APPLICATION OF ARTIFICIAL NEURAL NETWORK IN PREDICITON OF METHANE GAS HYDRATE FORMATION RATE

MEGAT NAIMPUTRA BIN MGT RODZEP

CHEMICAL ENGINEERING

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By

Megat Naimputra Bin Mgt Rodzep

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Dissertation submitted in partial fulfillment of
the requirements for the
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Universiti Teknologi PETRONAS
32610, Bandar Seri Iskandar,
Perak Darul Ridzuan

CERTIFICATION OF APPROVAL

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Approved by,

_____

(Dr Bhajan Lal)

UNIVERSITI TENOLOGI PETRONAS

BANDAR SERI ISKANDAR, PERAK

September 2015

CERTIFICATION OF ORIGINALITY

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

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MEGAT NAIMPUTRA BIN MGT RODZEP

ABSTRACT

This work aims to use Artificial Neural Network (ANN) in prediction of methane gas hydrate formation. There are a lot of thermodynamic modelling have been developed and applied in prediction of the formation gas hydrate however there is still none yet proven model that can predict the formation rate of methane gas hydrate. This study emerges as to build a kinetic model consume time and are very complex due to stochastic behavior of gas hydrate. Therefore, ANN methods show the best potential technology to be used for development of model to predict the formation rate of gas hydrate. The aims of this study are to develop artificial kinetic models by using ANN that can predict the growth rate of formation of methane gas hydrate. To determine the best configuration to be used in ANN involving the number of layers and number of hidden neurons to be used in ANN models. In this study, pressure and temperature are used as the model's input with the growth rate of methane gas hydrate as the model's output. The result shows every ANN model has different best configuration in prediction of methane gas hydrate. From the study also few limitation of ANN also addressed.

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

The discovery of gas hydrates is long way back in 18th century by Sir Humphrey Davy. Gas hydrates or clathrate is crystalline solid compounds that are formed in mixture of water and volatile liquids or non- or slightly polar low molecular weight gases. Hydrate form when hydrogen bonded water molecules form cage like structure, known as cavities in the crystalline lattice or the host [1, 2]. In these cavities hydrate-forming molecule or guest molecules are trapped and stabilize the hydrate structure. General conditions for gas hydrates formation are high pressure, low temperature and gas composition of the guest molecules in supersaturated solution[1].

The structure of gas hydrate varies depending on the gas molecules that are trapped within the cavities. Common gases that form gas hydrates are methane, ethane, propane and carbon dioxide. These guest molecules form different type or structure of gas hydrates depending on their sizes and shape. Currently, three different hydrate structures are known and well-studied as in the Figure 1.1; cubic structure I (sI), cubic structure II (sII) and hexagonal structure H (sH). These structures form depending on the guest molecules that are trapped within the cavities. The unit cell of sI hydrate consist of 46 water molecules forming two small cavities and six large cavities[1, 2]

.

The small cavity has the shape of pentagonal dodecahedron (5^{12}), while large cavity has the shape of a tetradecahedron ($5^{12}6^2$). The sII hydrate unit cell consists of 136 water molecules forming sixteen small cavities and eight large cavities. Similarly to sI shape, structure of sII small cavity is also pentagonal dodecahedron (5^{12}) but the large cavity has the shape of hexadecahedron ($5^{12}6^4$). In sH structure, the unit cell is divided into three small cavities of (5^{12}), two medium ($4^3 5^6 6^3$) and one large cavity of ($5^{12}6^8$) as shown in Figure 1.1.

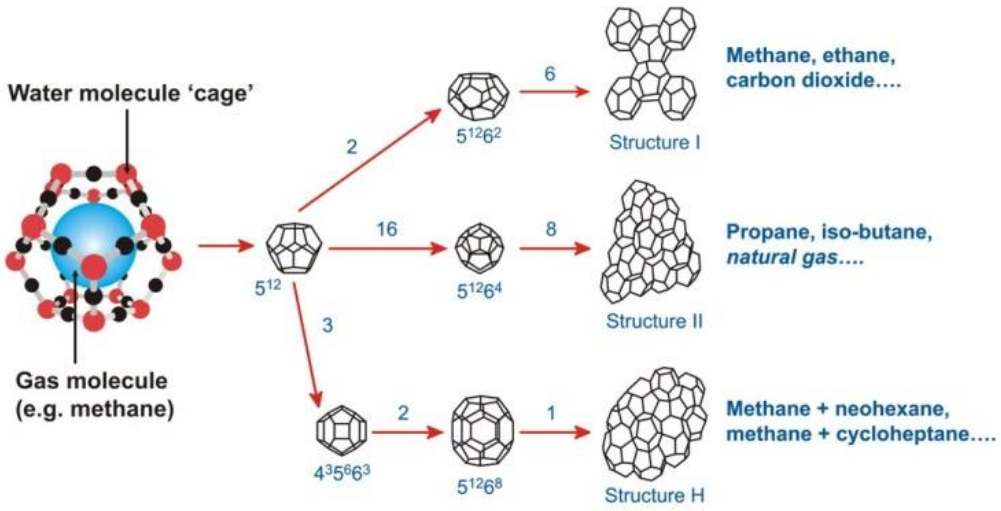

Figure 1.1: Common Structures of Gas Hydrates

Gas hydrate is considered as new energy sources aside from fossil fuel as it is abundantly found in onshore and offshore. It is estimated, approximately 200,000 trillion cubic feet of methane could exist in hydrates form in the U.S. permafrost regions and its surrounding waters However, further study on how to extract the methane from gas hydrate is need. Gas hydrate is also considered as a technology for storage and transportation of gases such as hydrogen gas etc.

In contrary, due to low temperature and high pressure conditions that exist in deep offshore and deep well drilling in oil and gas industries, gas hydrate easily formed and plugs oil and gas production pipeline, facilities and drilling wells. This is a major problem to flow assurance in oil and gas industry. When gas hydrates form

it causes pipeline plugging and to remove the plugging is very expensive. The prevention of hydrate formation requires a vast amount of money as much 10-15% of production cost and the removal cost of this hydrate from an offshore pipeline somehow around $2-$4 million [3, 4].

Water removal, heating, depressurization and chemical inhibition are the available gas hydrate mitigation methods. Currently, chemical inhibition is used due to economic applicability advantage. Gas hydrate inhibition is study can be categorized in two different areas, thermodynamics and kinetics; Thermodynamic inhibition concentrate on measuring the pressure-temperature condition at which three phases, liquid-hydrate-vapor (L-H-V) are in equilibrium and aimed in shifting the L-H-V equilibrium curve to low temperature and high pressure region. Figure 1.2 show the concentration of thermodynamic inhibitor used in industry and typical inhibitor are methanol but it requires up until 60 wt% concentration.

