# ADAPTIVE NEURAL FUZZY INFERENCE SYSTEMS FOR HYDROGEN ADSORPTION ISOTHERM PREDICTION

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# Adaptive Neural Fuzzy Inference System for Hydrogen Adsorption Prediction

by

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Dissertation submitted in partial fulfillment of

the requirements for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the

Chemical Engineering Programme

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Approved by,

A.P Dr. Suzana Yusup
Project Supervisor

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK

July 2009

# 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.**

Jj.

**JUFRI AFIQ JOLAN**

ABSTRACT

This report is basically to discuss about the basic concept and implementation of Artificial Neural Fuzzy Inference System (ANFIS) in predicting the hydrogen adsorption isotherm. The objective of this project is to create an ANFIS that is able to predict the hydrogen adsorption isotherm. The challenge in this project is to develop the ANFIS that is able to predict the hydrogen adsorption isotherm at the highest accuracy.

ANFIS is developed by using MatLab R2008a. This software which is a mathematical power tool has the ability to develop the ANFIS. This is because the software has the Fuzzy Logic Toolbox which is the basic requirement in building the system.

The basic system is developed to receive two inputs which are temperature and pressure from users and gives one output which is the hydrogen adsorption value. Three membership functions are provided for each input which is then used in determining the output of the system.

Multiple training data are given to the basic system in order to mature it. Upon completion, the system is then tested with test data and output from the system is analyzed. Calculations of the output percentage error are carried out. From here, the ANFIS membership functions for each input are fine tuned in order to reduce output percentage error in order to increase the prediction accuracy of the system.

As a result, the ANFIS is able to give prediction data with an error less than 5% which desirable in this project.

# ACKNOWLEDGEMENT

First and foremost, I would like to praise Allah the Almighty for with His blessings and guidance tha I am able to successfully complete my Final Year Research Project. Sincerely, I would like to express my deepest gratitude to the individuals that have taken the time and effort to assist and guide me in completing the project. Without the cooperation and help of these individuals, it will be hard for me to finish this project.

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# CHAPTER 1

# PROJECT BACKGROUND

## 1. BACKGROUND OF STUDY

Neuro Fuzzy (NF) computing is a popular framework for solving complex problems. If we have knowledge expressed in linguistic rules, we can build a Fuzzy Inference System (FIS), and if we have data, or can learn from a simulation (training) then we can use Artificial Neural Networks (ANN). For building a FIS, we have to specify the fuzzy sets, fuzzy operators and the knowledge base. Similarly for constructing an ANN for an application the user needs to specify the architecture and learning algorithm. An analysis reveals that the drawbacks pertaining to these approaches seem complementary and therefore it is natural to consider building an integrated system combining the concepts. While the learning capability is an advantage from the viewpoint of FIS, the formation of linguistic rule base will be advantage from the viewpoint of ANN.

By combining both ability of ANN and also FIS, therefore we have a new method called Adaptive Neural Fuzzy Inference Systems (ANFIS). This ANFIS has the capability in creating a model which is useful in prediction for a given input. The model constructions begin with the learning of the raw data which is done by ANN and the reasoning of the data which is given by FIS. As a result, a mathematical model with a high accuracy can be produced.

The term *neuro-fuzzy system* is used for approaches which display the following properties [17]:

- A neuro-fuzzy is based on a fuzzy system which is trained by learning algorithm derived from neural network theory. The (heuristical) learning procedure operates on local information, and causes only local modifications in the underlying fuzzy system.

- A neuro-fuzzy system can be viewed as a 3-layer feedforward neural network. The first layer represents input variables, the middle (hidden) layer represents fuzzy rules and the third layer represents output variables. Fuzzy sets are encoded as (fuzzy) connection weights. It is not necessary to represent a fuzzy system like this to apply a learning algorithm to it. However, it can be convenient, because it represents the data flow of input processing and learning within the model.
- A neuro-fuzzy system can be always (i.e.\ before, during and after learning) interpreted as a system of fuzzy rules. It is also possible to create the system out of training data from scratch, as it is possible to initialize it by prior knowledge in form of fuzzy rules.
- The learning procedure of a neuro-fuzzy system takes the semantical properties of the underlying fuzzy system into account. This results in constraints on the possible modifications applicable to the system parameters.

