



**Artificial Neural Network predictive model for Hydrogen production using
Biomass gasification in a pilot plant**

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Dissertation submitted in partial fulfilment of the requirement for the
Bachelor of Engineering (Hons)
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CERTIFICATION OF APPROVAL

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(Chemical Engineering)

Approved by,

Dr. Haslinda Bt Zabiri

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

September 2014

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

Mohamed Mustafa Suliman

ABSTRACT

The growth in population nowadays has led to an increase in the consumption of the fossil fuels like oil and gas, which leads to depletion and shortage in the supply of the oil and gas. Also it will lead to an increase in the pollution and greenhouse effects in the environment. The need for a reliable, affordable and clean energy supply rises as it is very important for society, economy and the environment. Hydrogen production from biomass gasification is considered a very promising clean energy option for reduction of greenhouse gas emissions and energy dependency.

The complexity of the biomass gasification process has led the researchers to develop models to simplify the process and save time and energy. A lot of models have been developed like the equilibrium model, kinetic model and the Artificial Neural Network (ANN) model. ANN models are simple to use, easy to generate and require a short period of time to get acceptable results depending on the pool of previous experimental data comparing to the other models that need power, time, a lot of assumptions and calculations to obtain good results.

The main objectives of this study are: 1- to design and develop an Artificial Neural Network (ANN) model for the hydrogen production from biomass gasification process. 2- To evaluate the results of the model and validate them with the previous experimental data. 3- To compare the results of the simulation with different ANN models with the SIMCA-P software model.

To achieve the goal of this study, four (4) ANNs have been developed after performing a preliminary analysis which was done by SIMCA-P11 and SIMCA-P13 software to determine the factors that affect the hydrogen production and also as it has a linear modelling for the process which is compared to the results of the ANNs. ANNs performed better in the prediction process with a mean squared error (MSE) of 5.4%. This validate that the ANN modelling is better for the purposes of prediction comparing to the other models available.

ACKNOWLEDGEMENT

All the thanks due to Allah, The Most Gracious and The Most Merciful for His continuous, endless and great blessings and guidance throughout my life and my studies. Everything we do, does not only affect us or done only by us, some of the people around us have affected our decision and by that what we do will affect them as well.

Looking at the semesters, I would like to start by saying and giving my utmost appreciation and deep gratitude towards my supervisor Dr. Haslinda Bt Zabiri for her consistent guidance, immeasurable support, and encouragement throughout the course of this project.

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1. CHAPTER 1: INTRODUCTION

1.1 Background of study

The high and increasing demand for the fuels for transportation and energy production and the rise in the environmental concerns about the pollution and greenhouse effects, and with the diminishing crude oil reserves, have led the researchers to focus on renewable energy.

Korpela, S. A. (2006) mentioned that the oil production for the companies outside the OPEC is decreasing due to the heavy exploitation and utilization of fossil fuels. The worldwide growth in industry, economy and population has led to a great increase in the global energy demand and consumption, and this rate will increase rapidly in the future.

Hydrogen production from biomass has become an attractive and important option in energy generation. Hydrogen is considered the best substitute for fossil fuels with the high heating value (HHV) for different usages as in transportation, home usage, and heating. In Malaysia, agricultural waste is foreseen as the best biomass feedstock for hydrogen production due to the rapid growth in the agriculture sector over the years. The utilization of agricultural waste as hydrogen feedstock will anticipate both future shortage in petroleum supply and landfill disposal problem of the agricultural residues.

1.2 Problem statement

1.2.1 Problem identification

Biomass gasification process is a very complex process that depends on complex chemical reactions, partial oxidation of pyrolysis products and char, conversion of tar and hydrocarbons and the water gas shift reaction in order to produce the syngas. This complicated process needs a model that can evaluate the process and to be used in prediction of the results. Modelling is a very powerful and useful tool for designing and optimizing the biomass gasification process. Some of the models used in the biomass gasification process are the kinetic, equilibrium and artificial neural network models. The first two models need power and time and a lot of assumptions and calculations to obtain good results, but the ANN models which are simple to use, easy to generate and

require a short period of time to get acceptable results depending on the pool of previous experimental data.

From the literature review done, various models of ANN have been developed for the purposes of modelling the process of biomass gasification and prediction of the product gas composition or the factors that affect the composition of the product gas. Table 1.1 shows the summary of the findings of the previous researches on ANN modelling for biomass gasification. For those models, the feedstock used varied from wood, a mixture of wood, Paper, Kitchen garbage, PE plastic, and Textile and Poplar sawdust, pine sawdust, comminuted sugar bagasse and cotton stem. Puig-Arnavat, M. et al (2013) used data for two different reactors, one Circulating Fluidized Bed gasifier (CFB) and one Bubbling Fluidized Bed gasifier (BFB), Xiao et al. (2009) used a lab-scale fluidized-bed gasifier is equipped with a stainless steel tube (31 mm inside diameter and 560 mm height), which is surrounded by an electric heater (about 2 kW), and Guo et al. (2001) a reactor which was made of stainless steel tube, 150 mm in inner diameter and 1360 mm in height. It was heated by a cylindrical electrical heating element, capable of delivering up to 12 kW of power.

For this study the ANN model is developed to investigate the biomass gasification as conducted by Moghadam et al. (2013) and Moghadam et al. (2014) as they used a palm kernel shell (PKS) and polyethylene waste blend as a feedstock for a catalytic steam gasification process and the pilot unit they used consists of two cylindrical reactors made of Inconel 625. The fluidized bed gasifier has the height of 2500 mm and internal diameter of 150 mm and 200 mm in gasification and free board zone, respectively. The fixed bed gasifier height is 2500 mm and internal diameter of 150 mm. The gasifiers equipped with four individual electrical heaters and eight thermocouples for controlling the temperature profile across each reactor.

Table 1.1: Findings of previous researches on ANN modelling for biomass gasification

Author	Year	Title	Objective	Findings				
				Biomass used	Modelling	Data	Results	Conclusion
Maria Puig-Arnava, J. Alfredo Hernández, Joan Carles Bruno, Alberto Coronas	2013	Artificial neural network models for biomass gasification in fluidized bed gasifiers	To obtain two models that can predict the producer gas composition and the gas yield from biomass composition and few operating parameters, like thermodynamic equilibrium models do, but avoiding the high complexity of kinetic models.	Wood	Two ANN models are presented: - one for Circulating Fluidized Bed gasifier (CFB) - one for Bubbling Fluidized Bed gasifier (BFB) Both models determine the product gas composition (CO,CO ₂ ,H ₂ ,CH ₄) and gas yield	Published experimental data from other authors has been used to train the ANNs.	- For CFB: Experimental and simulated values for CO, CO ₂ , H ₂ , CH ₄ , and gas yield were compared satisfactorily through a linear regression model for each. All the R ² values are higher than 0.99 except for H ₂ composition which is 0.98. The ANN passed with a 99.8% of confidence level. - For BFB: All the R ² values are higher than 0.99 except for CO ₂ composition which is 0.98. The ANN passed with a 99.8% of confidence level.	The results showed how the percentage composition of the product gas and the gas yield for a CFB or BFB gasifiers can be successfully predicted. Additional experimental data is needed to enlarge the database to improve the developed models.
Gang Xiao, Ming-jiang Ni,	2009	Gasification characteristics of MSW and an ANN	To predict the gasification characteristics, the LHV of gas,	Mix of 5 different organic materials:	An ANN was developed to predict the gasification characteristics. The	Data was gathered from the experiments they conducted	The relative errors in the training, validating data are within ±15% and ±20%, respectively, and predicting relative errors of an industrial sample	They concluded that the result of the ANN in predicting the

Yong Chi, Bao-sheng Jin, Rui Xiao,		prediction model	gasification products and gas yield	Wood, Paper, Kitchen garbage, PE plastic, Textile	inputs of the ANN in the input layer were: the percentage of the five different kinds of the organic component, equivalence ration (ER) and temperature	for the different types of the organic materials and MSW.	below $\pm 25\%$.	gasification characteristics of MSW is feasible and produced acceptable results
Bing Guo, Dingkai Li, Congming Cheng, Zi-an Lu, Youting Shen	2001	Simulation of biomass gasification with a hybrid neural network model	To predict the yield and gas composition of the different gasification processes	Poplar sawdust, pine sawdust, comminut ed sugar bagasse and cotton stem	They developed four identical, in topological structure, neural networks to determine the gas production rate as a function of the bed temperature (T) and gasification time (t_g) for the four major gas species	Data was gathered from the experiments they conducted for the different types of the biomass used as feedstock	The model-predicted production rates of major gas species for the feedstocks are generally in good agreement with the experimental data	They concluded that the gasification profiles obtained by the neural networks are reflecting the real gasification process for each of the types of the different biomass feedstocks used

1.2.2 Significance of the project

By doing this study and developing the ANN model for the hydrogen production using a biomass gasification process, the author will experiment the efficiency of the ANN in predicting the result of the process and validating the results with the published ones. This will be helpful to the researchers at Green Technology MOR, UTP as the project is done according to the pilot plant facility there and their published data. Also the model can be used for other different process in the future, helps for future control studies for the process and helps saving time, energy and money.

1.3 Objectives and scope of study

1.3.1 Objectives

The objectives of the study are:

- To design and develop an Artificial Neural Network (ANN).
- To model and simulate the hydrogen production process using biomass gasification using the developed ANN.
- To validate the results with the actual experimental data.
- To compare the results of the simulation with different ANN models with the SIMCA-P software model.

1.3.2 Scope of study

The scope of study for this project covers the following:

- Understanding the gasification process – biomass gasification, types of biomass used in the process and the gaseous products of the process
- Understanding the basic elements of the gasification pilot plant – reactors system, feeding system and the gas analyzer
- Designing the ANN and writing the coding and learning to use SIMCA-P for data analysis
- Obtaining data from previous experiments conducted

2. CHAPTER 2: LITERATURE REVIEW

In this section, previous work concerning the biomass gasification, hydrogen and artificial neural network models will be discussed. The summary of the literature review done on ANN modelling and its findings can be found in Table 1.1.

2.1 Fuel Depletion and global energy:

Nowadays, the high and increasing demand for the fuels for transportation and energy production and the rise in the environmental concerns about the pollution and greenhouse effects, and with the diminishing crude oil reserves, have led the researchers to focus on renewable energy.

Korpela, S. A. (2006) mentioned that the oil production for the companies outside the OPEC is decreasing due to the heavy exploitation and utilization of fossil fuels. The worldwide growth in industry, economy and population has led to a great increase in the global energy demand and consumption, and this rate will increase rapidly in the future.

Lee et al. (2007) discussed about the energy crises of 1973 and 2005 and that it was triggered by a shortage of petroleum crude supply in the global market, mainly driven by increased transportation fuel needs. That led to an increase in the demand and need for alternative transportation fuels. Cleaner-burning and more efficient fuels are going to be in high demands. Substantial attention has been given to the renewable energy as it does not get depleted or used up over the years. The author also briefed about the benefits of renewable energy which are numerous and they include:

1. Environmental cleanness without pollutant emission
2. Non-depletive nature
3. Availability throughout the world
4. No cause for global warming
5. Waste reduction
6. Stabilization of energy costs
7. Creation of jobs

Zerta et al. (2008) reported the world energy consumption trend and projection over the next 80 years as shown in Figure 2.1. The percentages of each energy form are presented in Figure 2.2 (Khatib, 2012). From these figures, it can be seen that currently 14% of the worldwide energy consumption is supplied from biomass energy and liquid biofuels.

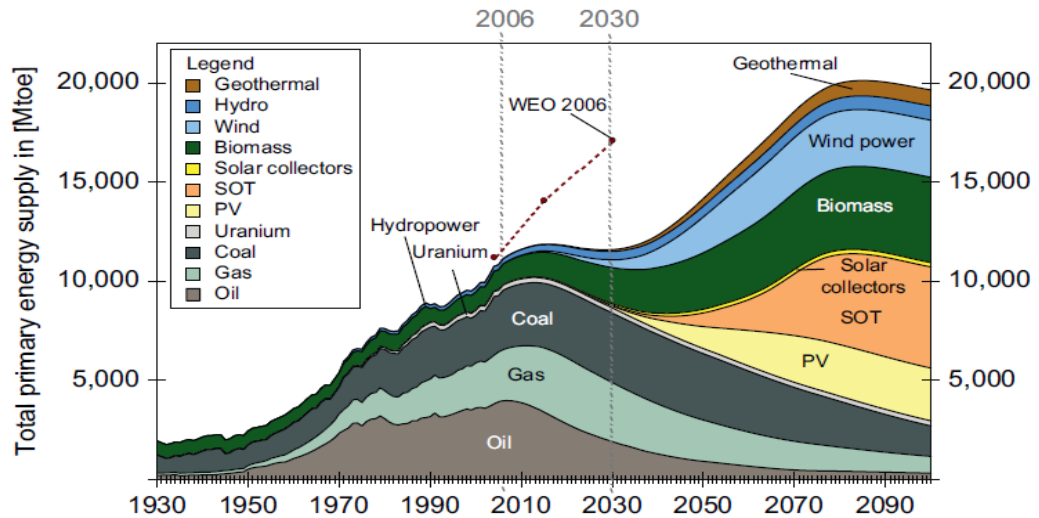


Figure 2.1: Worldwide energy consumption of fuel types from 1930-2090 (Zerta et al. 2008)

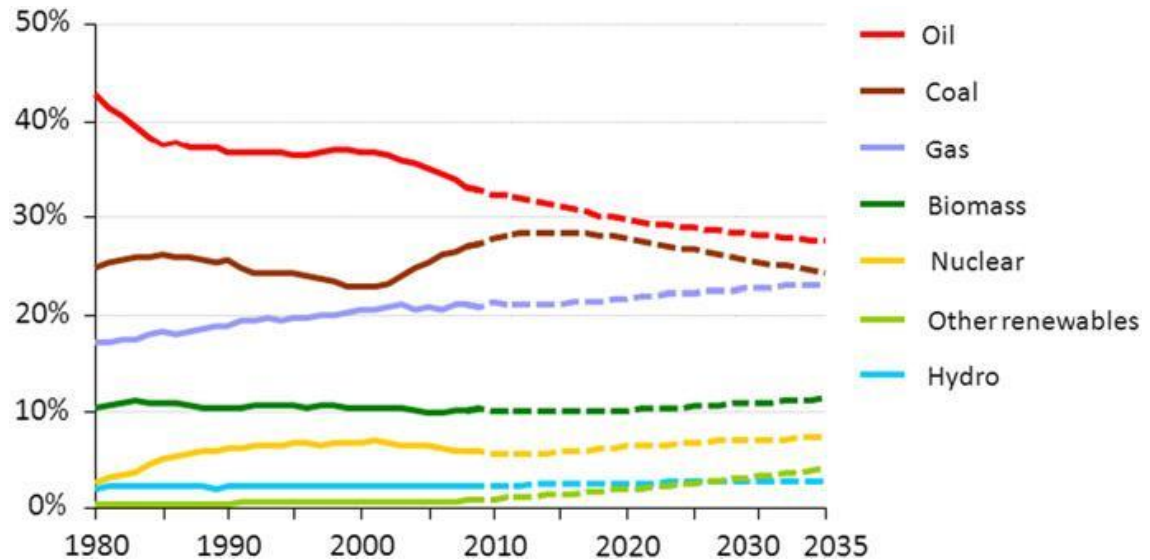


Figure 2.2: Percentage of main energy sources from 1980-2035(Khatib 2012)

2.2 Biomass Gasification and Hydrogen

McKendry, P. (2002) defined “Biomass” as a term that covers a wide range of materials that can be used as fuel or raw materials which have in common that they are all derived from recently living organisms. The previous definition excludes the traditional fossil fuels, although they also are derived from Plants as coal or animal life as in oil and gas; it has taken millions of years to be converted to their current form.