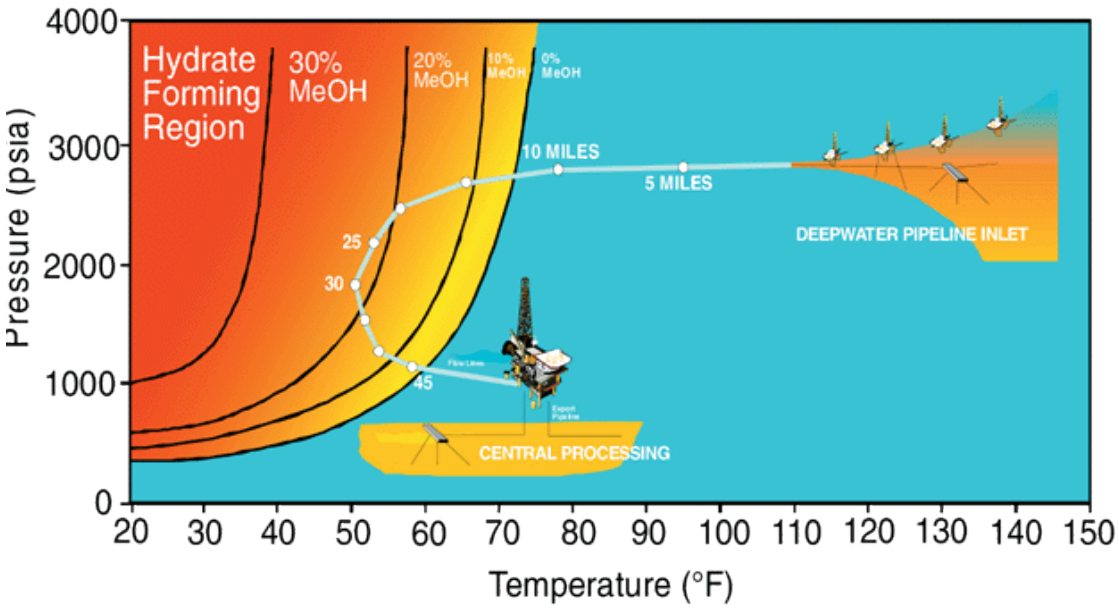

Figure 1.2: Formation of Gas Hydrates at equilibrium phase

Whereas in kinetic inhibition of hydrate concentrate on delaying the induction time and /or crystal growth of hydrate formation, polymers are commonly applied for kinetic inhibition and are used at less concentrations (> 2 wt%).

In order to enhance the mitigation of gas hydrate formation in pipelines, understanding and modeling of gas hydrate formation and growth kinetics becomes a necessity. While extensive studies are available are on thermodynamics of gas hydrate, no acceptable model or well established model has been developed for the kinetics of gas hydrates, thus making the thermodynamics of gas hydrate well understood than kinetics. There have been few attempts in modeling of kinetics of gas hydrates but there is still no good result due to the stochastic nature of hydrate formation. Also, not only the stochastic nature but gas hydrate formation depends on factors such as subcooling, experimental apparatus and stirring speed.

Kinetics of hydrate depends on induction time and crystallization of hydrate growth. Induction time is the time taken for crystal nuclei to form and when nuclei have reached the requisite critical size they will grow and form hydrate crystals[5, 6]. The growth or formation process refers to the growth of a stable hydrate nuclei till it become solid hydrates. Mass and heat transfer are essential in hydrate growth process although most of the nucleation parameters such as surface area, agitation, gas composition and displacement from equilibrium conditions are at stable region. Figure 1.3 shows a plot of gas consumed verses time for a typical gas hydrate kinetic experiment indicating various stages in the experiment. The induction time is stochastic or unpredictable thus require extra attention and difficulty in modeling but hydrate growth process is quite predictable and therefore give a relief for hydrate formation modeling.

Artificial Neural Networks (ANN) are quite simple where it is an electronic models inspired based on the biological nervous system[7]. The brain basically learns from experience and so does ANN. It is a proof that some problems are beyond the scope of present computers are indeed solvable by this system[8]. This

modeling also assures a less technical way toward developing machine solutions. This innovative approach of solving problems also provides a smoother degradation during system overload than its traditional counterparts.

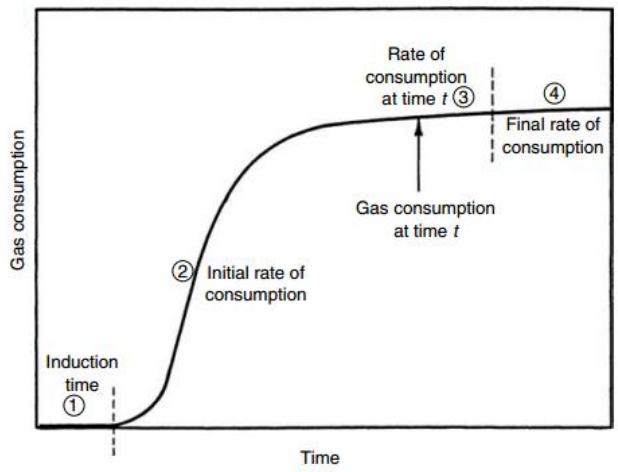

Figure 1.3: Gas Consumption vs. time for hydrate formation

Therefore, the application of ANN in prediction of methane gas hydrate formation rate is crucial for better understanding the formation rate of a gas hydrate. If this application of ANN successfully can predict the formation rate the studies for prevention gas hydrate formation and plug can be studies well. When a gas hydrate formation can be predicted the inhibitor quality for kinetic inhibition will be improved and the result will be more accurate. This work therefore seeks to develop an ANN model to predict the formation rate of pure methane gas hydrate.

1.2 Problem Statement

Gas hydrate plug oil and gas pipeline, the understating and modeling of kinetics gas hydrate formation growth is necessary for mitigating hydrate plugs problems. While extensive studies are available are on thermodynamics of gas hydrate, no acceptable model or well established model has been developed for the kinetics of gas hydrates. Therefore, this work seeks to develop an ANN model to predict the growth rate of formation of pure methane gas hydrate.

1.3 Objectives

The objectives of this research are:

1. To develop artificial kinetic models by using ANN that can predict the growth rate of formation of methane gas hydrate.
2. To determine the best configuration to be used in ANN involving the number of layers and number of hidden neurons to be used in ANN models

1.4 Scope of Study

The scopes of study for this research are directed towards developing an artificial kinetic model by using neural network starting from training of ANN models to the testing and compare the performance and result from the model. ANN in the Matlab software is used for the modelling and experimental data in open literature are used to train and verify the model.

