทเทียมที่เหมาะสมที่สุดประกอบด้วยจำนวน 1 และ 3 โหนดในชั้นซ่อนที่ 1 และ 2 ตามลำดับ ซึ่งให้ MSE และ IAE ของการทำนายรวมต่ำที่สุด (MSE/IAE = 0.037/3.394)

ในงานวิจัยนี้ได้ใช้วิธีการตัดตัวแปรอินพุตเพื่อเพิ่มประสิทธิภาพการทำนายของโครงข่ายประสาทเทียมโดยใช้วิธี Partial modeling ด้วยวิธีนี้ตัวแปรอินพุตที่ส่งผลต่อการทำนายน้อยที่สุดสามารถระบุได้ด้วยการพิจารณาค่าความคลาดเคลื่อนของเอาท์พุตแต่ละตัว จากผลการศึกษาพบว่าในกรณีนี้ %TSC มีผลต่อการทำนายค่าเอาท์พุตน้อยที่สุดโดยเฉพาะต่อค่าสีและค่า PRI เทียบกับตัวแปรอินพุตอื่นๆ ดังนั้นจึงอาจไม่พิจารณาตัวแปร %TSC ทั้งนี้เนื่องจากค่า %TSC มีความสัมพันธ์กับค่า %DRC ดังนั้นในส่วนนี้ได้ออกแบบโครงข่ายประสาทเทียมที่ประกอบด้วยจำนวน 1 และ 3 โหนดในชั้นซ่อนที่ 1 และ 2 ตามลำดับ (TANSIG) ใหม่โดยพิจารณาเพียง 3 อินพุต คือ ปริมาณกรดอะซิติก เวลาที่ใช้ในการจับตัวและ %DRC จากผลการจำลองพบว่าประสิทธิภาพการทำนายเพิ่มขึ้นซึ่งให้ค่า MSE/IAE ของการทำนายรวมเท่ากับ 0.037/3.260

ในส่วนสุดท้าย ได้ศึกษาหาสภาวะดำเนินการที่ดีที่สุดบนพื้นฐานของแบบจำลองโครงข่ายประสาทเทียมที่สร้างขึ้นจาก 3 อินพุตโดยการวิเคราะห์กราฟพื้นผิวตอบสนอง จากผลการจำลองพบว่า สภาวะดำเนินการที่ดีที่สุดที่ให้ค่าสี ($\approx$ 3) และค่า MV (> 58 ML(1+4) 100^{o}C) ยอมรับได้คือ สภาวะดำเนินการที่ปริมาณกรดอะซิติก 0.2-0.22% โดยปริมาตรต่อน้ำหนักเนื้อยางแห้ง และเวลาที่ใช้ในการจับตัว 1.2-1.5 ชั่วโมง อย่างไรก็ตามค่า MV ของยางแผ่นมีแนวโน้มเพิ่มขึ้นเมื่อเก็บไว้เป็นเวลานาน อีกทั้งในกรณีนี้พบว่าค่า P_0 และ PRI มีค่าสูงกว่าเกณฑ์มาตรฐานในทุกกรณี

Thesis Title Development of Artificial Neural Network model for pale crepe rubber processing

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ABSTRACT

Pale crepe is a high quality rubber sheet since it has white/pale color (Lovibond color ≤ 3). It is produced from a particular type of rubber latex, RRIM 600, and used as raw material for manufacturing required-color products such as rubber soles, plaster, sport equipment, and medical devices etc. Even the pale crepe rubber has higher value added than RSS No.1, however it has been found that this process has not been widely used in Thailand because of high cost of the bleaching agent. To solve these problems, this work focuses on the pale crepe rubber processing with a fractional coagulation instead of the color bleaching. The objective of this study is to develop an artificial neural network (ANN) for pale crepe rubber produced by fractional coagulation, and to determine the optimal process conditions based the obtained ANN through response surface analysis.

The activities of this study are divided into three parts: the experimental results, ANN design for pale crepe rubber process, and the optimum operating conditions determination based the obtained ANN model. In the first part, the experiment has been carried out to produce pale crepe rubber via fractional coagulation method, 1% by wt. of acetic acid has been used to coagulate the latex fractionally. Effects of acetic acid amount and coagulation time have been investigated on the rubber properties; Lovibond color, Mooney viscosity (MV), initial plasticity (P_0) and Plasticity Retention Index (PRI). The proper operating condition should be at 0.15% vol./wt. of acetic acid, and coagulation time of 2 hrs to give the property requirement: rubber color ≤ 3, MV > 60, P_0 > 35 and PRI > 60.

In the second part, a network model has been designed by varying 1-2 hidden layers by varying their number of nodes (1 to 10). ANN model has feed-forward scheme with four input variables such as (1) acetic acid amount, (2) fractional coagulation time, (3) %dry rubber content (%DRC) of diluted latex, and (4) the corresponding %total solid content (%TSC). Four rubber properties, such as (1) rubber color, (2) MV, (3) P_0, and (4) PRI have been predicted via using linear transfer functions (PURELIN). The ANN has been trained using the Levenberg-Marquardt algorithm with 30 experimental data sets, 80% for training and 20% for testing. Effects of hidden layer, transfer function, and input variable selection have been investigated on the network prediction performance.

For one hidden layer ANN model structure, seven transfer functions such as TANSIG, LOGSIG, HARDLIM, HARDLIMS, SATLINS, POSLIN and RADBAS have been investigated in the hidden layer to retrieve the properties of pale crepe rubber. It has been found in the simulation results that the network model with 6 nodes, and the RADBAS transfer function gives the minimum overall MSE and IAE of the output prediction, MSE/IAE = 0.029/3.109. Moreover, the effect of the hidden layer has also investigated. The network model with two hidden layers (TANSIG) has been designed in the optimal manner providing the ANN model with 1 and 3 nodes in hidden layer 1 and 2 respectively gives minimum overall MSE and IAE (MSE/IAE = 0.037/3.394).

A variable selection approach such a partial modeling has been further applied in this research for the model improvement. The insignificant input variable has been chosen by considering their corresponding output variances. It has been found that %TSC has smallest effects on all process outputs in this case, especially Lovibond color and PRI compared to the other inputs. Therefore, %TSC could be ignored since it varies according to %DRC, it has then been chosen as the insignificant variable and further eliminated. New network model with 1 and 3 nodes in hidden layer 1 and 2 respectively (TANSIG) has been trained with three inputs, the acetic acid amount, the coagulation time and %DRC. The network structure with three input variables gives the overall MSE/IAE is 0.037/3.260. It can be seen that the ANN prediction can be improve by removing the less affect input variable.

Finally, the optimal operating conditions have been chosen based the network model with three input variables by considering the response surface plots. It has been found in the simulation results that the conditions providing acceptable color ($\approx$ 3) and MV (> 58 ML(1+4) 100^{o}C) at the same time are under the acetic acid amount of 0.2-0.22% vol./wt. dry rubber and coagulation time is 1.2-1.5 hr. It is noted that the MV of rubber sheet could be increased over time during storage. In this case, the predicted values of P_0 and PRI are higher than the product requirement in all cases. The optimal condition from the ANN model is related with the optimal condition from experimental data.

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CHAPTER 1

INTRODUCTION

1.1 Introduction

Rubber is an important industrial crop of Thailand. Three biggest rubber producers over the world are Thailand, Indonesia and Malaysia respectively. Top three Thailand's export markets are China, Japan and Malaysia. The most exported natural rubber are Block Rubber, Ribbed Smoked Sheet (RSS) and Concentrated Latex (Altering Risk to Opportunity (AFET), 2011). The important quality according to Standard of Thai Rubber (STR) is its color, more white and clear, higher value added. Pale crepe is a high quality rubber sheet since it has white/pale color (Lovibond color ≤ 3). It is produced from a particular type of rubber latex, RRIM 600, and used as raw material for manufacturing required-color products such as rubber soles, plaster, sport equipment, and medical devices etc.

Nowadays, pale crepe product has not the exact standard in Thailand; it has only the standard set by the manufacturer corresponding to the customer demand. Pale crepe rubber processing is normally achieved by the steps shown in Figure 1.1 (Singthuean, R., et al, 2011). The good quality fresh latex of RRIM600 is firstly preserved by adding 0.03-0.06% wt./vol. rubber latex of 2% sodium sulfite (Na_2SO_3). Afterward the preserved latex is diluted to obtain 25% dry rubber content (DRC) by adding pure water, and further exhibited an enzymatic reaction by adding 0.05-0.08% wt./wt. dry rubber of 5% sodium metabisulfite ($Na_2S_2O_5$). The latex is next bleached by using 0.1-0.2% wt./wt. dry rubber of a bleaching agent in order to achieve the product color-requirement, and then oagulated by adding 0.3-0.35% wt./wt. dry rubber of 2% formic acid. The coagulated rubber is rolled by using two-roll mill machine and lastly dried under the temperature of 35-40^{O}C for 3-4 days.

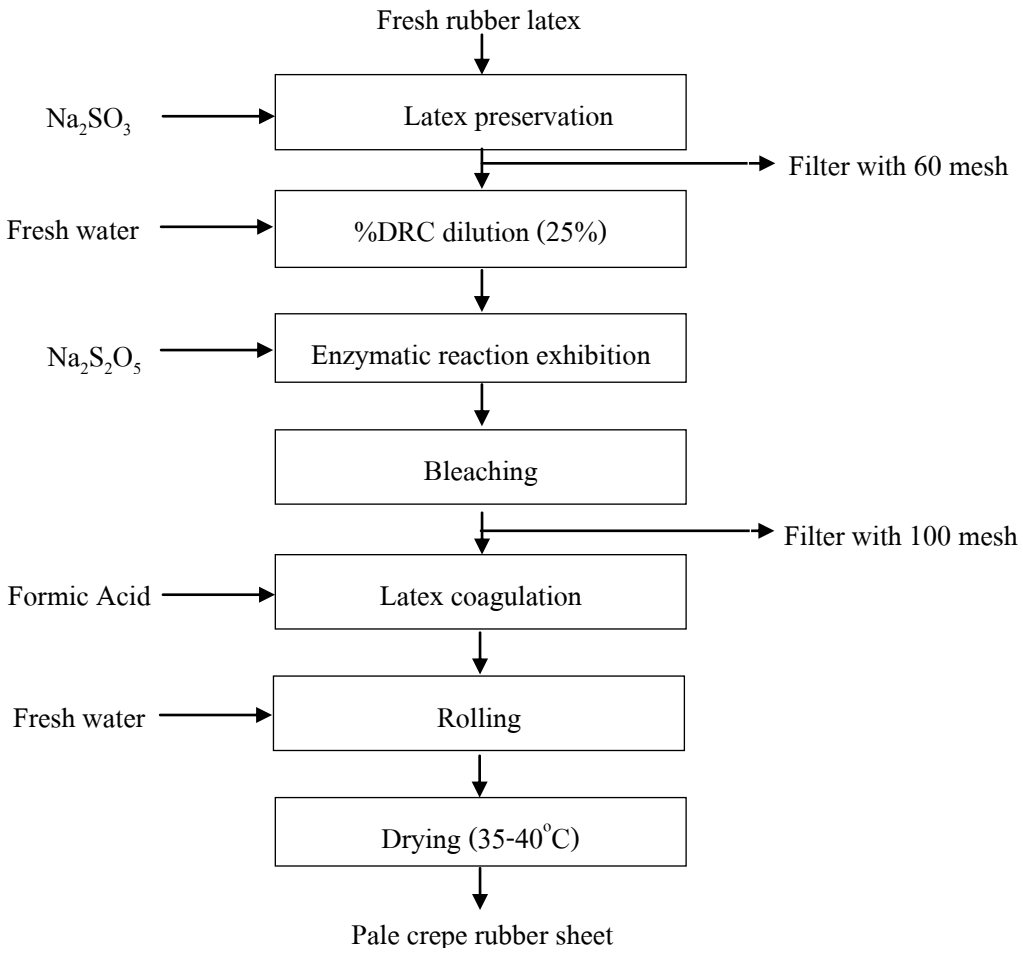


Figure 1.1 Pale crepe rubber processing

Even the pale crepe rubber has higher value added than RSS No.1; however, it has been found that this process has not been widely used in Thailand because of high cost of the bleaching agent. Cureobleach that is imported from Sri Lanka has cost of 1,500-2,000 bath per liter with minimum 50 liters per time. In addition sulfer-containing bleaching agent is effluvial and bad for producer's health. To solve these problems, this work focuses on the pale crepe rubber processing with a fractional coagulation instead of the color bleaching. In this study, a pale crepe rubber production is achieved by the following steps:

(1) Latex preservation

(2) % dry rubber content (DRC) dilution (varying 25-29% DRC and 27-32% total solid content, TSC)

(3) Enzymatic reaction exhibition

(4) Fractional coagulation (varying acetic acid of 0-0.45% v/w dry rubber and coagulation time of 1-3 hr.)

(5) Latex coagulation

(6) Drying at 35-40^{o}C for 3 days

In this work, the operating conditions in a fractional coagulation step has been designed in the optimal manner in order to achieve the required properties of the pale crepe rubber sheet corresponding to STR standard, this work focuses on determining the optimal operating conditions based artificial neural network (ANN) model achieving rubber sheet property requirement such as minimum color, Mooney viscosity (MV) > 60, initial plasticity (P_0) > 35 and plasticity retention index (PRI) > 60.

1.2 Research objectives

The overall objectives of this research are:

1) To develop an artificial neural network (ANN) for pale crepe rubber produced by fractional coagulation.

2) To determine the optimal process conditions based the obtained ANN through response

surface analysis.

1.3 Scopes of research work

To achieve the above objective, the following research scopes have been identified:

1) To understand the artificial neural network with feed-forward network for multilayer network and supervised training.

2) To design the artificial neural network through MATLAB program.

3) To determine the optimal conditions through response surface analysis.

4) To study the pale crape rubber production from RRIM 600 by fractional coagulation and fractional coagulation with color pigment bleaching.

5) To analyze the rubber physical quality such as Lovibond color, Mooney viscosity (ISO 289/ASTM D1646) and plasticity (ASTM D3194).

6) To design the optimal conditions based the following decision variables for optimization design such as minimum Lovibond color, Mooney viscosity > 60, initial plasticity (P_0) > 35 and plasticity retention index (PRI) > 60.

1.4 Expected benefits

1) To obtain an artificial neural network for pale crape rubber production by fractional coagulation.

2) To acquire an optimal process conditions based the obtained artificial neural network through response surface analysis.

CHAPTER 2

LITERATURE REVIEW

2.1 Artificial Neural Network (ANN) for rubber industries

Mooney viscosity is one of the important properties of rubber. It can guarantee the quality of product required by the rubber properties. Padmavathi, G. et al., (2005) studied a reliable model predicting product quality using ANN to developed model to predict Mooney and solution viscosity of PBR from process variables. The input-output data collected from plant history is confined into two types of neural networks which are a multi layered feeds forward neural network with a sigmoid transfer function and generalized regression neural network (GRNN). The ANN structures are presented as followed:

- There are 11 inputs of ANN input variables.
- There is one output of ANN output variable.
- The transfer function of multi-layered feeding forward neural network is the tan-sigmoid (TANSIG) transfer function in the hidden layer and the linear (PURELIN) transfer function in output layer and using Levenberg-Marquardt as training function.
- The transfer function of GRNN is radius basis (RADBAS) in hidden layer and linear transfer (PURNLIN) function in output layer.

GRNN is significantly able to predict Mooney and solution viscosity better than feed forward neural network and the prediction from the reactor outlet was deviated by MSE is 0.0252

Demirhan,E., et al, (2006) studied the properties of SBR-1712 type synthetic rubber compounding by using feed forward neural network trained with the back propagation algorithm called associative neural network (ASNN). This type improves prediction ability of feed forward neural network by means of explicit correction of the bias. The aim of this study is to prepare SBR-1712 rubber compound with different furnace carbon black to measure their properties.

A set of data containing 30 examples were chosen for neural network study, 25 of them were used to develop a model and 5 randomly selected examples were used for testing the model validation. Steps for data analysis are as following:

1. Analyze of all descriptors, ANNs analysis of the training set with 14 descriptors are resulted in a model with very good statistical qualities. The five compounds in the external test set were accurately predicted.
2. Use pruning methods for the analysis of observed weight. Some descriptors were determined as non-significant ones and were eliminated by the pruning algorithms, only five descriptors were selected.

Application of pruning method to analyze data set slightly improves the prediction ability of ANNs for the training set. Basically, itis not improved for the purpose of the test set. It can be said that the model is robust and predictive.

Thodesen, C., et al, (2009) explored the utilization of the statistical regression and neural network approaches in predicting the viscosity values of crumb rubber modified (CRM) binder at various temperature. The regression and a series of neural network model have been developed to predict the viscosity values of various CRM binders. The importance and sensitivity analysis of input variables were performed in neural network to evaluate the influences of each independent variable on the viscosity of CRM binders. The regression model was developed into two parts, first the effects of the addition of crumb rubber to the virgin binders, second, the effects of temperature on binder.

Neural network model was used to develop the predictive models of the viscosity values of asphalt mixture considering the interaction of complicated variables. Six parameters from asphalt binder, crumb rubber and test conditions (asphalt binder source, binder grade, rubber source, test temperature, rubber gradation, and rubber content) were expressed as independent variables to yield the viscosity values. There were 276 viscosity value data. 187 of them were selected as the training data and 89 were used as the testing data set.

The regression basing models on two variables of the asphalt binders could effectively predict the viscosity values of binder at various testing temperature and mixing type. The neural network approach can effectively create a feasible predictive model.

Nascimento, C.A.O. et al., (2000) study the optimization method using neural network which has been applied in the process of nylon-6,6 polymerization in a twin-screw extruder reactor. The process variables are presented as followed:

- There are 7 inputs of ANN input variables e.g. temperature, pressure of the vacuum system, flow rate, pressure in the extruder head, amine end-group concentration, carboxyl end-group concentration and screw rotation speed
- There are 3 inputs of ANN output variables e.g. degree of filling, the amine end-groups and the carboxyl end groups.
- There are 44 training data sets from the pilot plant that have been randomly split into two groups for the learning set (80%) and testing (20%) of the neural network.

The best ANN model is fed forward network with one hidden layer each of which is constituted by four neurons and the activation function used is the sigmoidal function.

2.2 ANN with variable sensitivity analysis

Despagne, F., et al., (1998) proposed two new methods based on the estimation of the contribution of each input variable to the variance of the predicted response. The first method is variance propagation. The second method is partial modeling and comparing the new methods with previous comparative e.g. Hinton diagram and saliency estimation. The synthetic data set consists of three data sets. Each set comprises of 60 data sets which were used as a training set and 40 data sets which was used for testing. Industrial data sets have been evaluated on three real data sets:

Set 1: minor mineral compound in polymer (30 data sets for learning and 10 data set for testing)

Set 2: hydroxyl number in polyether polyols (40 data sets for learning and 10 data set for testing)

Set 3: octane number in gasoline (80 data sets for learning and 52 data set for testing)

The feed forward ANN model is obtained one input layer with 3 nodes, one hidden layer with 2 nodes and the activation function is the hyperbolic tangent.

Anderson, F.O. et al., (2000) studied two methods variable influence and contribution in neural network models are examined. First is variable sensitivity analysis method: sequential zeroing of weight (SZW) the second is systematic variation of variables (SVV). The synthetic data sets 100 data sets have been used with 60 data sets as a training set and 40 data sets as a testing set. The real data sets evaluated on three real data sets:

Set 1: a study of octane number by NIR (45 data sets for learning and 15 data sets for testing)

Set 2: response in a reactor with feed rate (data set 32 experiments)

Set 3: methanol-tetrahydrofuran-water system (data set 35 experiments)

The multilayer feed forward ANN model is obtained with one hidden layer each of which is constituted by 10 neurons and the activation function used is the hyperbolic tangent.

Gestal, M., et al., (2004) studied two different genetic algorithms (GAs) intended to select a small number of wave number which are to be used to develop classification models, “pruned search” and “fixed search” and compare results of different assays. Two different ways of variable selection will be applied to get a small set of variables which cope with the most important features of the original data set. They will be used to classify apple beverages according to the percentage of apple juice they have. One is procruster rotation and the second based on the concept idea of GA. The laboratory standards were split into two groups with different amount of juice. The first set held 2-20% juice. It contained total of 173 standard samples, of which 134 were dedicated to train the model and 39 were used for validation. The second set contained 25-100% juice. It had 130 standard samples of which 86 were used for training and 44 for validation.

Generally, when the GA works with only ‘n’ variables (fixed search), it may happen that good solutions are broken down into new individuals which cannot survive and the GA algorithm behaves as if only mutation is performed. With the pruned approach, the GA seems to focus on discarding irrelevant information when an individual possesses those ‘n’ variables that give an optimal solution, the resulting individuals will clearly be worse, the total amount of variables can be reduced. Procruster selected variable could be related to specific characteristics of the three sugars. None of GA searches gave pair of variables with clear chemical meaning.

2.3 Optimization based ANN (surface analysis)

Maridass, B. et al., (2004) presented the result of the study on devulcanization and recycling of post factory gum natural rubber based on waste rubber powder using a counter rotating twin screw extruder with L/D = 8 to establish a functional relationship between the factors (extruder screw speed and extruder barrel temperature) and various properties like tensile strength, elongation at break (%), modulus, hardness, tear strength, swelling ratio and to establish the optimum processing screw speed and barrel temperature. For the RSM design, 10 combinations were chosen from an experimental design based on central composite rotatable design (CCRD). The data obtained from the six responses were tensile strength, elongation at break (%), maximum torque, shorehardness, tear strength and swelling index (%). The data were fitted into mathematical model by regression analysis. The model equation was used to draw two dimensional contour plots and three dimensional response surface. According to the contour plot and response surface, the maximum torque is obtained at lower screw speeds and decreases with increasing screw speed since the barrel temperature has no significant effect on the torque value. Moreover, the increase in the extruder barrel temperature shows an increase in the tensile strength. In addition, the level of extension depends on the degree of crosslinking of rubber matrix. A small degree of crosslinking gives higher elongation. Furthermore, as the degree of crosslinking increases, hardness also progressively increases. Additionally, the optimal tear strength is at the middle of the experimental region. Besides, swelling increases with in the barrel temperature as well as the screw speed.

The ANOVA analysis of all responses gave the coefficient of determination (R^2) to be higher than 0.89 suggesting that the model is a good fit.

Yingyong, R. et al., (2012) studied a simulation of beta-carotene recovery from palm oil esterification product using a high vacuum distillation technology. The simulation studies have been divided into two parts; first, process modeling using Response Surface Methodology (RSM). It consists of a box behnken design which has been employed to study the split fraction response of ethylesters of palm oil, diglyceride and carotene. Moreover, the independent variables are the temperature, feed flow rate and pressure. To confirm the point, the result shows that the most

important parameter is temperature, feed flow rate and pressure. The second part, ANN contain a set of data simulated by Aspen plus which have been used to feed ANN with three inputs of temperature, feed flow rate and pressure and one output of a split fraction of carotene in the residue product. The data contains 25 runs (15 runs same as used for RSM design and additional 10 runs) which it is randomly split into learning set 80% and testing set 20%. The model have two hidden layers with three nodes each, their transfer function are tan-sigmoid. ANN training results then give comparable agreement with MSE=1.6×10^{-6} and SSE=2.32×10^{-6}.

This work aimed at comparing the performance of RSM and ANN for the determination of the optimal operating conditions of the high vacuum distillation for carotene recovery. The optimal range of the operating conditions based ANN is larger than RSM.

Sinha, K. et al., (2013) studied microwave-assisted extraction of yellow-red natural dye from seeds of Bixa Orellana (Annatto) with surface methodology (RSM) and ANN were used to develop predictive model for simulation and optimization of the dye extraction process. The studies have been divided into two parts:

The 1st RSM design: a standard RSM design was used to identify the relationship between the responses function (total amount of dye extracted) and the process variables (solvent pH, extraction time and amount of Annatto seeds used in extraction). A total of 20 experiments were performed in duplicate accordingto the CCD matrix and the average values were used in data analysis. The adequacy of the developed model and statistical significance of the regressioncoefficients were tested using the analysis of variance (ANOVA). The interaction among the different independent variables and their corresponding effect on the response was studied by analyzing theresponse surface contour plots.