Klass, D.L. (2004) discussed about the sources of biomass as the term includes various natural and derived materials, such as wood and herbaceous species, woody wastes (e.g. from forest thinning and harvesting, timber production and carpentry residues), agricultural and industrial residues, waste paper, municipal solid waste, sawdust, grass, waste from food processing, animal wastes, aquatic plants and industrial and energy crops grown for biomass.

2.2.1 Hydrogen

Hydrogen production from biomass has become an attractive and important option in energy generation. Hydrogen is considered the best substitute for fossil fuels with the high heating value (HHV) for different usages as in transportation, home usage, and heating. In Malaysia, agricultural waste is foreseen as the best biomass feedstock for hydrogen production due to the rapid growth in the agriculture sector over the years. The utilization of agricultural waste as hydrogen feedstock will anticipate both future shortage in petroleum supply and landfill disposal problem of the agricultural residues.

Palm kernel shell is one of the best potential biomass feedstock available. In Malaysia in 2000, the palm kernel shell generated reached up to 471 thousand tones, and potential power generation from the utilization of palm kernel shell was about 77.65 MW. The oil-palm solid wastes (including shell, fiber, and empty fruit bunch) are cheap and abandoned materials produced during the palm oil milling process. For every ton of oil-palm fruit bunch being fed to the palm oil refining process, about 0.07 tons of palm shell, 0.146 tons of palm fiber, and 0.2 tons of empty fruit bunch are produced as the solid wastes (Abdullah, S. S. & Yusup, S. 2010; Esfahani et al. 2012).

2.2.2 Biomass properties

Proximate and ultimate analyses are normally the first steps in evaluating the feedstock solid fuels before the gasification process. Proximate analysis gives the fuel characteristics in terms of mass percentage of moisture, volatile matters, fixed carbon and ash content in the solid fuel.

It is performed by heating the raw material to a set temperature, the solid fuel decomposition takes place at this temperature to generate volatile gaseous substances. The moisture content is the water molecules that physio-chemically bond to the solid fuel material; however, the moisture content can be removed by heating without any chemical reactions occurring. The volatile matters that are released from biomass decomposition reactions contain a series of gaseous molecules of hydrogen, carbon monoxide, carbon dioxide and other hydrocarbons. The decomposition rate and released gas composition are affected by temperature and heating rate. The decomposition reactions are also termed as pyrolysis or de-volatilization. The remaining solid from de-volatilization of the solid fuel is called char, which consists of fixed carbon and ash. The ash content is defined as the mass percentage (or weight percentage, wt %) of the remaining solid to the chars after char complete combustion.

Ultimate analysis gives the elemental constitution of a particular fuel in mass fraction or weight percentage (wt %) in a dry ash-free basis (daf). Ultimate analysis is performed by complete combustion of the fuel normally on the oven-dried material. Composition of the combustion final products is analyzed and the main elements of the solid fuel are determined.

Moghadam et al. (2013) have published the results of the proximate and ultimate analysis of the experiment he conducted, he used biomass feedstock as Palm Kernel Shell (PKS) mixed with High Density Polyethylene (HDPE). The biomass feedstock (PKS) was obtained from local palm oil factory. The PE waste was from high density polyethylene (HDPE) plastic waste grade 2. Samples were pulverized and sieved into a specific particle size between 1-2 mm. The results of the analysis are shown in table 2.1

Table 2.1: Proximate and ultimate analysis (Moghadam et al. 2013)

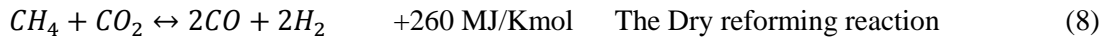
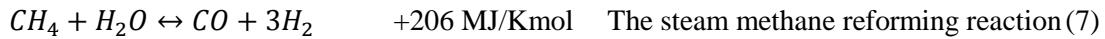
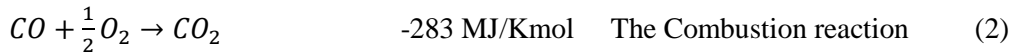
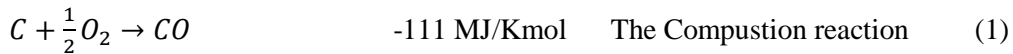
Proximate Analysis (wt% wet basis)	PKS	HDPE	Ultimate analysis (wt% dry basis)	PKS	HDPE
Moisture content	12.00	0.00	C	49.23	85.71
Volatile matter	30.53	99.67	H	5.04	14.29
Fixed carbon	48.50	0.00	O	44.94	0.00
Ash	8.97	0.33	N	0.74	0.00
Holocellulose	54.30	-	S	0.05	0.00
Alpha-cellulose	29.60	-	Density (kg/m ³)	733	1194
Lignin	59.30	-	HHV (MJ/kg)	24.97	45.98

2.2.3 Biomass Gasification

Puig-Arnavat, M. et al (2013) defined gasification as it is a partial thermal oxidation, which results in a high proportion of gaseous products (carbon dioxide, water, carbon monoxide, hydrogen, and gaseous hydrocarbons), small quantities of char (solid product), ash and condensable compounds (tars and oils). Steam, air or oxygen, are supplied to the reaction as oxidizing agents. The gas produced can be standardized in its quality and is easier and more versatile to use than the original biomass e.g. it can be used to power gas engines and gas turbines, or used as a chemical feedstock to produce liquid fuels. Gasification adds value to low or negative-value feedstock by converting them to marketable fuels and products. In the same study by they claimed that the biomass gasification is very efficient and clean process that converts biomass feedstock to different products for many applications. The modern usage of biomass now gives a promising future for reducing energy dependency and greenhouse gas emissions to the environment; as the biomass is considered to be a CO₂-neutral. Biomass gasification is considered in different and advanced applications in some of the developing countries, and also it can be used for rural electrification in isolated installations or in growing states. The availability, ability for continuous power generation and synthesis of

different fuels and chemicals make the biomass to be the renewable energy source that can replace the fossil fuels.

Esfahani et al. (2012) reported that the gasification reaction is the result of chemical reactions between carbon in the char and steam, carbon dioxide and hydrogen in the reactor, as well as chemical reactions between the evolved gases. The gasification process, in principle, involves a wet basis, carbon, carbon monoxide, carbon dioxide, hydrogen, water and methane from the following reactions:



Moghadam et al. (2013) and Moghadam et al. (2014) mentioned in his study for the biomass gasification about the process of the gasification, starting with the gasification pilot plant as can be seen in Figure 2.3 below. The pilot plant consists of a cylindrical reactor made of (Inconel 625). The measurements of the fluidized bed gasifier used are about 2500 mm in height, 150 mm in internal diameter, and 200 mm in gasification and free board zone. The reactor has four electrical heaters and temperature controllers are used to control the temperature of the reactor. For measuring the temperature, there are eight thermocouples installed in the gasifier reactor as the following, two in the dense bed, four in the gasification zone and two in the free board zone. The feedstock for his study was mixed with Ni catalyst.

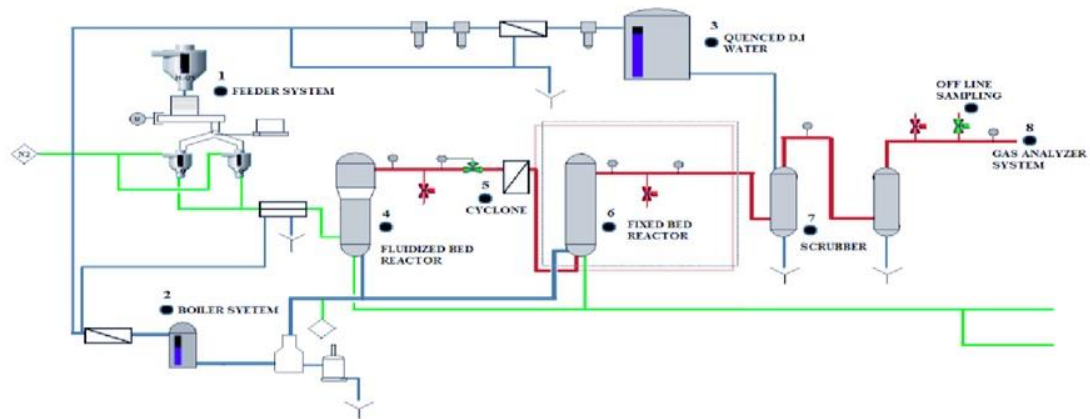


Figure 2.3: Process flow diagram of pilot plant catalytic steam gasification system. (Moghadam et al. 2013)

1- Feeding system. 2- Boiler system. 3- Quenched D.I. water system. 4- Fluidized bed gasifier. 5- Cyclone. 6- Fixed bed gasifier. 7- Scrubber system. 8- Gas analyzer system.

The feedstock is fed to the fluidized bed gasifier with a rate of 1.2 kg/h using a variable speed screw feeder and two swing lock hopper. Water is used to cool the feeding system to avoid any clogging. A super heater is used to superheat the steam supplied by the boiler to about 270 °C and it is used as the gasifying agent in the process. The gas produced from the reactor passes through a cyclone and then to a scrubber to remove all fly ash and tar residual. Then a sample of the gas passes to the gas analyzers (Teledyne 7500, 7600 and 4060) to determine the amount of H₂, CO, CO₂, CH₄, N₂, O₂, H₂S, and NO₂ in the produced gas.

2.3 Artificial Neural Network Modelling

Biomass gasification process is a very complex process that depends on complex chemical reactions, partial oxidation of pyrolysis products and char, conversion of tar and hydrocarbons and the water gas shift reaction in order to produce the syngas. This complicated process needs a model that can evaluate the process and to be used in prediction of the results.

Modelling is a very powerful and useful tool for designing and optimizing the biomass gasification process. Some of the models used in the biomass gasification process are the kinetic, equilibrium and artificial neural network models. The kinetic and equilibrium models require and use differential equations and to be solved using

programming software needs power and time to acquire the accurate predictions needed for the process.

Neural networks are seen as contributing a brain-based neurologically inspired, and biologically plausible approach to cognitive modelling (Lappi. 2007). They are inspired by the natural neurons as they receive signals through synapses, then the neuron will be activated and emits a signal which might be sent to another synapse or to activate another neuron as can be seen in figure 2.4. An ANN also composed of a lot of neurons or nodes (interconnected processing elements) to solve problems and they are like humans they learn by example and previous experiments.

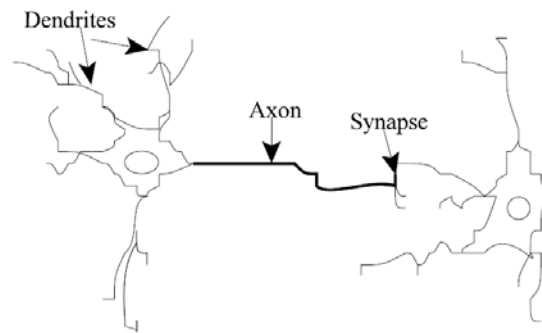


Figure 2.4: Natural neurons (Rojas. 1996)

Artificial neural networks (ANN) have been reported to be used in a lot of fields like, pattern recognition, signal processing, function approximation and process simulation (Guo et al. 2001).

Guo et al. (2001) mentioned in his study that Artificial neural network (ANN) model offers an alternative way to model the biomass gasification process and to predict the composition of the product gas and gas yield, as the ANN model does not require a comprehensive understanding of the details of the process. The working principle of the ANN is that it transforms the inputs into outputs based on established and previous input-output relationships. These relationships are found from previous and observed experimental data.

The ANN architecture or topology talks about how the neurons are organized and interconnected and how the information passes through the network. The ANN

architecture is composed mainly from three parts or layers, the first is the input layer this is where the inputs of the process are defined and then the information will pass to the second part the hidden layer/s (it can be one layer or more than one depending on the complexity of the problem or the process) where the information of the inputs is processed and then sent to the third part or what is called the output layer to deliver and show the outputs of the process. Figure 2.5 shows the three layers and how the neurons are arranged into the layers (hidden layers) and the connection between the layer, activation function and learning method, the pervious data from experiments make the learning process to find the relationship between the inputs and outputs (Kalogirou. 2002).