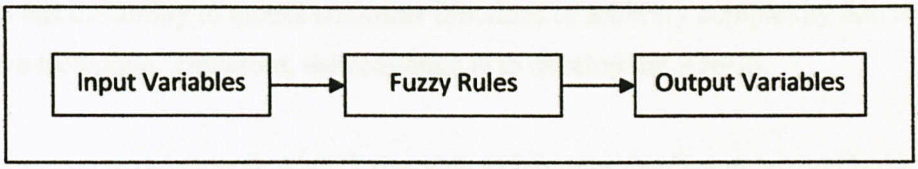


Figure 1: Basic concept of Neuro Fuzzy

## 2. PROBLEM STATEMENT

Hydrogen gas has the potential to replace oil and gas for vehicles. This is because combustion of hydrogen will give steam as the product, which is pollution free. The drawback is that hydrogen has low energy content compared to its volume. Thus the problem is to provide hydrogen storage for hydrogen-based transportation system. Carbon based materials are found as a promising adsorbent for hydrogen due to its high surface area and light weight. Thus it will give a low volume in hydrogen storage.

Many researchers have come out with different types of model in describing the behavior of gas adsorption in microporous adsorbent. However, those models are based on the assumptions made due to several reasons such as adsorption at supercritical condition, types of carbon surface and structures as well as interaction of hydrogen molecules and adsorbent molecules [15].

As a result, hydrogen can be predicted based on model developed such as Grand Canonical Monte Carlo, Ono-Kondo fit model, Linear Comprehensive Supercritical Adsorption Model, Dubinin-Astakhov equation, and Langmuir Model. However, each model has its own limitations due to several assumptions made. Hence, a new approached in adsorption model is introduced to improve and simplify the predicted model.

Unlike any other models, an assumption-free model of hydrogen adsorption can be developed using neuro-fuzzy system or specifically Adaptive Neuro Fuzzy Inference System (ANFIS) which implies Takagi-Sugeno-Kang method of fuzzy inference system. Such programming has been used before in predicting methane adsorption onto activated carbon and also many other prediction case studies. This is because ANFIS has the ability to model nonlinear functions or arbitrary complexity due to its adaptive technique. Therefore, the challenge is to develop the ANFIS.

It is important to develop an ANFIS that able to interpret the data given precisely. This because if the system unable to learn to improve its interpretation ability, it will cause the system to give wrong prediction which is undesirable. So, an error free ANFIS is required.

## 2.1 Significant of the Project

This project will be able to ease the researcher in determining the adsorption isotherm of Hydrogen at various temperature and pressure onto various type of activated carbon. Success in this project will lead to the ability to predict the adsorption isotherm of Hydrogen at various temperature and pressure. Not only that, this project also can be brought forward to predict the adsorption isotherm of other substance other than Hydrogen itself.

## 3. OBJECTIVES AND SCOPE OF STUDY

The objectives of the study are:

- To predict hydrogen adsorption isotherm onto activated carbon at various temperature range and various pressure range by using ANFIS.
- To acquire prediction data for Hydrogen adsorption isotherm on activated carbon.
- To compare results between ANFIS prediction and real data.

The ANFIS will be developed using MatLab R2008a which contains a Fuzzy Logic Toolbox. The ANFIS applies the technology of neural network to produce fuzzy logic rules and membership functions automatically. In fuzzy logic, there are two methods which are Takagi-Sugeno-Kang and the other one is Mamdani. Takagi-Sugeno-Kang is similar to Mamdani in many aspects. The main difference between Takagi-Sugeno-Kang and Mamdani is that Takagi-Sugeno-Kang output membership is either linear or constant. As for ANFIS, it will implements Takagi-Sugeno-Kang FIS.