CHAPTER 2

LITERATURE REVIEW

2.1 Previous Kinetic Modelling

The first kinetic modeling was developed by Englezos et al. by combing crucial key factors of hydrate formation and it was tested under isothermal and isobaric condition. The model indicates the formation is depending on appearance of nuclei and its growth. However, the growth is dependent on interfacial area, pressure, temperature and the degree of supercooling[9]. The model can be summarized as three-step process transport of the gas from bulk of the gas phase to liquid bulk phase, diffusion of gas from the bulk of water phase and liquid film to hydrate crystal-liquid interface through a laminar diffusion layer around the hydrate particle, and "Reaction" at the interface, which is adsorption process describing how the gasses incorporated to the cavities of water structure and stabilization of framework of the structure. The global rate of reaction used in Englezos et al. is as equation (1)

$$R_y(t) = K(f - f_{eq}) \tag{1}$$

Even though this Englezos et al. model is proven but there are lots of shortcoming where it only fitted with structure I growth model which are methane, ethane and carbon dioxide. Also the model is very sensitive to number of moles consumed at the turbidity point, to which is not easy access. The calculation of critical

radius is assumed at equilibrium pressure not system pressure thus it indicates force imbalance. Another problem was that; the predictions were accurate only for duration of 80min.

Later in 1993, Skovborg modified Englezos model by simply replace one parameter inside the model. In Englezos et al. model particle population balance is used but in Skovborg model it is replace by a simple reaction between total surface area of the hydrate particles with the amount of gas consumed [10]. Skovborg made an analysis over Englezos et al. model and pointed out that rate of reaction, K* simply insensitive because by increasing and decreasing the value of K* with all other parameter remain the same does bring significant agreement between the model and the results of experiment. Skovoborg assume that this result is because of one of the parameter that controlling diffusion is assigned wrongly.

The basis for such a model is, in the water bulk phase equilibrium exists between the liquid water with some dissolved gas and the hydrate particle in other word the interface is equilibrium between liquid phase and gas phase; Gas is transported from the gas-water interface to the water bulk phase according to simple-film theory.

The mass transfer and total gas consumption are stated in equation (2) and the extended or simplified model is stated as equation (3). This simplified model yield satisfactory result for the data.

$$\frac{dn}{dt} = K_L A_{(g-l)} C_{w0} (x_{int} - x_b) \tag{2}$$

$$\frac{dn_{tot}}{dt} = \sum_{i=1}^{NG} \frac{dn_i}{dt} = C_{w0} \sum_{i=1}^{NG} K_L^i A_{(g-l)} (x_{int}^i - x_b^i) \tag{3}$$

In 2012, Zare Nezhad et al. come out with a kinetic model for formation of hydrate in isothermal-isochoric systems. The model is based on based on the time variations of reaction chemical potential of hydrates former such as methane, ethane, propane and etc. The model consider homogenous reaction between gas and water proceeding in an isochoric system at a fixed temperature [11]. The result shows that at high agitation intensities when the intrinsic kinetic is rate controlling, the trends of normalized gas consumption profiles of different pure gas hydrate formation processes follow a unique path. The proposed model can be conveniently used for studying the energy conversion processes via gas hydrate formation in isothermal–isochoric systems.

Recently, Nazari et al. (2013) developed a kinetic model for gas hydrate mitigation in the absence/presence of low-dosage water-soluble ionic liquid for methane. A Five step mechanism is resolved for this kinetic modeling of methane hydrate formation [12] as follow: Dissolution of methane molecules in the aqueous phase; Clathrate and labile cluster formation by dissolved methane and water molecules; Formation of crystal unit cell by clusters; Formation of a crystal nucleus by unit cells; Formation of hydrate crystal

From all these steps the mechanism, general rate of formation is derived from equation (4)

$$r_i = \frac{dc_i}{dt} = k c_i^{\alpha} c_j^{\beta} \tag{4}$$

This Nazari et al. model however experimented to test the Ionic Liquids (IL) effect on the formation of gas hydrate and the results are showing ILs is affecting the formation of hydrate but still can be studies further.

Kinetic of gas hydrate is a very complex to be modeled and showing an accurate result from a kinetic model is nearly impossible because of the formation of hydrates is very ambiguous and formation depended on different driving forces. Furthermore, growth rate is dependent on the composition and testing conditions for the gas hydrate formation. Therefore, emerge the new technologies that can help prediction of gas hydrate.

2.2 Artificial Neural Network

An Artificial Neural Network (ANN) is an information processing paradigm such as the brain and how its process information or pattern [13]. The key component of this paradigm is the novel information processing system structures. It is composed of large number neurons (highly interconnected processing elements) functioning in unison to solve a specific problem. ANN is like people and it learns by experience and example. An ANN is designed for a specific application, such as data classification or pattern recognition, through learning processes. Learning in the biological systems comprises the adjustments to the synaptic connections that exist in between the neurons.

A neuron is a device that comprise with numerous inputs and one output[14]. The operation of a neuron has two modes; the mode for training and the mode of. In the training mode, neuron can be trained to identify or differentiate for particular input patterns. When it comes to the using mode, when a taught input data or pattern is detected by neuron at the input; its associated output turn out to be the current output. If the input pattern is not in the taught list of input patterns, the outcome will be determined by the firing rule. The rule will determine the output of the neuron configuration work. Figure 2.2 show how simple neuron configuration work.

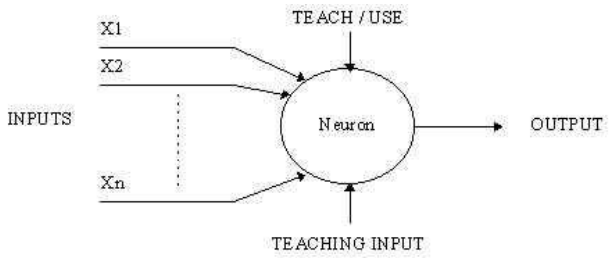

Figure 2.2: Simple Neurons Configuration

An important application of neural networks is pattern recognition. Pattern recognition can be implemented by using a feed-forward (Figure 2.3) neural network that has been trained accordingly. During training, the network is trained to associate outputs with input patterns. When the network is used, it identifies the input pattern and tries to output the associated output pattern. The power of neural networks comes to life when a pattern that has no output associated with it, is given as an input. In this case, the network gives the output that corresponds to a taught input pattern that is least different from the given pattern. Feed-forward ANNs (Figure 2.3) allow signals to travel one way only; from input to output. There is no feedback (loops) i.e. the output of any layer does not affect that same layer. Feed-forward ANNs tend to be straight forward networks that associate inputs with outputs. They are extensively used in pattern recognition. This type of organisation is also referred to as bottom-up or top-down.