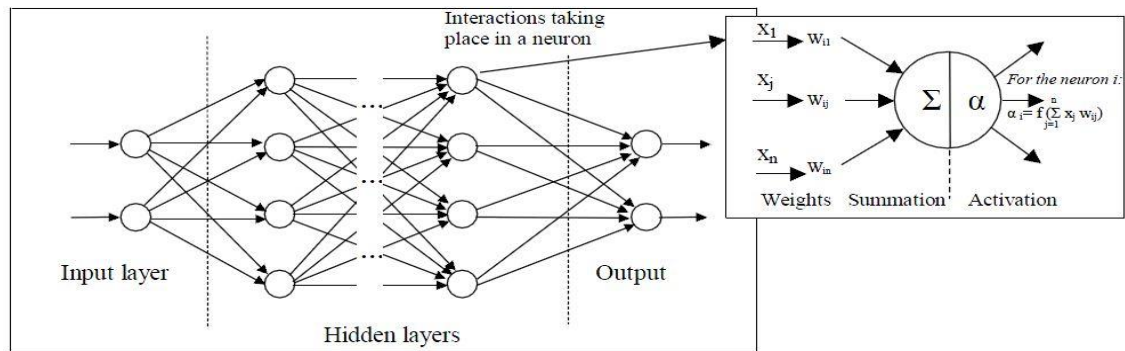


Figure 2.5: Schematic diagram of a multilayer neural network and how the information is processed (Kalogirou. 2002).

The layers are connected through a set of weights expressed as a two dimensional matrix, w_{ij} . In a neural network the value of a node in a hidden layer is a result of non-linear transfer function α which is the weighted sum over all the nodes in the previous layer plus a constant term b_1 which is referred to as the bias as the following equation (9):

$$\beta_i = \sum_j w_{ij} \alpha_{pj} + b_j \quad (9)$$

The subscript j refers to a summation of all the nodes in the previous layer of nodes, and the i subscript refers to the node position in the present layer, the p subscript refers to the input pattern. An algorithm called back-propagation is used to establish the weight values to be used to solve for the output and it will be changed in every run till getting the satisfied output value. Training a neural network begins with a set of training data

consisting of input data and its corresponding output data, then the weights will be adjusted until the sum of differences between the neural network outputs and the corresponding original output data is minimized and the error between the actual and the desired outputs of the network is reduced (Kalogirou et al. 1999).

Guo et al. (2001) conducted gasification on several types of biomass in fluidized bed gasifier at atmospheric pressure with steam as the fluidizing medium. Then they developed an artificial neural network model to predict the yield and gas composition of the gasification processes. Four types of biomass were used as feedstock: poplar sawdust, pine sawdust, comminuted sugar bagasse and cotton stem. The experiments were conducted at different gasification temperatures for each of the biomass feedstock. They developed four identical, in topological structure, neural networks to determine the gas production rate as a function of the bed temperature (T) and gasification time (tg) for the four major gas species. They concluded that the gasification profiles obtained by the neural networks are reflecting the real gasification process for each of the types of the different biomass feedstock used.

Xiao et al. (2009) have conducted an experiment of gasification of municipal solid waste (MSW). They used five different kinds of organic components: wood, paper, kitchen garbage, polyethylene (PE) plastic, and textile. The experiments were conducted at different temperature for each of the five kinds of the organic components. And they used three representative types of simulated MSW which were gasified in a fluidized bed. The lower heating value (LHV) of gas, gasification products and gas yield were reported. An ANN was developed to predict the gasification characteristics. The inputs of the ANN in the input layer were: the percentage of the five different kinds of the organic component, equivalence ratio (ER) and temperature. They concluded that the result of the ANN in predicting the gasification characteristics of MSW is feasible and produced acceptable results, as they found the relative errors in the training, validating data are within $\pm 15\%$ and $\pm 20\%$ respectively, and predicting relative errors of an industrial sample below $\pm 25\%$.

Puig-Arnava et al. (2013) developed two artificial neural network (ANN) models: one for Circulating Fluidized Bed gasifier (CFB), and one for Bubbling Fluidized Bed

gasifier (BFB). They were used to predict the producer gas composition and the gas yield from biomass composition and few operating parameters, like thermodynamic equilibrium models do, but avoiding the high complexity of kinetic models. Published experimental data from other authors has been used to train the ANNs. The results showed how the percentage composition of the product gas and the gas yield for a CFB or BFB gasifiers can be successfully predicted, as for the CFB Experimental and simulated values for CO, CO₂, H₂, CH₄, and gas yield were compared satisfactorily through a linear regression model for each. All the R² values are higher than 0.99 except for H₂ composition which is 0.98, while for BFB, all the R² values are higher than 0.99 except for CO₂ composition which is 0.98.

3. CHAPTER 3: METHODOLOGY

3.1 Research methodology

In any engineering problem, there are several approaches must be followed to solve the problem, one of those approaches is the modelling approach, which will be used here in this study. As it can be seen in the previous chapter, the modelling hasn't been used a lot in the biomass gasification process. So in this study, the author will use that model to predict the hydrogen yield from a biomass gasification process and validate the results with the experimental data. The author is using the data published by Moghadam et al. (2013) and Moghadam et al. (2014), and results are divided into three groups. The first will be used for training the neural network. The second group will be used for testing the neural network and finally the third will be used for validating the neural network with the experimental results. Below are the key milestone and Gantt chart of this project.

3.2 Key Milestone for FYP I

No	Activities	Date
1	Submission of the extended proposal	Week 6
2	Proposal Defence (oral presentation)	Week 8,9
3	Submission of Interim Draft Report	Week 13
4	Submission of Interim Report	Week 14

3.3 Gantt chart for FYP I

No	Detail/ Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Selection of Project Topic	█	█												
2	Preliminary Research Work		█	█	█	█									
3	Submission of Extended Proposal						█								
4	Proposal Defense								█	█					

3.6 Gantt chart for FYP II

No	Detail/ Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	
1	Project Work Continues: Starting the simulation with MATLAB ANN	█	█	█	█	█	█	█									
2	Submission of Progress Report								█								
3	Project Work Continues: Evaluating the results of the simulation and finding other models for comparison								█	█	█	█	█				
4	Pre-SEDEX											█					
5	Submission of Draft Report												█				
6	Submission of Dissertation (soft bound)													█			
7	Submission of Technical Paper														█		
8	Oral Presentation															█	
9	Submission of Project Dissertation (Hard bound)																█

3.7 Tools

The modelling process in this study will be carried out using artificial neural network on MATLAB 2012a, and a preliminary analysis of the data to see what factor affects the production of hydrogen in the biomass gasification process using SIMCA-P. Both softwares are available and licensed in UTP.

SIMCA-P is developed by Umetrics, which is mainly used for the methods of principle component analysis (PCA) and partial least square (PLS) regression. It is a kind of user-friendly software based on Windows: the operations of models in SIMCA-P are very convenient to handle and the results can be easily illustrated by plots and lists, which present the explanation of the models in kinds of forms.

MATLAB[®] is a high-level language and interactive environment for numerical computation, visualization, and programming. Using MATLAB, you can analyze data, develop algorithms, and create models and applications. The language, tools, and built-

in math functions enable you to explore multiple approaches and reach a solution faster than with spreadsheets or traditional programming languages, such as C/C++ or Java™. You can use MATLAB for a range of applications, including signal processing and communications, image and video processing, control systems, test and measurement, computational finance, and computational biology. More than a million engineers and scientists in industry and academia use MATLAB, the language of technical computing.

4. CHAPTER 4: RESULTS AND DISCUSSION

4.1 Data Collection

As a first step in this study which is collecting the data of hydrogen production from biomass gasification from the Green Technology MOR, UTP. The set included 34029 data point relating temperature, PE-PET (Polyethylene ratio to biomass feed), and steam to biomass feed to hydrogen composition of the produced gas.

As mentioned by Moghadam R.A (2014), the feedstock for the gasification process was Palm Kernel Shell (PKS) mixed with polyethylene which was obtained from a high-density polyethylene (HDPE). The proximate and ultimate analyses of the feedstock are reported in Table 2.1

The experiment was conducted according to Moghadam (2014); he found out that there are factors that affect the process of producing hydrogen and syngas, which are:

- 1- Temperature
- 2- Steam to feedstock ratio (S/F)
- 3- Polyethylene waste to biomass (P/B) ratio

Those variables have been studied to find their effect on the syngas produced and the composition of hydrogen produced.

In this study, the author will be using the same variables as input variables for the Artificial Neural Network and to study the relation to the output variable (Hydrogen composition), so that relation would help in the ANN by using the ANN for prediction purposes later on to find the expected composition of hydrogen that could be produced from a gasification process before running it and which could save time and energy if the simulation and the results of the ANN came positive, so that researchers could proceed with the experiment and if it came negative, they change some of the variables used. All this to save the money and not wasting the resources in experiments which are not sure if they would produce accepted results.

Effects of the variables on the hydrogen yield and syngas produced:

- Effect of temperature

Temperature exhibits the most crucial effect on catalytic steam gasification process and has major influence on the final product composition.

As observed, gasification reactions favored high temperature and the process was influenced by endothermic reactions. Increasing temperature with setting the other factors constant will increase the production of the syngas and give a high yield of produced hydrogen gas.

- Effect of steam/feedstock (S/F) ratio

S/F ratio is an influential parameter on the gasification process. Optimum S/F ratio is important for better conversion since too large S/F ratio does not always favor the syngas production and is not cost effective, as it involved a large amount of superheated steam being utilized.

Introducing an excess steam to gasification process increased the hydrocarbon cracking but excessive steam would lower the gasification temperature and consequently degraded the syngas quality and less hydrogen yield.

- Effect of polyethylene waste blending ratio

The results showed that the increased of polyethylene in the mixtures increased the conversion of the solid feedstock to gaseous products. This is because polyethylene degrades easily and faster compared to biomass at higher temperature.

Furthermore, polyethylene contains higher volatile matter, low ash content and absence of fixed carbon compared to biomass.

The experimental data obtained were about 34029 data points, for training the ANNs about 15000 data points (from data point no.1 to data point no. 15000) have been used, this purpose of this is to include a lot of different inputs and so the ANN would be able to predict better results if it falls in between those inputs, a set of 50 data points (from data point no. 20162 to data point no. 20212) have been used for testing the ANNs, the reason behind choosing this small number is that the graph would be clear and to differentiate better between the predicted and experimental data, because if we increased the number the graph would not be that clear for comparisons.

4.2 SIMCA-P13 results

A preliminary analysis was done for the data using SIMCA-P13 software described in the previous chapter.

The results of the analysis are shown below:

R^2

R^2 is the percent of variation of the training set – Y with PLS – explained by the model. R^2 is a measure of fit, i.e. how well the model fits the data. A large R^2 (close to 1) is a necessary condition for a good model, but it is not sufficient. You can have poor models (models that cannot predict) even with a large R^2 . You will get a poor R^2 when you have poor reproducibility (much noise) in the training data set, or when for other reasons X does not explain Y.

Q^2

Q^2 is the percent of variation of the training set – Y with PLS – predicted by the model according to cross validation. Q^2 indicates how well the model predicts new data. A large Q^2 ($Q^2 > 0.5$) indicates good predictivity. You will get a poor Q^2 when the data have much noise, or when the relationship X->Y is poor, or when the model is dominated by a few scattered outliers.

The figure 4.1 below shows that R^2 and Q^2 value is around 0.35 which might be considered as a poor R^2 but as long as the R^2 is not less than Q^2 then the model is still can get good and acceptable predictions.

The R^2 and Q^2 values can be seen in Figure 4.1 below.

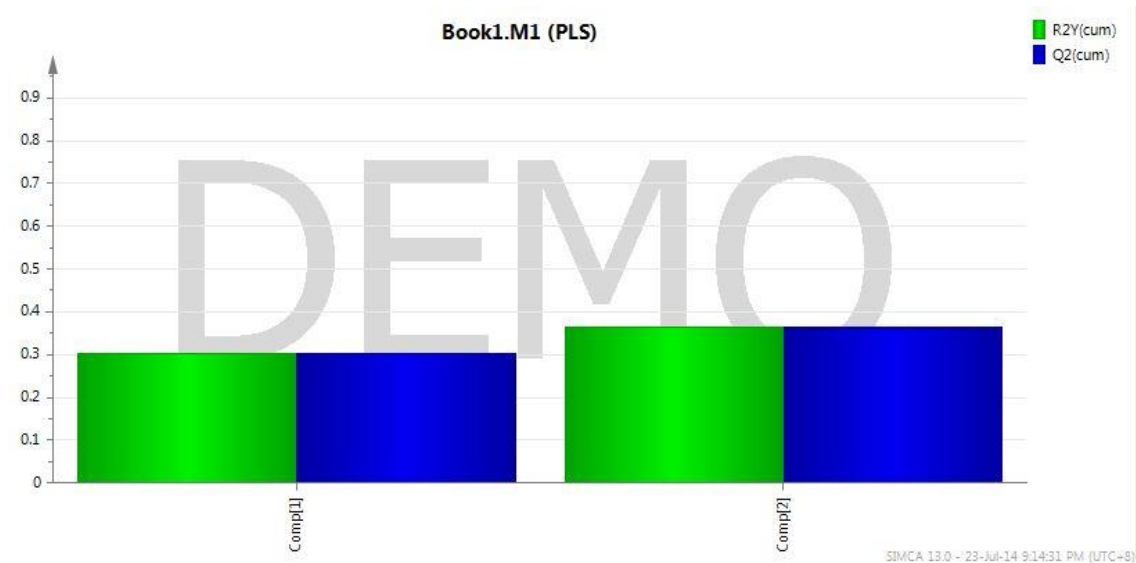


Figure 4.1: Summary of fit plot PLS

Figure 4.2 shows the scores t_1 , t_2 , etc., which are new variables summarizing the X-variables. The scores are orthogonal, i.e., completely independent of each other. There are as many score vectors as there are components in the model. The score t_1 (first component) explains the largest variation of the X space, followed by t_2 etc.