To create a complete fuzzy logic system, two methods are available in MatLab R2008a. First method is by using the ANFIS Graphic User Interface (GUI) Editor which is easy to set up the ANFIS and gives the basic needs for developing an ANFIS. The second method is by using the MatLab command line. By using the command line, the user will have more freedom to add various calculations in order to increase the integrity and reliability of the test on the developed ANFIS. This includes the calculation on other different model from ANFIS.

For this project, the author will use both ANFIS GUI Editor and also MatLab command line in developing the ANFIS. This is because by combining both methods, analysis and tuning of the ANFIS will be much better.

## 4. FEASIBILITY OF PROJECT

The student is required to develop a system which contains learning capabilities. Neuro-Fuzzy or Adaptive Neuro Fuzzy Inference System (ANFIS) is not a new finding. Therefore, the student should be able to gather a lot of data regarding this system from the net also there are a lot of case study that can be used as a starting point in order to help him to develop the system.

Furthermore, this system already being applied in the other project in UTP before, therefore, the student can request help from the expert of this system within UTP. With the help from the lecturers and the resources from UTP itself, this project will be able to finish within two semesters.

# CHAPTER 2

# LITERATURE REVIEW

In this chapter the author present about cooperative NF system and concurrent NF system followed by the different fused NF models. Some discussions and conclusions are provided towards the end.

The purpose of this literature review to further understands any available system that exists. From the existed system, comparisons are being made in order to find the advantages and the weaknesses of each system.

## 1. COOPERATIVE AND CONCURRENT FUZZY SYSTEMS

In the simplest way, a cooperative model can be considered as a preprocessor wherein ANN learning mechanism determines the FIS membership functions or fuzzy rules from the training data. Once the FIS parameters are determined, ANN goes to the background. The rule based is usually determined by a clustering approach (self organizing maps) or fuzzy clustering algorithms. Membership functions are usually approximated by neural network from the training data.
In a concurrent model, ANN assists the FIS continuously to determine the required parameters especially if the input variables of the controller cannot be measured directly. In some cases the FIS outputs might not be directly applicable to the process. In that case ANN can act as a post process or of FIS outputs. Figures 1 and Figure 2 depict the cooperative and concurrent NF models.