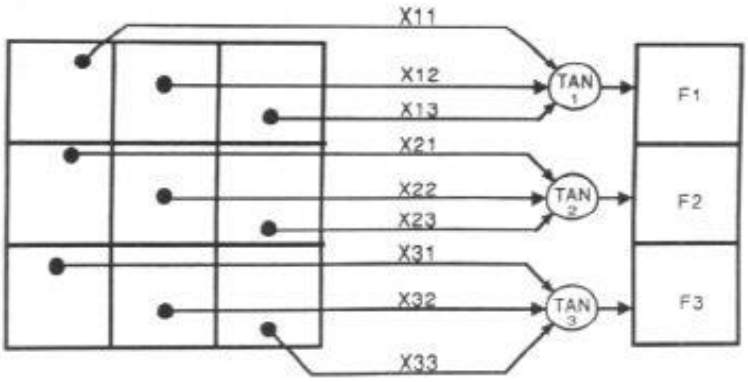

Figure 2.3: Example of Pattern Recognition of ANN

2.2.1 Multilayer perceptron

A multilayer perceptron (MLP) is a model that use feedforward artificial neural network to maps sets of inputs onto a set of relevant outputs. A MLP model contains of multiple layers of nodes, each node is a neuron (processing element) with a nonlinear activation function in a fixed graph, with each layer is completely connected to the next layer except the input nodes[7, 8, 14]. MLP employs a supervised learning technique for training of the network called backpropagation.

Learning occurs in the perceptron by changing connection weights after each piece of data is processed, based on the amount of error in the output compared to the expected result. This is an example of supervised learning, and is carried out through backpropagation, a generalization of the least mean squares algorithm in the linear perceptron.

Backpropagation is the abbreviation for backward propagation calculation of errors. This method is very common training of ANN. Backpropagation calculate the gradient of a loss function in the network with respect to all the weightage within the network. The gradient then fed to the optimization process which in turn applies to update the weights, in order to minimize the loss function. Backpropagation needs a known desired output for each input data in order to calculate the gradient.

When a specified training pattern is fed to the input layer, the weighted sum of the input to the j^{th} node in the hidden layer is given by

$$Net_j = \sum w_{ij} x_j + \theta_j \tag{5}$$

Equation (5) is to calculate the aggregate of input data to the neurons. The term is the weighted value from a bias node that frequently has 1 an output value. The "Net" term, also known as the action potential, is passed onto an appropriate activation function used to decide whether a neuron should fire. Since algorithm used for the activation function is differentiable, Sigmoid equation is used as the activation function,

$$O_j - X_k - \frac{1}{1+e^{Net_j}} \tag{6}$$

For error calculation and weight adjustment is backpropagation the equation used are as follows, If the value of the output node of actual activation, k, is Ok, thus the expected output for node k is t_k where in equation (3) Ok (1- Ok) is the derivative of Sigmoid function.

$$\delta_k - \Delta_k O_k(1 - O_k) \tag{7}$$

The formulas used to modify the weight, $w_{j,k}$, between the output node, k, and the node, j is:

$$\Delta w_{j,k} = l_r \delta_k x_k \tag{8}$$

Where $\Delta w_{j,k}$ is the change in the weight between nodes j and k, l_r is the learning rate.

For errors of the backpropagation, equation (9) is employed. Ideally, the error function should have a value of zero when the neural network has been correctly trained. This, however, is numerically unrealistic.

$$E - \frac{1}{2}\sum(\sum(t_k - O_k)^2) \tag{9}$$

2.2.2 ANN on Gas Hydrate Formation

Zahedi et al. has done a prediction of hydrate formation temperature with assessment by using two different methods. The assessment included statistical model and Artificial Neural Network. Statistical model used were Engineering Equation Solver (EES) and Statistical Package for Social Sciences (SPSS)[15]. Whereas, Multilayer Perceptron (MLP) is used to predict the hydrate formation temperature by ANN.

Statistical method used correlation to predict hydrate formation temperature such as Berge-correlation and Kobayashi and Sloan-correlation. For neural network the MLP used 70% of experimental data is used for training purposes and the rest of data are predicted to prove the prediction. From 203 experimental data point it is found out ANN can predict excellently the 30% of the data for the hydrate formation temperature.

On the other hand, Ghavipour et al. also studies the use of neural network in predicting the hydrate formation conditions. The experiments uses six different gas mixtures were done and more than 130 hydrate equilibrium points in the pressure range of about 450–3000 psia. The input for ANN training are the pressure and specific gravity of the gas mixture and in this neural network prediction 70% of data are used to train the network and the remaining is used to test the network[16].

The study also tests the four different methods of training in neural network for modelling (1) Levenberg-Marquadt backpropagation (2) gradient descent with momentum and adaptive learning rate backpropagation (3) scaled conjugate gradient back propagation (4) one-step secant back propagation. The study also uses variable of numbers of neuron and number of hidden layer for each of training method. The

result showing that using Levenberg-Marquadt backpropagation training, ANN can predict very well the formation with lowest mean square error.

From the literatures, it is proven that ANN is a technology that is showing promising attributes to predict the growth rate of methane gas hydrate by teaching the neural network with every data that has been collected through previous experiments on gas hydrate formation.

CHAPTER 3

METHODOLOGY

ANN has been used to predict the methane gas hydrate growth rate with pressure and temperature as inputs. To accurately predict the hydrate growth rate using ANN, a Multilayer Perceptron (MLP) was employed.

Levenberg-Marquardt backpropagation or trainlm was used to train the MLP. The trainlm training method is a dependable training method as its algorithm is designed to work with complex data based on theoretical assumption. Result produced by trainlm also much faster and accurate compared to other training method neural network provides. The training based on trainlm produce a lower mean square error thus proving its suitability for training of predicting growth rate of methane hydrate. The MLP models used in the work will be identified herein as; ANN model One, ANN model Two and ANN model Three.

The data used for this models prediction is the experimental result from Ma et al. [17] and Sun et al. [18] as shown in Table 1. The experiments were performed in semi-batch reactor under isothermal and isobaric conditions with at constant pressure. The experiment studied the gas hydrate formation kinetics on the gas/water interface.