Hence the scatter plot of t_1 vs t_2 is a window in the X space, displaying how the X observations are situated with respect to each other. This plot shows the possible presence of outliers, groups, similarities and other patterns in the data. The score plot is a map of the observations.

With a two-dimensional score plot, SIMCA draws the tolerance ellipse based on Hotelling's T^2 . Observations situated far outside the ellipse are outliers.

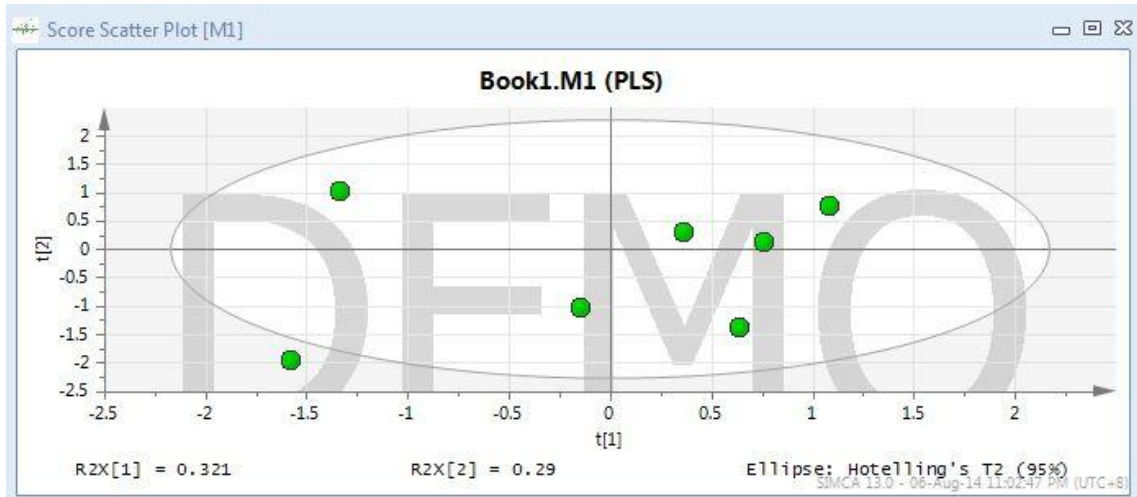


Figure 4.2: Score Scatter Plot.

The PLS loading weights plot (Figure 4.3) displays the relation between the X-variables and the Y-variables. To facilitate interpretation this plot is by default color coded according to the model terms.

The above w^*c plot is a superimposition of the w^* plot and the c plot, for the first and second components. The w^* 's are the loading weights that combine the X-variables to form the scores t . These weights are selected so as to maximize the correlation between T and U , thereby indirectly between X and Y . This plot of the X- and Y-loading weights (w^* and c) of one PLS component against another, 1 and 2, shows how the X-variables correlate with the Y-variables, and the correlation structure of the X's and Y's. X-variables with large w^* 's (positive or negative) are highly correlated with U (Y). These variables with large w^* 's, are situated far away from the origin (on the positive or negative side) on the plot. Hence we see how the responses vary in relation to each other, which ones provide similar information and their relationship to the terms in the model.

The figure shows that the X- variables (Temp and PE-PET) are much closer to the Y-variable (H_2), which means that those 2 are highly correlated and affects the product much more than the S/F.

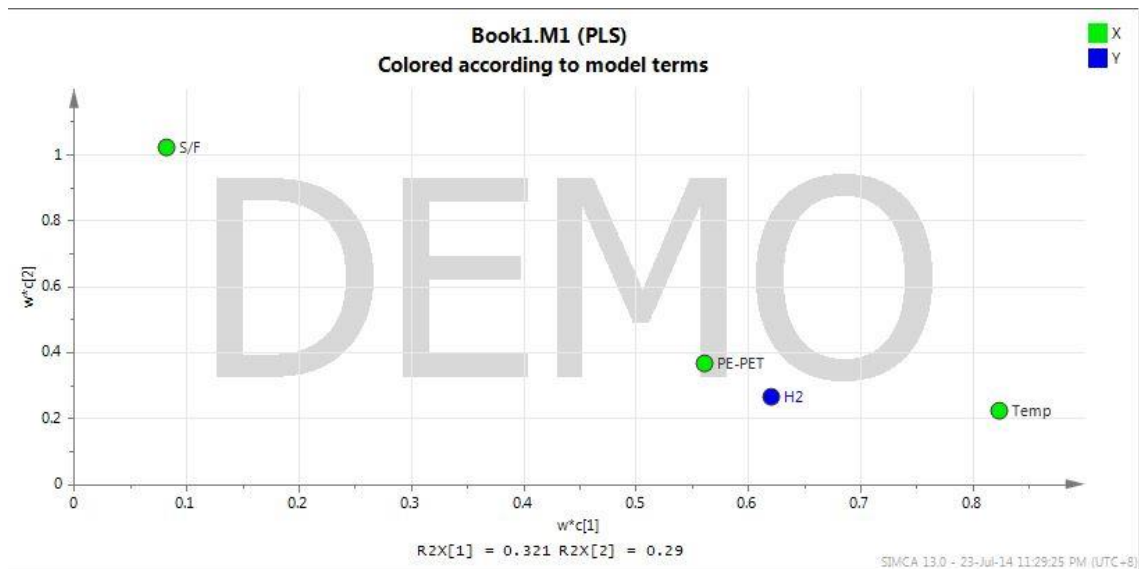


Figure 4.3: Loading weights plot.

The VIP (Variable Importance for the Projection) graph (Figure 4.4) shows the summary of the importance of the variables both to explain the inputs and to establish the correlation to the output. The VIP values are calculated for each input (x_k) by summing the squares of the Partial Least Squares (PLS) loading weights w_{ak} . The sum of squares of all VIP's is equal to the number of terms in the model. Hence, the average VIP is equal to 1.

VIP-values larger than 1 indicates “important” X-variables, and values lower than 0.5 indicate “unimportant” X-variables. The interval between 1 and 0.5 is a gray area, where the importance level depends on the size of the data set. So according to that and as can be seen from the figure above, Temperature is the most important factor or variable in the process of hydrogen production as it is value about 1.3. Then followed by the PE-PET with a value around 0.9, S/F (steam to feed ration) comes last with a value of 0.7. As long all those values above 0.5, it means that they all important to the process of hydrogen production but some factors have more effect than the others and there comes their importance to the process.

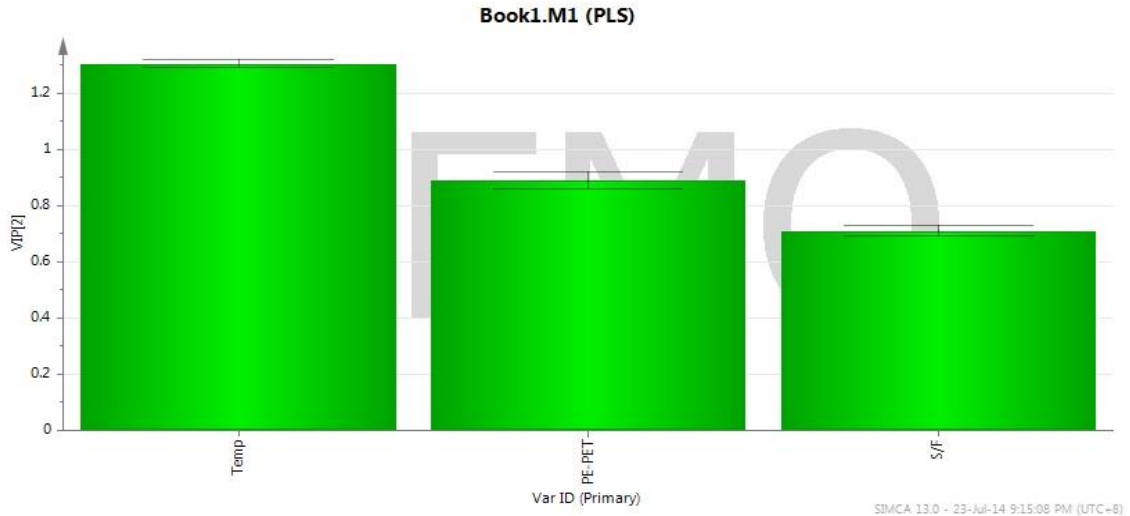


Figure 4.4: VIP Plot.

With PLS/OPLS/O2PLS models, Figure 4.5 displays the relationship between the first summary of all the Y-variables (u_1) and the first summary of all the X-variables (t_1).

- Strong relationship between X and Y is manifested by a small scatter around the diagonal line.
- The size of the scatter band is a measure of the variability.
- Look for curvature (curved line), outliers, groups and jumps.

An off-diagonal point is an observation that breaks the general correlation structure between X and Y.

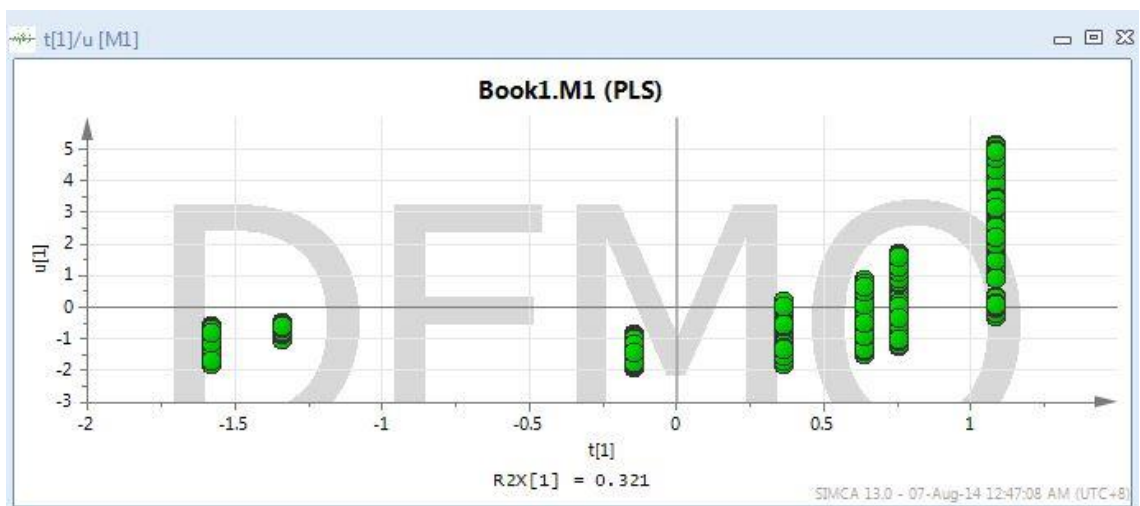


Figure 4.5: $t(1)$ vs $u(1)$ Plot.

The preliminary analysis done, shows the factors that affect the process of hydrogen production from biomass according to the data provided, where it can be seen clearly from figure 4.4, that Temperature has the highest effect on the hydrogen composition produced where increasing the temperature will increase the yield of hydrogen, coming secondly is the PE-PET and finally with a less effect on the hydrogen production the steam to feed ration (S/F).

Also, the analysis done for the data shows that the relation between the inputs and outputs is not linear as in figure 4.5 it does not show a straight line and also the value of R^2 as in figure 4.1 is not high as expected. All the mentioned before does not affect the process of predicting from the data but it just shows that a relation is non-linear and then the need for a model that is able to predict future results from a non-linear data.

Figure 4.6 shows the plot of the actual experimental data versus the predicted data using the SIMCA-P13 software. As it can be seen, the actual results are plotted with the black color and the predicted with the blue color, the data that have been plotted here are from the data point 20162 to 20212. The plot shows that the predicted data does not follow the same line of the actual experimental data, and this might be due to the reason mentioned before, that the model is non-linear while the software uses linear models to do the prediction process, and that is why the proposed model to solve this problem is the ANN using MATLAB, at the end of the simulation process, the author will compare the results to check the validity of all the models and which one promises better results.

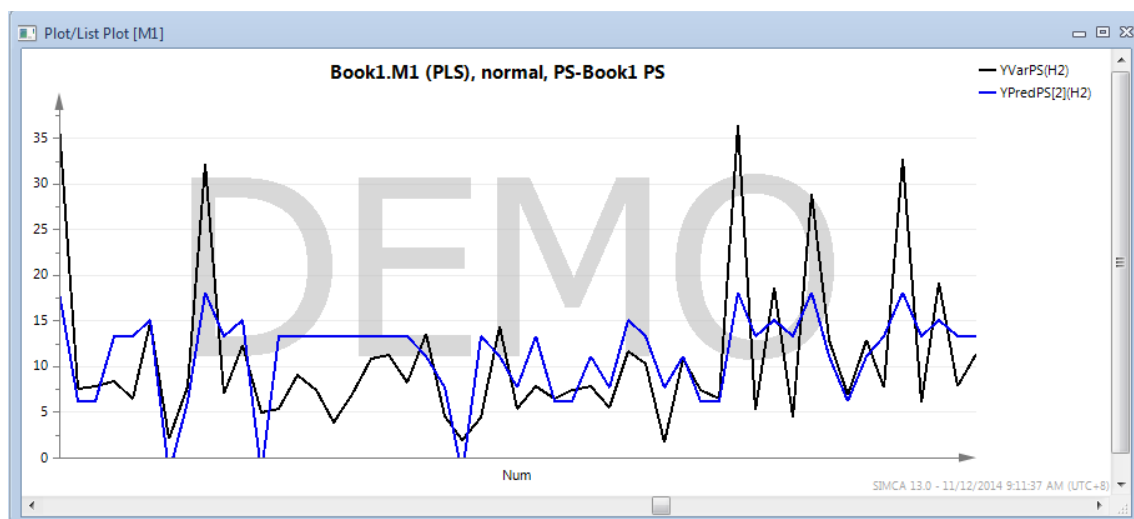


Figure 4.6: Actual experimental data vs predicted data using SIMCA-P13.