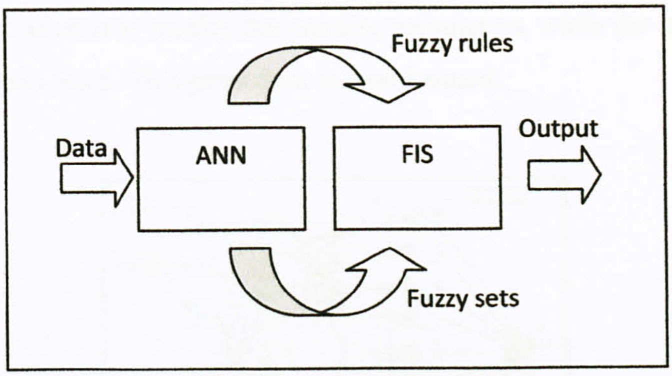

Figure 2: Cooperative Neural Fuzzy System

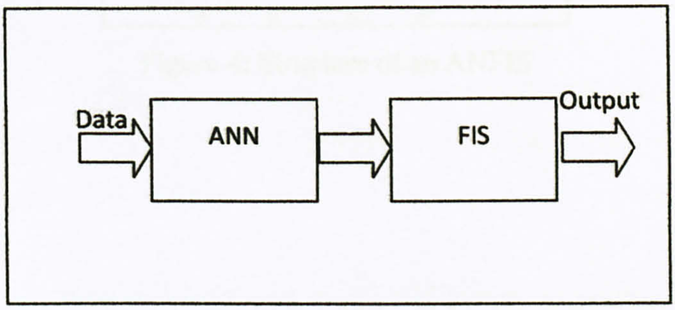

Figure 3: Concurrent Neural Fuzzy System

## 2. ADAPTIVE NEURAL FUZY INFERENCE SYSTEM (ANFIS)

ANFIS implements a Takagi Sugeno FIS and has a five layered architecture as shown in Figure 2. The first hidden layer is for fuzzifications of the input variables and T-norm operators are deployed in the second hidden layer to compute the rule antecedent part. The third hidden layer normalizes the rule strengths followed by the fourth hidden layer where the consequent parameters of the rule are determined. Output layer computes the overall input as the summation of all incoming signals. ANFIS uses backpropagation learning to determine premise parameters (to learn the parameters related to membership functions) and least mean square estimation to determine the consequent parameters. A step in the learning procedure has got two parts: In the first part the input patterns are propagated, and the optimal consequent parameters are estimated by an iterative least mean square procedure, while the premise parameters are assumed to be fixed for the current cycle through the training set. In the second part the patterns are propagated again, and in this epoch (training), backpropagation is used to modify the premise parameters, while the consequent parameters remain fixed. This procedure is then iterated.

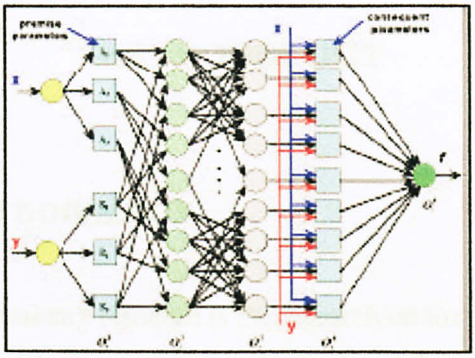

Figure 4: Structure of an ANFIS

# CHAPTER 3

# METHODOLOGY

## 1. RESEARCH METHODOLOGY

In this project, the preliminary research is the research on the previous project work that has the same application or concept as this project. The research is done in order to find out the information on how this system is implemented in various situations. This preliminary research is further improved by having discussions with the persons who have used this system before.

The second research methodology is by finding the information from the internet. The purpose of finding the information from the internet is to increase the knowledge on the system. This includes reading the case study and also how the system is implemented in various disciplines. Gathering the information from the internet also can help the author to know improvement that has been done by other people on this system and how to troubleshoot the system.

The third method of research is done by reading from journals, articles and also books. These materials are important in order to help the author to further understanding the basic concept of the system and also the theory behind it. Mastering the basic is the most important thing when working on a project.

## 2. PROJECT ACTIVITIES

For this project, the author use Adaptive Neural Fuzzy Inference System (ANFIS) which implement a Sugeno Fuzzy Inference System. At the beginning, a training data from literature are taken as the training data for the ANFIS. For hydrogen adsorption, the parameters that affect the amount of adsorption are temperature and pressure. Therefore, these two parameters are taken as the input for the ANFIS.

The data taken from the literature [15] are based on temperatures at 173K, 213K and 253K. The data are as below:

| No. | Temperature (K) | Pressure (MPa) | Adsorption (mmol/g) | No. | Temperature (K) | Pressure (MPa) | Adsorption (mmol/g) |
|---|---|---|---|---|---|---|---|
| 1 | 173 | 0.1232 | 1.450 | 9 | 173 | 2.0112 | 19.2718 |
| 2 | 173 | 0.224 | 2.9016 | 10 | 173 | 2.4032 | 21.8538 |
| 3 | 173 | 0.3136 | 4.03 | 11 | 173 | 2.8176 | 24.03 |
| 4 | 173 | 0.4928 | 6.3702 | 12 | 173 | 3.3136 | 26.209 |
| 5 | 173 | 0.7056 | 8.224 | 13 | 173 | 3.7056 | 28.1434 |
| 6 | 173 | 0.9408 | 11.209 | 14 | 173 | 4.224 | 30.1612 |
| 7 | 173 | 1.2464 | 13.3852 | 15 | 173 | 4.7392 | 31.9344 |
| 8 | 173 | 1.5824 | 16.3702 | 16 | 173 | 5.2128 | 33.3852 |