The 2ndANN design: The input of the ANN model was identical to the factor considered in RSM approach, namely, pH, extraction time and amount of Annatto seeds. The amount of dye extracted was considered as response (output) for ANN modeling. The ANN model use tan-sigmoid transfer function (TANSIG) at hidden layer and a linear transfer function (PURNLIN) at output layer. This work used the root mean square error (RMSE), coefficient of determination (R^2) and absolute average deviation (AAD) to compare the performance of the RSM and ANN model. In this study, the ANN model has higher predictive capability than RSM model.

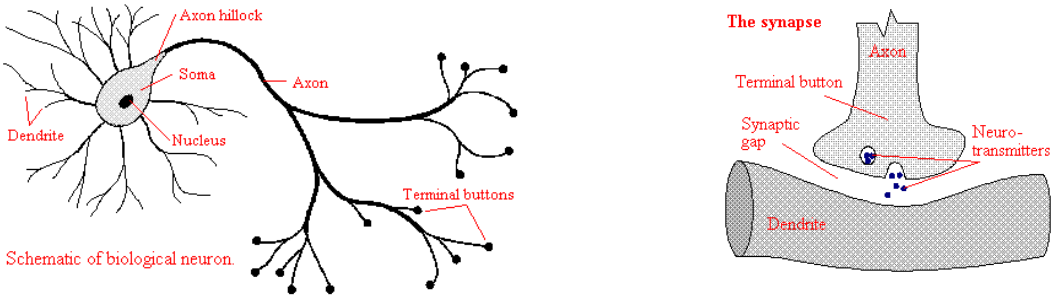
CHAPTER 3

THEORY

3.1 Artificial Neural Network (ANN)

3.1.1 Introduction to Artificial Neural Network

Artificial neural network (ANN) is a computational model based on the structure and functions of biological neuron networks. Information that flows through the network affects the structure of the ANN because a neural network changes or learns, in a sense based on that input and output. ANNs are considered nonlinear statistical data modeling tools where the complex relationships between inputs and outputs are modeled or patters are found. ANN is also knows as a neural network.



(a) Biological neuron (b) Neuron connection

Figure 3.1.1 Schematic of biological neuron

From Figure 3.1.1, in human brain, a typical neuron collects signals from others through a host of fine structures called *dendrites*. The neuron sends out spikes of electrical activity through a long, thin stand known as an *axon*, which splits into thousands of branches. At the end

of each branch, a structure called a *synapse* converts the activity from the axon into electrical effects that inhibit or excite activity from the axon into electrical effects that inhibit or excite activity in the connected neurons. When a neuron receives excitatory input that is sufficiently large compared with its inhibitory input, it sends a spike of electrical activity down its axon. Learning occurs by changing the effectiveness of the synapses so that the influence of one neuron on another changes (Fraser, N., 1998).

3.1.2 Mathematical model of Artificial Neural Network

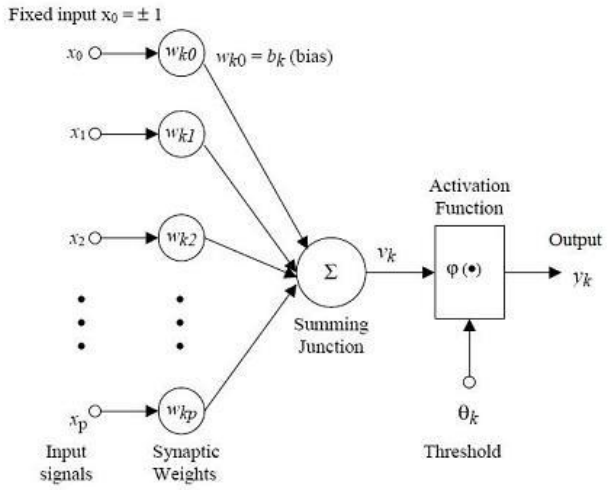


Figure 3.1.2 ANN mathematical modeling

A detailed mathematical model of a neuron is shown in Figure 3.1.2. Model may include an externally applied *threshold* that has the effect of lowering the net input of the activation function. On the other hand, the net input of the activation function may be increased by employing a *bias* term rather than a threshold. The scalar input x_0, x_1, …, x_p is transmitted through a connection that multiplies its strength by the scalar weight w_{k0}, w_{k1}, …, w_{kp} and sum with bias by the summing junction. The transfer function net input v_k is the argument of the transfer function with takes the argument v_k and produces the output y_k. In mathematical term, can describe a neuron **k** by writing the following equations:

$$v_k = \sum_{x=1}^{p}\left(w_{kp}x_p + b_k\right) \quad (3.1.1)$$

and

$$y_k = f(v_k) \quad (3.1.2)$$

where $x_0, x_1, \ldots, x_p$ are inputs

$w_{k0}, w_{k1}, \ldots, w_{kp}$ are the synaptic weights of neuron k

v_k is the linear combiner output

b_k is the bias term

f is the activation function

and y_k is the output signal of the neuron

3.1.3 Artificial Neural Network structure

Neural network architecture defines its structure including number of hidden layer, number of hidden nodes and number of output nodes. The hidden layers provide the network with its ability to generalize. For the hidden nodes there is no magic formula for selecting the optimum number of hidden nodes. A rough approximation can be obtained by the geometric pyramid rule. The basic structures of neural network are as following:

3.1.3.1 Type of neural network

There are wide variety of neural network and their architectures. Types of neural networks range from simple Boolean networks (perceptions) to complex self-organizing network (Kohonen networks). There are also many other types of neural networks like Hopefield network, Pulse networks, Radial Basis Function Networks, Boltzmann machine. The most important class of neural networks for real world problem solving includes

- Multilayer Perceptron (MLP)

The most popular form of neural network architecture, a multilayer perceptron has any number of input, one or more hidden layers with any number of nodes, use liner combination function in the input layers, uses generally sigmoid activation function in the hidden layers, has

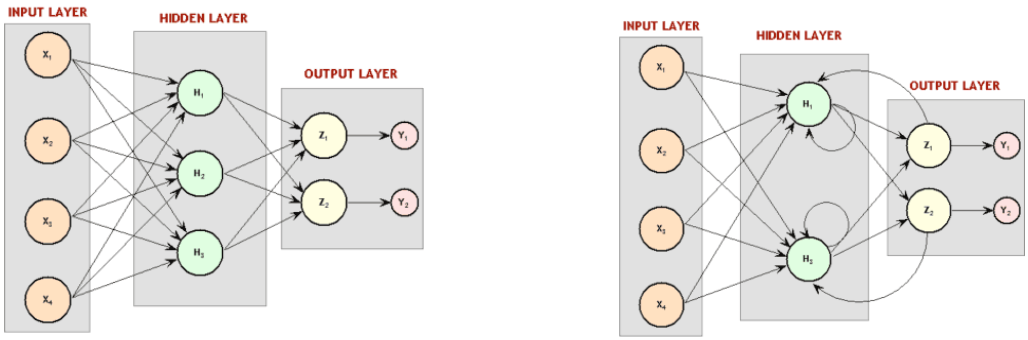
any number of outputs with any activation function and has connections between the input layer and the first hidden layer, between the hidden layers and between the last hidden layer and the output layer.

- Radial Basis Function Networks (RBF)

Radial basis function networks are also feed-forward but have only one hidden layer. A RBF network has any number of inputs, typically has only hidden layer with any number of units, uses radial combination functions in the hidden layer, has any number of outputs with any activation function, has connections between the input layer and the hidden layer, and between the hidden layer and the output layer.

3.1.3.2 Network architecture

There are several types of architecture of ANN. However, the two most widely used ANN are discussed below:



(a) Feed-forward network (b) Recurrent network

Figure 3.1.3 ANN structure

- **Feed-forward Networks**

Feed-forward ANNs allow signals to travel one way only; from input to output. There is no feedback (loop) i.e. the output of any layer does not affect that same layer. They are extensively used in pattern recognition.

- **Feedback/Recurrent Networks**

Feedback networks can have signals traveling in both directions by introducing loops in the networks. Feedback networks are dynamic; their ‘state’ is changing continuously until they reach an equilibrium point. They remain at the equilibrium point until the input changes and a new equilibrium needs to be found.

3.1.3.3 Weight adjusting

The most significant property of a neural network is that it can learn from environment, and it can improve its performance through learning. Learning is a process by which the free parameters of a neural network i.e. synaptic weights and thresholds are adapted through a continuous process of simulation by the environment in which the network is embedded.

- **Supervised learning**

This case, every input pattern that is used to train the network is associated with an output pattern, which is the target or the desired pattern. A teacher is assumed to be present during the learning process, when a comparison is made between the network’s computed output and the correct expected output to determine the error. The error can then be used to change network parameters, which result in an improvement in performance.

- **Unsupervised learning**

With unsupervised learning, there is no feedback from the environment to indicate if the outputs of the network are correct. The network must discover features, regulations, correlations, or categories in the input data automatically. For most varieties of unsupervised learning the targets are the same as inputs. In other words, unsupervised learning usually performs the same task as an auto-associative network, compressing information from the input.

3.1.3.4 Activation function

Activation functions are mathematical formula that determines the output of a processing node. Each unit takes its net input and applies an activation function to it. The purpose of the transfer function is to prevent output from reaching very large value which can paralyze neural network and thereby inhibit training. The most commonly used activation functions are in table 3.1.

3.1.3.5 Model building

Multilayer feed-forward neural network or multilayer perceptron (MLP) is very popular and is used more than other neural network type for a wild variety of tasks. Multilayer feed-forward neural network by back propagation is based on supervised learning. The characteristics of MLP are as following:

(i) Has any number of input

(ii) Has one or more hidden layers with any number of nodes. The internal layer are called ‘hidden’ because they only receive internal input (input from other processing unit) and produce internal output (output to other processing units).

(iii) Uses linear combination function in the hidden layer and output layers.

(iv) Use generally sigmoid activation function in the hidden layer.

(v) Has any number of outputs with any activation function

(vi) Have connections between the input layer and the first hidden layer, between the hidden layer, and between the last hidden layer and the output layer.

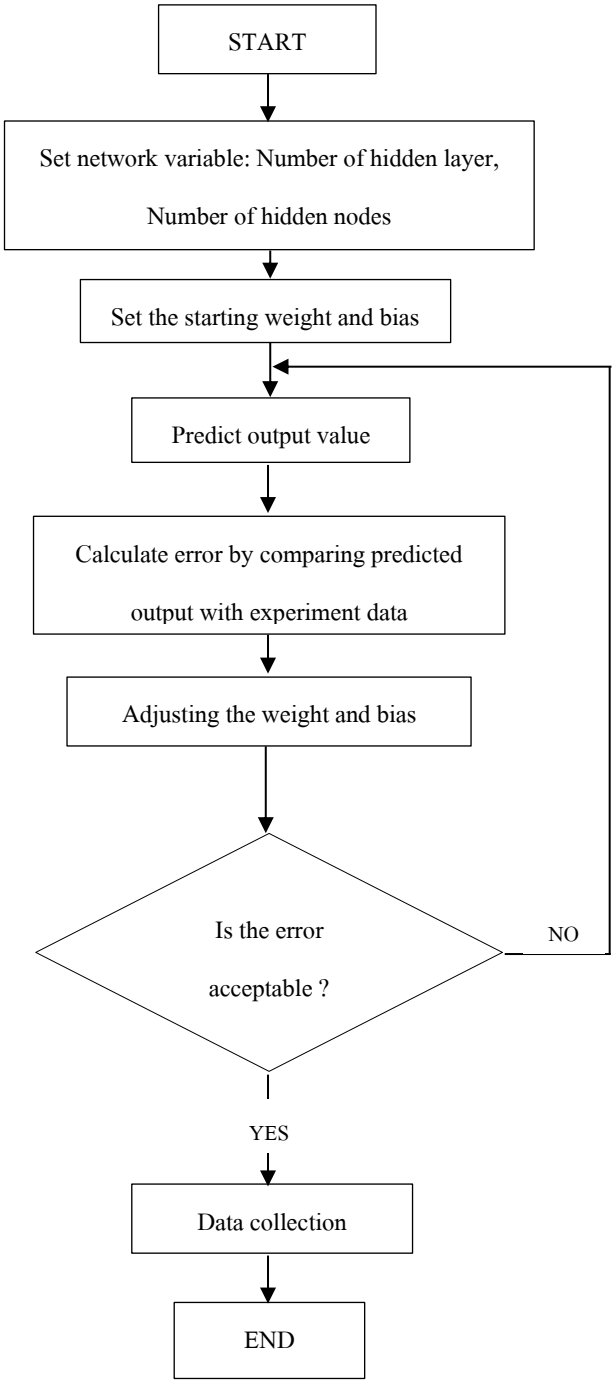
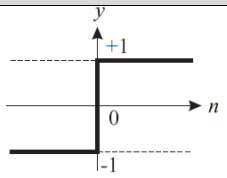
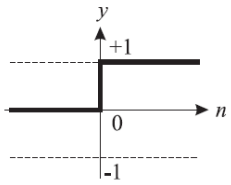
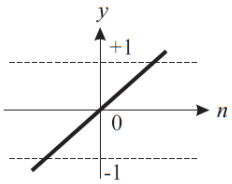
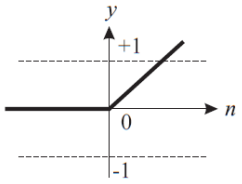
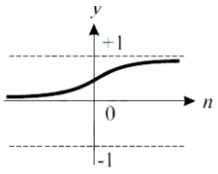
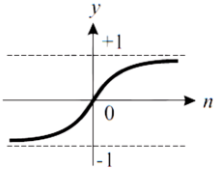


Figure 3.1.4 Function of Artificial Neural Network

Table 3.1.1 Transfer function

function	equation	graph
Symmetrical hard limit	$y = -1$ if $n < 0$ $y = +1$ if $n \geq 0$	
Hard limit	$y = 0$ if $n < 0$ $y = 1$ if $n \geq 0$	
Linear	$y = n$	
Positive linear	$y = 0$ if $n < 0$ $y = n$ if $n \geq 0$	
Log-sigmoid	$y = \frac{1}{1 + e^{-n}}$	
Hyperbolic tangent sigmoid	$y = \frac{e^{n} - e^{-n}}{e^{n} + e^{-n}}$	

3.2 Variable Selection

Variable selection is a highly informative explanatory variable that is dissimilar to other input variables. Consequently, the optimal input variable set will contain the fewest input variables required to describe the behavior of the output variable, with a minimum degree of redundancy and with no uninformative variables. Identification of an optimal set of input variables will lead to a more accurate, efficient, cost-effective and more easily interpretable ANN model.

3.2.1 Hinton Diagram

The Hinton diagram provides a compact visual display of the weight and biases related to a particular unit in a network. The diagram for a unit shows the signs and magnitudes of all of the incoming and outgoing weights as well as the sign and magnitude of the unit's bias. Each weight is represented by a box drawn on the diagram. The area of the box represents the weight's magnitude while the color of the box indicates the sign of the weight. Typically, white boxes indicate positive weights and black boxes indicate negative weight. The diagram is organized so that each unit in the network has an assigned position in the diagram. Typically, output units occupy position of a box in a diagram indicates the unit at the other end of the weight. A bias for a given unit is drawn in that unit's diagram in the position where weights to and from the unit are shown in that unit's diagram in the position where weights to and from the unit are shown in the other diagrams.

Hinton diagrams help in understanding an ANN by providing a concise visual representation of the network's weights and biases. Each diagram makes it easy to see the signs and magnitudes of the weights that contribute to a unit's activation and the relative influence of the unit's activation on the units at the next level in the network (Craven, M.W., et al., 1991).

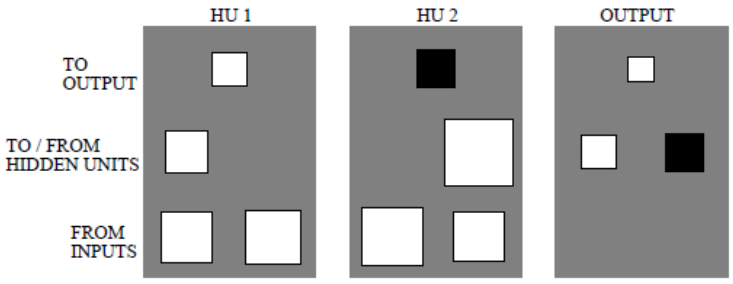


Figure 3.2.1 Hinton diagram

3.2.2 Partial modeling

Partial modeling is proposed for estimating experimentally the sensitivity of each input variable. A model response $y = f(x_1, x_2)$ as a function of two orthogonal input variables. The exact form of the relationship is unknown, therefore using ANN to model this relationship, with a set of ns training samples. To illustrate the procedure, considering the simple ANN displayed in Fig 3.2.2. At the end of the training, a set of weights that determine the ANN model. In order to estimate the relative contribution of each input variable to the variance of the predicted response, first project the ns samples from the training set no the final ANN model, setting all input variables but the first to zero. In the present example, only variable x_2 is set to zero. Obtaining a vector $\hat{y}(x_1)$, the response predicted by the ANN model using only input variable x_1(fig 3.2.2b). Repeat the procedure, now setting x_1 to zero, to obtain the vector $\hat{y}(x_2)$ (fig 3.2.2c). Using the respective variances of $\hat{y}(x_1)$ and $\hat{y}(x_2)$ to estimate the sensitivity of input variable x_2 and x_2 respectively (Despagne, F., et al., 1998).

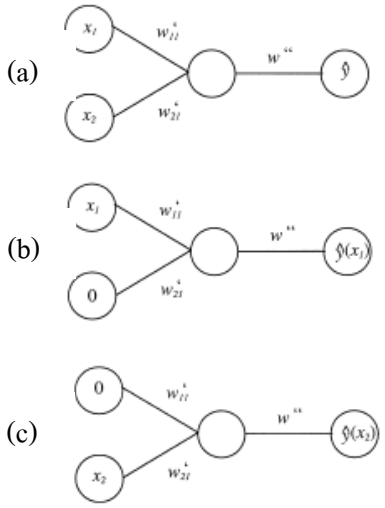


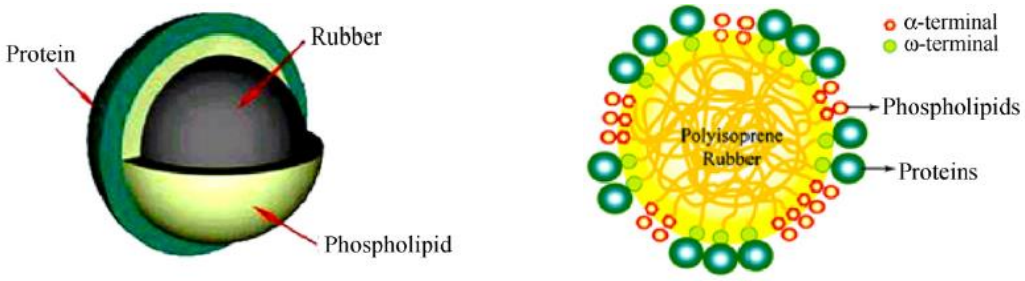
Figure 3.2.2 Illustration of the principle of partial modeling:

(a) Full model, (b) partial modeling of variable 1, (c) partial modeling of variable 2.

3.3 Natural rubber

3.3.1 Natural rubber composition

Fresh *Hevea brasilliensis* Latex has high stability because the rubber particles surrounded by protein and phospholipid lipid has characteristics of a spherical particle size 0.1-2 microns (μm). The arrangement of protein and phospholipids on the surface of rubber particles has 2 forms as shown in figure 3.3.1. In 1979, Gomez, J.B., et al., has been presented the first arrangement (Figure 3.3.1a) the rubber particle has been surrounded by phospholipid layer in inner layer and protein layer in outer layer, it has double layer. In 2011, Nawamawat, S., et al., has been presented the second arrangement (Figure 3.3.1b) the rubber particle has been surrounded by thin film of protein and phospholipid and confirm the arrangement by various technique such as Atomic Force Microscopy and Confocal Laser Scanning Microscopy.



(a) Gomaz, J.B., et al., 1979 (b) Nawamawat, S., et al., 2011

Figure 3.3.1 Structural arrangement of proteins and phospholipids on the surface of the rubber particles.

Protein and phospholipid particle surrounded affect the stability of rubber particle, rubber particle has positive charge from amino group and negative charge from carboxylic group on protein and phospholipid particle, respectively. If pH > 5.0 rubber particle has more negative charge cause high stability and colloids, if pH is in the range 3.0-5.0 rubber particle has lose the stability and has rubber coagulation (Nawamawat, K., et al., 2011).

Rubber latex has important component 30-36% is rubber phase, 5-6% is non-rubber component and the rest is water. Despite the non-rubber components, but it is most important because it determines the properties of natural rubber. non-rubber could be divided into 4 groups such as protein and amino acid, lipids, carbohydrate and metal ions. Protein defines properties stiffening, tear strength, heat build-up and dynamic crack growth. Lipids define vulcanization and crystallization. Carbohydrates sugar group indicated the quality of the latex by measurement of the volatile fatty acids, VFA, which is caused by the hydrolysis of bacteria and metal ions affecting the stability of the latex (Jitlada, S. et al., 2011).

CHAPTER 4

MATERIAL AND METHODOLOGY

4.1 Material

4.1.1 Raw material

1. Fresh rubber latex, RRIM 600

4.1.2 Chemical

1. Sodium sulfite, Na_2SO_3
2. Sodium metabisulfite, $Na_2S_2O_5$
3. Acetic acid
4. Formic acid

4.2 Equipment

4.2.1 Analysis tools

1. Lovibond color measurement

The color of the raw rubber is compared and matched as closely as possible with that of standard color slides. The raw rubber is tested in the form of a moulded disc of standard thickness. Color matching is carried out under diffuse daylight illumination against a matt white background, preferable by use of a comparator which holds the test pellets and comparison slide

in convenient juxtaposition. The standard colored glasses used are calibrated in color index units according to the intensity of their color. The numerically higher index values have deeper color. The basis of calibration is the 'Lovibond color scale' in amber units.

2. Mooney viscometer

The test consists of determining the torque necessary to rotate a disc in a cylindrical chamber filled with rubber under specified conditions. A number proportional to this torque is taken as an index of the viscosity of the rubber. The Mooney viscometer (a shearing-disk viscometer) is used.

3. Rapid plasticity

A disc-shaped test pellet shall be rapidly compressed between small parallel platens to a fixed thickness of 1 mm and held thus for 15 s to reach approximate temperature equilibrium with the platens. It shall then be subjected to a constant compressive force of 10±0.1 kgf for 15 s; its thickness at the end of this period in 0.01 mm units shall be taken as the measure of plasticity.

4.3 Laboratory Equipment

1. Beakers
2. Sieve size 60 and 100 mesh
3. Weighing machine
4. Microwave
5. Desiccator
6. Oven
7. Rubber rolling machine

4.4 Methodology

4.4.1 Activity 1: Effect of acetic acid amount and coagulation

In this section, pale crepe production has been divided into 2 processes:

Pretreatment and %DRC dilution processes

1. Adding 0.05% wt./vol. of rubber latex of 2% wt./vol. Sodium Sulfite, Na_2SO_3 into the rubber latex for preservation.
2. Stirring latex for 5 min under speed of 100 rpm.
3. Filtering the latex with 60 meshes to remove all contaminates.
4. Diluting %DRC to 25%, and further stirring for 5 min under speed of 100 rpm.
5. Adding 0.05% wt./wt. of dry rubber content of 5% wt./vol. of Sodium metabisulfite, $Na_2S_2O_5$ into 1,000 ml. of the sample latex for reduction of an enzymatic reaction, and stirring for 5 min. under 100 rpm.

Fractional coagulation and drying process

6. Fractionally coagulating by varying 1% wt./vol. of acetic acid of 0, 0.15, 0.30 and 0.45% vol./wt. dry rubber, and setting the fractional coagulation time of 1, 2 and 3 hr.
7. Filtering with 100 meshes, and then adding 0.35% wt./wt. of dry rubber content of 2% of Formic acid, and then stirring for 5 min.
8. Setting the coagulation time of 30 min, and rolling with a crepr machine.
9. Drying the rubber sheets under the temperature of 35-40^{o}C for 3-4 days.