Table 1: Experimental data of methane hydrate growth rate from Ma et al [17] and Sun et al. [18]

Temperature T(K)	Pressure P (MPa)	Rate R(mm²/s)	Temperature T(K)	Pressure P (MPa)	Rate R(mm²/s)
276.3	8.73	3.886	281.3	8.04	0.09946
276.2	8.25	3.396	281.6	8.3	0.10498
276.2	7.88	3.157	278.8	6.7	0.12199
276.2	7.43	2.747	281.6	8.65	0.14215
276.2	7.09	2.363	281.4	8.5	0.14728
276.2	6.85	1.996	282.1	8.98	0.16202
276.2	6.54	1.841	281.6	8.8	0.14571
276.2	6.23	1.409	278.8	6.9	0.19019
276.2	5.62	0.864	281.6	8.95	0.23662
276.1	5.14	0.586	278.1	6.7	0.28314
276.1	4.93	0.38	281.6	9.1	0.25738
276.1	4.83	0.371	281.9	9.5	0.26543
276.1	4.79	0.328	278.8	7.5	0.37292
278.1	5.15	0.02794	281.8	10.35	0.38424
276.6	4.55	0.03143	278.1	7.4	0.38963
280.4	6.85	0.03385	278.1	7.55	0.35412
281.1	7.33	0.0445	278.4	7.9	0.48592
280.4	7.1	0.05983	277.9	8.1	0.6587
282.4	8.31	0.06448	277.9	8.5	0.81643
281.4	7.66	0.07096	278.1	8.9	0.77055
280.6	7.21	0.07535	277.8	9.12	1.61606
282.5	8.45	0.07815	277.4	9.57	1.9065
278.9	6.3	0.08491	277.9	10.3	1.8975
282.6	8.73	0.09026	277.9	10.7	1.86085
281.4	8.12	0.09356			

From data in Table 1, the ANN models will be tested based on the numbers of neurons configured in each ANN model as shown in Table 2. Also for

consistency, a constant 70% of the data was used training, 15% for validation and another 15% for testing or verification in all the ANN models with different neurons.

Table 2: ANN models and sets of configurations

ANN Model	Number of Layer	Number of Neurons
One	1	1
		3
		5
		8
		10
		12
		15
Two	2	1
		3
		5
		8
		10
		12
		15
Three	3	1
		3
		5
		8
		10
		12
		15

Table 3 shows the training parameters used in this work. Based on the parameters stated, the models will be trained until it satisfies the set parameter and ready for prediction. After completing the training, the models performance is evaluated.

Table 3: Set parameters of all ANN Models Training

Iterations	1000
Minimum gradient	1E -10
Validation Check	1000

The performance of every model is evaluated with two factors the Regression Values (R^2) and Mean Square Errors (MSE). R^2 values measure the correlation between predicted data from ANN models with the experimental data from previous studies. An R value of 1 means a close relationship, 0 a random relationship. The R^2 value is given by the equation:

$$R^2 = bX + a \tag{10}$$

Where R^2 = Correlation between predicted values with literature experimental values, bX = gradient of the R^2 of predicted values with literature experimental values. α = y-intercept.

Mean Square Error (MSE) is calculated using equation (11). MSE is the average squared difference between outputs and targets. Lower MSE values give better predictions.

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \tilde{y}_i)^2 \tag{11}$$

3.1 ANN Model Prediction procedure

The ANN models in this were created using Matlab software, all ANN models was modelled to undergo training process, validation and testing process to predict the growth rate of methane gas hydrate. The summaries on how ANN Models are created and trained with the analysis of result validation for prediction are as follow;

1. An input data consisting of temperature and pressure obtained from experimental data Table 1 was created in an excel file.
2. Target data using the growth rate of methane hydrate obtained from experimental data Table 1 was also created in an excel file.
3. After which the nntool command in Matlab software lunched, showing the Neural Network work space environment.
4. The input data in the excel file was imported as *input* for neural network and likewise the target data file as targets for the output of the neural network.
5. The type of ANN model was selected based on the number of layers as indicated earlier, then the number of neuron in each layer was also selected accordingly in Table 2. In addition, the training method is also selected (trainlm (Levenberg-Marquardt Backpropagation)).
6. The network parameters are set for training, validation and testing.
7. The network starts training the models until the set parameters are satisfied.
8. The R^2 values for training, validation and testing of the network are check.
9. The ANN predicted outputs are plotted against experimental data from previous study and R^2 values and MSE values for each ANN models are calculated.
10. The procedure is repeat for all configurations as in Table 1.

CHAPTER 4

RESULT AND DISCUSSION

Focusing to show the ability of ANN in predicting gas hydrate growth rate, three ANN models with different configurations of varying number of hidden layers and neurons per layer were developed. In ANN, the training and validation testing performances are very critical on improving ANN prediction. Predictions comprise of 1, 3, 5, 8, 10, 12 and 15 neurons number in each hidden layer of ANN. The result of training, validation, testing and overall predictions for each neural network (NN) model in this work are presented.

4.1 ANN model Training, Validation and Testing

Correlation coefficient (R^2) was employed to assess the training performance of the models in this work; Table 4 shows the R^2 values for the training of each ANN model. From Table 4, the models show very strong correlation ($R^2 > 0.9$) in their training performance except configuration of 1 neuron per layer in model One and 3 neurons in model Two that has R^2 values of (0.44181 and 6.6×10^{-35}) respectively. This occurs when the neural network fails to pick the data for training accordingly. Hence, the two configurations result is not valid. For the rest of model configurations, the high training performance may be attributed to the increasing number of layers and neurons therefore improving the NN learn and prediction ability.

Table 4: Training's result of all ANN models.

ANN Model	Number of Layer	Number of Neurons	Regression (R^2)
One	1	1	0.44181
		3	0.99912
		5	0.99888
		8	0.99691
		10	0.98619
		12	0.99045
		15	0.99342
Two	2	1	0.96031
		3	6.16E-35
		5	0.99427
		8	0.99543
		10	0.98546
		12	0.98564
		15	0.99628
Three	3	1	0.98702
		3	0.99837
		5	0.99934
		8	0.99514
		10	0.99965
		12	0.97542
		15	0.99956

Next to training is validation of the ANN models. This is important to evaluate the training process of the models. Similarly, the R^2 values for validation the model is presented in Table 5. The validation process showed similar results as the training process, with almost all the model shows $R^2 > 0.9$ except the same two configurations in model One and Two as in the training process. Since it has been identified the configurations are unable to perform the prediction the result for validation and testing is void. On the other hand, with impressive R^2 values showed from others models configuration in each model validates that the models are well trained with the inputs data.

Table 5: Validation's result of all ANN models.

ANN Model	Number of Layer	Number of Neurons	Regression (R^2)
One	1	1	0.58546
		3	0.99169
		5	0.99956
		8	0.99907
		10	0.99994
		12	0.99897
		15	0.99988
Two	2	1	0.99887
		3	0.00E+00
		5	0.99406
		8	0.99977
		10	0.99715
		12	0.98848
		15	0.99997
Three	3	1	0.97086
		3	0.99966
		5	0.99837
		8	0.99999
		10	0.96845
		12	0.99381
		15	0.99931

After validation of models, the models undergo testing process to see the actual performance of the model in predicting the growth rate of methane gas hydrate. The testing performance is presented in Table 6. Excellent testing result showed by the models with $R^2 > 0.97$ shows that the configurations used in each model are well fitted for the predictions. To identify the best configurations, the mean square errors for overall prediction is calculated and analyzed. The failure of 1 neuron in model One and 3 neurons in model Two also shows that in the neural network there is possibility of randomness and inability of the network to process the data.