Table 1: Literature data for adsorption at 173K

| No. | Temperature (K) | Pressure (MPa) | Adsorption (mmol/g) | No. | Temperature (K) | Pressure (MPa) | Adsorption (mmol/g) |
|---|---|---|---|---|---|---|---|
| 1 | 213 | 0.4256 | 2.2568 | 9 | 213 | 2.9520 | 13.4658 |
| 2 | 213 | 0.5936 | 3.5464 | 10 | 213 | 3.4256 | 15.6448 |
| 3 | 213 | 0.8176 | 4.2718 | 11 | 213 | 3.7840 | 17.5792 |
| 4 | 213 | 1.0448 | 5.6448 | 12 | 213 | 4.3024 | 19.6748 |
| 5 | 213 | 1.3360 | 6.8538 | 13 | 213 | 4.7952 | 21.4508 |
| 6 | 213 | 1.6384 | 8.8688 | 14 | 213 | 5.4256 | 23.0628 |
| 7 | 213 | 2.0784 | 10.0806 | 15 | 213 | 5.7952 | 24.6748 |
| 8 | 213 | 2.4928 | 11.8538 | | | | |

Table 2: Literature data for adsorption at 213K

| No. | Temperature (K) | Pressure (MPa) | Adsorption (mmol/g) | No. | Temperature (K) | Pressure (MPa) | Adsorption (mmol/g) |
|---|---|---|---|---|---|---|---|
| 1 | 253 | 0.4368 | 1.4508 | 8 | 253 | 2.9072 | 13.4658 |
| 2 | 253 | 0.6496 | 2.4986 | 9 | 253 | 3.4256 | 15.6448 |
| 3 | 253 | 0.952 | 3.3852 | 10 | 253 | 3.8176 | 17.5792 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 4 | 253 | 1.224 | 4.2718 | 11 | 253 | 4.3024 | 19.6748 |
| 5 | 253 | 1.6496 | 5.0806 | 12 | 253 | 4.7616 | 21.4508 |
| 6 | 253 | 2.0112 | 6.3702 | 13 | 253 | 5.3472 | 23.0628 |
| 7 | 253 | 2.4256 | 7.6598 | | 253 | 5.8288 | 16.209 |

Table 3: Literature data for adsorption at 253K

The ANFIS is then created. Two methods are available in MatLab for the development of the ANFIS which are from Matlab command line or ANFIS Editor Graphic User Interface (GUI).