The dried rubber sheets have been further analyzed their properties such as Lovibond color, Mooney viscosity (MV), Initial plasticity (P_0) and Plasticity Retention Index (PRI). The average property values from 3 repeated data have been presented with standard deviation of 3 samples.

4.4.2 Activity 2: ANN design

In this section, ANN design has been divided in to 2 parts:

Part 1: ANN model with 1 hidden layer has been trained by varying a number of nodes from 1 to 10 nodes. The optimum model structure has been chosen by considering the overall Mean Square Error (MSE) and Integral Absolute Error (IAE) of the output predictions. Effect of activation functions has also been investigated.

Part 2: ANN model with 2 hidden layers has been trained by varying a number of hidden layer, 1 and 2 hidden layers; and its number of nodes from 1 to 10 nodes. The network model structure has been chosen in the optimum way by minimizing the overall MSE and IAE of the output prediction. Comparison of the predicted outputs and the experimental data has also been illustrated by considering the effects of acetic acid amount and coagulation time.

4.4.3 Activity 3: Input variable analysis (Partial modeling)

The ANN model obtained from the previous section has been further identified the insignificant input variable by using the partial modeling approach. The insignificant input variable has been identified by considering its corresponding sensitivity index (variance). A new network without the insignificant input variable has been trained and tested; the comparison of the predicted variables and experimental data has been shown.

4.4.4 Activity 4: Optimum conditions determination

The optimum condition has been determined based on the network model, containing only the significant inputs and 2 hidden layers, by considering the surface plots of all responses. In this work, the optimal operating conditions have been chosen by considering the rubber sheet properties: minimum rubber color, Mooney viscosity (MV) > 60, initial plasticity (P_0) > 35 and Plasticity Retention Index (PRI) > 60.

CHAPTER 5

PALE CRAPE RUBBER PROCESSING

5.1 Process Description

Pale crepe is a high quality rubber sheet since it has white/pale color (Lovibond color < 4). It is produced from a particular type of rubber latex, RRIM 600. Pale crepe rubber production process has been divided into 2 processes as seen in Figure 5.1.1:

Pretreatment and %DRC dilution processes

1. Adding 0.05% wt./vol. of rubber latex of 2% wt./vol. Sodium Sulfite, Na_2SO_3 into the rubber latex for preservation.
2. Stirring latex for 5 min under speed of 100 rpm.
3. Filtering the latex with 60 meshes to remove all contaminates.
4. Diluting %DRC to 25%, and further stirring for 5 min under speed of 100 rpm.
5. Adding 0.05% wt./wt. of dry rubber content of 5% wt./vol. of Sodium metabisulfite, $Na_2S_2O_5$ into 1,000 ml. of the sample latex for reduction of an enzymatic reaction, and stirring for 5 min. under 100 rpm.

Bleaching and drying process

6. Filtering with 100 meshes, then adding a bleaching agent and stirring for 5 min.
7. Adding 0.35% wt./wt. of dry rubber content of 2% of Formic acid, and then stirring for 5 min.
8. Setting the coagulation time of 30 min, and rolling with a crepr machine.
9. Drying the rubber sheets under the temperature of 35-40^{o}C for 3-4 days.

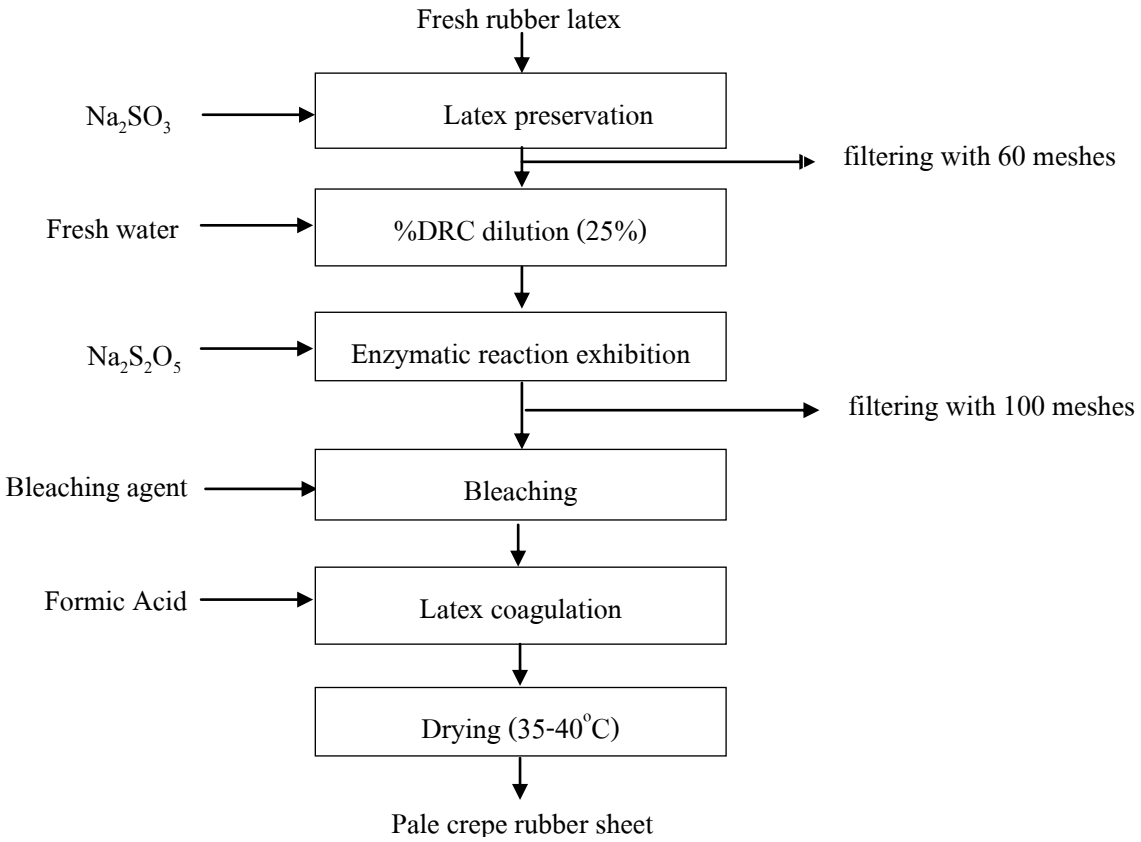


Figure 5.1.1 Pale crepe rubber process flow chart

In this work, pale crepe rubber production is achieved by the following steps:

1. Latex preservation
2. % dry rubber content (DRC) dilution by varying randomly with 25-29%DRC and 27-32% total solid content, TSC
3. Enzymatic reaction exhibition
4. Fractional coagulation by varying 1% wt./vol. of acetic acid of 0, 0.15, 0.30 and 0.45% vol./wt. dry rubber, and the fractional coagulation time of 1, 2 and 3 hr.
5. Latex coagulation of 30 mins.
6. Drying the rubber sheets under the temperature of 35-40°C for 3-4 days.

Artificial neural network (ANN) has been firstly designed to estimate the dried rubber properties by using the full input data consisting of initial %DRC, %TSC (step 2), the amount of 1% wt./vol. acetic acid and the fractional coagulation time (step 4). Effects of a number of layers and nodes as well as the corresponding activation functions have been investigated. The optimum network model has been further improved by eliminating insignificant variables through a variable selection approach. In order to achieve the required properties of the pale crepe rubber sheets, this work focuses lastly on determining the optimal operating conditions based the partial ANN model by considering the rubber sheet properties: minimum rubber color, Mooney viscosity (MV) > 60, initial plasticity (P_0) > 35 and Plasticity Retention Index (PRI) > 60.

5.2 Experimental results

In this section, the experiment has been carried out to produce pale crepe rubber via a fractional coagulation method, 1% by wt of acetic acid has been used to coagulate the latex (RRIM 600) fractionally. Effects of acetic acid amount and coagulation time have been investigated on the rubber properties; Lovibond color, MV, P_0 and PRI. In this study, the acetic acid amount and the coagulation time have been varied 0.15%, 0.30% and 0.45% vol./wt. of dry rubber, and 1, 2 and 3 hr.

Table 5.2.1 Effect of acetic acid on rubber color

Acid amount (% vol./wt.)	Coagulation time (hr.)		
	1	2	3
0.00	3.7±0.3	3.7±0.3	3.7±0.3
0.15	3.3±0.3	3.0±0.0	3.3±0.3
0.30	3.7±0.3	3.8±0.3	4.3±0.3
0.45	3.8±0.3	3.8±0.3	4.5±0.5

Table 5.2.1 and Figure 5.2.1 shows the effect of acetic acid on rubber color in Lovibond unit. Each error bar has been plotted by using standard deviation of 3 samples. It could be seen from the experimental results that the rubber color is significantly decreased at 0.15% vol./wt., 2 hrs and increased at 0.30% and 0.45% vol./wt., 3 hrs. This might be because lutoid particles containing carotenoids in the rubber latex has been destroyed under low pH condition resulting in a dark rubber sheet. Then the proper operating condition should be at 0.15% vol./wt. of acetic acid, and coagulation time of 2 hrs.

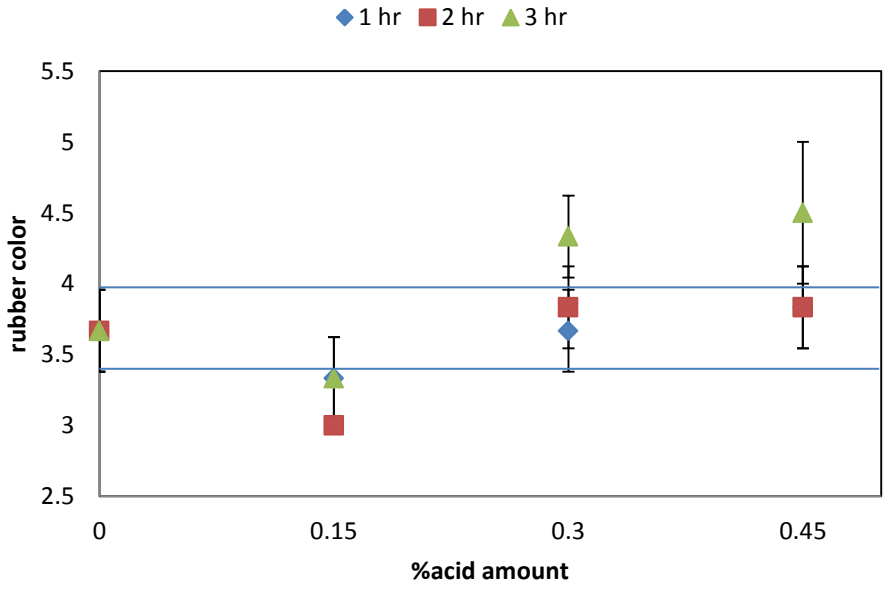


Figure 5.2.1 Effect of acetic acid on rubber color

Table 5.2.2 and Figure 5.2.2 show the effect of acetic acid on Mooney viscosity (MV). Each error bar has been plotted by using standard deviation of 3 samples. It could be seen from the experimental results that MV is significantly decreased at 0.45% vol./wt., 1-2 hrs (MV < 60). This might be because the rubber sheet has lower %DRC resulting in lower MV under lower pH condition. Then the proper operating condition could be at 0.15% or 0.3% vol./wt. of acetic acid, and coagulation time of 1-3 hrs.

Table 5.2.2 Effect of acetic acid on Mooney viscosity, ML 1+4 (100°C)

Acid amount (% vol./wt.)	Coagulation time (hr.)		
	1	2	3
0.00	61.0±2.3	61.0±2.3	61.0±2.3
0.15	59.0±2.5	59.5±1.8	61.8±3.8
0.30	62.7±0.6	66.2±6.9	68.2±4.4
0.45	57.3±0.6	56.3±0.6	60.1±0.9

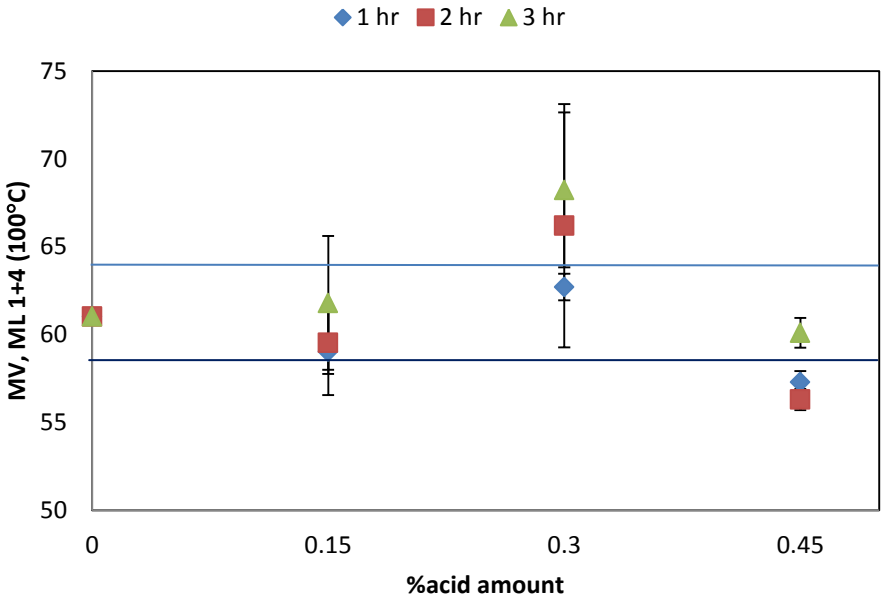


Figure 5.2.2 Effect of acetic acid on Mooney viscosity

Table 5.2.3 Effect of acetic acid on P_0

Acid amount (% vol./wt.)	Coagulation time (hr.)		
	1	2	3
0.00	55.5±1.0	55.5±1.0	55.5±1.0
0.15	51.7±1.0	50.8±0.3	55.5±2.2
0.30	50.7±1.3	56.5±1.3	59.0±2.3
0.45	48.2±0.3	50.3±1.0	50.0±1.0

Table 5.2.3 and Figure 5.2.3 show the effect of acetic acid on initial plasticity (P_0). Each error bar has been plotted by using standard deviation of 3 samples. It could be seen from the experimental results that P_0 is significantly decreased at 0.15% vol./wt., 1-2 hrs, 0.30% vol./wt., 1 hrs 0.45% vol./wt., 1-3 hrs, but increased at 0.30% vol./wt., 3 hrs. This might be because the rubber sheet has lower %DRC resulting in lower P_0 under lower pH condition. Then the proper operating condition could be at 0.15 – 0.45% vol./wt. of acetic acid, and coagulation time of 1-3 hrs since they give P_0 over the property requirement (P_0>35).

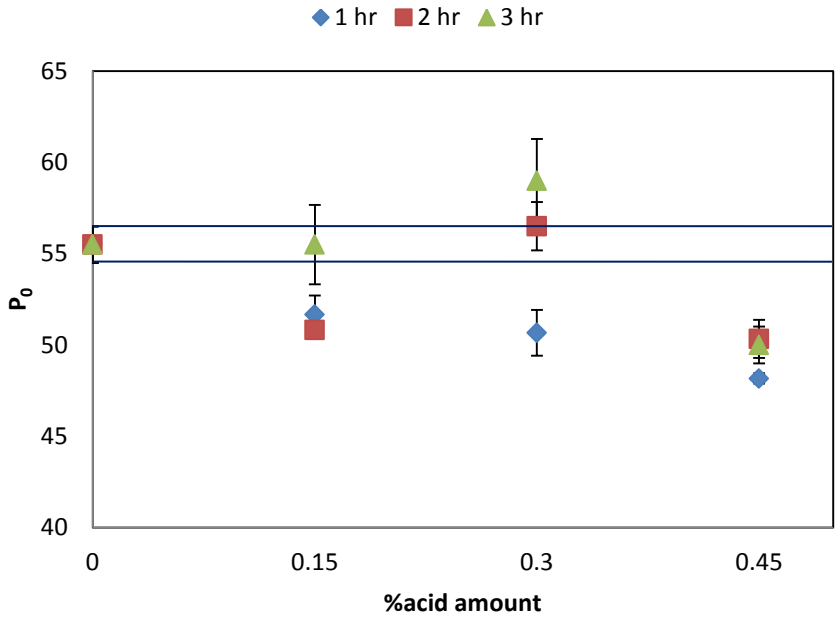


Figure 5.2.3 Effect of acetic acid on P_0

Table 5.2.4 Effect of acetic acid on PRI

Acid amount (% vol./wt.)	Coagulation time (hr.)		
	1	2	3
0.00	92.8±1.8	92.8±1.8	92.8±1.8
0.15	93.2±2.5	93.8±2.0	92.8±2.1
0.30	92.1±0.8	82.8±6.7	89.9±1.8
0.45	91.3±1.6	88.4±1.6	92.7±1.2

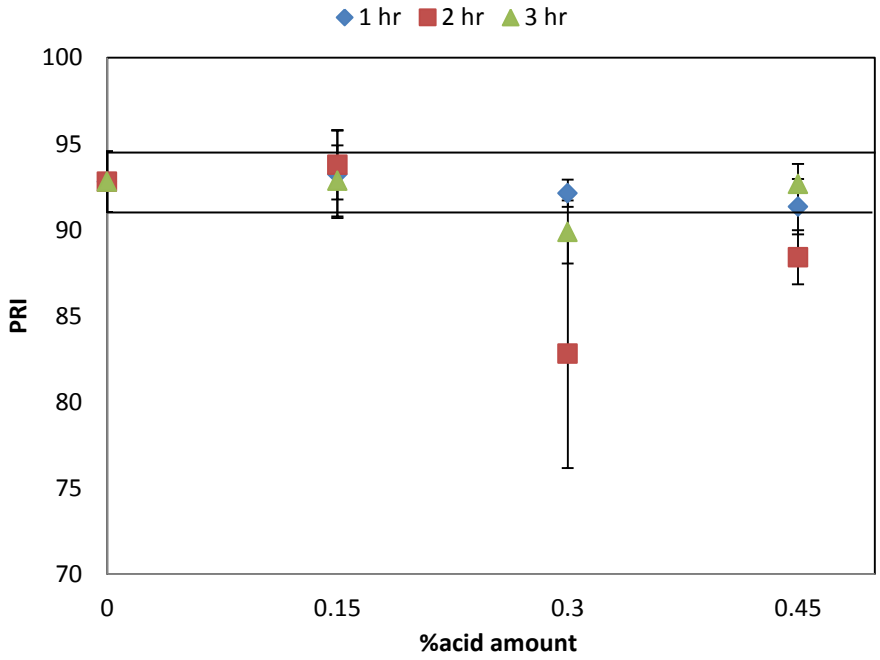


Figure 5.2.4 Effect of acetic acid on PRI

Table 5.2.4 and Figure 5.2.4 show the effect of acetic acid on plasticity retention index (PRI). Each error bar has been plotted by using standard deviation of 3 samples. It could be seen from the experimental results that PRI is significantly decreased at 0.30% vol./wt., 2 hrs 0.45% vol./wt., 2 hrs. This might be because the rubber sheet has lower %DRC resulting in lower ability of oxidation inhibition (P_{30}) under lower pH condition. Then the proper operating condition could be at 0.15 – 0.45% vol./wt. of acetic acid, and coagulation time of 1-3 hrs since they give PRI over the property requirement (PRI>60).

5.3 Artificial Neural Network design for Pale Crepe Rubber Process

5.3.1 Fully-input model structure

According to the process, the network model has been designed for 1-2 hidden layers by varying their number of nodes (1 to 10). In this research, Artificial Neural Network (ANN) model has feed-forward scheme with four input variables such as (1) acetic acid amount, (2) fractional coagulation time, (3) %dry rubber content (%DRC) of diluted latex, and (4) the corresponding %total solid content (%TSC). Four rubber properties, such as (1) rubber color, (2) Mooney viscosity (MV), (3) initial plasticity (P_0), and (4) Plasticity Retention Index (PRI) have been predicted via using linear transfer functions (PURELIN). The ANN has been trained using the Levenberg-Marquardt algorithm with 30 experimental data sets, data matrix [4×30]; 80% for training (training matrix, [4×24]) and 20% for testing (testing matrix, [4×6]).

$$\text{Overall MSE} = \frac{1}{m}\sum_{j=1}^{k}\sum_{i=1}^{n}\left(y_{ij} - y'_{ij}\right)^2 \tag{5.3.1}$$

$$\text{Overall IAE} = \sum_{j=1}^{k}\sum_{i=1}^{n}\left|y_{ij} - y'_{ij}\right| \tag{5.3.2}$$

$$\text{MSE}_\text{j} = \frac{1}{n}\sum_{i=1}^{n}\left(y_{ij} - y'_{ij}\right)^2 \tag{5.3.3}$$

$$\text{IAE}_\text{j} = \sum_{i=1}^{n}\left|y_{ij} - y'_{ij}\right| \tag{5.3.4}$$

where y_{ij} is the i^{th} experimental outputs, j

y'_{ij} is the i^{th} predicted outputs, j

k and n is a total number of outputs, and a number of testing data respectively

m is $n \times k$

In this research, the performance of the ANN model has been identified by using the values of mean square error (MSE) and integral absolute error (IAE). General overall MSE and IAE equations for multiple-inputs multiple-outputs (MIMO) system are shown in Equations (5.3.1) and (5.3.2) respectively. In addition individual MSE and IAE equations for each output are shown in Equations (5.3.3) and (5.3.4) respectively.

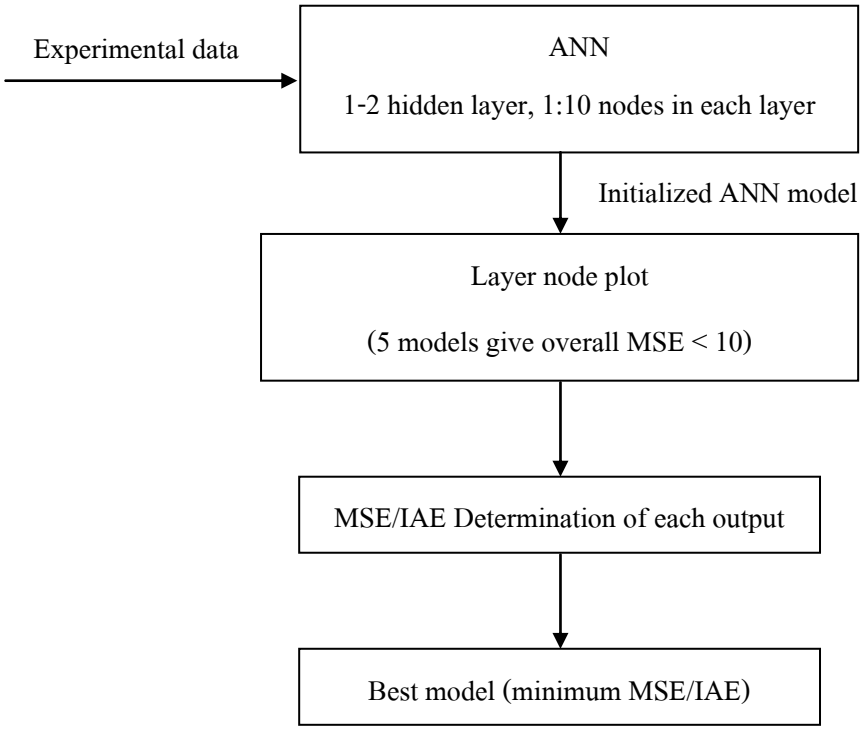


Figure 5.3.1 Analytical Artificial Neural Network (ANN) flow chart

5.3.1.1 ANN design with 1 hidden layer

5.3.1.1.1 Effect of layer node

In this section, ANN model has been trained with 1 hidden layer, the number of nodes is varying from 1 to 10 nodes. It has been found from the Figure 5.3.2 that the minimum overall MSE is in the range of hidden node 1-6 in this case. However it should be noted that in cases of high hidden nodes (higher than 6 nodes), the training approach has been terminated due to reaching the maximum training iterations (20 iterations in this case). Six ANN structures are then chosen arbitrarily as [1], [2], [3], [4], [5] and [6]. Table 5.3.1 shows MSE and IAE values of four models prediction. It has been found in the simulation results that the optimal network structure could have 1 node in hidden layer give minimum overall MSE and IAE of the output prediction.