Table 6: Testing's result of all ANN models.

ANN Model	Number of Layer	Number of Neurons	Regression (R^2)
One	1	1	0.34534
		3	0.99981
		5	0.99933
		8	0.98599
		10	0.99989
		12	0.99894
		15	0.99989
Two	2	1	0.99997
		3	0.00E+00
		5	0.99917
		8	0.99997
		10	0.99443
		12	0.99995
		15	0.97373
Three	3	1	0.99962
		3	0.98754
		5	0.98896
		8	1
		10	0.98026
		12	0.99711
		15	0.98376

4.2 ANN models overall prediction

Overall performance of prediction of growth rate of methane gas hydrate by all models is presented Table 7. The performance consists of the R^2 values and MSE produced by each configuration in the models. The MSE of each configuration from the models is then plotted in Figure 4.1 to find the best configuration in every model employed for the prediction.

Table 7: Overall performance of all ANN Models

ANN Model	Number of Layer	Number of Neurons	Regression (R)	MSE
One	1	1	1E-14	4.31E-01
		3	0.99976	7.1548E-04
		5	0.998	5.9945E-04
		8	0.9943	1.9925E-03
		10	0.9836	5.1934E-03
		12	0.9876	3.9554E-03
		15	0.9932	2.0092E-03
Two	2	1	0.9725	8.5551E-03
		3	6.00E-16	4.31E-01
		5	0.9904	2.9082E-03
		8	0.9945	1.6978E-03
		10	0.9728	8.9651E-03
		12	0.9978	6.8455E-03
		15	0.9942	1.7396E-03
Three	3	1	0.9786	6.3832E-03
		3	0.9969	9.1557E-04
		5	0.998	6.0818E-04
		8	0.992	2.5083E-03
		10	0.998	5.9371E-04
		12	0.9544	1.5071E-02
		15	0.9961	1.2864E-03

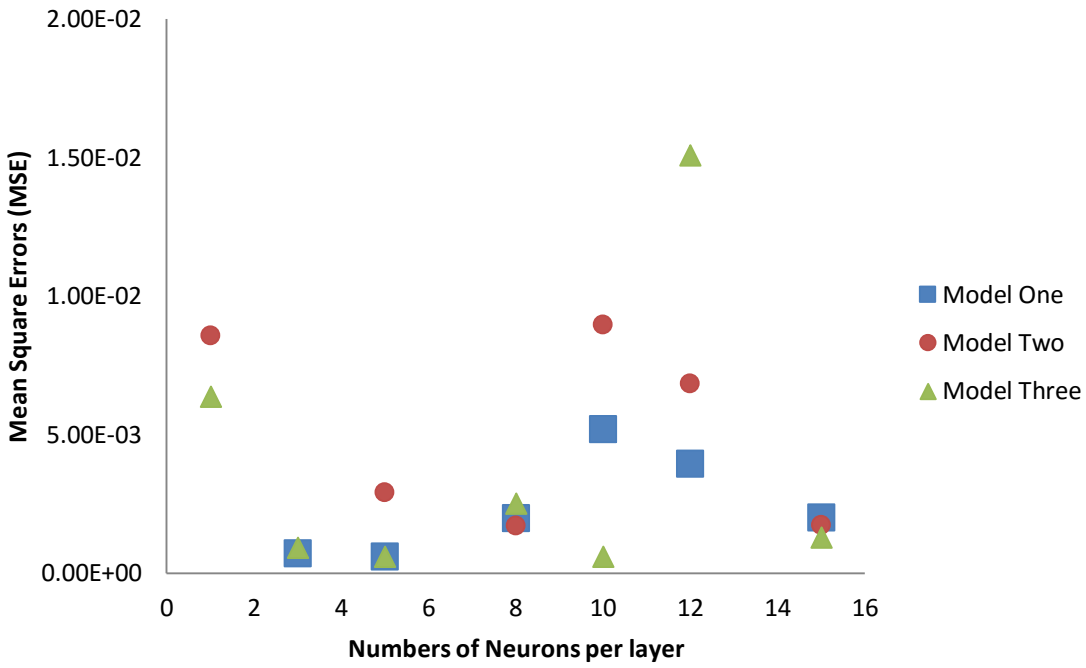

Figure 4.1: Means Square Errors (MSE) against number of neurons in ANN models

Overall, all models show impressive result of prediction may be because of number of training for each model has been contributing to its efficiency of predicting the growth rate of methane gas hydrate. For each model the best configuration is determined by the lowest MSE produced in each model with the R^2 values produced by models' testing. This is because the actual performance of the model is shown from testing the model with training data and MSE of overall shows the successfulness of data selection by NN for training and validation.

For ANN model One the best configurations is five neurons in a hidden layer of NN with R^2 from testing is 0.999 and MSE of 5.995E-04. Whereas, in ANN model Two eight neurons in each layer shows the lowest MSE of 1.698E-03 and R^2 values of 0.999 and lastly in ANN model Three, the best configuration is with five neurons per layer produce R^2 values of 0.989 and MSE of 5.9371E-04.

The challenges in this work is to set the best configuration to predict the growth rate is erratic because by using excessive hidden neurons can cause network over-fitting or in other word the network over-estimate the complexity of the prediction target outputs. Similarly, this problem happens when a network has very low number of hidden neurons that cause under-fitting of network. Bias/ or dilemma in determining the best number of neurons in the layers cause the capability of network to predict an output decreases.

Limitation for this model prediction is that the prediction only valid from the range of input data means the prediction of growth rate of methane gas hydrate is only valid in the range of input pressure and temperature. The NN cannot extrapolate the prediction in areas where pressure or temperature is not trained as input data.

Also in this work, the selections of data by NN are not specified as nntool function in Matlab does not specify data which 70% of the data used for training and 30% of the data used for validation and testing of the models. Therefore, the result obtained from the network varies every time training is done.

CHAPTER 5

CONCLUSION

In conclusion, three ANN models have been developed and tested to predict the formation rate of methane gas hydrate. The results from all the models to identify best configuration for every model is presented where the best for ANN model One is five neurons in a layer with R^2 values of 0.999 and MSE of 5.995E-04 whereas, for ANN model Two the best is configuration of eight neurons in each layers with MSE of 1.698E-03 and R^2 values of 0.999 and lastly ANN model Three with the best configuration comprise of five neurons produce R^2 values of 0.989 and MSE of 5.9371E-04. There are some limitations in the work where two of configuration from the models unable to select the data properly that resulting randomness in prediction of the network. Also, the models only can predict growth rate of methane gas hydrate based on the range of input pressure and temperature only and lastly the selection of data for training, validation and testing of the model are randomly selected therefore produce different result when running the network.