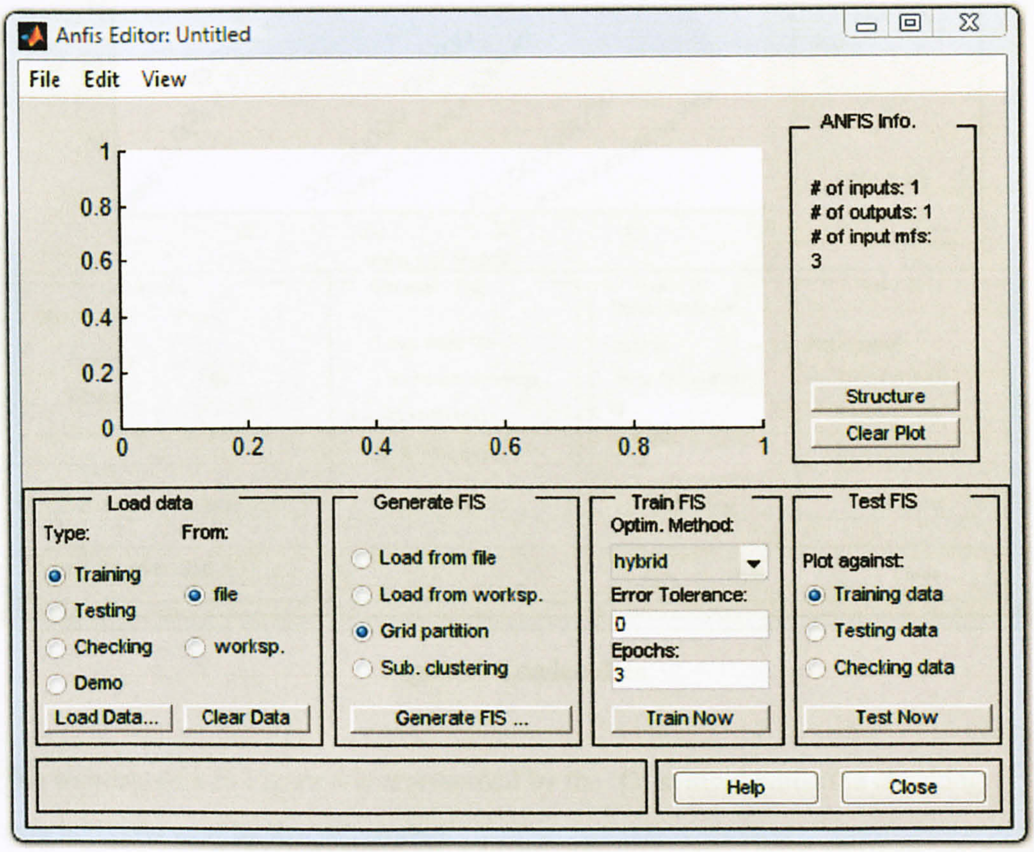


Figure 5: ANFIS Editor GUI

For this project, both methods are used in order to increase the integrity of the final results of the simulation. The above ANFIS Editor window is opened by entering the command below in the Matlab command window:

```
anfisedit
```

For the ANFIS Editor GUI method, the training and checking data for the hydrogen adsorption isotherm are both loaded into the editor. The amount of training data is roughly about 80% from the checking data which coming from the literature data in Table 1, Table 2 and Table 3. The loaded data in the ANFIS Editor is shown in the figure below:

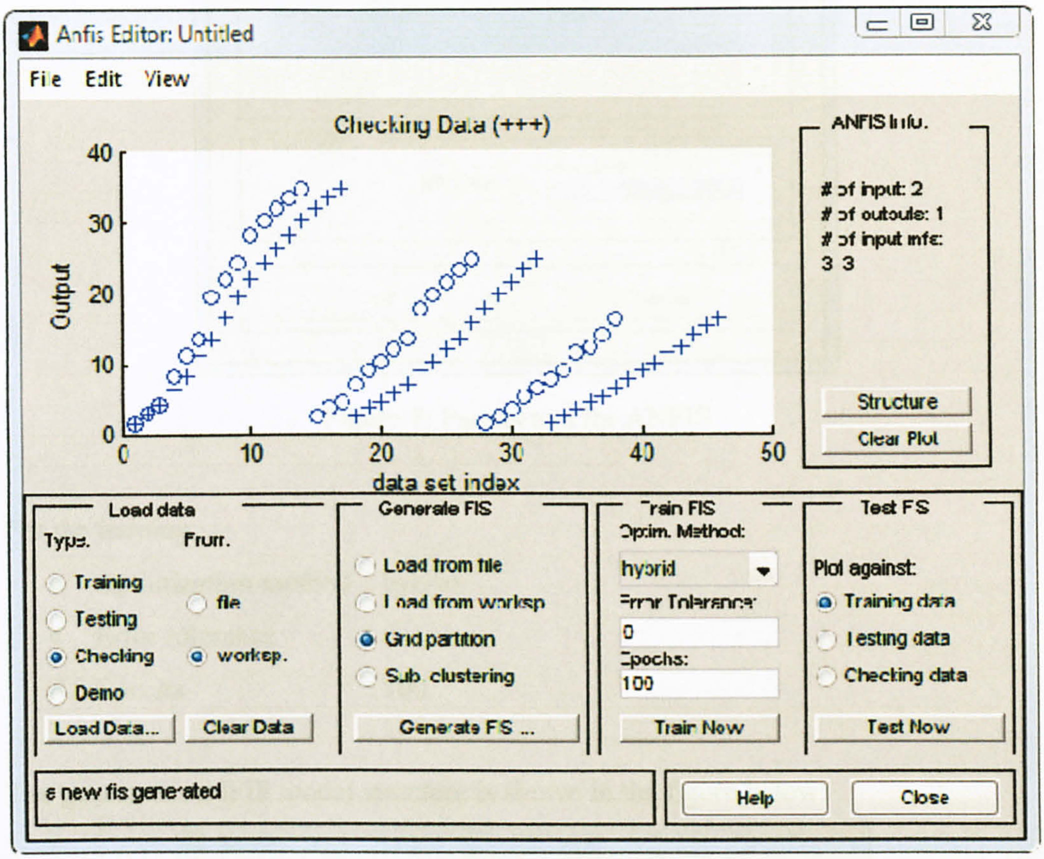


Figure 6: Loaded data

The training data in Figure 6 is represented by the 'O' symbol while the checking data is represented by the '+' symbol.

The ANFIS is generated based on grid partition. The parameters for both inputs are as below:

- Number of Membership Functions : 3 for each input
- Input Membership Functions type : Gaussian Bell
- Output Membership Functions type : Linear

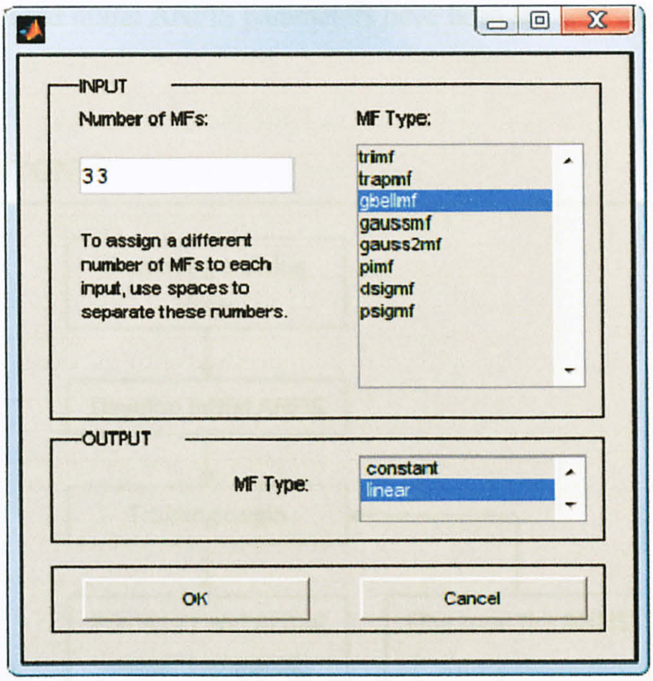


Figure 7: Parameters for ANFIS

For the training:

- Optimization method : hybrid
- Error tolerance : 0
- Epochs : 100

The generated ANFIS model structure is shown in the figure below:

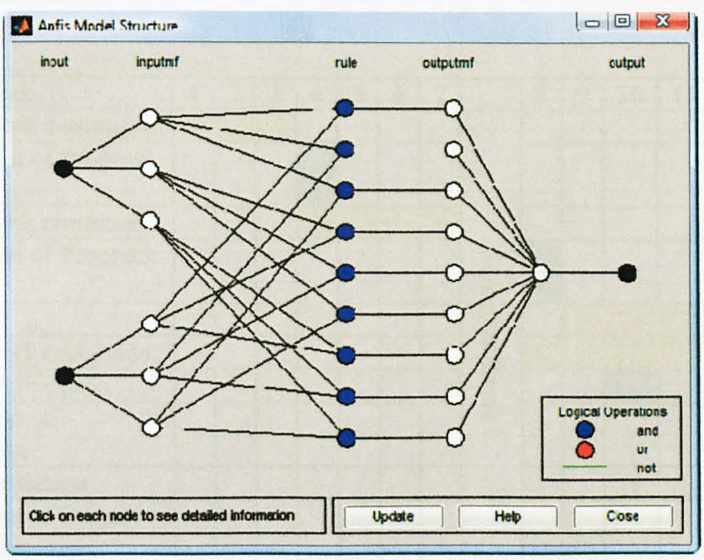


Figure 8: ANFIS Model Structure

After all the required initial ANFIS parameters have been set, training of the ANFIS can be started.