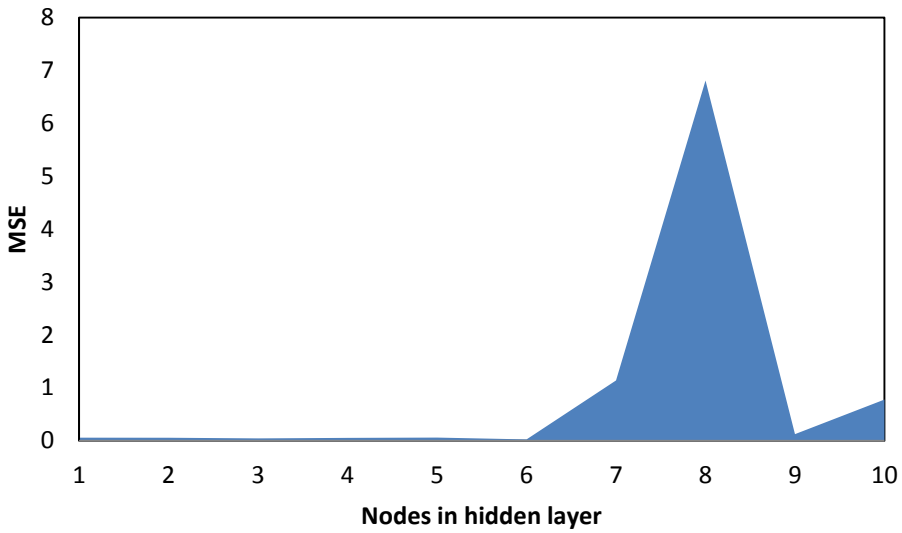


Figure 5.3.2 Overall MSE response according to ANN design with 1 hidden layer

Table 5.3.1 Performances of ANN model with 1 hidden layer, MSE and IAE

Structure	1 node		2 nodes		3 nodes		4 nodes		5 nodes		6 nodes	
	MSE	**IAE**	**MSE**	**IAE**	**MSE**	**IAE**	**MSE**	**IAE**	**MSE**	**IAE**	**MSE**	**IAE**
Color	0.021	0.584	0.038	1.070	0.230	2.057	0.323	3.179	0.925	5.431	0.030	0.942
MV	0.060	1.285	0.050	1.261	0.078	1.447	0.324	2.646	0.308	2.697	0.058	1.335
P_0	0.007	0.402	0.018	0.560	0.132	1.318	0.326	2.552	0.276	2.703	0.016	0.582
PRI	0.137	1.591	0.143	1.784	0.137	1.916	0.100	1.720	0.287	2.741	0.102	1.546
Overall	0.056	3.862	0.062	4.715	0.144	6.737	0.268	10.097	0.449	13.572	0.052	4.406

5.3.1.1.2 Effect of transfer function

In this section, the ANN model has been trained and tested using Levenberg-Marquardt algorithm (TRAINLM) with the different transfer function such as TANSIG, LOGSIG, HARDLIM, HARDLIMS, SATLINS, POSLIN and RADBAS to retrieve the properties of pale crepe rubber. The ANN model has 1 hidden layer; the number of nodes has been varied from 1 to 10 nodes. General overall MSE for multiple-inputs multiple-outputs (MIMO) system are shown in Table 5.3.2.

Table 5.3.2 Effect of nodes on prediction performance (overall MSE) with different transfer functions

nodes	Transfer functions						
	TANSIG	LOGSIG	HARDLIM	HARDLIMS	SATLINS	POSLIN	RADBAS
1	0.056	0.056	0.064	0.064	0.057	0.063	0.061
2	0.054	0.054	0.064	0.064	0.052	0.051	0.037
3	0.043	0.145	0.064	0.064	0.041	0.041	0.769
4	0.052	0.052	0.064	0.064	0.066	0.064	0.103
5	0.057	0.051	0.064	0.064	0.040	0.052	0.060
6	0.023	0.066	0.064	0.064	0.043	0.050	0.060
7	1.138	0.168	0.064	0.064	0.036	0.051	59.692
8	6.807	0.099	0.064	0.064	0.033	0.042	0.064
9	0.123	0.128	0.064	0.064	0.061	0.047	0.293
10	0.776	0.134	0.064	0.064	0.052	0.036	0.032

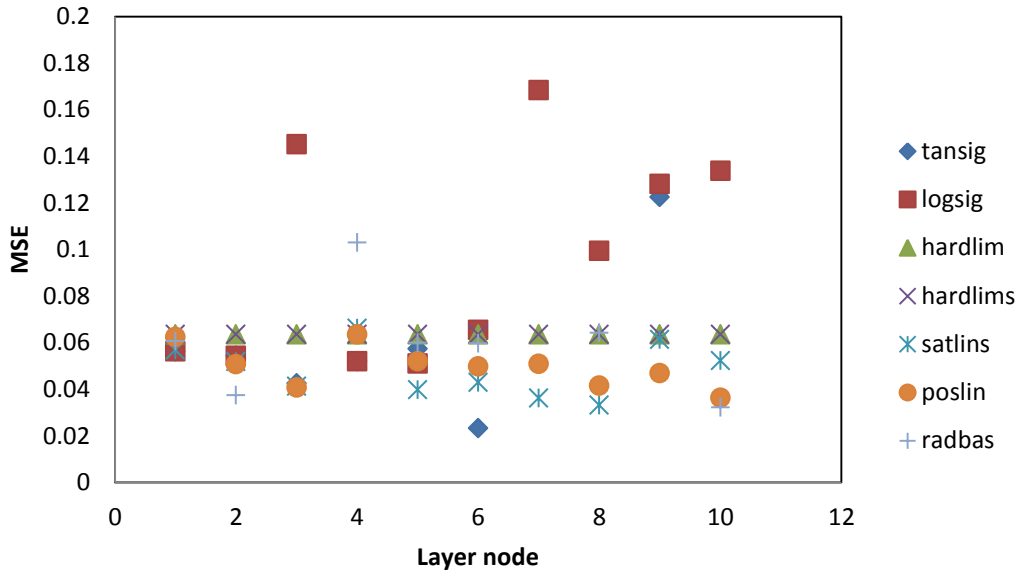


Figure 5.3.3 MSE of each transfer function for MIMO system

It has be seen from the simulation results that ANN with the transfer function of TANSIG (6 nodes) gives the smallest MSE (0.023). However, SATLINS, POSLIN and RADBAS (8, 10, 10 nodes respectively) give insignificantly different values of MSE, 0.033, 0.036 and 0.032 respectively. Then, the prediction error of five network structures (one hidden layer) with TANSIG, LOGSIG (5 nodes), SATLINS, POSLIN and RADBAS has been next evaluated separately for each output as shown in Table 5.3.3 and Figure 5.3.4 – 5.3.7. Figure 5.3.4 – 5.3.7 show effect of five different transfer functions on prediction color, MV, P_0 and PRI respectively. It could be seen from the simulation results that RADBAS transfer function gives the minimum MSE (0.023) and IAE (0.583) values for the color prediction.

Figure 5.3.5 shows the MSE of MV prediction. It could be seen from the simulation results that POSLIN transfer function gives the minimum MSE (0.036) and IAE (1.029) values for MV prediction. In this case, LOGSIG gives highest prediction error with MSE/IAE = 0.067/1.354. Figure 5.3.6 shows the MSE value of P_0 output. It could be seen from the simulation result that POSLIN transfer function gives the minimum MSE (0.008) and IAE (0.423) values for P_0 prediction. However, TANSIG, LOGSIG, RADBAS and SATLINS also provide acceptable

prediction errors with MSE/IAE = 0.021/0.543, 0.018/0.532, 0.014/0.586 and 0.016/0.625 respectively.

Table 5.3.3 Effect of transfer functions on output prediction performances

Output	TANSIG		LOGSIG		SATLINS		POSLIN		RADBAS	
	MSE	IAE	MSE	IAE	MSE	IAE	MSE	IAE	MSE	IAE
Color	0.032	0.900	0.048	1.107	0.030	0.899	0.027	0.895	0.023	0.583
MV	0.058	1.382	0.067	1.354	0.047	1.211	0.036	1.029	0.040	0.990
P_0	0.021	0.543	0.018	0.532	0.016	0.625	0.008	0.423	0.014	0.586
PRI	0.018	0.590	0.054	1.147	0.051	1.050	0.059	1.117	0.041	0.951
Overall	0.033	3.415	0.046	4.141	0.036	3.786	0.032	3.464	0.029	3.109

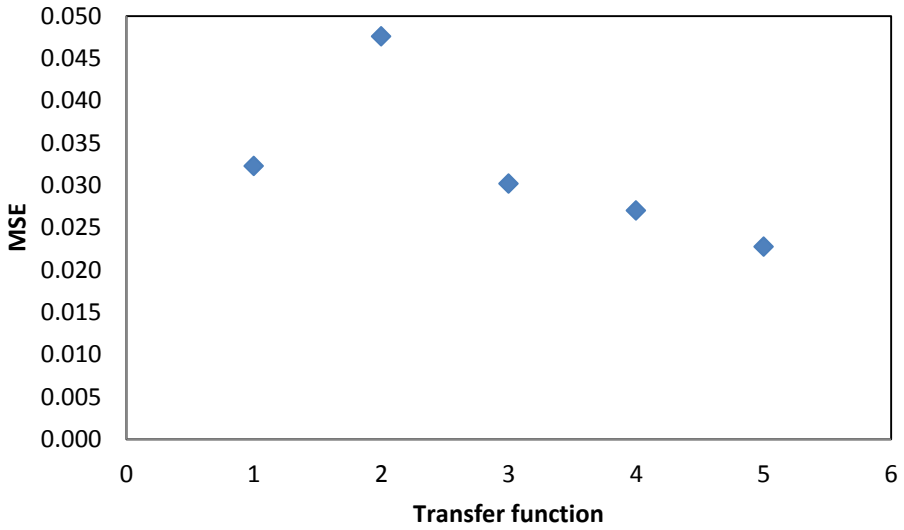


Figure 5.3.4 Effect of transfer function on color prediction

1 = TANSIG, 2 = LOGSIG, 3 = SATLINS, 4 = POSLIN, 5 = RADBAS

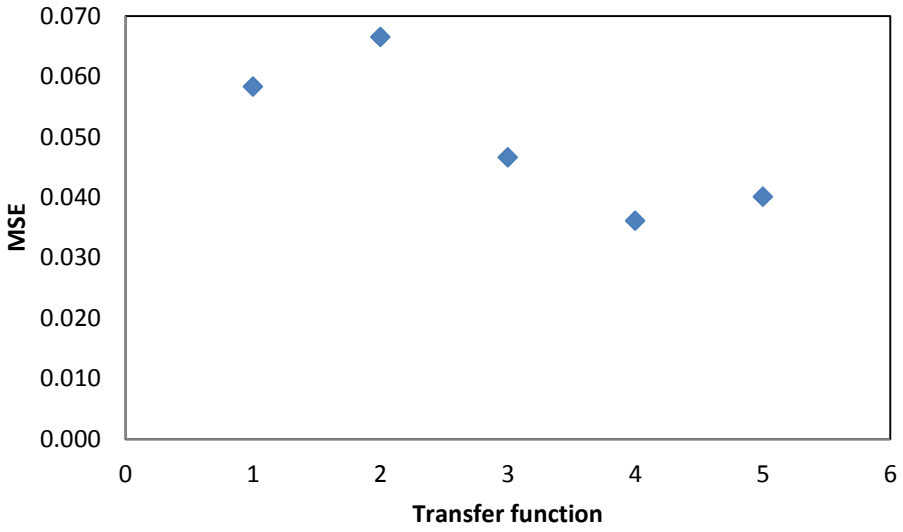


Figure 5.3.5 Effect of transfer function on MV prediction

1 = TANSIG, 2 = LOGSIG, 3 = SATLINS, 4 = POSLIN, 5 = RADBAS

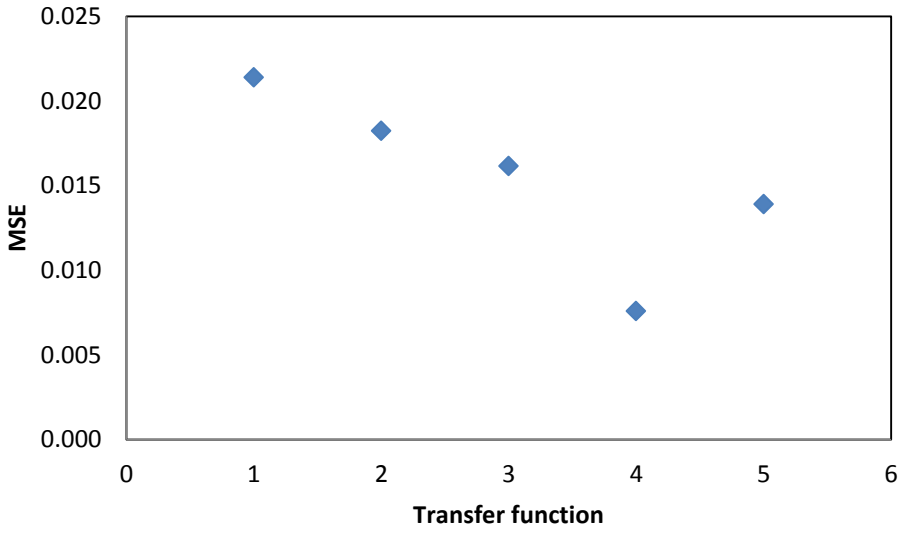


Figure 5.3.6 Effect of transfer function on P_0 prediction

1 = TANSIG, 2 = LOGSIG, 3 = SATLINS, 4 = POSLIN, 5 = RADBAS

.

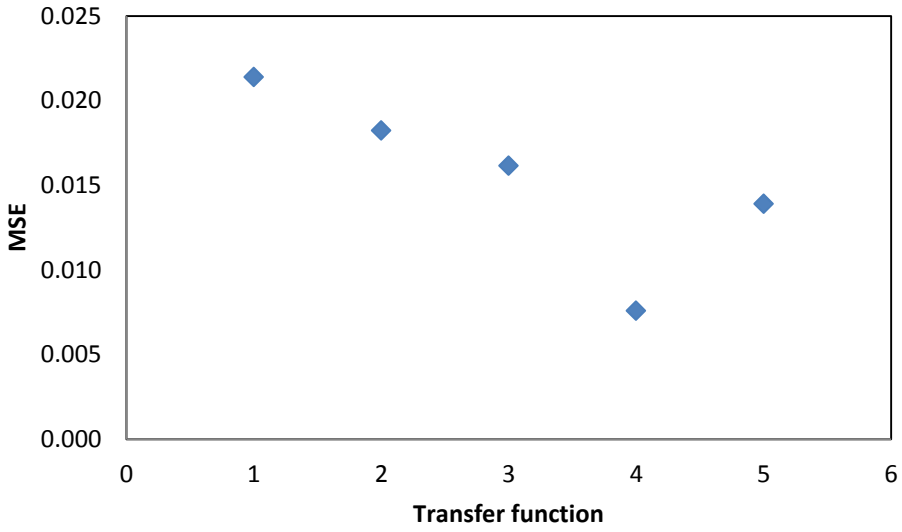


Figure 5.3.7 Effect of transfer function on PRI prediction

1 = TANSIG, 2 = LOGSIG, 3 = SATLINS, 4 = POSLIN, 5 = RADBAS

Figure 5.3.7 shows the MSE of PRI output. It could be seen from the simulation result that TANSIG transfer function give the minimum MSE (0.018) and IAE (0.590) values for PRI prediction. In this case, POSLIN gives highest prediction error with MSE/IAE = 0.059/18.141. It could be concluded in this section that ANN models with RADBAS transfer function give good overall prediction performance, MSE/IAE = 0.029/3.109 as shown in Table 5.3.3. In this case, different activation functions show insignificant effects on the output prediction because the operating range is too small. However, it should be noted that the activation functions should be chosen according to the process output responses.

5.3.1.2 ANN design with 2 hidden layers

In this section, ANN model has been designed in the optimal way by plotting MSE surface and its contour plot with node number of layer 1 and 2 as shown in Figure 5.3.8 and Figure 5.3.9, respectively. The ANN has been trained using Levenberg-Marquardt algorithm with TANSIG transfer function (mostly used) and the rubber properties have been predicted via using linear transfer functions (PURELIN). The overall mean square error (MSE) is calculated by Equation 5.3.1. It has been found in the simulation results that for MSE < 10, the network structure could have [1-4, 2-4] nodes for layer [1, 2] respectively, and [6-10, 1-10] nodes for layer [1, 2] respectively.

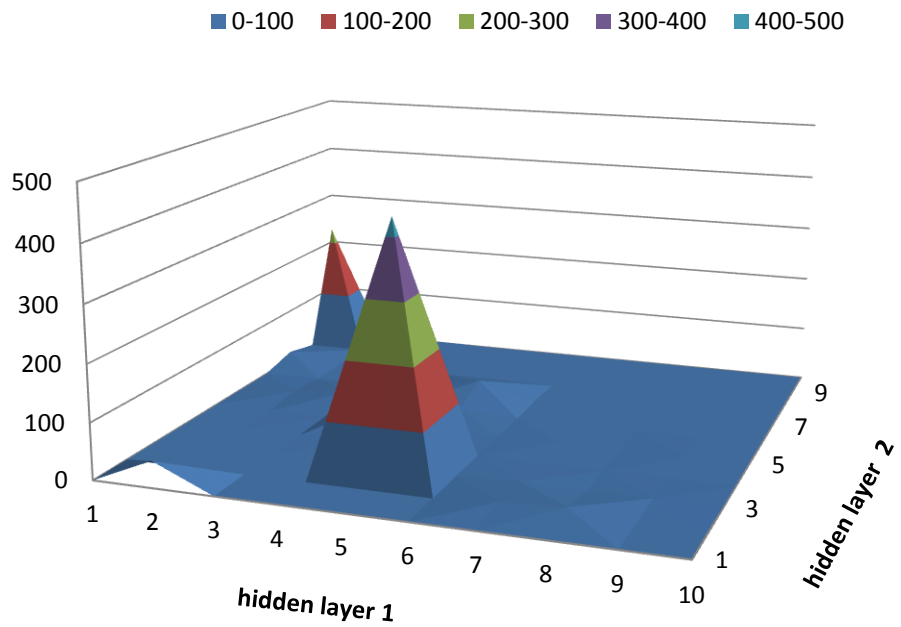


Figure 5.3.8 Overall MSE response according to (fully) ANN node tuning

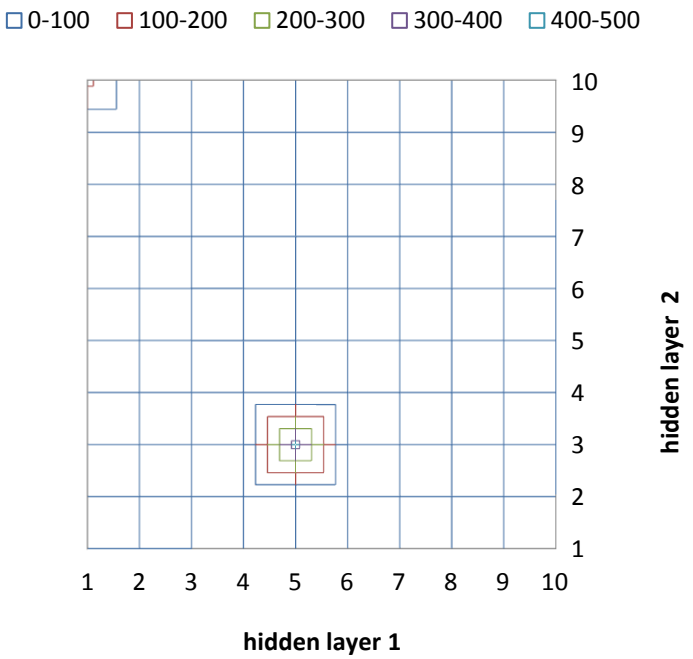


Figure 5.3.9 Overall MSE contour plot according to (fully) ANN node tuning

In order to minimizing the prediction error of each property, the optimal network structure has been chosen by considering MSE and integral absolute error (IAE) of the predicted output individually, Equation (5.3.3) and Equation (5.3.4) respectively. Figure 5.3.10, 5.3.12, 5.3.14 and 5.3.16 show IAE surface plots for rubber property predictions such as color, MV, P_0 and PRI respectively. In addition Figure 5.3.11, 5.3.13, 5.3.15 and 5.3. 17 show IAE contour plots for rubber property predictions such as color, MV, P_0 and PRI respectively. It could be seen that the ANN structure, [nodes for layer 1, nodes for layer 2] that gives good performance of rubber color, MV, P_0 and PRI could be [1-4, 1-3], [5-7, 1-2], and [8-10, 6-10].