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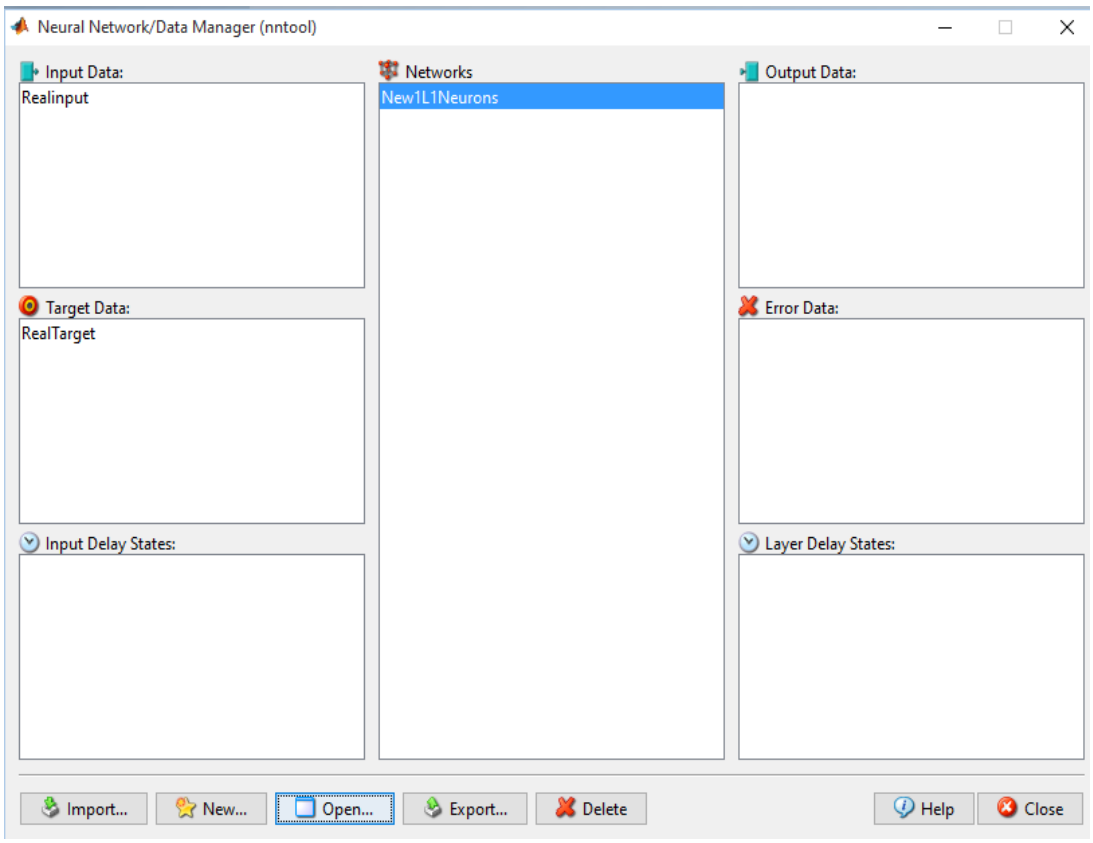
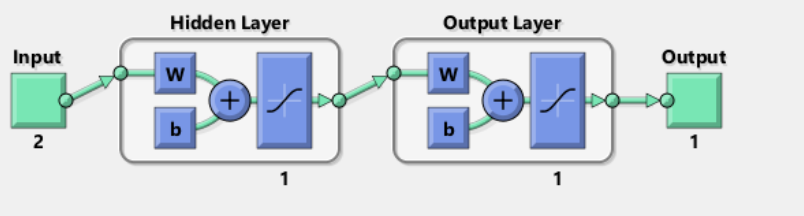
APPENDICES

ANN configuration tools

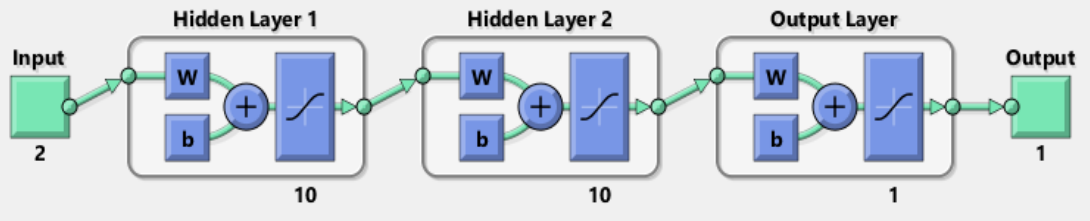


ANN Models

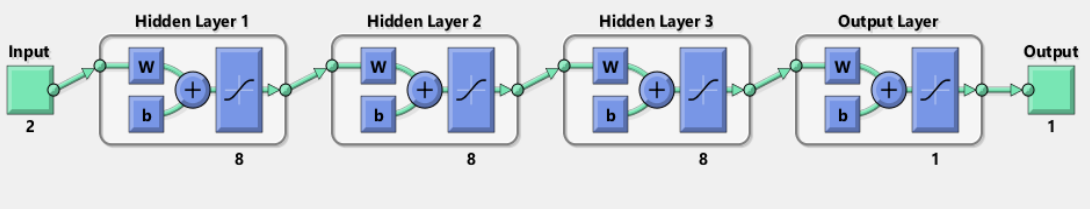
ANN model One: Example configuration of 1 hidden neuron in a layer



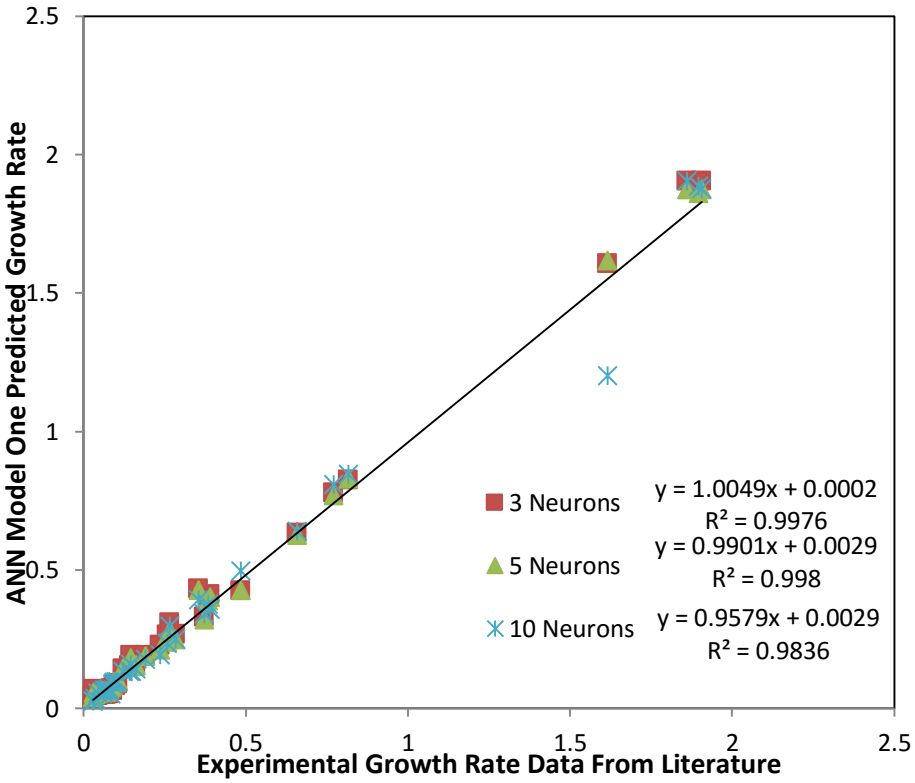
ANN model Two: Example configuration of 10 hidden neuron in each layer