4.3 MATLAB's ANN (NEWFF Functions) results

After finishing the analysis of the data by SIMCA-P13 software, the author started to use the MATLAB Neural Network (ANN) to simulate the process. As have been mentioned before the data set has been divided to parts, one for training the neural network and another one for testing the network. A Newff Function has been used as the ANN for the simulation process; it has been divided into three (3) layers: Input layer, Hidden layer and Output layer. A different number of Neurons has been assigned to the hidden layer in order to check for a better output results. A Mean Squared Error (MSE) function has been used to evaluate the error percentage between the actual experimental results and the predicted results of the ANN.

Here are some of the results, using around 15000 data point for the training and 50 data point for the testing of the network. The training set is from data point no. 1 to the data point no. 15000, and the testing set from the data point no. 20162 to the data point no. 20212. The rest will be shown in appendix A.

In order to know the best Transfer functions to be used in this ANN layers (for input and hidden layer) a comparison have been made between the three transfer functions (Logsig, Tansig, Purelin) as can be seen in table 4.1 and the best combination to be used in the ANN is to have the Input Layer TF as Tansig and the Hidden Layer TF as Purelin, because they have the lowest MSE percentage and this combination have been used in order to produce the following results.

Table 4.1: A comparison between combinations of Transfer Functions (TF).

Input Layer TF	Hidden Layer TF	MSE Percentage
Logsig	Tansig	5.466 %
	Purelin	5.484 %
	Logsig	116 %
Purelin	Tansig	12.19 %

	Purelin	43.16 %
	Logsig	116 %
Tansig	Tansig	5.459 %
	Purelin	5.442 %
	Logsig	116 %

❖ For 5 Hidden neurons: Current MSE: 5.500%

Figure 4.7 shows the ANN training window for the newff function with Five (5) Hidden neurons in the Hidden layer. It also shows the number of iterations needed to reach the desired result which was 72 iterations.

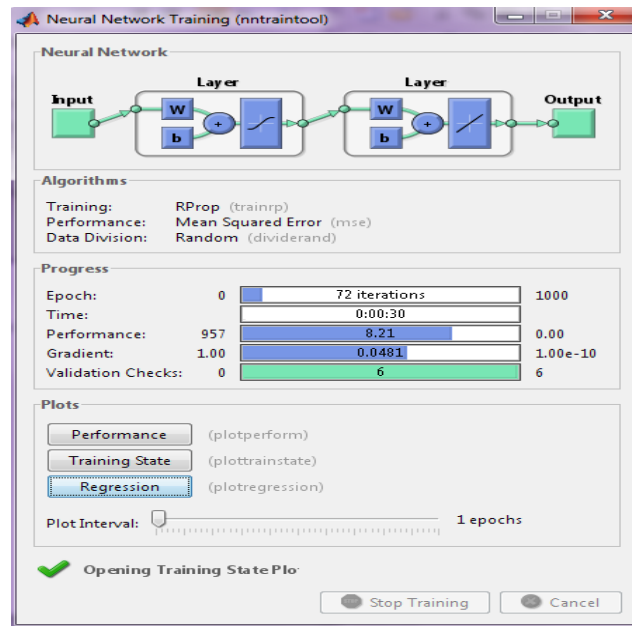


Figure 4.7: ANN training window.

After the training of the ANN stops it produces the following graphs as in Figure 4.8, Figure 4.9 and Figure 4.10.

Figure 4.8 shows the performance of the ANN with relation to the MSE with the iterations number. Comparing the training set with the validation and testing sets and it also shows the best performance that gives the minimum error value.

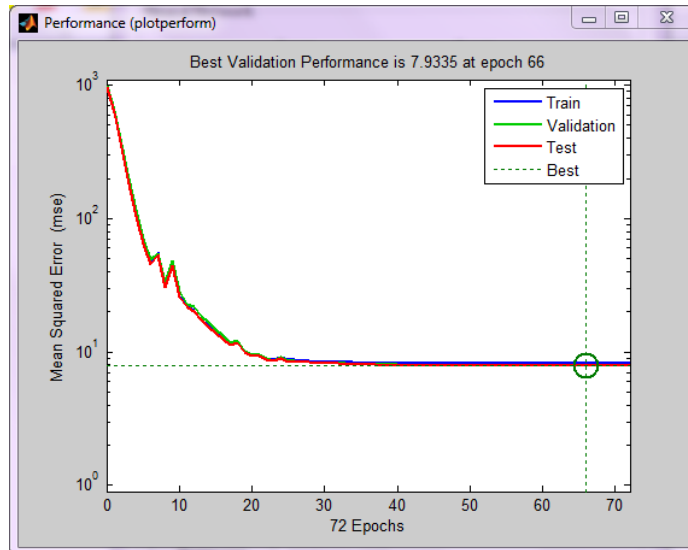


Figure 4.8: ANN Performance Plot.

Figure 4.9 shows the plot of regression of the ANN, also comparing the different sets of the training, validation and testing sets. Also it shows the overall plot of the three sets with the regression (R) value.

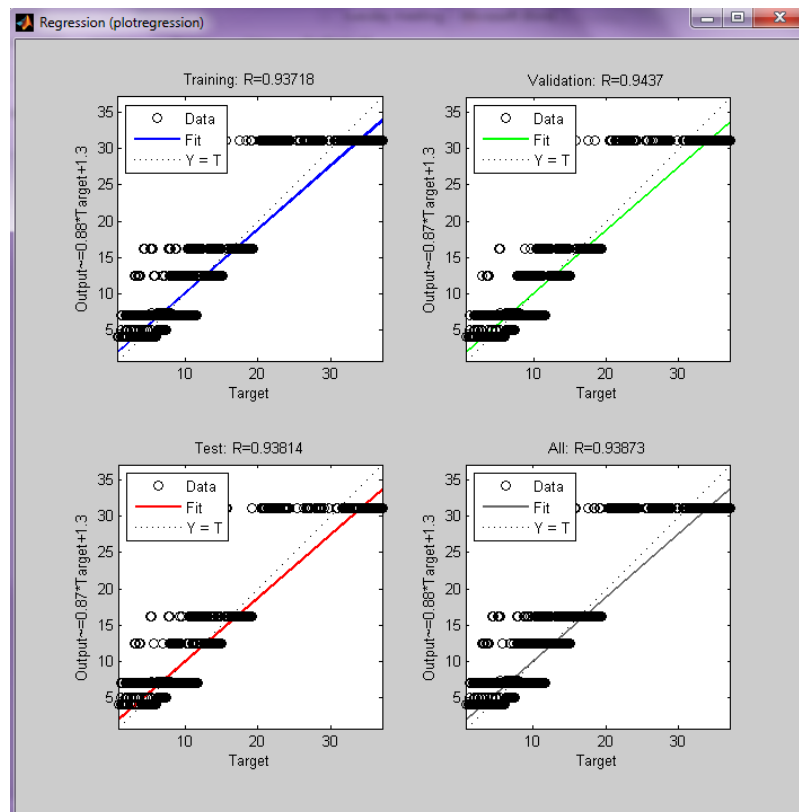


Figure 4.9: ANN's Regression Plot.

Figure 4.10 shows the final output of the ANN, as it plots the Actual experimental data and the ANN predicted results. After the iteration the minimum MSE error found was 5.50%. The graph shows that the predicted results almost the same as the actual experimental results but only differs in a small part (the range of data points between 20173 and 20180), but for the other point even if it is not the same but still gives a correct directional change, meaning if the actual plot is going up then the predicted is going up also, which will give an expectation how the results would be.

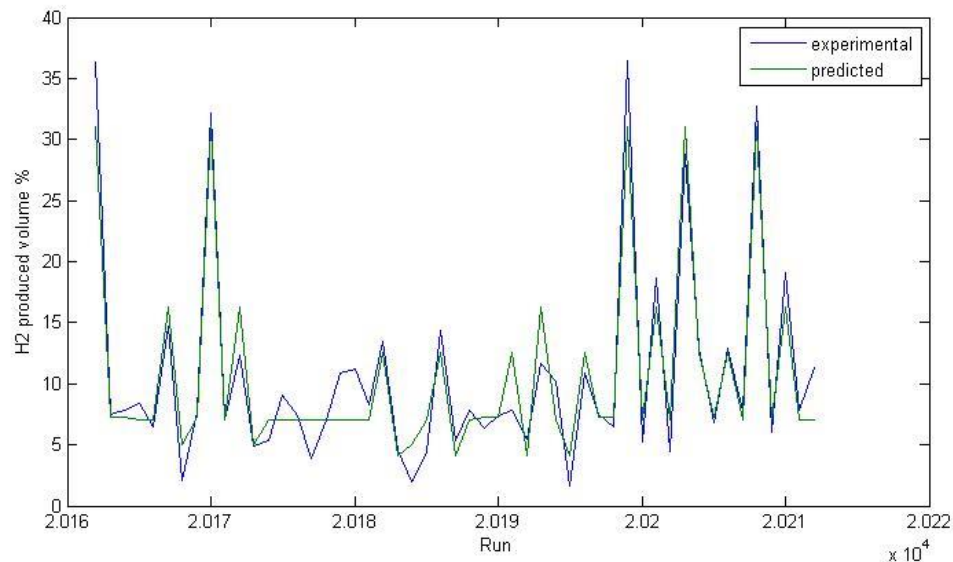


Figure 4.10: ANN's plot between the actual experimental data and the predicted data.

4.4 MATLAB's ANN (NEWFF Function with normalized data) results

Another way of running the simulation is by normalizing the data to be in the range between [-1 and 1], which is a common way of running the ANN and sometimes it will help in giving better results. The author has used the method of normalizing the data and ran the simulation. The result produced after the normalization was the same as the previous results in terms of the error or the graph for the 5 hidden neurons:

- ❖ For 5 Hidden neurons: Current MSE: 5.500%

Figure 4.11 shows the ANN training window for the newff function with Five (5) Hidden neurons in the Hidden layer and with the normalized data. It also shows the

number of iterations needed to reach the desired result which was 102 iterations more than the newff function without normalizing the data.

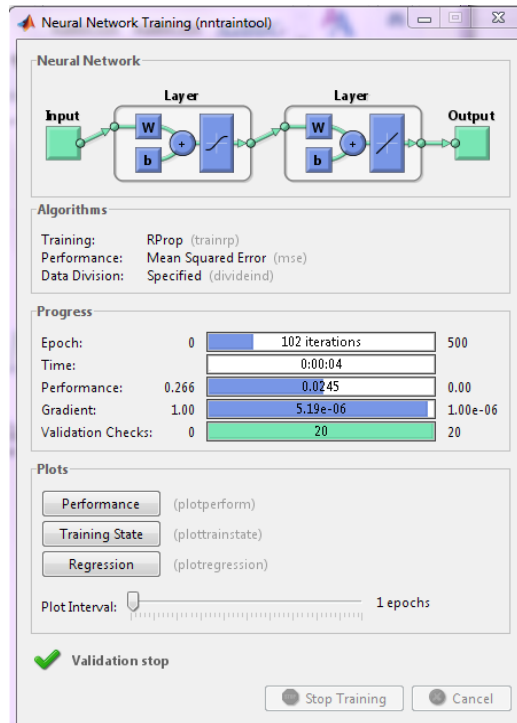


Figure 4.11: ANN training window (normalized data).

Figure 4.12 shows the plot of regression of the ANN, also comparing the different sets of the training, validation and testing sets. Also it shows the overall plot of the three sets with the regression (R) value. It shows a slight difference with the value of the overall R value with 0.9388 comparing to the previous model where R was 0.93873

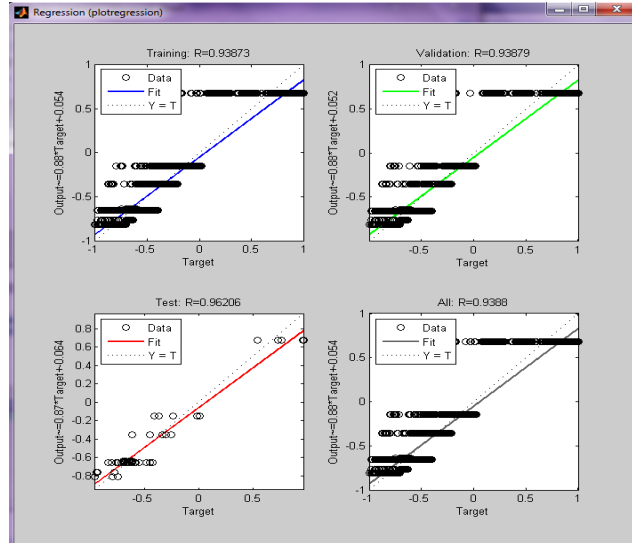


Figure 4.12: ANN's Regression Plot (normalized data).

Figure 4.13 shows the final output of the ANN, as it plots the Actual experimental data and the ANN predicted results. After the iteration the minimum MSE error found was 5.50%. The percentage error and the graph look the same as the previous model without the normalization of the data, which shows that the normalization did not change the output of the ANN but differed in the way to reach it, where was a slight difference in the number of iterations and the value of R.

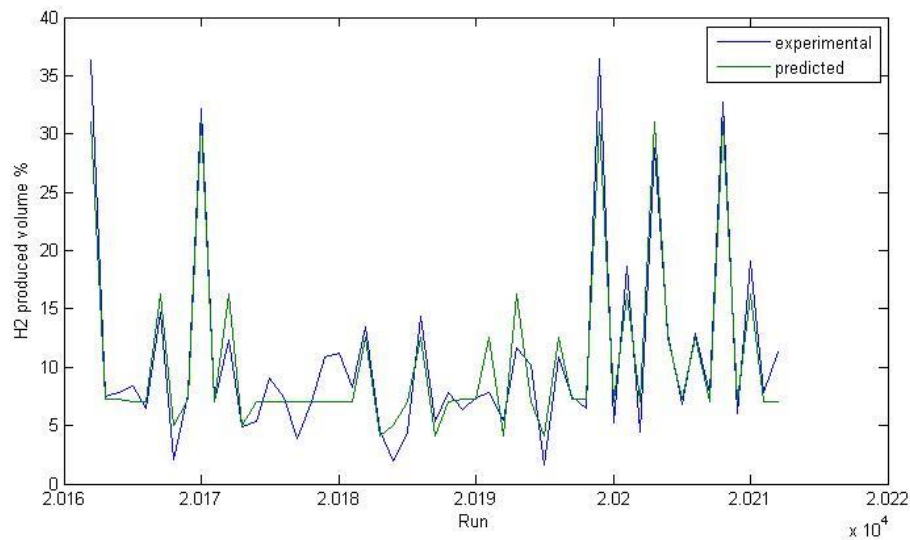


Figure 4.13: ANN's plot between the actual experimental data and the predicted data (normalized data).