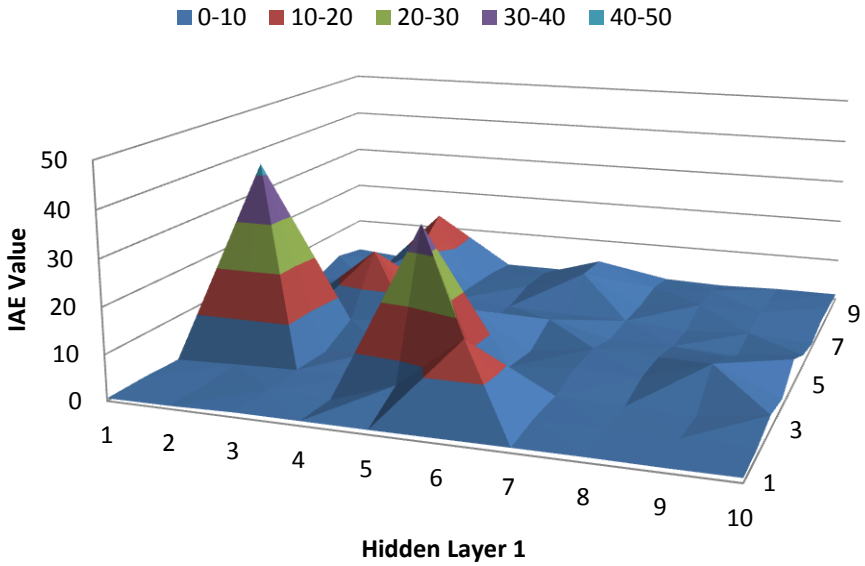


Figure 5.3.10 IAE surface plot for color prediction according to (fully) ANN node tuning

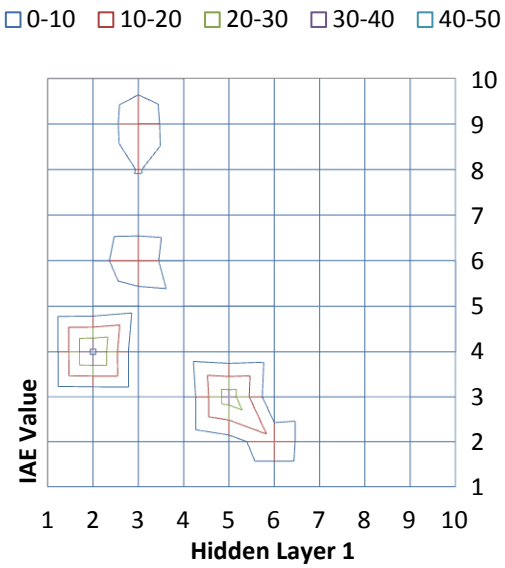


Figure 5.3.11 IAE contour plot for color prediction according to (fully) ANN node tuning

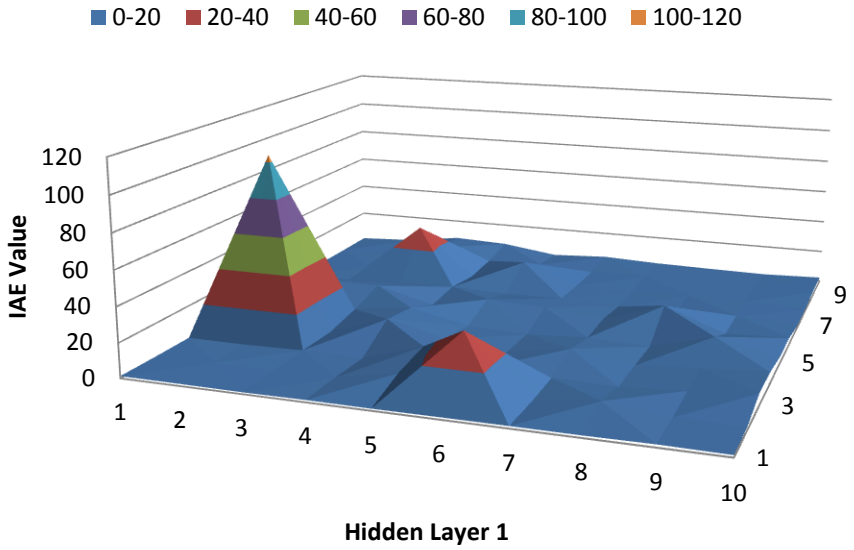


Figure 5.3.12 IAE surface plot for MV prediction according to (fully) ANN node tuning

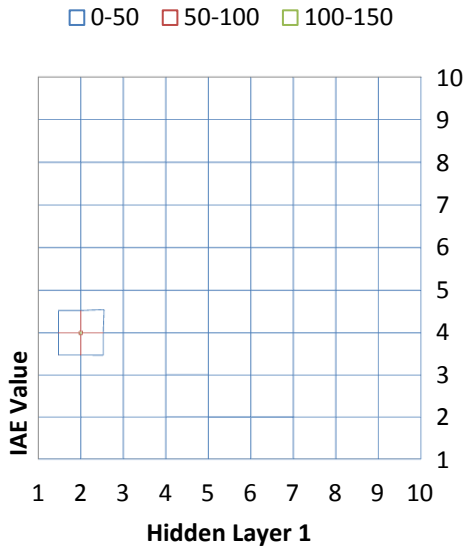


Figure 5.3.13 IAE contour plot for MV prediction according to (fully) ANN node tuning

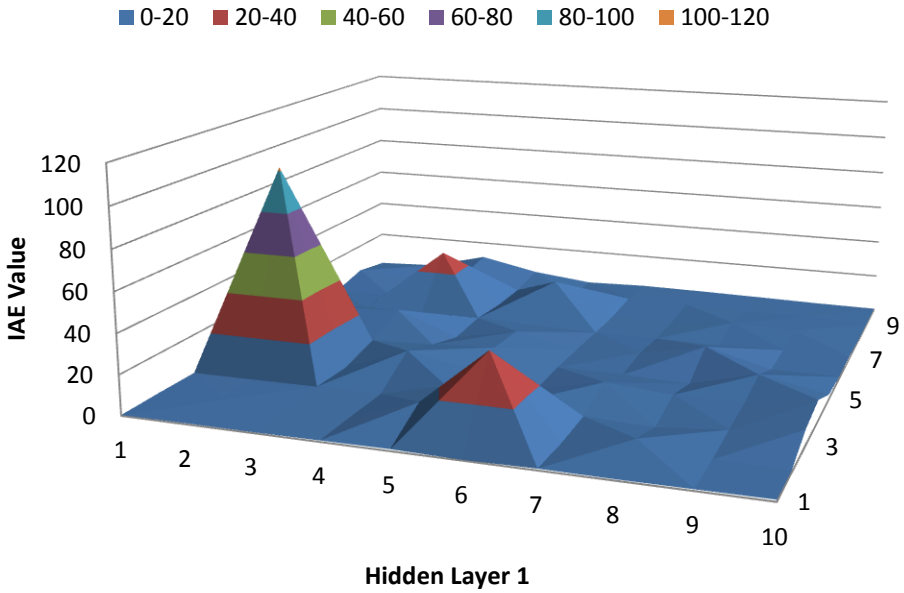


Figure 5.3.14 IAE surface plot for P_0 prediction according to (fully) ANN node tuning

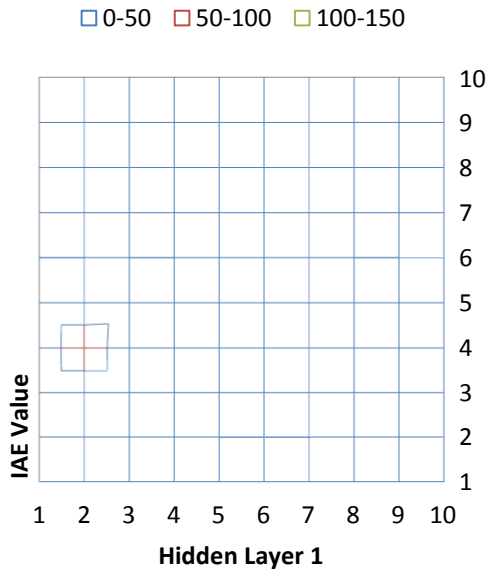


Figure 5.3.15 IAE contour plot for P_0 prediction according to (fully) ANN node tuning

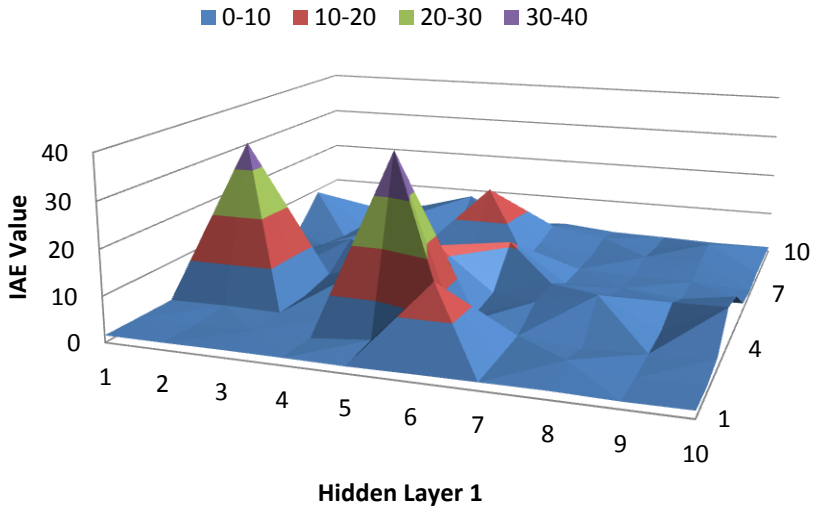


Figure 5.3.16 IAE surface plot for PRI prediction according to (fully) ANN node tuning

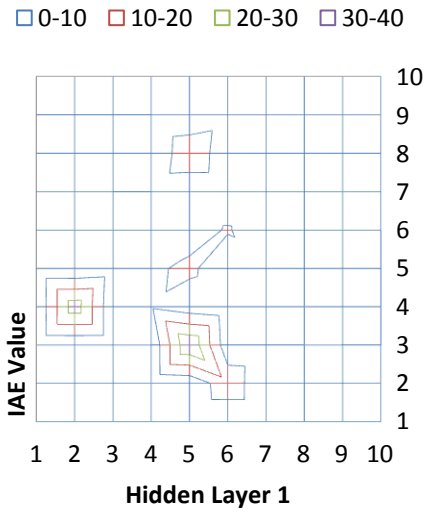


Figure 5.3.17 IAE contour plot for PRI prediction according to (fully) ANN node tuning

From Figures 5.3.8-5.3.17, five ANN structures are then chosen arbitrarily as with nodes of [8,10], [1,3], [3,2], [6,1] and [10,7] for layer [1,2]. Table 5.3.4 shows MSE and IAE values of five models prediction. Figures 5.3.18 – 5.3.21 show the comparison of the predicted outputs and the experimental testing data for the ANN model structures, [1,3], [3,2], [6,1] and [10,7]

respectively. It has been found in this work that ANN model structure with 1 and 3 nodes in layer 1 and 2 respectively gives minimum overall MSE/IAE (0.037/3.394) of the output prediction. The ANN with structure of [1,3] gives smallest IAE values of color and MV prediction (0.452 and 1.124 respectively), but structure of [10,7] gives smallest IAE values of P_0 and PRI (0.451 and 1.081).

Table 5.3.4 Performances of (fully) ANN model, MSE and IAE

Structure	8,10		1,3		3,2		6,1		10,7	
	MSE	IAE	MSE	IAE	MSE	IAE	MSE	IAE	MSE	IAE
color	0.159	1.642	0.008	0.452	0.040	0.984	0.036	0.952	0.077	1.462
MV	0.124	1.683	0.046	1.124	0.085	1.383	0.157	2.092	0.010	1.637
P_0	0.037	0.754	0.015	0.559	0.039	0.857	0.079	1.119	0.013	0.451
PRI	0.044	1.077	0.079	1.259	0.108	1.630	0.114	1.598	0.042	1.081
Overall	0.091	5.156	0.037	3.394	0.068	4.854	0.096	5.761	0.058	4.632

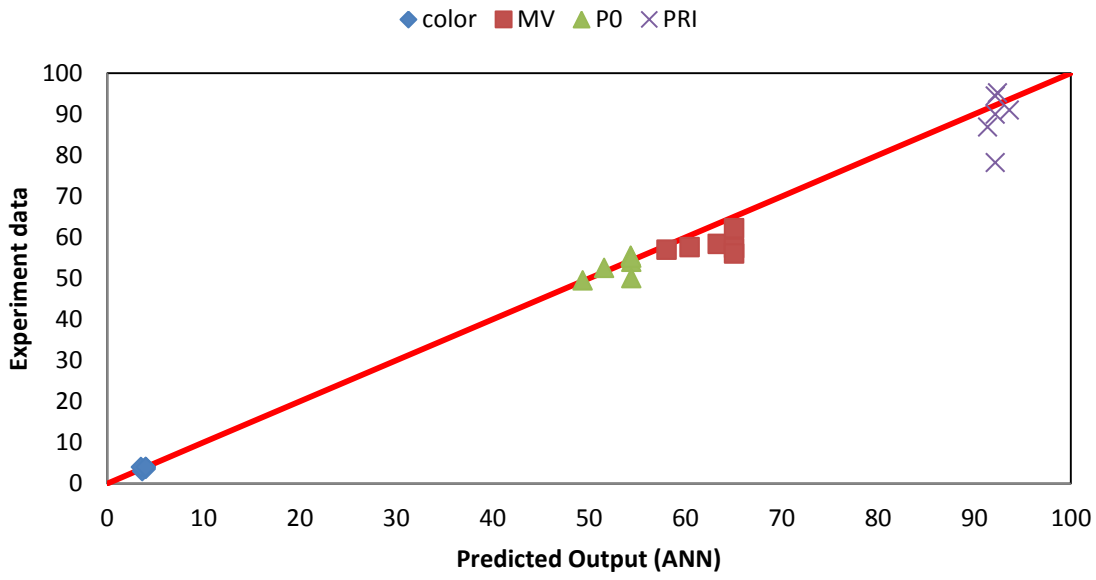


Figure 5.3.18 Comparison of the predicted and experimental outputs for ANN structure [1,3]

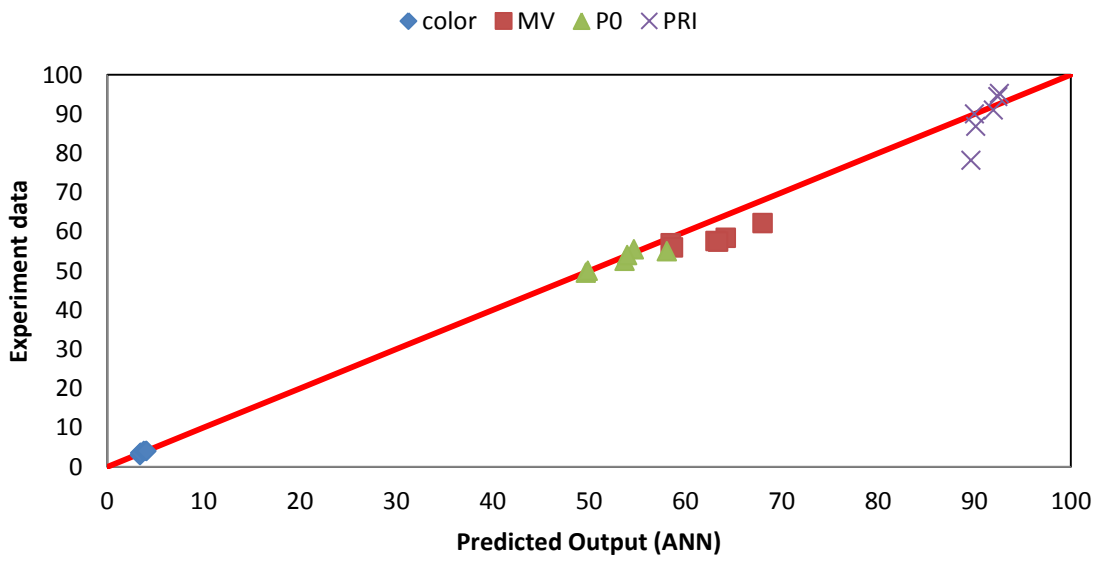


Figure 5.3.19 Comparison of the predicted and experimental outputs for ANN structure [3,2]

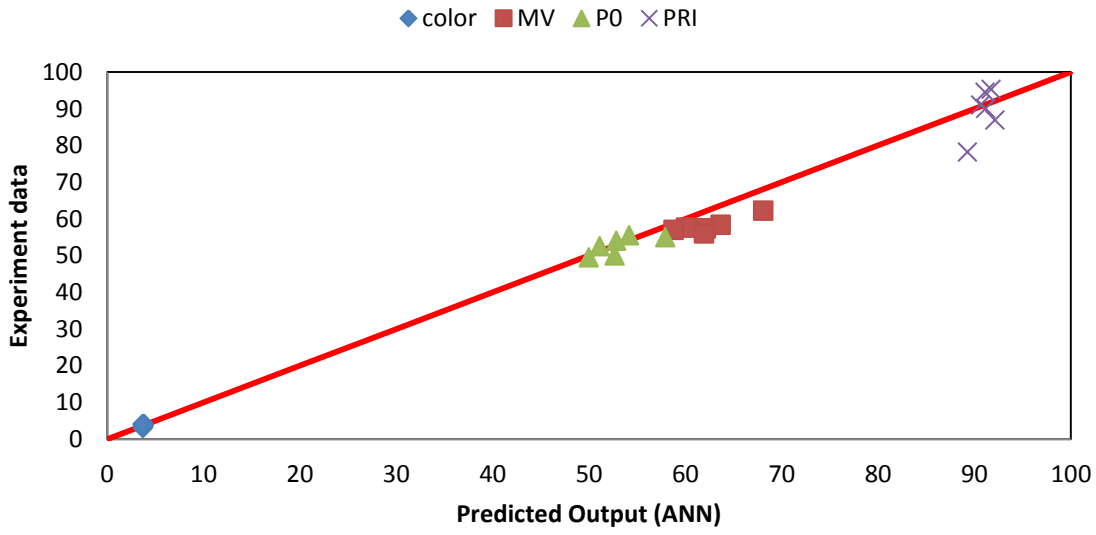


Figure 5.3.20 Comparison of the predicted and experimental outputs for ANN structure [6,1]

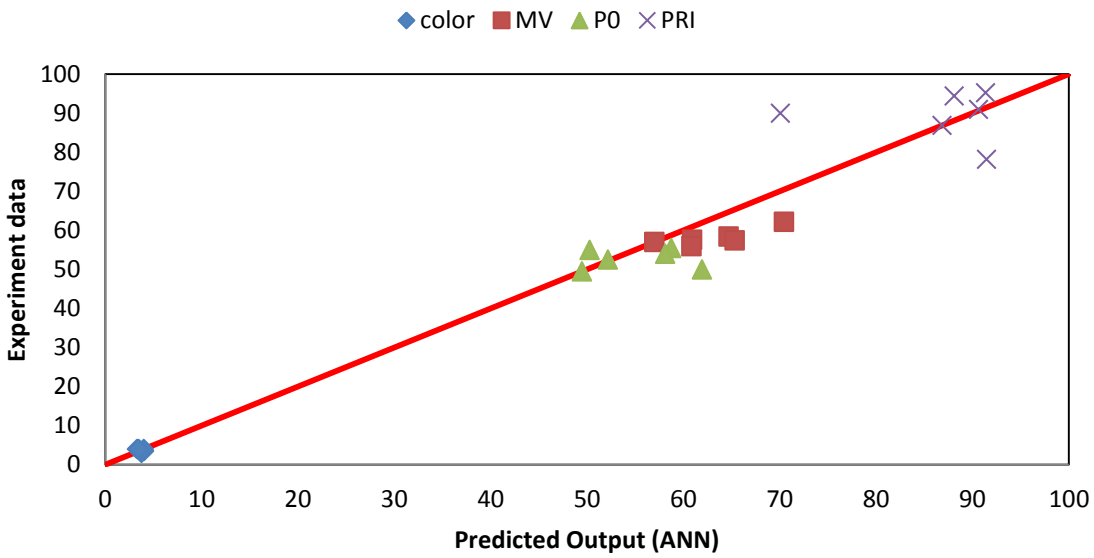


Figure 5.3.21 Comparison of the predicted and experimental outputs for ANN structure [10,7]

This part shows the comparison of the experiment and predicted data by considering the effect of acetic acid amount and coagulation time. The rubber properties such as Lovibond color, MV, P_0 and PRI have been predicted by using ANN model with structure of [1,3] nodes for layer 1 and 2 respectively. The transfer functions TANSIG and PURELIN have been used in the hidden layers and the output layer respectively. The acetic acid amount and the coagulation time have been varied 0.15%, 0.30% and 0.45% vol./wt. of dry rubber, and 1, 2 and 3 hr.

Figure 5.3.22 shows the comparison of the predicted and experimental Lovibond color. It could be seen from the results that the predicted rubber color are smaller than the actual data about 0.1 – 1 Lovibond unit in all conditions. However, the network model gives acceptable trend of the rubber color as seen in the Figure 5.3.22.

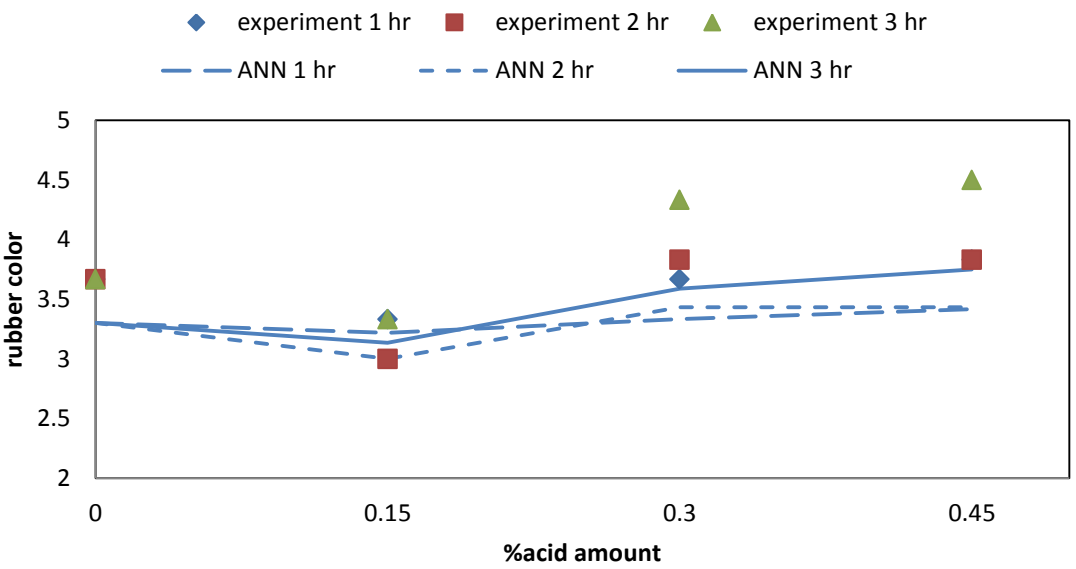


Figure 5.3.22 Comparison of the predicted and experimental rubber color, ANN with [1,3]

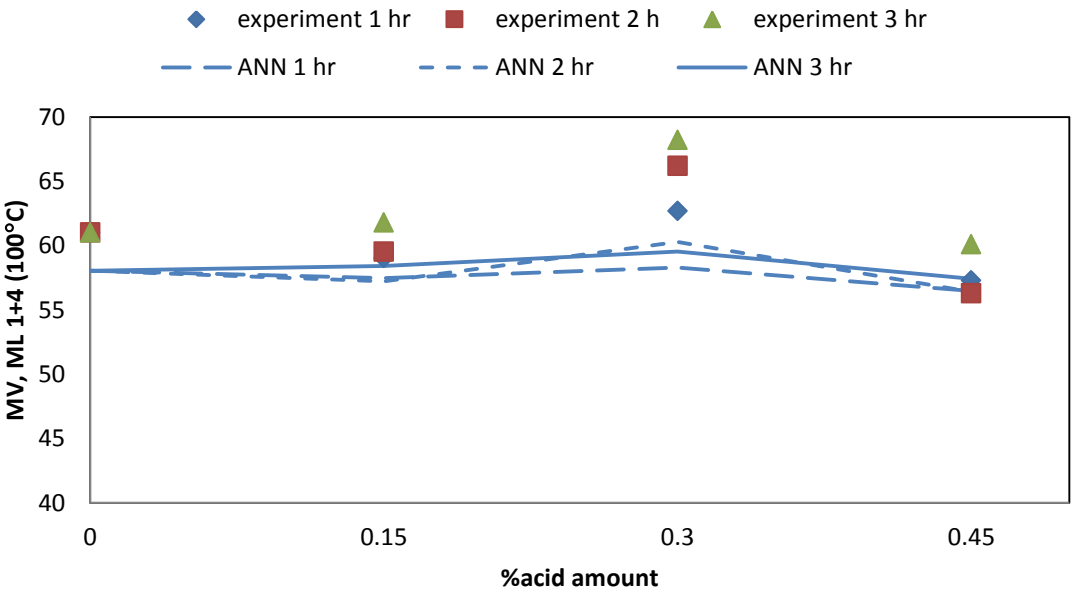


Figure 5.3.23 Comparison of the predicted and experimental MV, ANN with [1,3]

Figure 5.3.23 shows the comparison of the predicted and experimental MV. It could have seen that the predicted outputs provided by ANN model with 2 hidden layers [1,3] are smaller than the experimental results about 2-10 ML 1+4 (100°C) in all conditions. Figure 5.3.24 shows the comparison of the predicted and experimental initial plasticity (P_0). It could have seen that the predicted outputs provided by ANN model with structure of [1,3] relate with the experimental results. However, the predicted data are smaller than the experimental data about 1 – 5 values of P_0. Figure 5.3.25 shows the comparison of the predicted and experimental plasticity retention index (PRI). It could have seen that the predicted outputs provided by ANN model relate with the experimental result. However the predicted PRI are slightly different with the experimental ones only about 1 – 2%.