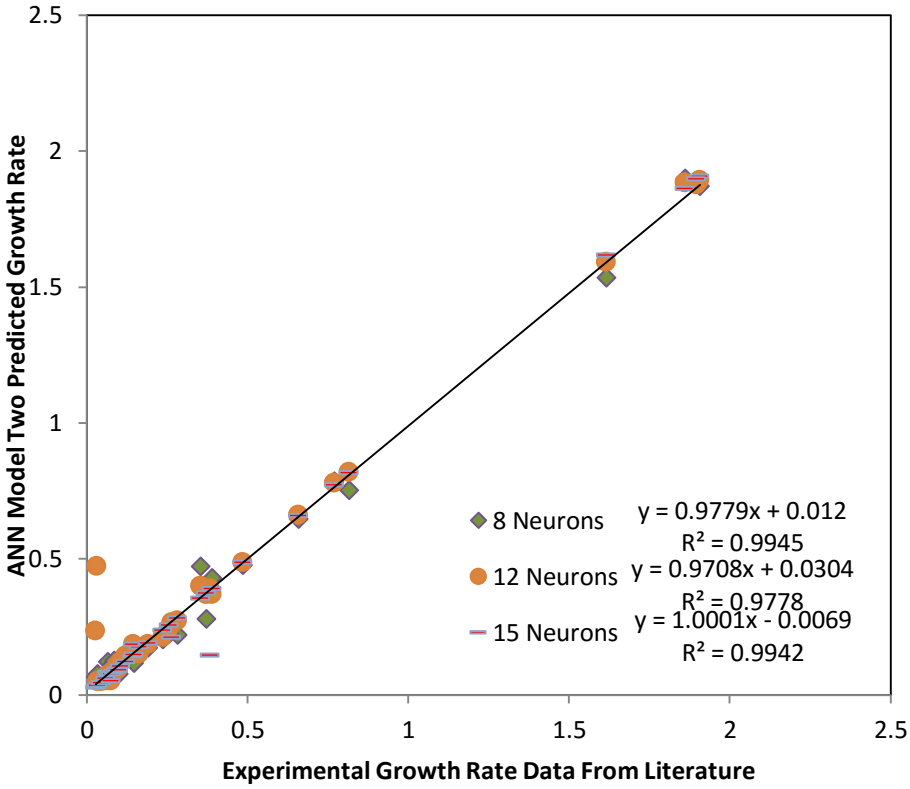


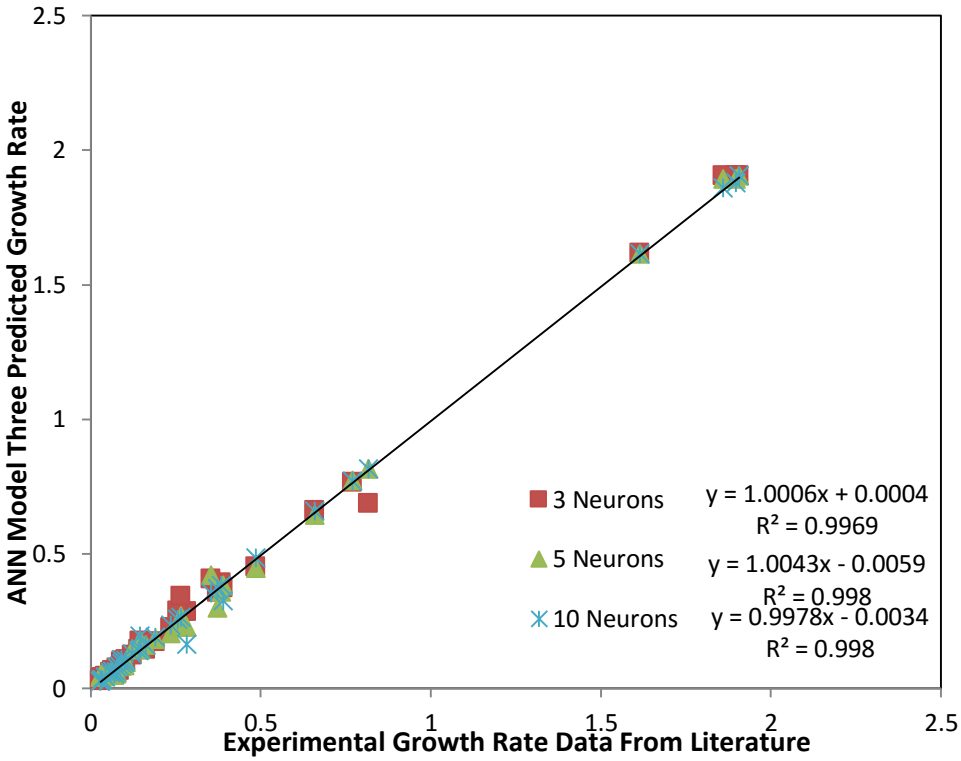
ANN model Three: Example configuration of 8 hidden neuron in each layer



Regression (R^2) values of all models






ANN Model Three Predicted Growth Rate
Experimental Growth Rate Data From Literature
0
0.5
1
1.5
2
2.5
3 Neurons
y = 1.0006x + 0.0004
R² = 0.9969
5 Neurons
y = 1.0043x - 0.0059
R² = 0.998
10 Neurons
y = 0.9978x - 0.0034
R² = 0.998

Gantt Chart & Key Milestone

Table A: Gant Chart & key milestone for FYP1 & FYP 2

No	Detail Work (FYP1)	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														
5	Project Work Continues														
6	Submission of Interim Report														

No	Detail Work (FYP2)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	Project Work Continues															
2	Submission of Progress Report															
3	Pre-SEDEX															
4	Submission of Draft Final Report															
5	Submission of Dissertation (soft bound)															
6	Submission of Technical Paper															
7	Viva															
8	Submission of Project Dissertation (Hard Bound)															