4.5 MATLAB's ANN (NEWFIT Function) results

The newfit function gave the same result as the newff function as they both have the same task and coding just a small different only when using a 1-input to output relations to draw the fit plot, but when using more than 1-input like the case here, it will not be possible to draw the fit plot but the results will still be the same. Figure 4.14 shows the performance of the ANN with relation to the MSE with the iterations number. Comparing the training set with the validation and testing sets and it also shows the best performance that gives the minimum error value which was around the 30th epoch.

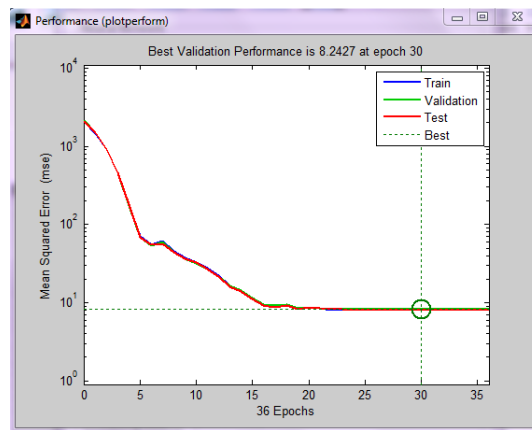


Figure 4.14: Performance Plot.

Figure 4.15 shows the plot of regression of the ANN, also comparing the different sets of the training, validation and testing sets. Also it shows the overall plot of the three sets with the regression (R) value, also the values does not differ much with the previous ANNs functions.

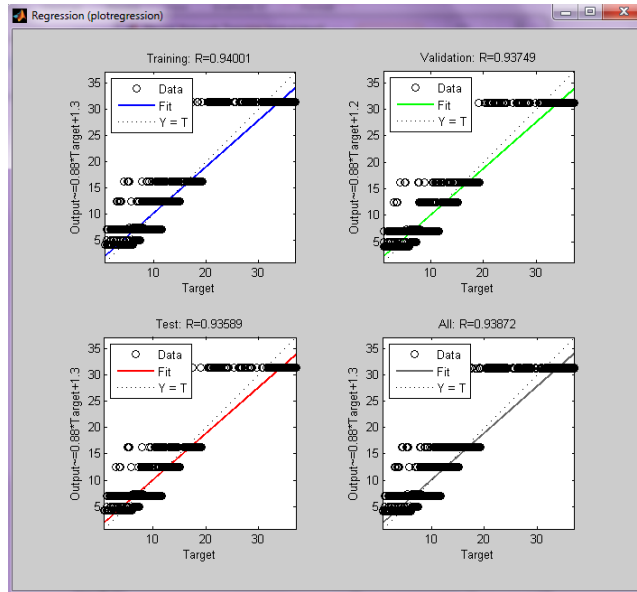


Figure 4.15: Regression Plot

Figure 4.16 shows the final output of the ANN, as it plots the Actual experimental data and the ANN predicted results produced by the newfit function. As it can be noticed, it does not vary much from the previous plots by the other functions. It only differs in the error percentage calculated by a very small margin.

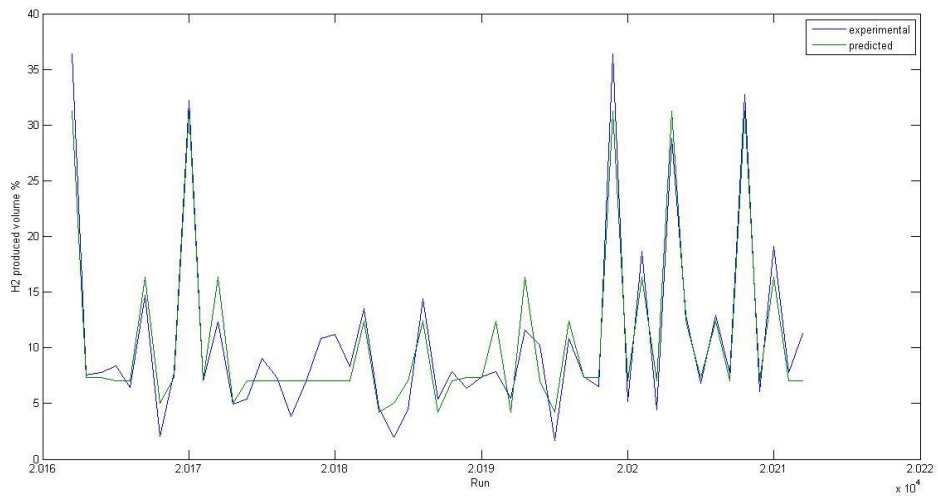


Figure 4.16: ANN's plot between the actual experimental data and the predicted data

4.6 MATLAB's ANN (NEWNARX Function) results

The newnarx function gives almost the same results as the newff function, producing the same graph and but with a little difference of the error percentage. Also the training takes much more time than the newff function, as for the newnarx function what it does is that it calculates for all of the data with inputs and outputs for one iteration only in the next iteration it will consider the result of the outputs of the first iteration with the inputs for the second iteration thus the longer time in the training process.

❖ For 5 Hidden neurons: Current MSE: 5.406%

Figure 4.17 shows the training window of the newnarx function, one of the differences that could be noticed is the longer time this ANN takes to produce the result because of the reason mentioned before.

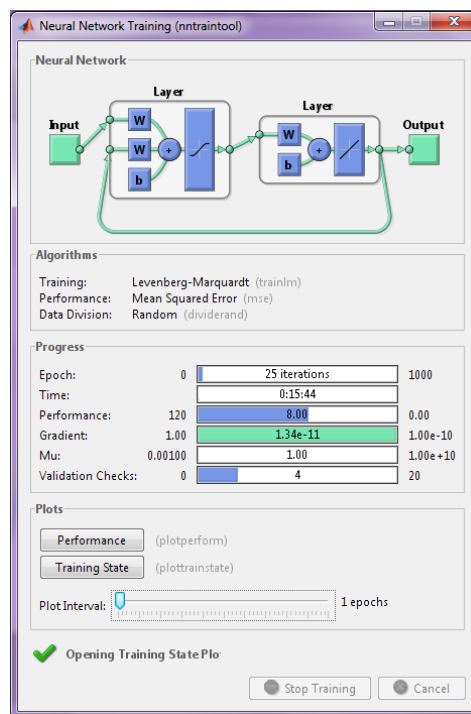


Figure 4.17: ANN training window (newnarx function).

Figure 4.18 shows the training state plot vs epochs, where it shows the plot for the gradient, mu, and validation checks at 25th epoch which is the number of iteration for this ANN function.

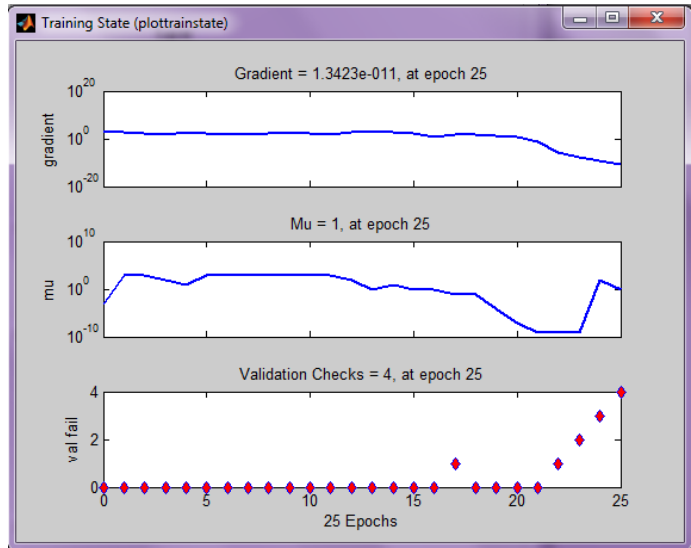


Figure 4.18: Training State Plot.

Figure 4.19 shows the performance of the ANN with relation to the MSE with the iterations number. Comparing the training set with the validation and testing sets and it also shows the best performance that gives the minimum error value. At the 25th epochs (iteration) the error at its minimum for this ANN function for the training, validation and testing sets.

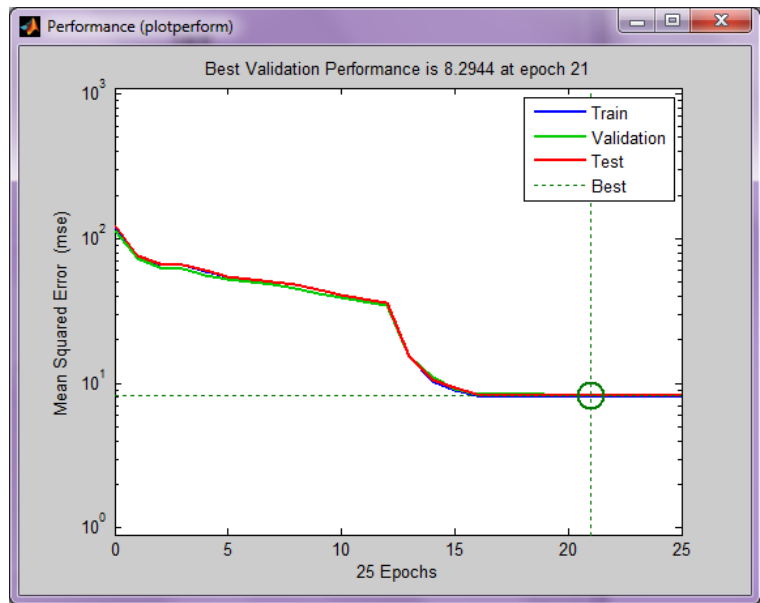


Figure 4.19: Performance Plot.

Figure 4.20 shows the final output of the ANN, as it plots the Actual experimental data and the ANN predicted results. As it can be noticed, it does not vary much from the previous plots by the other functions. It only differs in the error percentage calculated by a very small margin.

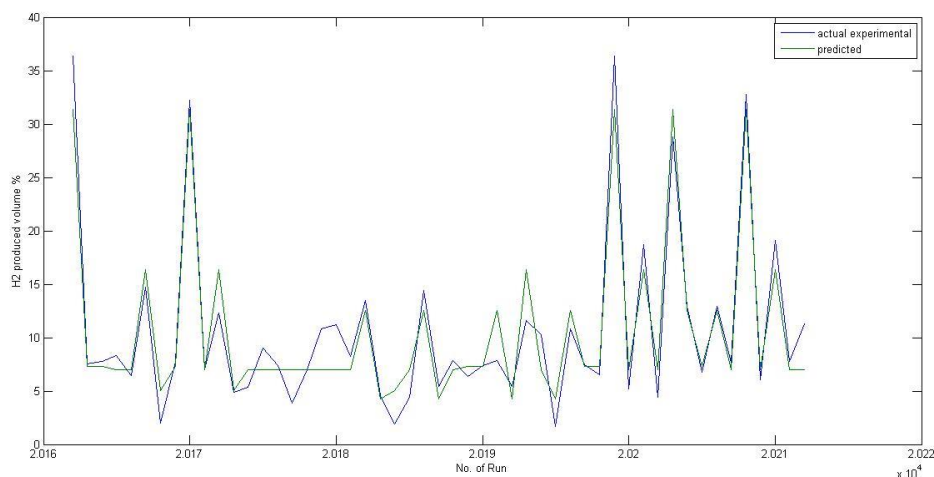


Figure 4.20: ANN's plot between the actual experimental data and the predicted data

From all the plots produced by the ANNs and SIMCA-P, a straight line is shown for the predicted data between data point no. 20174 to data point no. 20181, the reason for this straight line is that the input data for those data points have the same data for Temperature, PE/Biomass ratio and S/F ration, so for the models and according to the relationship established, they establish that it would produce the same output. Hence, the straight line is shown for the predicted data in that range.

As the performance of the ANNs is statistically measured by the mean square error (MSE) and regression coefficient (R^2), and from the figures above, the MSE is calculated and explained, whereas the R^2 is shown in the graphs but not mentioned as a tool of validating the ANNs. When the value of R^2 gets closer to value of 1.0, it shows that the model is successful and that the predicted data is almost the same as the experimental data. For all the ANNs in this study, it can be seen that the value of R^2 from the figures above (figure 4.9, 4.12, 4.15) is about 0.94 which shows that the models of the ANNs are successful for the prediction process.

After simulating all the ANNs, table 4.2 summarizes the efficiency of each function of the ANN that was used in this project by the number of hidden neurons used and it shows the MSE percentage at each number of the hidden neurons. From the table, it can be noticed that the error percentage varies from 5.4% to 5.5% which could be considered almost the same and it shows that using any of these functions to run the ANN would produce almost the same result and comparing the graphs from all these functions with the one produced by SIMCA-P software, it can be shown clearly that the ANN has produced better results in prediction the hydrogen yield of the process of biomass gasification.

Table 4.2: A comparison between different types of ANN Functions.

Type of ANN Function	Hidden Layer Neurons	MSE Percentage
Newff	5	5.500 %
	10	5.401 %
	15	5.425 %
Normalized newff	5	5.500 %
	10	5.401 %
	15	5.425 %
newfit	5	5.413 %
	10	5.471 %
	15	5.503 %
Newnarx	5	5.406 %
	10	5.460 %
	15	5.498 %

5. CHAPTER 5: CONCLUSION AND RECOMMENDATION

In conclusion, the research study promises good results and if they study goes as planned and achieves its objectives, it will bring a great benefit to the students and researchers in Universiti Teknologi PETRONAS (UTP) as it will help them to model their processes and to know the results that might come out of that process. As the biomass gasification is the hope for the future energy resources, this research might bring more attention to the technologies related to this field and the production of renewable energy resources to help the development in the countries with a lot of agricultural waste as Malaysia. This project is feasible when taking into account the time constraint and the capability of the student with the help of the supervisor.