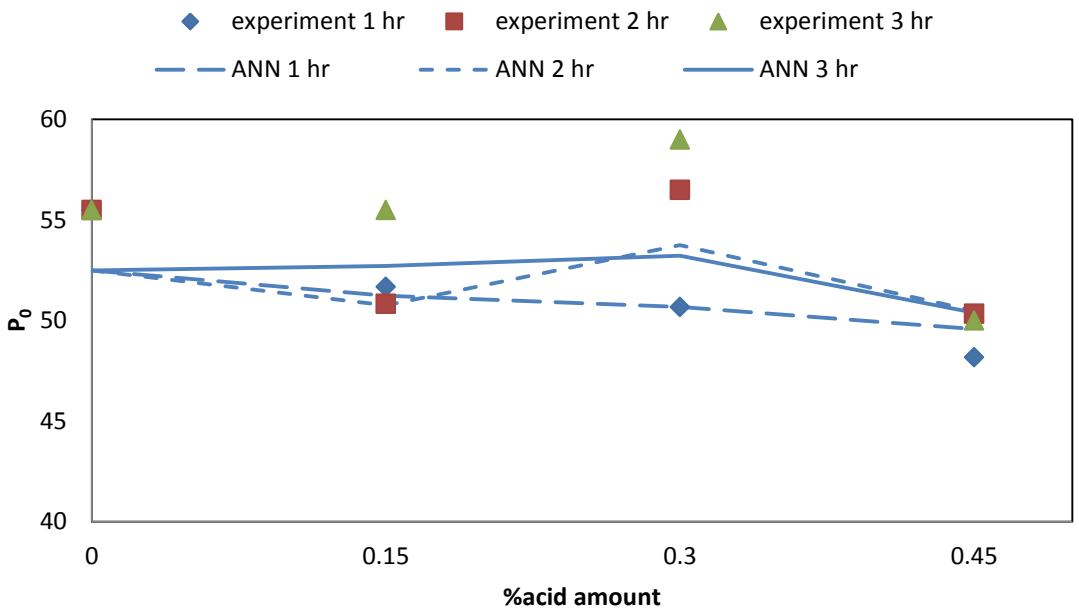


Figure 5.3.24 Comparison of the predicted and experimental P_0, ANN with [1,3]

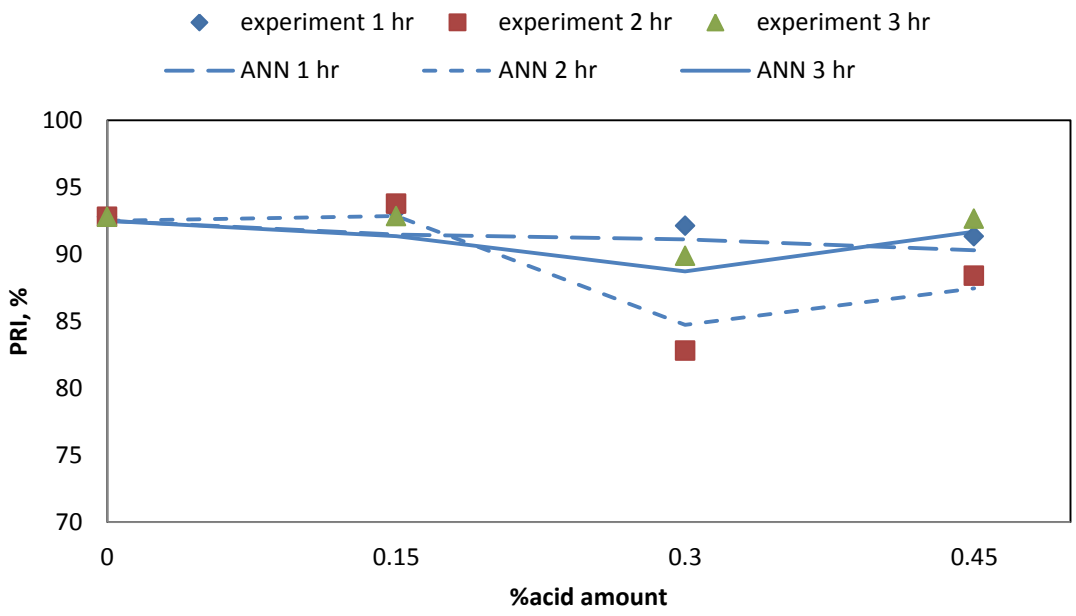


Figure 5.3.25 Comparison of the predicted and experimental PRI, ANN with [1,3]

5.3.2 Input variable analysis (Partial modeling)

Since the performance of ANN model strongly depends on the training data sets, significant input variables should then be carefully chosen to give good performance of the model. Insignificant input variables might give poor prediction results, a variable selection approach such a partial modeling (Despagne, F., et al., 1998) has been further applied in this section for the model improvement. In this case, the sensitivity (S_i) of the predicted responses, $\sigma^2_{\hat{y}(x_1)}$ has been determined as shown in Equation (5.3.5).

$$S_i = \sigma^2_{\hat{y}(x_i)} \tag{5.3.5}$$

According to the partial modeling approach presented by Despagne,F., et al., 1998 all ANN inputs but the first (x_1= acetic acid amount) are firstly set to zero ($x_2, x_3, x_4 = 0$). The procedure is next repeated by setting $x_1, x_3, x_4$to zero, to obtain $\sigma^2_{\hat{y}(x_2)}$ and so on.

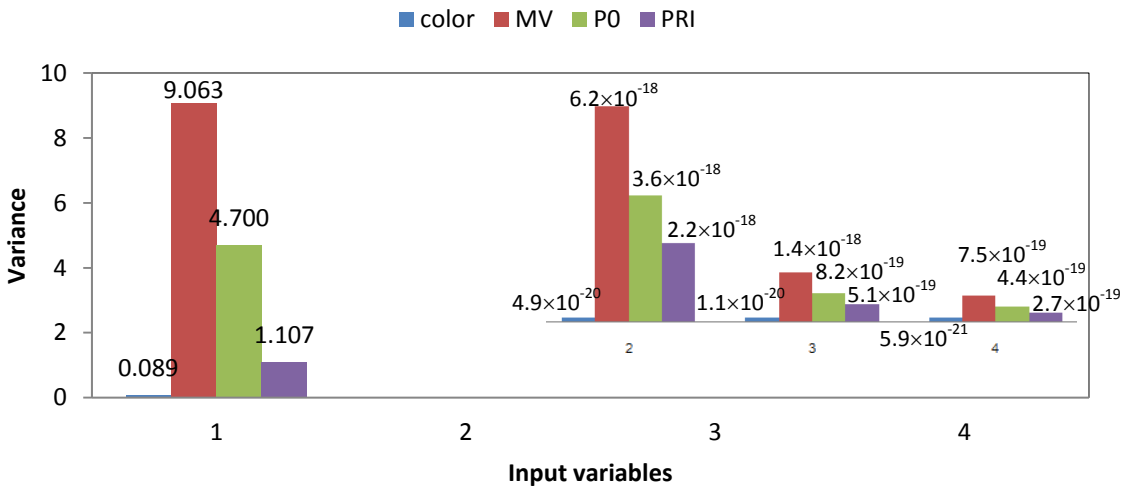


Figure 5.3.26 Sensitivity of the predicted output corresponding to input variables

1 = acetic acid amount, 2 = coagulation time, 3 = %DRC, 4 = %TSC

In this section, the fully ANN model obtained from the section 5.3.1 with four input variables, and the structure of [1,3] has been further identified the insignificant input variable by using the partial modeling approach. The sensitivity bar plot in this case has been shown in Figure 5.3.26. It can be seen that the acetic acid amount has largest effects on predicted outputs, MV (9.063), P_0 (4.700), PRI (1.107) and Lovibond color (0.089) respectively. The other three input variables such as the coagulation time, %DRC and %TSC have significantly smaller than the acid amount. Moreover, %TSC has smallest effects on all process outputs, especially Lovibond color and PRI compared to the other inputs. This might be because %TSC is normally higher than %DRC around 3% - 5% in which non-rubber consisting of color pigments is the difference of %TSC and %DRC. Therefore, %TSC could be ignored since it varies according to %DRC, it has then been chosen as the insignificant variable and further eliminated.

5.3.3 Partial-inputs model structure

In this section, new network model has been trained with three inputs, the acetic acid amount, the coagulation time and %DRC. The network structure has been chosen with two hidden layers, 1 node for layer 1 and 3 nodes for layer 2 with hyperbolic tangent sigmoid transfer function (TANSIG). The linear transfer functions (PURELIN) are used in the output layer. Figure 5.3.27 shows the comparison of the predicted and experimental outputs in case of three – inputs ANN model. The overall MSE/IAE are shown in Table 5.3.5.

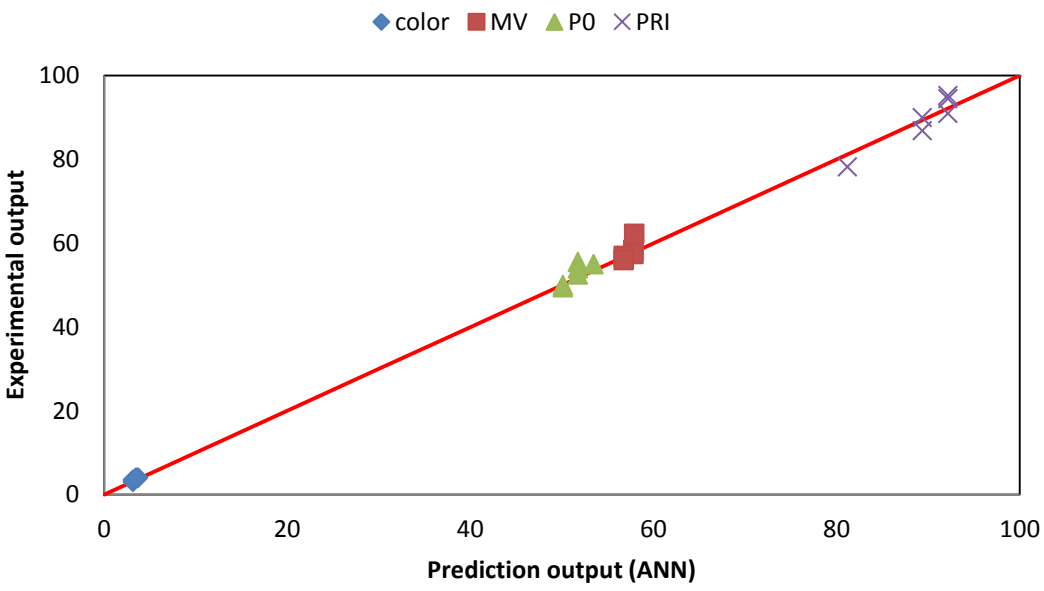


Figure 5.3.27 Comparison of the predicted and experimental outputs for ANN with 3 inputs

Table 5.3.5 Performances of (3-inputs) ANN model with structure of [1,3]

Structure	1,3	
	MSE	**IAE**
color	0.003	0.264
MV	0.053	1.218
P0	0.006	0.405
PRI	0.083	1.372
Overall	0.037	3.260

Figure 5.3.27 shows the validation of ANN (partial) model. The predicted of each output variable has been grouped. The accuracy between the experimental and predicted output are accepted. It has been found that overall MSE/IAE is 0.037/3.260 for ANN with 3 input variables. The ANN prediction can be improved by removing the less affect input variable, in which the predicted color and P_0 are significantly improved in this case.

5.4 Optimum conditions determination

By applying the input variable selection, the output prediction of the ANN model has been improved as seen in previous part. The optimum conditions have been further evaluated by considering the surface plots of the responses as shown in Figure 5.3.28 – Figure 5.3.31. It can be seen that P_0 and PRI values are higher than the properties requirement ($P_0 > 35$ and PRI > 60) in all cases if the process operates at %DRC = 27.17. It could be seen that MV is higher than the standard, MV> 60 ML(1+4) 100°C if the process operates under the acetic acid amount of 0.25-0.28% vol./wt. dry rubber and coagulation time in range of 0.1-0.6 hr. Moreover, MV values are higher than 58 ML(1+4) 100°C in the acetic acid amount of 0.2-0.27% vol./wt. dry rubber and coagulation time in range of 0.1-1.5 hr.

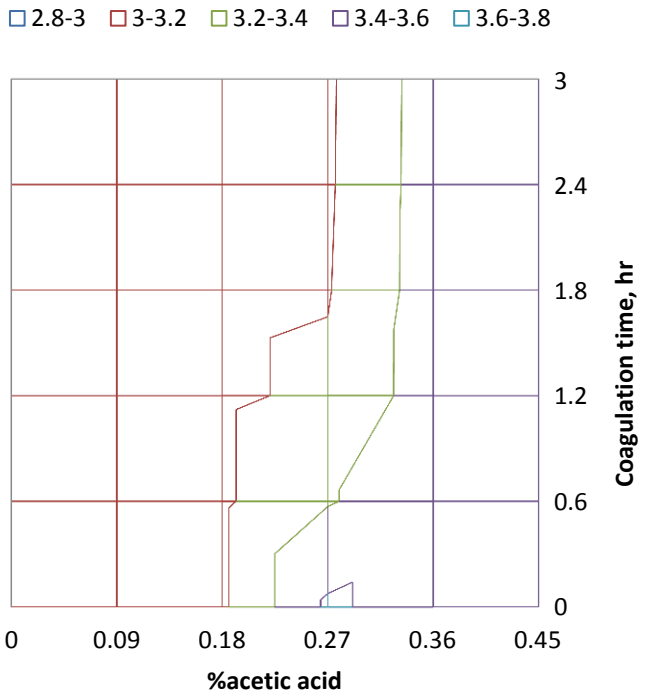


Figure 5.3.28 Response surface of predicted Lovibond color

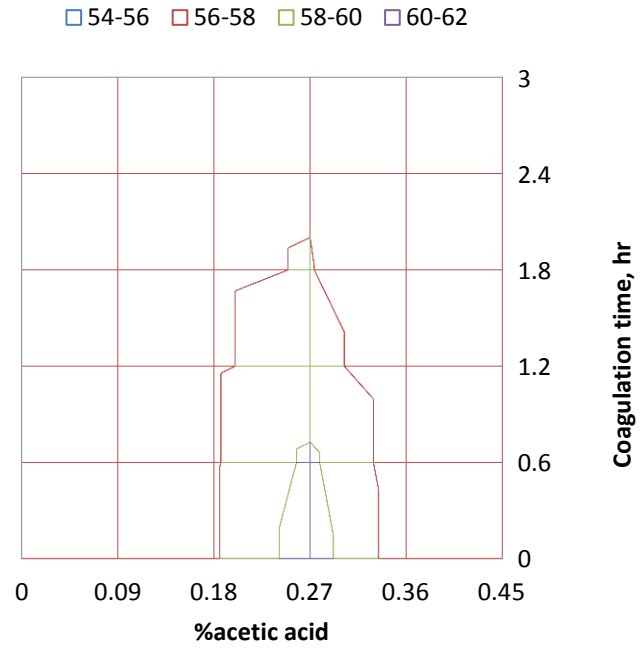


Figure 5.3.29 Response surface of predicted MV

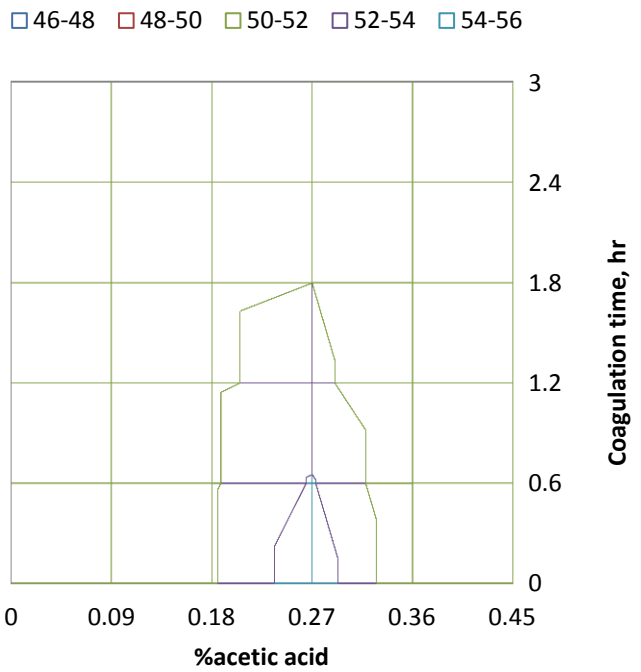


Figure 5.3.30 Response surface of predicted P_0

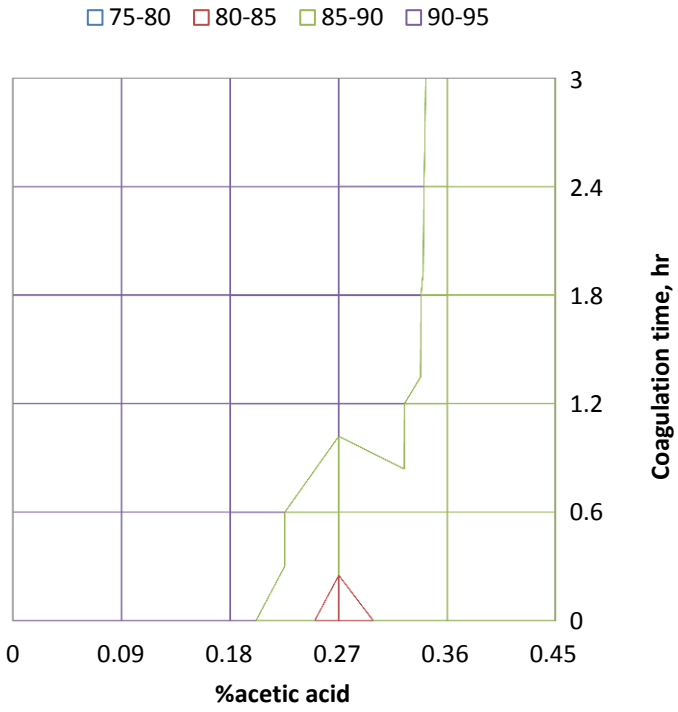


Figure 5.3.31 Response surface of predicted PRI

The Lovibond color has slightly higher than the product specification (≈ 3) in (1) the acetic acid amount of 0.01-0.2% vol./wt. dry rubber and coagulation time in range of 0.1-1.8 hr, (2) the acetic acid amount of 0.01-0.22% vol./wt. dry rubber and coagulation time in range of 1.2-3 hr and (3) the acetic acid amount of 0.01-0.27% vol./wt. dry rubber and coagulation time in range of 1.8-3 hr. By considering the predicted responses, it has been found that the conditions providing acceptable color (≈ 3) and MV (> 58 ML(1+4) 100^{o}C) at the same time are under the acetic acid amount of 0.2-0.22% vol./wt. dry rubber and coagulation time is 1.2-1.5 hr. MV of rubber sheet could be increased over time during storage. The optimal condition from the ANN model is related with the optimal condition from experimental data.

CHAPTER 6

CONCLUSIONS AND RECOMENDATIONS

6.1 Experimental results

The experiment has been carried out to produce pale crepe rubber via fractional coagulation method, 1% by wt. of acetic acid has been used to coagulate the latex (RRIM 600) fractionally. Effects of acetic acid amount and coagulation time have been investigated on the rubber properties; Lovibond color, MV, P_0 and PRI. The acetic acid amount and the coagulation time have been varied 0.15%, 0.30% and 0.45% vol./wt. of dry rubber, and 1, 2 and 3 hrs. From the experimental results, it could be seen that the rubber color is significantly decreased at 0.15% vol./wt., 2 hrs and increased at 0.30% and 0.45% vol./wt., 3 hrs. MV is significantly decreased at 0.45% vol./wt., 1-2 hrs (MV < 60). P_0 is significantly decreased at 0.15% vol./wt., 1-2 hrs, 0.30% vol./wt., 1 hrs 0.45% vol./wt., 1-3 hrs, but increased at 0.30% vol./wt., 3 hrs. PRI is significantly decreased at 0.30% vol./wt., 2 hrs 0.45% vol./wt., 2 hrs. Then the proper operating condition should be at 0.15% vol./wt. of acetic acid, and coagulation time of 2 hrs to give the property requirement: minimum rubber color, MV > 60, P_0 > 35 and PRI > 60.

6.2 Artificial Neural Network design for Pale Crepe Rubber Process

6.2.1 Fully-input model structure

The ANN model has been designed for 1-2 hidden layers by varying their number of nodes (1 to 10). Artificial Neural Network (ANN) model has feed-forward scheme with four input variables such as (1) acetic acid amount, (2) fractional coagulation time, (3) %dry rubber content (%DRC) of diluted latex, and (4) the corresponding %total solid content (%TSC). Four rubber properties, such as (1) rubber color, (2) Mooney viscosity (MV), (3) initial plasticity (P0), and (4) Plasticity Retention Index (PRI) have been predicted via using linear transfer functions (PURELIN). The ANN has been trained using the Levenberg-Marquardt algorithm with 30 experimental data sets, data matrix [4×30]; 80% for training (training matrix, [4×24]) and 20% for testing (testing matrix, [4×6]). The performance of the ANN model has been identified by using the values of mean square error (MSE) and integral absolute error (IAE).

6.2.1.1 Effect of layer node

ANN model has been trained with 1 hidden layer, the number of nodes is varying from 1 to 10 nodes. It has been found in the simulation results that the optimal network structure could have 1 node in hidden layer give minimum overall MSE and IAE of the output prediction with MSE = 0.056 and IAE = 3.862.

6.2.1.2 Effect of transfer function

The ANN model has been trained and tested using Levenberg-Marquardt algorithm (TRAINLM) with the different transfer function such as TANSIG, LOGSIG, HARDLIM, HARDLIMS, SATLINS, POSLIN and RADBAS to retrieve the properties of pale crepe rubber. The ANN model has 1 hidden layer; the number of nodes has been varied from 1 to 10 nodes. The ANN models with RADBAS transfer function give good overall prediction performance, MSE/IAE = 0.029/3.109.

6.2.2 ANN design with 2 hidden layer

ANN model has been designed in the optimal way by plotting MSE surface and its contour plot with node number of layer 1 and 2. The ANN has been trained using Levenberg-Marquardt algorithm with TANSIG transfer function and the rubber properties have been predicted via using linear transfer functions (PURELIN). It has been found in this work that ANN model structure with 1 and 3 nodes in layer 1 and 2 respectively gives minimum overall MSE/IAE (0.037/3.394) of the output prediction.

6.2.3 Input variable analysis (Partial modeling)

The fully ANN model structure of [1,3] has been further identified the insignificant input variable by using the partial modeling approach. It can be seen that the acetic acid amount has largest effects on predicted outputs, MV (9.063), P_0 (4.700), PRI (1.107) and Lovibond color (0.089) respectively. The other three input variables such as the coagulation time, %DRC and %TSC have significantly smaller than the acid amount. Moreover, %TSC has smallest effects on all process outputs, especially Lovibond color and PRI compared to the other inputs because %TSC is normally higher than %DRC around 3% - 5% in which non-rubber consisting of color pigments is the difference of %TSC and %DRC. Therefore, %TSC could be ignored since it varies according to %DRC, it has then been chosen as the insignificant variable and further eliminated.

6.2.4 Partial-inputs model structure

New network model has been trained with three inputs, the acetic acid amount, the coagulation time and %DRC. The network structure has been chosen with two hidden layers, 1 node for layer 1 and 3 nodes for layer 2 with hyperbolic tangent sigmoid transfer function (TANSIG). The linear transfer functions (PURELIN) are used in the output layer. It has been found that overall MSE/IAE is 0.037/3.260 for ANN with 3 input variables. The ANN prediction

can be improved by removing the less affect input variable, in which the predicted PRI are significantly improved in this case.

6.3 Optimum condition determination

By applying the input variable selection, the output prediction of the ANN model has been improved as seen in previous part. The optimum conditions have been further evaluated by considering the surface plots of the responses. It has been found that the conditions providing acceptable color ($\approx$ 3) and MV (> 58 ML(1+4) 100^{o}C) at the same time are under the acetic acid amount of 0.2-0.22% vol./wt. dry rubber and coagulation time is 1.2-1.5 hr. MV of rubber sheet could be increased over time during storage. The optimal condition from the ANN model is related with the optimal condition from experimental data.

6.4 Recommendation

It is quite difficult to provide pale crepe rubber color <3 via fractional coagulation then it should be fractional coagulation coupled with color bleaching.

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APPENDIX A

NEURAL NETWORK

NETWORK FUNCTION

A feed-forward backpropagation network (NEWFF)

Syntax

net = newff(P,T,S,TF,BTF,BLF,PF,IPF,OPF,DDF)

Description

NEWFF(P,T,S,TF,BTF,BLF,PF,IPF,OPF,DDF) takes,

P - RxQ1 matrix of Q1 representative R-element input vectors.

T - SNxQ2 matrix of Q2 representative SN-element target vectors.

Si - Sizes of N-1 hidden layers, S1 to S(N-1), default = []. (Output layer size SN is determined from T.)

TFi - Transfer function of ith layer. Default is 'tansig' for hidden layers, and 'purelin' for output layer.

BTF - Backpropagation network training function, default = 'trainlm'.

BLF - Backpropagation weight/bias learning function, default = 'learngdm'.

PF - Performance function, default = 'mse'.

IPF – Row cell array of input processing functions. Default is {'fixunknowns', 'remconstantrows', 'mapminmax'}.

OPF - Row cell array of output processing functions. Default is {'remconstantrows', 'mapminmax'}.

DDF - Data division function, default = 'dividerand'; and returns an N layer feed-forward backprop network.

The transfer functions TF{i} can be any differentiable transfer function such as TANSIG, LOGSIG, or PURELIN.

The training function BTF can be any of the backpropagation training functions such as TRAINLM, TRAINBFG, TRAINRP, TRAINGD, etc.

WARNING: TRAINLM is the default training function because it is very fast, but it requires a lot of memory to run. If you get an "out-of-memory" error when training try doing one of these:

(1) Slow TRAINLM training, but reduce memory requirements, by setting NET.trainParam.mem_reduc to 2 or more. (See HELP TRAINLM.)

(2) Use TRAINBFG, which is slower but more memory efficient than TRAINLM.

(3) Use TRAINRP which is slower but more memory efficient than TRAINBFG.

The learning function BLF can be either of the backpropagation learning functions such as LEARNGD, or LEARNGDM.

The performance function can be any of the differentiable performance functions such as MSE or MSEREG.

Examples

```
load simplefit_dataset
net = newff(simplefitInputs,simplefitTargets,20);
net = train(net,simplefitInputs,simplefitTargets);
simplefitOutputs = sim(net,simplefitInputs);
```

Algorithm

Feed-forward networks consist of Nl layers using the DOTPROD weight function, NETSUM net input function, and the specified transfer functions. The first layer has weights coming from the input. Each subsequent layer has a weight coming from the previous layer. All layers have biases. The last layer is the network output. Each layer's weights and biases are initialized with INITNW.

Adaption is done with TRAINS which updates weights with the specified learning function. Training is done with the specified training function. Performance is measured according to the specified performance function.

TRAINING FUNCTION

Levenberg-Marquardt backpropagation (TRAINLM)

Syntax

[net,tr] = trainlm(net,tr,trainV,valV,testV)

info = trainlm('info')

Description

TRAINLM is a network training function that updates weight and bias states according to Levenberg-Marquardt optimization. TRAINLM is often the fastest backpropagation algorithm in the toolbox, and is highly recommended as a first choice supervised algorithm, although it does require more memory than other algorithms.

TRAINLM (NET,TR,TRAINV,VALV,TESTV) takes these inputs,

NET - Neural network.

TR - Initial training record created by TRAIN.

TRAINV - Training data created by TRAIN.

VALV - Validation data created by TRAIN.

TESTV - Test data created by TRAIN and returns,

NET - Trained network.

TR - Training record of various values over each epoch.

Each argument TRAINV, VALV and TESTV is a structure of these fields:

X - NxTS cell array of inputs for N inputs and TS timesteps.

X{i,ts} is an RixQ matrix for ith input and ts timestep.

Xi - NxNid cell array of input delay states for N inputs and Nid delays.

Xi{i,j} is an RixQ matrix for ith input and jth state.

Pd - NxSxNid cell array of delayed input states.

T - NoxTS cell array of targets for No outputs and TS timesteps.

T{i,ts} is an SixQ matrix for the ith output and ts timestep.

Tl - NlxTS cell array of targets for Nl layers and TS timesteps.

Tl{i,ts} is an SixQ matrix for the ith layer and ts timestep.

Ai - NlxTS cell array of layer delays states for Nl layers, TS timesteps.

Ai{i,j} is an SixQ matrix of delayed outputs for layer i, delay j.

Training occurs according to training parameters, with default values:

net.trainParam.show	25 Epochs between displays
net.trainParam.showCommandLine	0 generate command line output
net.trainParam.showWindow	1 show training GUI
net.trainParam.epochs	100 Maximum number of epochs to train
net.trainParam.goal	0 Performance goal
net.trainParam.max_fail	5 Maximum validation failures
net.trainParam.mem_reduc	1 Factor to use for memory/speed trade off.
net.trainParam.min_grad	1e-10 Minimum performance gradient
net.trainParam.mu	0.001 Initial Mu
net.trainParam.mu_dec	0.1 Mu decrease factor
net.trainParam.mu_inc	10 Mu increase factor
net.trainParam.mu_max	1e10 Maximum Mu
net.trainParam.time	inf Maximum time to train in seconds

TRAINLM is the default training function for several network creation functions including NEWFF, NEWCF, NEWTD, NEWDTDNN and NEWNARX. TRAINLM('info') returns useful information about this function.

Algorithm

TRAINLM supports training with validation and test vectors if the network's NET.divideFcn property is set to a data division function. Validation vectors are used to stop training early if the network performance on the validation vectors fails to improve or remains the same for

MAX_FAIL epochs in a row. Test vectors are used as a further check that the network is generalizing well, but do not have any effect on training.

TRAINLM can train any network as long as its weight, net input, and transfer functions have derivative functions. Backpropagation is used to calculate the Jacobian jX of performance PERF with respect to the weight and bias variables X. Each variable is adjusted according to Levenberg-Marquardt,

jj = jX * jX

je = jX * E

dX = -(jj+I*mu) \ je

where E is all errors and I is the identity matrix.

The adaptive value MU is increased by MU_INC until the change above results in a reduced performance value. The change is then made to the network and mu is decreased by MU_DEC.

The parameter MEM_REDUC indicates how to use memory and speed to calculate the Jacobian jX. If MEM_REDUC is 1, then TRAINLM runs the fastest, but can require a lot of memory. Increasing MEM_REDUC to 2, cuts some of the memory required by a factor of two, but slows TRAINLM somewhat. Higher states continue to decrease the amount of memory needed and increase training times.

Training stops when any of these conditions occurs:

1) The maximum number of EPOCHS (repetitions) is reached.

2) The maximum amount of TIME has been exceeded.

3) Performance has been minimized to the GOAL.

4) The performance gradient falls below MINGRAD.

5) MU exceeds MU_MAX.

6) Validation performance has increased more than MAX_FAIL times since the last time it decreased (when using validation).

LEARNING FUNCTION

Gradient descent w/momentum weight/bias learning function (LEARNGDM)

Syntax

[dW,LS] = learngdm(W,P,Z,N,A,T,E,gW,gA,D,LP,LS)

[db,LS] = learngdm(b,ones(1,Q),Z,N,A,T,E,gW,gA,D,LP,LS)

info = learngdm(code)

Description

LEARNGDM is the gradient descent with momentum weight/bias learning function.

LEARNGDM(W,P,Z,N,A,T,E,gW,gA,D,LP,LS) takes several inputs,

W - SxR weight matrix (or Sx1 bias vector).

P - RxQ input vectors (or ones(1,Q)).

Z - SxQ weighted input vectors.

N - SxQ net input vectors.

A - SxQ output vectors.

T - SxQ layer target vectors.

E - SxQ layer error vectors.

gW - SxR gradient with respect to performance.

gA - SxQ output gradient with respect to performance.

D - SxS neuron distances.

LP - Learning parameters, none, LP = [].

LS - Learning state, initially should be = [] nd returns,

dW - SxR weight (or bias) change matrix.

LS - New learning state.

Learning occurs according to LEARNGDM's learning parameters, shown here with their default values.

LP.lr - 0.01 - Learning rate

LP.mc - 0.9 - Momentum constant

LEARNGDM(CODE) returns useful information for each CODE string:

'pnames' - Returns names of learning parameters.

'pdefaults' - Returns default learning parameters.

'needg' - Returns 1 if this function uses gW or gA.

Examples

Here we define a random gradient G for a weight going to a layer with 3 neurons, from an input with 2 elements. We also define a learning rate of 0.5 and momentum constant of 0.8;

```
gW = rand(3,2);
lp.lr = 0.5;
lp.mc = 0.8;
```

Since LEARNGDM only needs these values to calculate a weight change (see Algorithm below), we will use them to do so. We will use the default initial learning state.

```
ls = [];
[dW,ls] = learngdm([],[],[],[],[],[],[],gW,[],[],lp,ls)
```

LEARNGDM returns the weight change and a new learning state.

Network Use

You can create a standard network that uses LEARNGD with NEWFF, NEWCF, or NEWELM.

To prepare the weights and the bias of layer i of a custom network to adapt with LEARNGDM:

1) Set NET.adaptFcn to 'trains'. NET.adaptParam will automatically become TRAINS's default parameters.

2) Set each NET.inputWeights{i,j}.learnFcn to 'learngdm'.

Set each NET.layerWeights{i,j}.learnFcn to 'learngdm'.

Set NET.biases{i}.learnFcn to 'learngdm'.

Each weight and bias learning parameter property will automatically be set to LEARNGDM's default parameters.

To allow the network to adapt:

1) Set NET.adaptParam properties to desired values.

2) Call ADAPT with the network.

Algorithm

LEARNGDM calculates the weight change dW for a given neuron from the neuron's input P and error E, the weight (or bias) learning rate LR, and momentum constant MC, according to gradient descent with momentum:

dW = mc*dWprev + (1-mc)*lr*gW

The previous weight change dWprev is stored and read from the learning state LS.

TRANSFER FUNCTIONS

1. Hyperbolic tangent sigmoid transfer function (TANSIG)

Syntax

A = tansig(N,FP)

dA_dN = tansig('dn',N,A,FP)

INFO = tansig(CODE)

Description

TANSIG is a neural transfer function. Transfer functions calculate a layer's output from its net input.

TANSIG(N,FP) takes N and optional function parameters,

N - SxQ matrix of net input (column) vectors.

FP - Struct of function parameters (ignored) and returns A, the SxQ matrix of N's elements squashed into [-1 1].

TANSIG('dn',N,A,FP) returns derivative of A w-respect to N.

If A or FP are not supplied or are set to [], FP reverts to the default parameters, and A is calculated from N.

TANSIG('name') returns the name of this function.

TANSIG('output',FP) returns the [min max] output range.

TANSIG('active',FP) returns the [min max] active input range.

TANSIG('fullderiv') returns 1 or 0, whether DA_DN is SxSxQ or SxQ.

TANSIG('fpnames') returns the names of the function parameters.

TANSIG('fpdefaults') returns the default function parameters.

Examples

Here the code to create a plot of the TANSIG transfer function.

```
n = -5:0.1:5;
a = tansig(n);
plot(n,a)
```

Here we assign this transfer function to layer i of a network.

```
net.layers{i}.transferFcn = 'tansig';
```

Algorithm

```
a = tansig(n) = 2/(1+exp(-2*n))-1
```

This is mathematically equivalent to TANH(N). It differs in that it runs faster than the MATLAB implementation of TANH, but the results can have very small numerical differences. This function is a good trade off for neural networks, where speed is important and the exact shape of the transfer function is not.

2. Logarithmic sigmoid transfer function (LOGSIG)

Syntax

```
A = logsig(N,FP)
dA_dN = logsig('dn',N,A,FP)
INFO = logsig(CODE)
```

Description

LOGSIG(N,FP) takes N and optional function parameters,

N - SxQ matrix of net input (column) vectors.

FP - Struct of function parameters (ignored) and returns A, the SxQ matrix of N's elements squashed into [0, 1].

LOGSIG('dn',N,A,FP) returns SxQ derivative of A w-respect to N.

If A or FP are not supplied or are set to [], FP reverts to the default parameters, and A is calculated from N.

LOGSIG('name') returns the name of this function.

LOGSIG('output',FP) returns the [min max] output range.

LOGSIG('active',FP) returns the [min max] active input range.

LOGSIG('fullderiv') returns 1 or 0, whether DA_DN is SxSxQ or SxQ.

LOGSIG('fpnames') returns the names of the function parameters.

LOGSIG('fpdefaults') returns the default function parameters.

Examples

Here is code for creating a plot of the LOGSIG transfer function.

```
n = -5:0.1:5;
a = logsig(n);
plot(n,a)
```

Here we assign this transfer function to layer i of a network.

```
net.layers{i}.transferFcn = 'logsig';
```

Algorithm

logsig(n) = 1 / (1 + exp(-n))

3. Hard limit transfer function (HARDLIM)

Syntax

```
A = hardlim(N,FP)
dA_dN = hardlim('dn',N,A,FP)
INFO = hardlim(CODE)
```

Description

HARDLIM is a neural transfer function. Transfer functions calculate a layer's output from its net input.

HARDLIM(N,FP) takes N and optional function parameters,

N - SxQ matrix of net input (column) vectors.

FP - Struct of function parameters (ignored) and returns A, the SxQ boolean matrix with 1's where N >= 0.

HARDLIM('dn',N,A,FP) returns SxQ derivative of A w-respect to N.

If A or FP are not supplied or are set to [], FP reverts to the default parameters, and A is calculated from N.

HARDLIM('name') returns the name of this function.

HARDLIM('output',FP) returns the [min max] output range.

HARDLIM('active',FP) returns the [min max] active input range.

HARDLIM('fullderiv') returns 1 or 0, whether DA_DN is SxSxQ or SxQ.

HARDLIM('fpnames') returns the names of the function parameters.

HARDLIM('fpdefaults') returns the default function parameters.

Examples

Here is how to create a plot of the HARDLIM transfer function.

```
n = -5:0.1:5;
a = hardlim(n);
plot(n,a)
```

Here we assign this transfer function to layer i of a network.

```
net.layers{i}.transferFcn = 'hardlim';
```

Algorithm

hardlim(n) = 1, if n >= 0

= 0, otherwise

4. Symmetric hard limit transfer function (HARDLIMS)

Syntax

```
A = hardlims(N,FP)
dA_dN = hardlims('dn',N,A,FP)
INFO = hardlims(CODE)
```

Description

HARDLIMS is a neural transfer function. Transfer functions calculate a layer's output from its net input.

HARDLIMS(N,FP) takes N and optional function parameters,

N - SxQ matrix of net input (column) vectors.

FP - Struct of function parameters (ignored) and returns A, the SxQ +1/-1 matrix with +1's where N >= 0.

HARDLIMS('dn',N,A,FP) returns SxQ derivative of A w-respect to N.

If A or FP are not supplied or are set to [], FP reverts to the default parameters, and A is calculated from N.

HARDLIMS('name') returns the name of this function.

HARDLIMS('output',FP) returns the [min max] output range.

HARDLIMS('active',FP) returns the [min max] active input range.

HARDLIMS('fullderiv') returns 1 or 0, whether DA_DN is SxSxQ or SxQ.

HARDLIMS('fpnames') returns the names of the function parameters.

HARDLIMS('fpdefaults') returns the default function parameters.

Examples

Here is how to create a plot of the HARDLIMS transfer function.

```
n = -5:0.1:5;
a = hardlims(n);
plot(n,a)
```

Here we assign this transfer function to layer i of a network.

```
net.layers{i}.transferFcn = 'hardlims';
```

Algorithm

hardlims(n) = 1, if n >= 0

= -1, otherwise

5. Linear transfer function (PURELIN)

Syntax

A = purelin(N,FP)

dA_dN = purelin('dn',N,A,FP)

INFO = purelin(CODE)

Description

PURELIN is a neural transfer function. Transfer functions calculate a layer's output from its net input.

PURELIN(N,FP) takes N and optional function parameters,

N - SxQ matrix of net input (column) vectors.

FP - Struct of function parameters (ignored) and returns A, an SxQ matrix equal to N.

PURELIN('dn',N,A,FP) returns SxQ derivative of A w-respect to N.

If A or FP are not supplied or are set to [], FP reverts to the default parameters, and A is calculated from N.

PURELIN('name') returns the name of this function.

PURELIN('output',FP) returns the [min max] output range.

PURELIN('active',FP) returns the [min max] active input range.

PURELIN('fullderiv') returns 1 or 0, whether DA_DN is SxSxQ or SxQ.

PURELIN('fpnames') returns the names of the function parameters.

PURELIN('fpdefaults') returns the default function parameters.

Examples

Here is the code to create a plot of the PURELIN transfer function.

```
n = -5:0.1:5;
a = purelin(n);
plot(n,a)
```

Here we assign this transfer function to layer i of a network.

```
net.layers{i}.transferFcn = 'purelin';
```

Algorithm

a = purelin(n) = n

6. Saturating linear transfer function (SATLIN)

Syntax

A = satlin(N,FP)

dA_dN = satlin('dn',N,A,FP)

INFO = satlin(CODE)

Description

SATLIN is a neural transfer function. Transfer functions calculate a layer's output from its net input.

SATLIN(N,FP) takes N and optional function parameters,

N - SxQ matrix of net input (column) vectors.

FP - Struct of function parameters (ignored) and returns A, the SxQ matrix of N's elements clipped to [0, 1].

SATLIN('dn',N,A,FP) returns SxQ derivative of A w-respect to N.

If A or FP are not supplied or are set to [], FP reverts to the default parameters, and A is calculated from N.

SATLIN('name') returns the name of this function.

SATLIN('output',FP) returns the [min max] output range.

SATLIN('active',FP) returns the [min max] active input range.

SATLIN('fullderiv') returns 1 or 0, whether DA_DN is SxSxQ or SxQ.

SATLIN('fpnames') returns the names of the function parameters.

SATLIN('fpdefaults') returns the default function parameters.

Examples

Here is the code to create a plot of the SATLIN transfer function.

```
n = -5:0.1:5;
a = satlin(n);
plot(n,a)
```

Here we assign this transfer function to layer i of a network.

```
net.layers{i}.transferFcn = 'satlin';
```

Algorithm

a = satlin(n) = 0, if n <= 0

= n, if 0 <= n <= 1

= 1, if 1 <= n

7. Symmetric saturating linear transfer function (SATLINS)

Syntax

```
A = satlins(N,FP)
dA_dN = satlins('dn',N,A,FP)
INFO = satlins(CODE)
```

Description

SATLINS is a transfer function. Transfer functions calculate a layer's output from its net input.

SATLINS(N,FP) takes N and optional function parameters,

N - SxQ Matrix of net input (column) vectors.

FP - Row cell array of function parameters (ignored) and returns values of N truncated into the interval [-1, 1].

SATLINS('dn',N,A,FP) returns SxQ derivative of A w-respect to N.

If A or FP are not supplied or are set to [], FP reverts to the default parameters, and A is calculated from N.

SATLINS('name') returns the name of this function.

SATLINS('output',FP) returns the [min max] output range.

SATLINS('active',FP) returns the [min max] active input range.

SATLINS('fullderiv') returns 1 or 0, whether DA_DN is SxSxQ or SxQ.

SATLINS('fpnames') returns the names of the function parameters.

SATLINS('fpdefaults') returns the default function parameters.

Examples

Here is the code to create a plot of the SATLINS transfer function.

```
n = -5:0.1:5;
a = satlins(n);
plot(n,a)
```

Here we assign this transfer function to layer i of a network.

```
net.layers{i}.transferFcn = 'satlins';
```

Algorithm

a = satlins(n) = -1, if n <= -1

= n, if -1 <= n <= 1

= 1, if 1 <= n

8. Radial basis transfer function (RADBAS)

Syntax

A = radbas(N,FP)

dA_dN = radbas('dn',N,A,FP)

INFO = radbas(CODE)

Description

RADBAS is a neural transfer function. Transfer functions calculate a layer's output from its net input.

RADBAS(N,FP) takes N and optional function parameters,

N - SxQ matrix of net input (column) vectors.

FP - Struct of function parameters (ignored) and returns A, an SxQ matrix of the radial basis function applied to each element of N.

RADBAS('dn',N,A,FP) returns SxQ derivative of A w-respect to N.

If A or FP are not supplied or are set to [], FP reverts to the default parameters, and A is calculated from N.

RADBAS('name') returns the name of this function.

RADBAS('output',FP) returns the [min max] output range.

RADBAS('active',FP) returns the [min max] active input range.

RADBAS('fullderiv') returns 1 or 0, whether DA_DN is SxSxQ or SxQ.

RADBAS('fpnames') returns the names of the function parameters.

RADBAS('fpdefaults') returns the default function parameters.

Examples

Here we create a plot of the RADBAS transfer function.

```
n = -5:0.1:5;
a = radbas(n);
plot(n,a)
```

Here we assign this transfer function to layer i of a network.

```
net.layers{i}.transferFcn = 'radbas';
```

Algorithm

a = radbas(n) = exp(-n^2)

APPENDIX B

RUBBER PROPERTIES ANALYSIS

1. Determination of color

1.1 Explanatory Notes

The color of the raw rubber is compared and matched as closely as possible with that of standard color slides. The raw rubber is tested in the form of a moulded disc of standard thickness. Color matching is carried out under diffuse daylight illumination against a matt white background, preferable by use of a comparator which holds the test pellets and comparison slide in convenient juxtaposition. The standard colored glasses used are calibrated in color index units according to the intensity of their color. The numerically higher index values have deeper color. The basis of calibration is the 'Lovibond color scale' in amber units.

1.2 Apparatus

(a) Hydraulic press: The press should be capable of exerting a pressure of not less than 500 p.s.i. on the cavity areas of the mould during the entire period of moulding. The platen temperatures shall be capable of being maintained at $150^{O}C \pm 3^{O}C$

(b) Mould: A stainless steel or aluminium mould 1.6 ± 0.05 mm thick having holes approximately 14 mm diameter. Two mould covers of similar material and at least 1.6 mm in thickness are required.

1.3 Procedure

1.3.1 Test pellet preparation

Take a test portion of 15 ± 5 g from the homogenised sample and pass three times between the roll mills at room temperature with the nip adjusted so that the final sheet thickness is 1.6 mm to 1.8 mm. After the initial pass, the rubber is rolled and passed endwise through the rolls. Fold the rubber from the second pass and pass it lengthwise through the rolls for the last

time. This final sheet, which should be uniform in texture and free from holes, shall immediately be doubled and the two halves pressed together lightly by hand. Cut two test pellets from the doubled sheet with the punch and measure their thickness until two test pellets are obtained with thickness between 3.2 mm and 3.6 mm. The two test pellets shall then be laminated together by lightly pressing with the fingers. Pre-heat the test pellets in the mould betwenn two sheets of polyester or cellulose film using mould covers for 1 min. then apply not less than 500 p.s.i. pressure on the cavity areas of the mould, for 4±0.5 min at $150^{O}C \pm 3^{O}C$. The moulded test pellet shall be 1.6±0.2 mm thick and free of color contaminants.

1.3.2 Color determination

Determine the color of the test pellet by matching as closely as possible with the appropriate color standard. Color matching shall be carried out under diffuse daylight against a matt white background, preferably by using a comparator mounting which holds the test pellets and comparison color at a convenient distance apart. The cover is put on and the color matched for each sample in turn.

2. Determination of Mooney viscosity

2.1 Explanatory Notes

The test consists of determining the torque necessary to rotate a disc in a cylindrical chamber filled with rubber under specified conditions. A number proportional to this torque is taken as an index of the viscosity of the rubber. The Mooney viscometer (a shearing-disk viscometer) is used.

2.2 Calibration and Maintenance

The following system of checking and calibrating Mooney viscometer should be adopted:

1. Dead load calibration to check that zero reading for zero force and a reading of 100 for a pair of force of 100 N should be regularly carried out following RRIM method.

2. Dead load calibration by incremental loading to check the whole range of the meter's reading should be carried out at least once in about six months following RRIM method.

2.3 Procedure

2.3.1 Determination of Mooney viscosity

The temperature of test should be $100^{O}C \pm 1^{O}C$. Check the die temperature for stability. Place the rotor in the die cavity to heat up to test temperature; 2 min are normally sufficient to heat the rotor from ambient temperature. Remove the hot rotor from the die cavity. Before this, divide about 25 g of the homogenised rubber into two equal portions. Place the preheated rotor stem through the centre of one portion. Put this whole combination in the lower die cavity and place the second portion on top of the rotor. Close the die immediately. Measure the time from the instant the die is closed, as indicated by the appropriate lamp on the control panel. Start the motor 1 min after closing the die cavity. Record the initial dial gauge reading immediately. Take as the viscosity of the rubber the dial reading at the end of the fourth minute the instant when the motor is started.

2.4 Expression of results

A typical test on NR with the normal rotor speed with viscosity number 60 should be reported as follows:

60 *ML* (1+4) $100^{O}C$

where 60 is the Mooney viscosity;

M stands for Mooney viscosity;

L indicates the use of a large rotor;

1 is the pre-heating time in min;

4 is the reading time in min;

$100^{O}C$ is the test temperature.

3. Determination of Rapid plasticity and Plasticity Retention Index

3.1 Explanatory Notes

1. Rapid plasticity

A disc-shaped test pellet shall be rapidly compressed between small parallel platens to a fixed thickness of 1 mm and held thus for 15 s to reach approximate temperature equilibrium with

the platens. It shall then be subjected to a constant compressive force of 10±0.1 kgf for 15 s; its thickness at the end of this period in 0.01 mm units shall be taken as the measure of plasticity.