From the preliminary analysis done, the data shows a good ability to obtain results using a prediction model like the ANN. SIMCA-P13 acts as a linear tool and that explains that the software was not able to obtain good relation between the inputs and outputs of the process, and that means that a non-linear software tool like the ANN would be better in solving the model and obtain good results. Also the preliminary analysis showed the relation and effect between each input with the output (hydrogen composition), as increasing the temperature would affect by increasing the composition of hydrogen produced comparing to the PE-PET and S/F (steam to feed ratio).

From the results obtained from the ANNs model and different functions used, the percentage error produced was very small and comparing the graph of the predicted data vs the actual experimental data between the ANN model and SIMCA-P model, shows that the ANN is a good way of modelling the process of hydrogen production from biomass gasification, the MSE percentage obtained was in the range of 5.4% to 5.5% which could be considered a good value as to some of the constraints of the real process and the way in obtaining the experimental data.

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APPENDICES

Appendix A:

Here are the results of the ANN (NEWFF & NEWFF –with normalized data- functions) with different number of Hidden neurons and the associated MSE error percentage.

❖ For 10 Hidden neurons: Current MSE: 5.401%

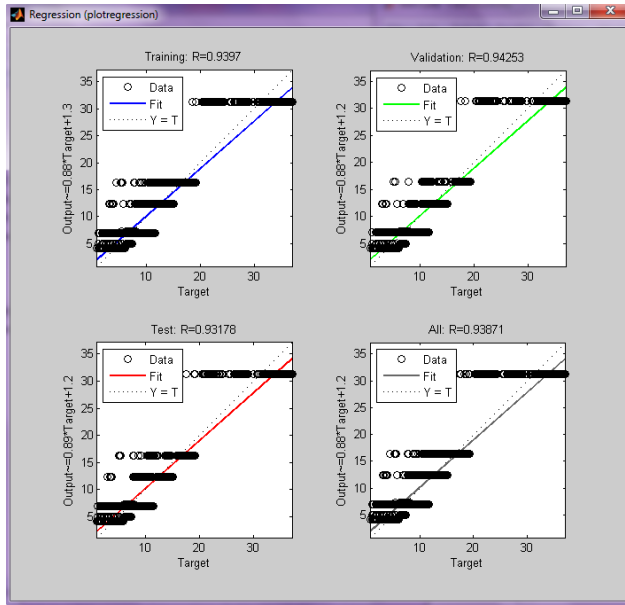


Fig A.1: Regression Plot

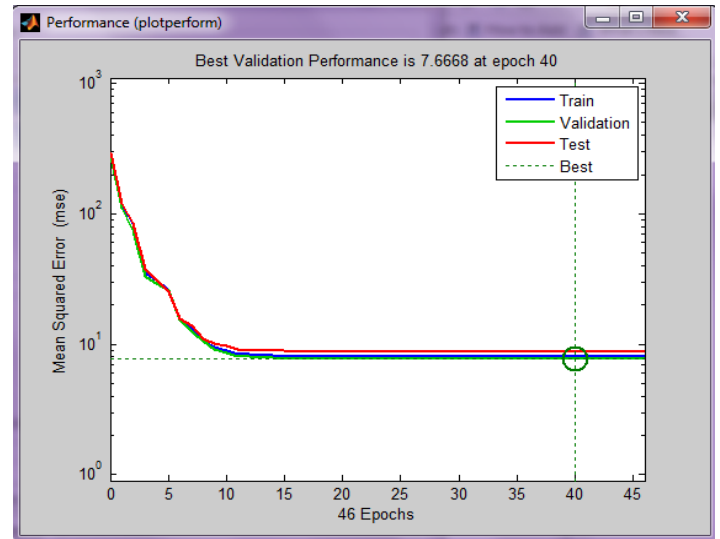


Fig A.2: Performance Plot

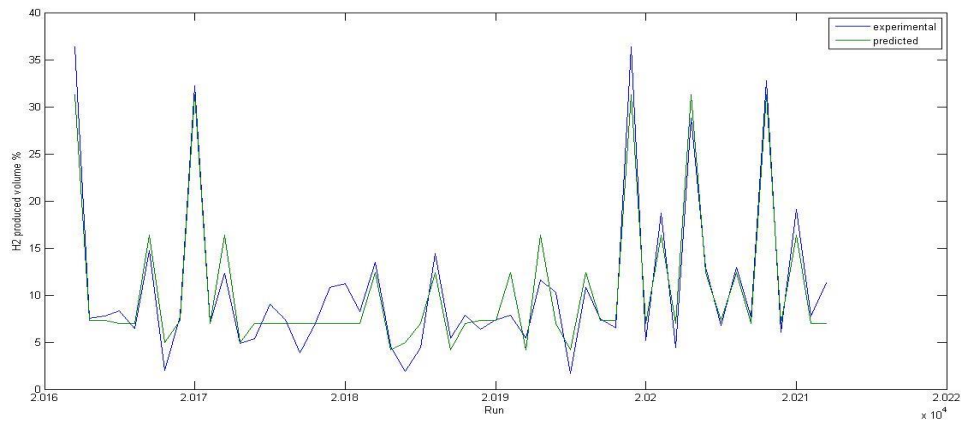


Fig A.3: Comparison between Actual experimental and predicted data

❖ for 15 Hidden neurons: Current MSE: 5.425%

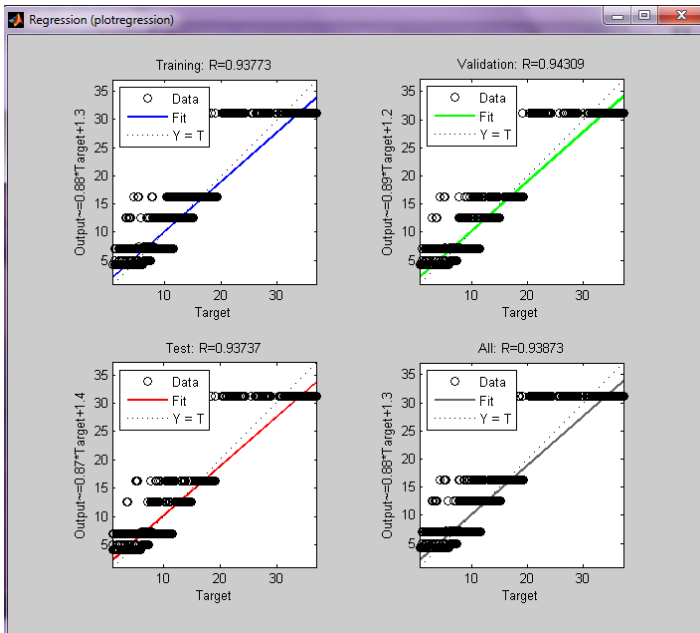


Fig A.4: Regression Plot

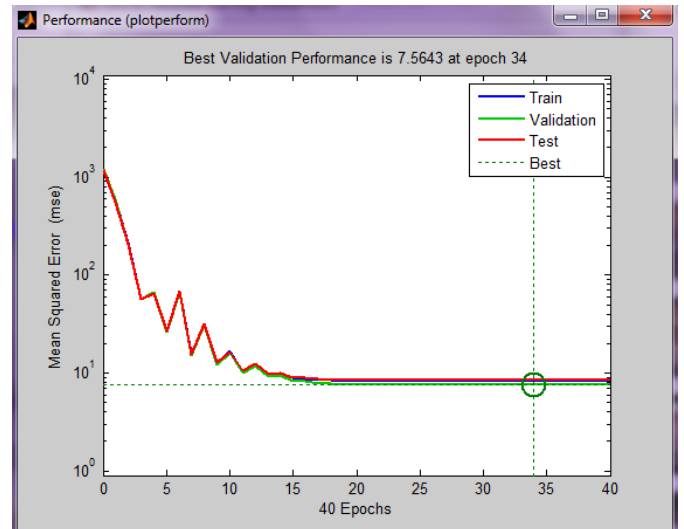


Fig A.5: Performance Plot

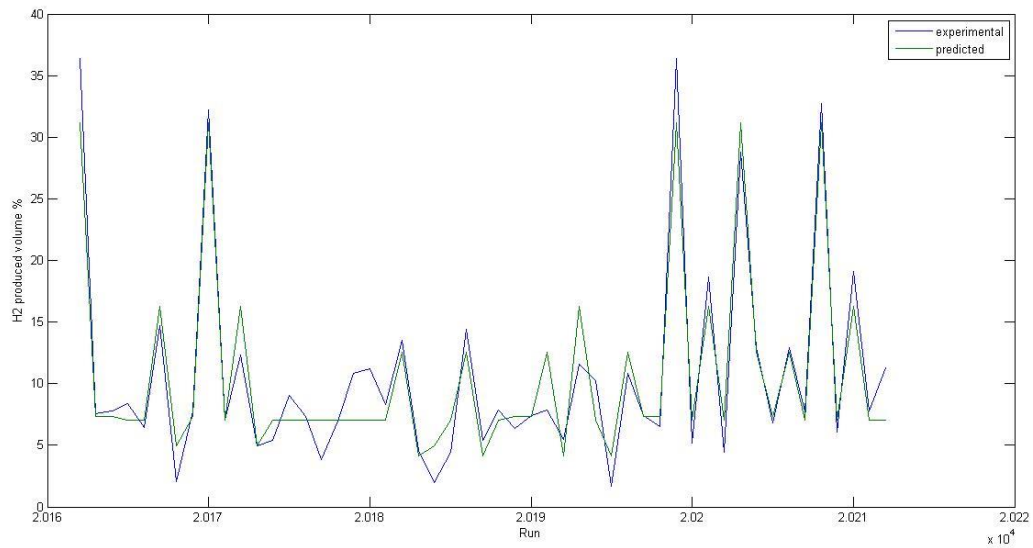


Fig A.6: Comparison between the actual experimental and predicted data

NEWFIT function with different number of neurons and the MSE percentage:

❖ For 10 Hidden neurons: Current MSE: 5.471%

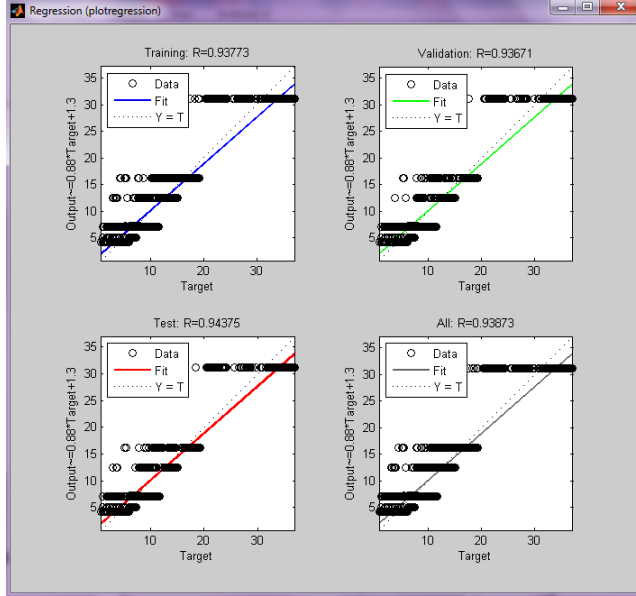


Fig A.7: Regression Plot

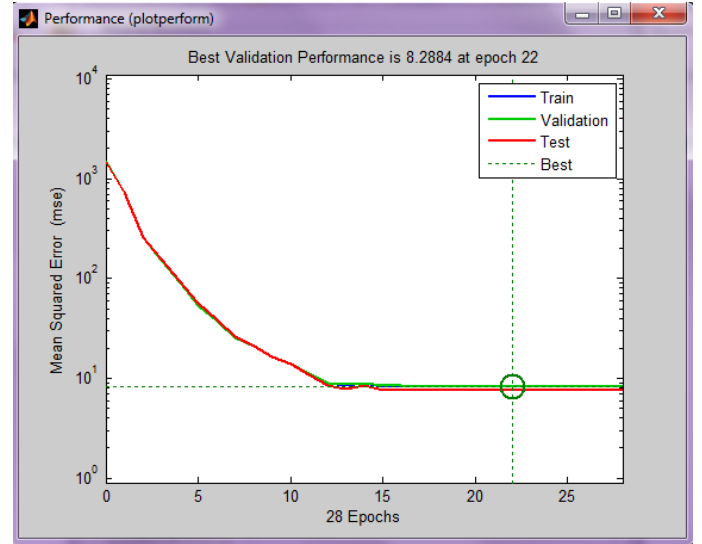


Fig A.8: Performance Plot

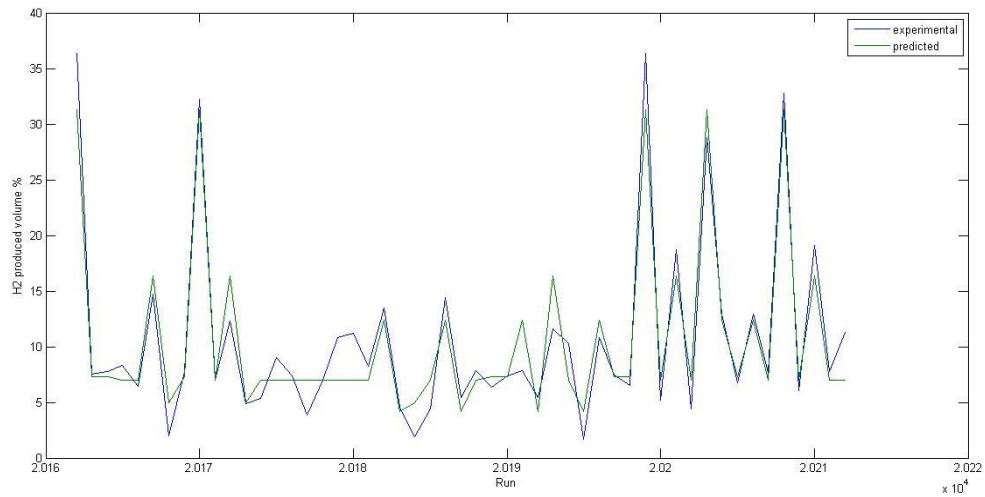


Fig A.9: Comparison between Actual experimental and predicted data

❖ for 15 Hidden neurons: Current MSE: 5.503%

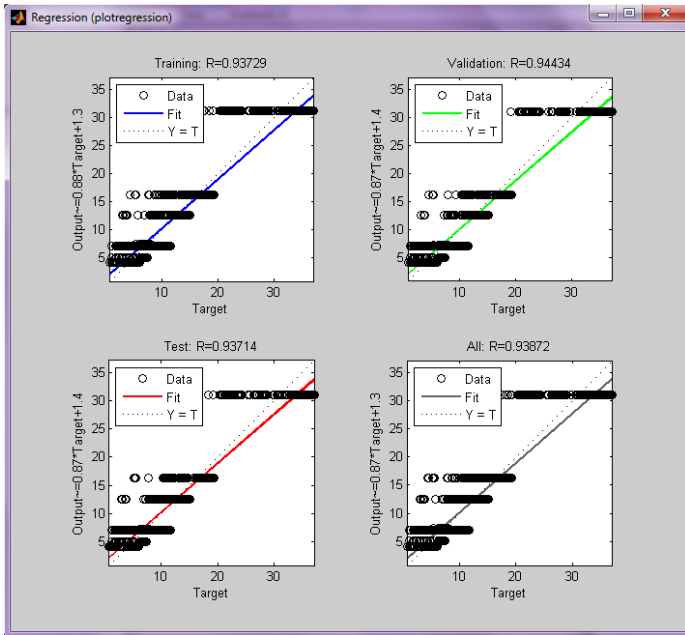


Fig A.10: Regression Plot

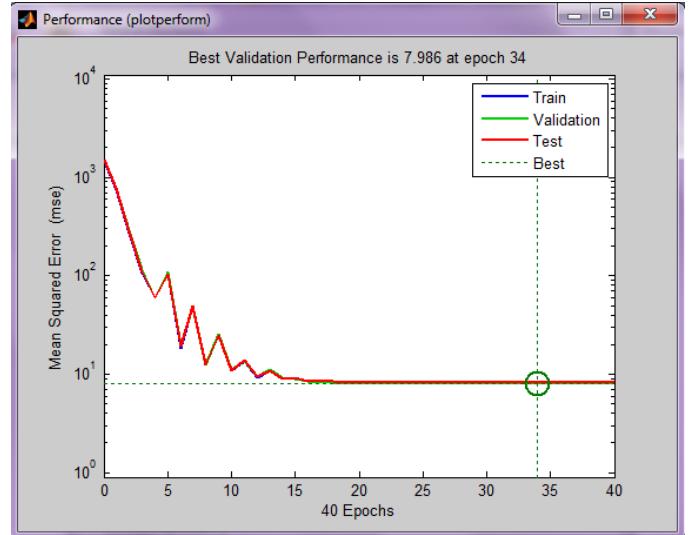


Fig A.11: Performance Plot

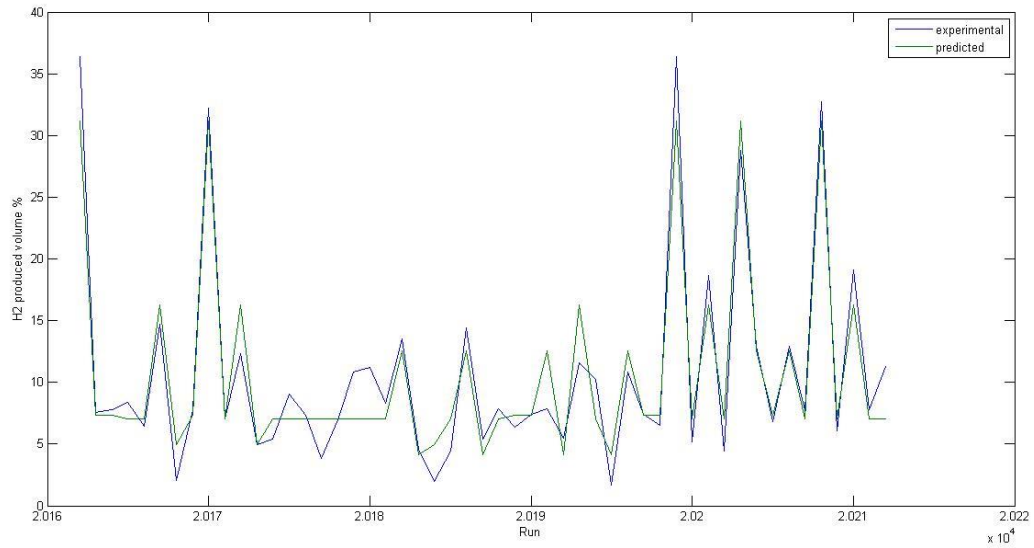


Fig A.12: Comparison between the actual experimental and predicted data

NEWNARX function with different neurons and MSE percentage:

❖ For 10 Hidden neurons: Current MSE: 5.460%

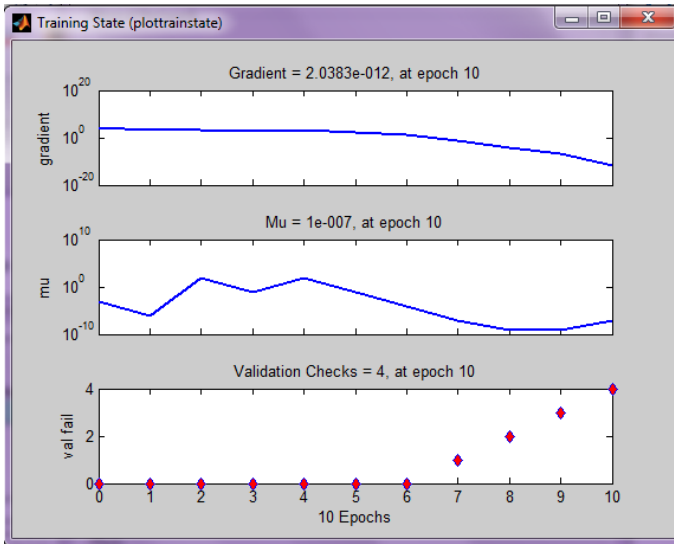


Fig A.13: Training state Plot

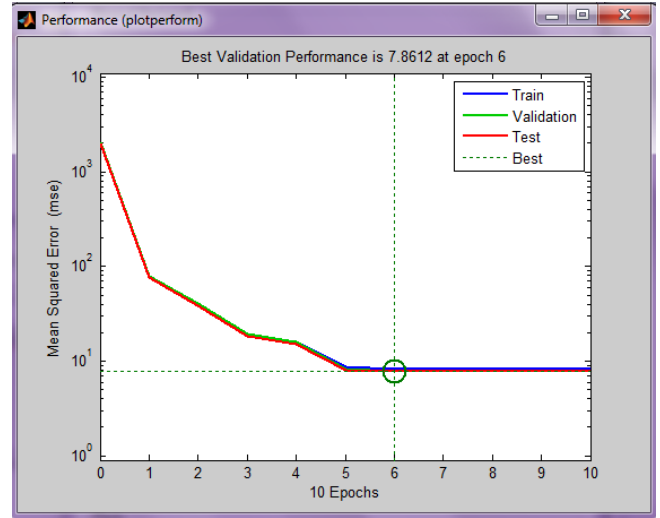


Fig A.14: Performance Plot

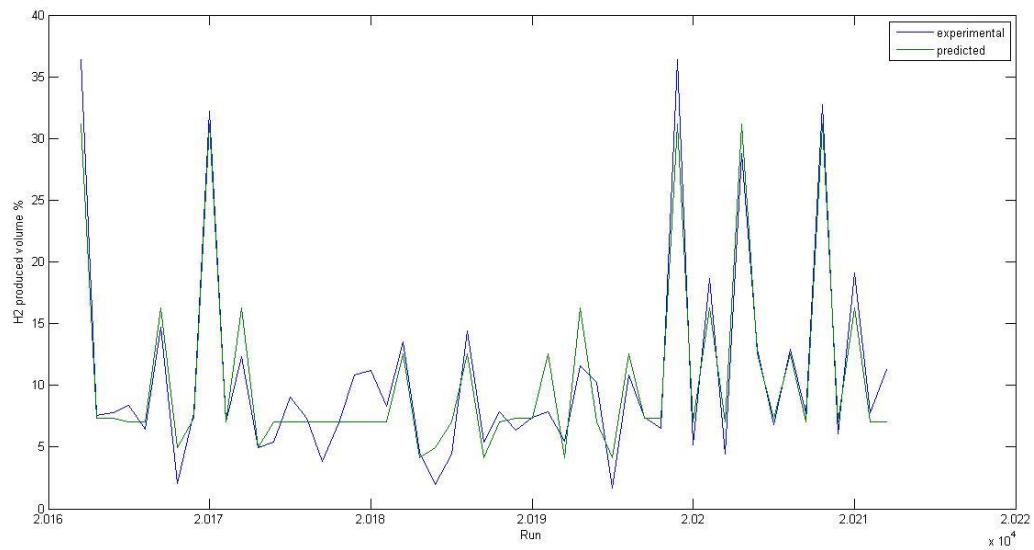


Fig A.15: Comparison between the actual experimental and predicted data

❖ For 15 Hidden neurons: Current MSE: 5.498%

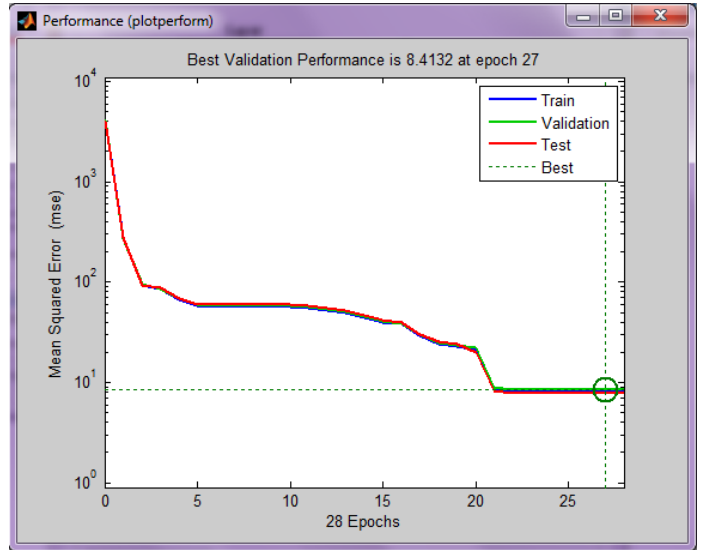
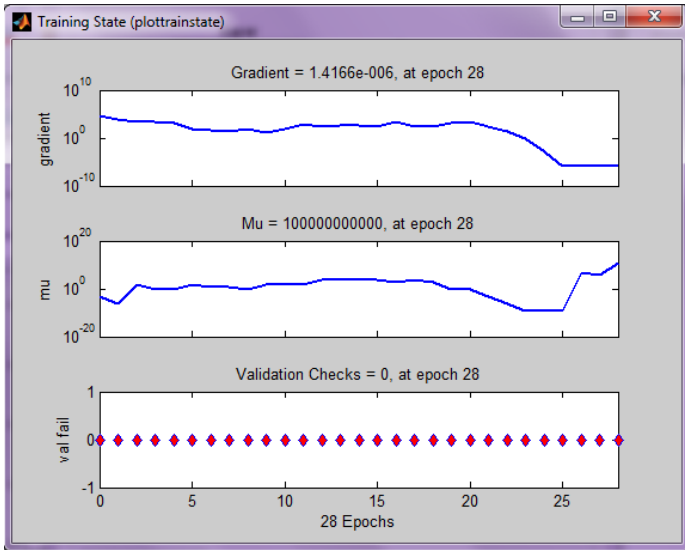


Fig A.16: Training state Plot

Fig A.17: Performance Plot

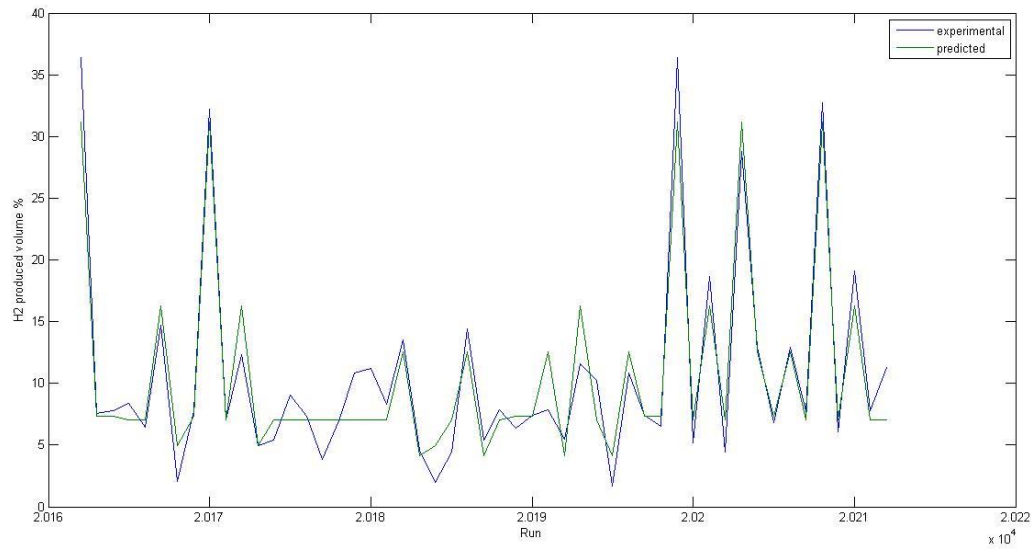


Fig A.18: Comparison between the actual experimental and predicted data