2. Plasticity Retention Index

The plasticity retention index (PRI) is a measure of the resistance of raw NR to oxidation. A high value of the index denotes high resistance to oxidation

The oxidation behavior of raw NR may have an important bearing on processing behavior and end product performance and the PRI test accordingly affords a convenient means of characterizing rubber in certain of these respects. The test involves measurements of the plasticity of NR testpieces before and after heating in air oven for 30±0.25 min at $140^{O}C \pm 0.5^{O}C$ using the parallel plate plastimeter with a platen 10 mm in diameter. The PRI is the percentage ratio of the plasticities after and before heating. The time and temperature of heating are such as to give adequate discrimination between rubbers and a reasonable speed of testing at a temperature similar to that attained in factory internal mixers. The value of the index is, howerver, virtually independent of the initial plasticity of the rubber. It is not independent of the test method. A different value will be obtained if, for example, the time or temperature of heating is altered or if a different type of plastimeter is used.

3.2 Equipment and Materials

(a) Parallel plate plastimeter: this is a standard equipment with a 10 mm platen and a process timer giving 15 s of pre-heating time.

(b) Punch, for the preparation of test pellets of approximately constant volume quickly and without difficulty. The punch shall compress a portion of the material to approximately 3 mm in thickness and shall cut out a disc approximately 13 mm in diameter.

(c) Thickness gauge: the gauge shall have a scale graduated in unit divisions of 0.01 mm.

(d) Lightweight aluminium tray, suitably marked for pellet identification.

(e) Oven, operating at $140^{O}C \pm 0.5^{O}C$. the oven shall be such that:

(i) The temperature fluctuation over a 30 min period is $\pm 0.5^{O}C$.

(ii) The temperature variation within the ageing region is $\pm 0.5^{O}C$.

(iii) It is an oven suitably designed for the testing of PRI.

(f) Approved cigarette paper, of about 0.03 mm thickness as authorized by RRIM.

3.3 Procedure

3.3.1 Preparation of test pellet

Pass a test portion of 20±5 g twice through the rolls of a cool mill with nip setting adjusted such that the final sheet thickness is 1.6 mm to 1.8 mm. The sheeted rubber piece is doubled after the first and final passes. If the sheet so obtained after two passes does not meet the thickness requirements, reject it and take a fresh test portion of the homogenised piece and repeat the operation by readjusting the nip setting. The final sheet which should be free from holes is immediately doubled and the two halves pressed lightly together by hand. Cut six test pellets from the doubled sheet with the punch. The test pellets should be a disc of rubber of thickness between 3.2 mm to 3.6 mm and approximately 13 mm in diameter. The test pellets are divided into two sets of three, one set each for plasticity determination before and after oven ageing.

The gauge steam pressure shall indicate 0.5-1 psi with free-flowing steam at the discharge end. Compress a disc-shaped test pellet, sandwiched between two pieces of cigarette paper each of approximate dimensions 40×35 mm, between the two parallel platens to a fixed thickness of 1.00±0.01 mm and hold it in the compressed state for 15±1s to reach approximate equilibrium. Then apply a constant compressive force of 10±0.1 kgf for 15±0.2s. The thickness at the end of this period is taken as the measure of rapid plasticity.

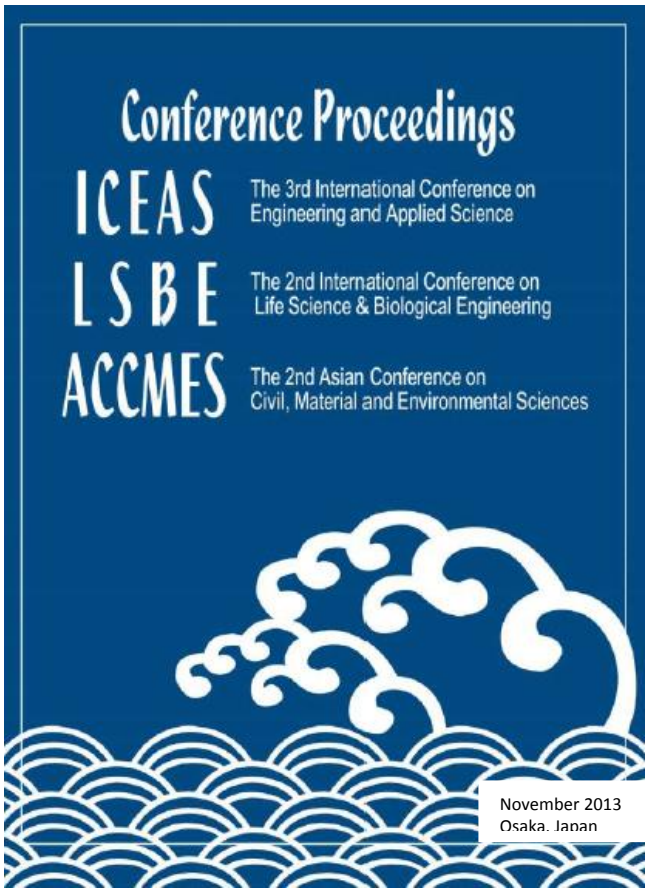
3.3.2 Determination of PRI

Ensure that the oven is not overloaded, *e.g.* with an excessive number of dishes or a thick plate which has a large thermal capacity; this could cause a prolonged temperature drop and might upset temperature uniformity.

Care should be taken that the test pellets are arranged within the temperature calibrated region of the oven. Before heating begins, check the oven temperature to ensure that it has been stable for at least 5 min. Quickly insert the tray with the dishes and test pellets, close the oven door, and start timing. It is necessary to ensure that the correct temperature is quickly regained and retained. After 30±0.25 min, remove the tray with the dishes and test pellets from the oven and allow to cool to room temperature.

APPENDIX C

CONFERENCE PROCEEDING



Optimal design based ANN with input variable selection for pale crepe rubber processing

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Abstract

This work focuses on determining the optimal operating conditions based on Artificial Neural Network model incorporated with input variable selection for pale crepe rubber processing in order to achieve its required properties. A fully feed-forward network model, with four input variables such as %acetic acid amount, fractional coagulation time, %DRC dilution and its corresponding %TSC, has been firstly developed in the optimal manner for a prediction of the rubber properties; rubber color, Mooney viscosity (MV), initial plasticity (P_0) and Plasticity Retention Index (PRI). Since the performance of the network model strongly depends on the training data sets, a variable selection approach such a partial modeling has been further applied for the model improvement. In this case, %TSC has been chosen as the insignificant variable by considering its sensitivity, and further eliminated. The final network model with three inputs has been used to determine the optimal operating conditions via response surface analysis.

Keywords: Neural network, Variable selection, Optimization, Modeling, Response surface analysis

1. Introduction

Artificial Neural Network (ANN) is *an information processing system which composes of a number of artificial processing units (or neurons) connected each other by simple weights.* It *is* the most successful technology which has been widely used in various applications such as chemical and biochemical processes. For example, *Nasciento and Guardani [1] have designed* feed-forward network *model for* a twin-screw extruder reactor with 7 inputs and 3 outputs. The training data set (44 data sets) from the pilot plant have been randomly split into two groups for the learning set (80%) and testing set (20%). The best neural model has one hidden layer which is constituted by 4 neurons, and the activation function used is the sigmoidal function. Another example is the application for predicting ink removal efficiency presented by Labidi, et.al. [2]. The network model, including of 3 inputs and 2 outputs, have been trained by 150 data sets with 135 learning set (90%) and 15 testing set (10%). The best network has two hidden layers each of which is constituted by 100

neurons, and the activation function for both layers that gives the best result is the sigmoidal function [2].

However, the network is a data-driven statistical model; an input variable selection is then the crucial issue for development of a suitable model in order to give a reasonable output prediction. The difficulty of selecting input variables arises due to a large number of available input variables; data redundancy; and less influential variables [3]. *Despagne and Massart have p*roposed two methods based on the variance estimation such as variance propagation and partial modeling. The methods have been compared with the previous comparative selection method such a magnitude approach (modified Hinton diagram) [4]. They have suggested that the partial modeling approach is particularly easy to implement with reasonable results. As seen in literatures, there are many research works focused on the input selection area [5].

This work aims to determine the optimal operating conditions based on the ANN model with input variable selection for pale crepe rubber processing. A fully feed-forward network model, with four input variables such as acetic acid amount, fractional coagulation time, %DRC dilution and the corresponding %TSC, has been firstly developed for a prediction of pale crepe rubber properties i.e. rubber color, Mooney viscosity (MV), initial plasticity (P_0) and Plasticity Retention Index (PRI). Since the performance of ANN model strongly depends on the training data sets, a variable selection approach such the partial modeling has been further applied for the model improvement. The developed model has been used to determine the optimal operating conditions via response surface analysis [6]. The prediction results through MATLAB program have been discussed.

2. Theory

2.1 Pale crepe rubber processing

Rubber is an important industrial crop of Thailand. Three biggest rubber producers over the world are Thailand, Indonesia and Malaysia respectively Top three Thailand's export markets are China, Japan and Malaysia. Natural rubber that has been mostly exported Block Rubber, Ribbed Smoked Sheet (RSS) and Concentrated latex. The most important quality according to Standard of Thai Rubber (STR) is its color, more white and clear, higher value added. Pale crepe is a high quality rubber sheet since it has white/pale color (Lovibond color < 3). It is produced from a particular type of rubber latex, RRIM 600, and used as raw material for manufacturing rubber soles, plaster, sport equipment, and medical devices.

Here, pale crepe rubber production is achieved by the following steps: (1) preservation by adding Na_2SO_3, (2) % dry rubber content (DRC) dilution (varying 25 – 29%DRC and 27 – 32% total solid content, TSC), (3) enzymatic reaction exhibition by adding $Na_2S_2O_5$, (4) fractional coagulation by varying acetic acid of 0 – 0.45% v/w dry rubber and coagulation time of 1– 3 hr, (5) latex coagulation, (6) drying at 35-40^{0}C for 3 days. In this work, the operating conditions in a fractional coagulation step has been designed in the optimal manner in order to achieve the required properties of the pale crepe rubber sheet corresponding to STR standard consisting of the Lovibond color < 3, Mooney viscosity (MV) > 60 ML (1+4) 100°C, initial plasticity (P_0) > 35 and Plasticity Retention Index (PRI) > 60 [8].

2.2 Artificial Neural Network (ANN)

ANN is purely data-driven model, it has been proven to be a universal approximator to identifying complex input-output relationships. The network model includes an externally applied threshold that has the effect of lowering the net input of the activation function. On the other hand, the net input of the activation function may be increased by employing a bias term rather than a threshold. In mathematical terms, a neuron, *k* can be described by writing the following pair of equations:

$$v_k = \sum_{j=1}^{p} (w_{kj} x_j) + b_k \quad (1)$$

$$y_k = f(v_k) \quad (2)$$

where $x_1, x_2, \ldots, x_p$ are the p^{th} inputs;
$w_{k1}, w_{k2}, \ldots, w_{kp}$ are the synaptic weights of neuron *k*;
v_k is the linear combiner output;
b_k is the bias term;
$f(.)$ is the activation function;
y_k is the output signal of the neuron.

2.3 Variable selection: Partial modeling

This method used for estimating experimentally the sensitivity of each input variable [4]. For example, ANN is used to find the relationship of a function of two input variables, $y = f(x_1, x_2)$ because the exact form of the relationship is unknown. To estimate the relative contribution of each input variable to the variance of the predicted response, the network model with all available input variables has to be preliminary designed. Afterward, setting all input variables but the first to zero ($x_2 = 0$) giving the predicted response as $\hat{y}(x_1)$. Then the procedure is repeated by setting x_1 to zero, to obtain the vector, $\hat{y}(x_2)$. The respective variances, σ^2 of $\hat{y}(x_1)$ and $\hat{y}(x_2)$ are further used to estimate the sensitivity, S_i of input variable x_1 and x_2 as shown in Eq.(3).

$$S_i = \sigma^2_{\hat{y}(x_i)} \quad (3)$$

The variance of each input variable will be further plotted in order to identify the insignificant variable.

3. Simulation results

3.1 Structure design of ANN (fully) model

In this section, the designed ANN model has feed-forward scheme with four (fully) input variables such as acetic acid amount, fractional coagulation time, %DRC dilution and the corresponding %TSC. Four rubber properties (rubber color, MV, P_0 and PRI) have been predicted via using linear transfer functions (purelin) in output layer. The model has been designed by varying a number of hidden layer (1 to 2) and its number of nodes (1 to 10) with hyperbolic tangent sigmoid transfer functions (tansig). The ANN has been trained using the Levenberg-Marquardt algorithm with 30 experimental data sets (80% training and 20% testing). The network has been trained using the Levenberg-Marquardt algorithm. It has been found in the simulation results that the minimum overall mean square error (MSE) calculated using Eq.(4) is in the range of 0.00 – 0.02. The optimal network structure could have 2 – 10 nodes in each hidden layers. However, it does not guarantee that the model could give the minimum prediction of all four rubber properties.

$$MSE = \sum_{i=1}^{n}\left[\frac{(c_i - \acute{c}_i)^2}{n} + \frac{(m_i - \acute{m}_i)^2}{n} + \frac{(p_i - \acute{p}_i)^2}{n} + \frac{(s_i - \acute{s}_i)^2}{n}\right] \quad (4)$$

$$IAE_k = \sum_{i=1}^{n}|y_i - \acute{y}_i| \quad (5)$$

where, c_i is % acetic acid amount, m_i is MV, p_i is P_0, s_i is PRI, and y_i is experimental output, $\acute{y}_i$ is predicted output and n is a total number of the experimental data sets.

In order to minimizing the prediction error of each property, the optimal network structure has been chosen by considering integral absolute error (IAE) of the predicted output individually, Eq.(5). It has been found from the IAE contour plots that the optimal network structure has 1 and 2 nodes in layer 1 and 2 respectively to guarantee the optimal prediction performance. Fig. 1 shows the comparison of the predicted and experimental testing data for all outputs, and IAE values are shown in Table 1.

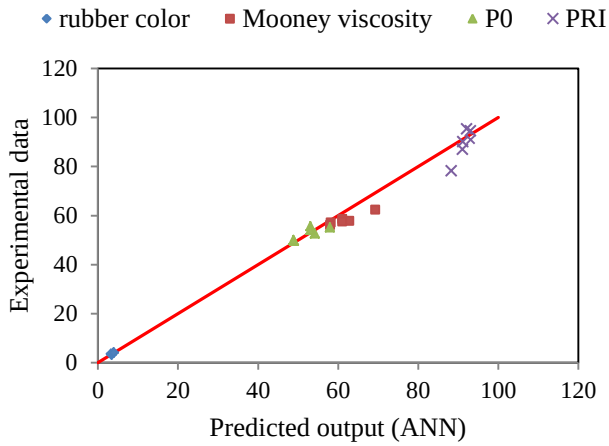


Figure 1: Comparison of predicted and experimental testing data for (four inputs)

Table 1: IAE values of ANN based full and reduced input variables

Output	IAE values (4 inputs)	IAE values (3 inputs)
Rubber color	0.888	1.251
Mooney viscosity	22.124	10.811
P0	9.527	5.432
PRI	22.029	16.131

3.2 Insignificant variable identification

Since the performance of ANN model strongly depends on the training data sets, a variable selection approach such a partial modeling has been further applied for the model improvement. In this case, the sensitivity of the predicted responses, $\sigma^2_{\hat{y}(x_1)}$ has been determined as Eq. (3) by firstly setting all ANN inputs but the first (x_1 = acetic acid amount) to zero ($x_2, x_3, x_4 = 0$). The procedure is repeated by setting x_1, x_3, x_4 to zero, to obtain $\sigma^2_{\hat{y}(x_2)}$ and so on. The sensitivity bar plot is shown in Fig. 2. It can be seen that the acetic acid amount, the coagulation time and %DRC have large effect on MV. Moreover, %DRC as well

as %TSC have small effects on Lovibond color and PRI compared to the others. This might be because non-rubber consisting of color pigments (non-rubber = %TSC - %DRC) is a minor component (≈ 3% – 5%) of the rubber latex. Therefore, %TSC has been chosen as the insignificant variable, and further eliminated.

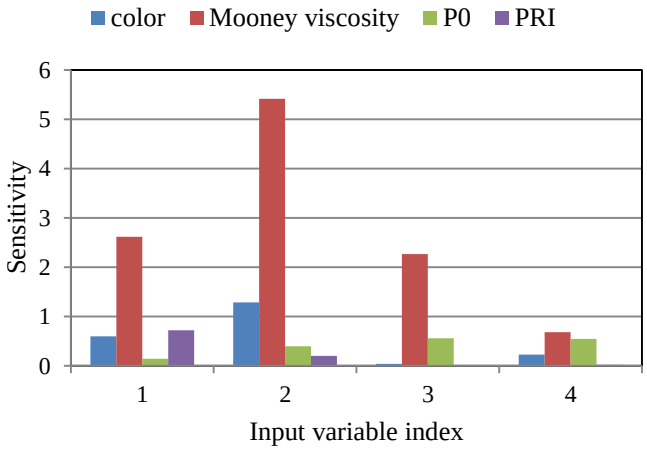


Figure 2: Sensitivities of the predicted output corresponding to each inputs, $\hat{y}(x_i)$: 1 = acetic acid amount, 2 = coagulation time, 3 = %DRC and 4 = %TSC

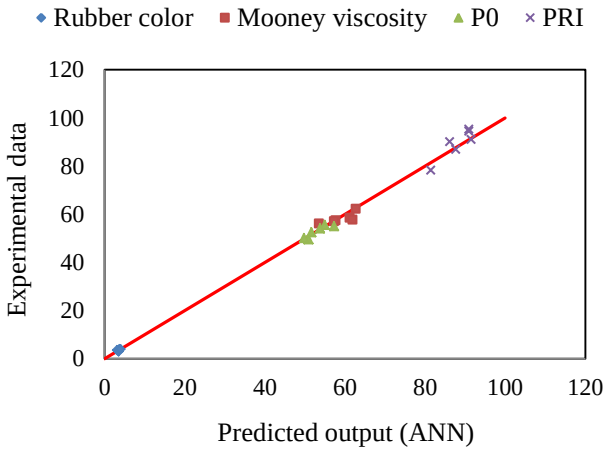
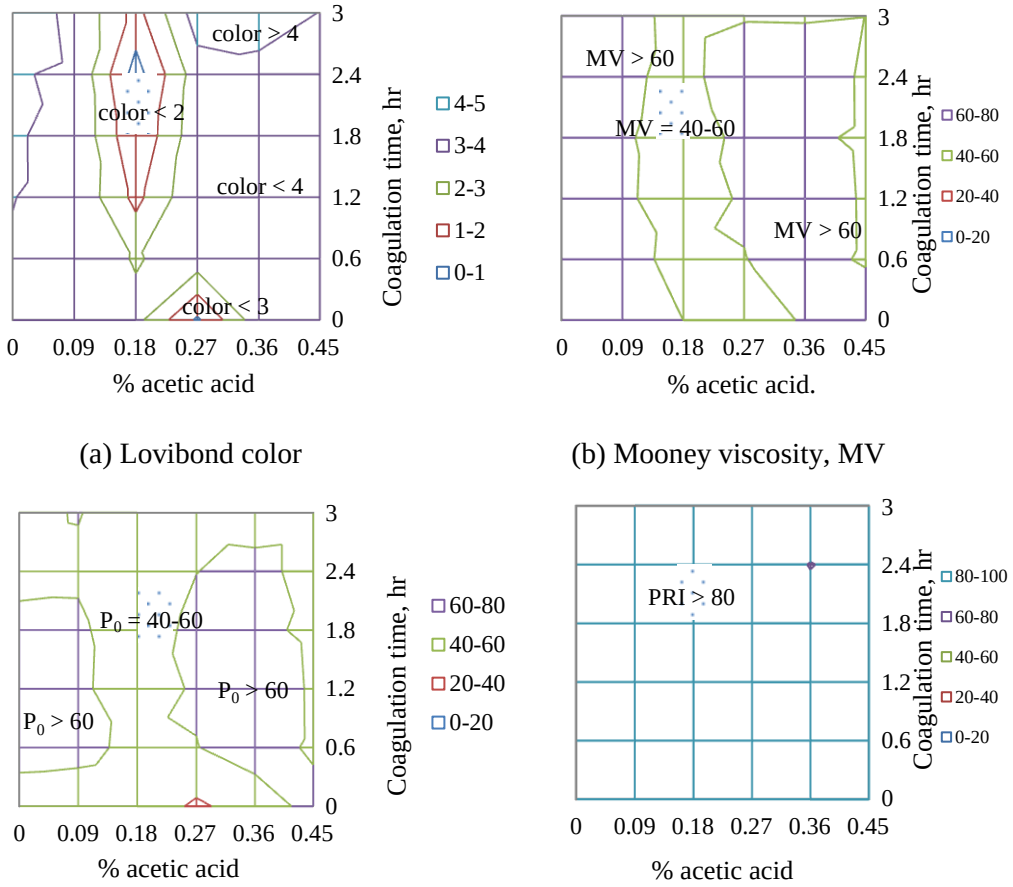


Figure 3: Comparison of predicted and experimental testing data for (three inputs)

New network model has been trained with three inputs, the acetic acid amount, the coagulation time and %DRC. The network structure has been chosen in the optimal manner by varying a number of the hidden layer (1 to 2) and its number of nodes (1 to 10) with hyperbolic tangent sigmoid transfer functions (tansig). The linear transfer functions (purelin) are used in the output layer. It has been found from the IAE contour plots that the optimal network structure has 3 and 7 nodes in layer 1 and 2 respectively.

3.3 Optimum condition determination

By applying the input variable selection, the output prediction of the ANN model is improved as seen by IAE values in Table 1. Even the IAE value of the predicted color is slightly higher than one obtained by ANN with full input variables. The optimum conditions have been further evaluated by considering the surface plots of the responses as shown in Fig. 4.



(a) Lovibond color

(b) Mooney viscosity, MV

(c) Initial plasticity, P_0

(d) Plasticity retention index, PRI

Figure 4: Predicted response surfaces based on ANN with three inputs by considering % acetic acid and coagulation time (%DRC = 27.17)

It can be seen in Fig. 4(a), 4(c) and 4(d) that the Lovibond color, P_0 and PRI values are higher than STR standard if the process operates at %DRC = 27.17, acetic acid amount of 0.17 – 0.22% v/w dry rubber and coagulation time in range of 1.8 – 2.4 hr, but MV is slightly lower than the standard, 40 – 60 ML(1+4) 100°C, Fig. 4(b). By considering the predicted responses, it has been found that there are not the conditions providing the color and MV over the standard at the same time. However, MV of the rubber sheet could be increased over time during storage. Therefore the optimal conditions have been chosen as shown in Table 2 by considering the rubber quality of the Lovibond color < 3, MV > 50 ML(1+4) 100°C, P_0 > 35 and PRI > 60.

Table 2: Optimal operating conditions

Acetic acid amount, % v/w dry rubber	Coagulation time, hr	%DRC
0.18	1.8	27 – 28
0.2	2	24 – 26
0.3	0.5	25 – 26

4. Conclusion

Rubber is an important industrial crop of Thailand. The most important quality according to Standard of Thai Rubber (STR) is its color, more white and clear, higher value added. Pale crepe is a high quality rubber sheet since it has white/pale color (Lovibond color < 3). In this work, a determination of the optimal operating conditions has been focused in order to achieve its required properties. The designed ANN model has feed-forward scheme with four (fully) input variables such as acetic acid amount, fractional coagulation time, %DRC dilution and the corresponding %TSC. Four rubber properties (rubber color, MV, P_0 and PRI) have been predicted. The model has been designed in the optimal manner obtaining 2 hidden layers with 1, 2 nodes respectively. Since the performance of ANN model strongly depends on the training data sets, a variable selection approach such a partial modeling has been further applied for the model improvement. The variance/sensitivity of each input variable has been considered to identifying an insignificant variable, which in this case %TSC has been chosen, and further eliminated. The final neural model with three inputs has 2 hidden layers with 3, 7 nodes respectively, and it has been used to determine the optimal operating conditions via response surface analysis.

Acknowledgments and Legal Responsibility

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