## 3. KEY MILESTONES

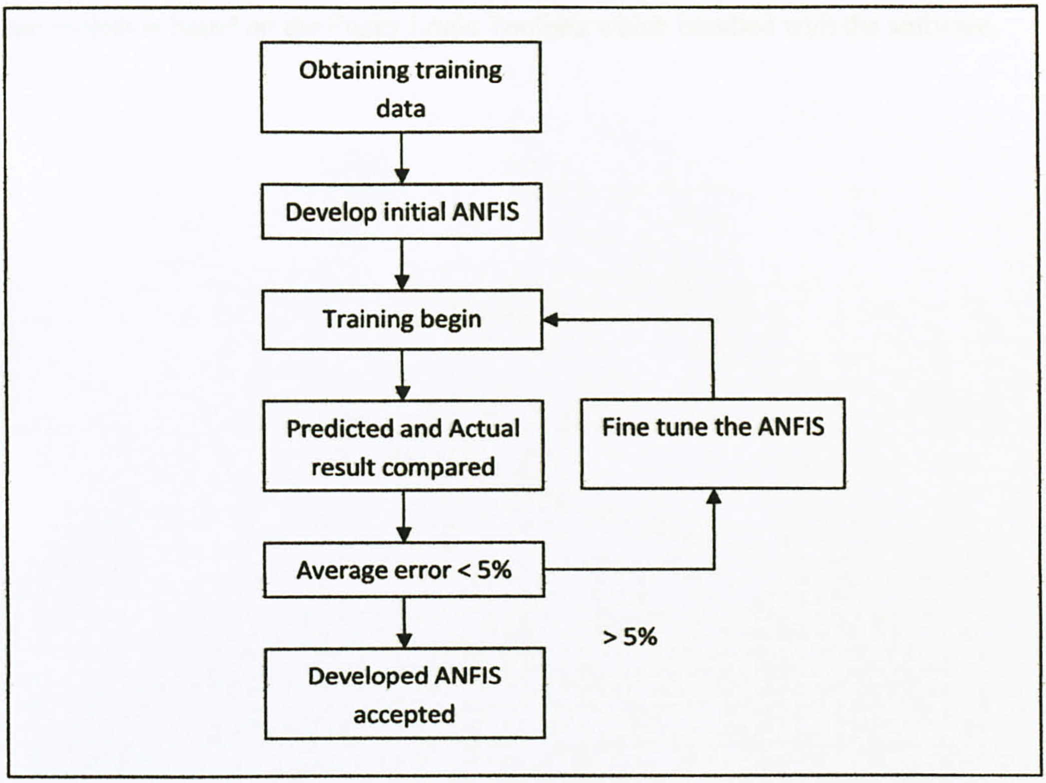


Figure 9: Key Milestones

## 4. GANTT CHART

| No | Detail/Week | 1 | 2 | 3 | 4 | 5 | 6 | 7 | | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Project work continues | | | | | | | | | | | | | | | |
| 2 | Submission of Progress Report 1 | | | | | | | | | | | | | | | |
| 3 | Project work continues | | | | | | | | | | | | | | | |
| 4 | Submission of Progress Report 2 | | | | | | | | | | | | | | | |
| 5 | Seminar | | | | | | | | Semester Break | | | | | | | |
| 6 | Project work continues | | | | | | | | | | | | | | | |
| 7 | Poster Exhibition | | | | | | | | | | | | | | | |
| 8 | Submission of Dissertation | | | | | | | | | | | | | | | |
| 9 | Oral Presentation | | | | | | | | | | | | | | | |
| 10 | Submission of Project Dissertation | | | | | | | | | | | | | | | |

Figure 10: Gantt chart

## 5. TOOLS

For this project, the software used is MatLab. Matlab is a powerful mathematic tool which able to compute a complex mathematical equation. The ANFIS developed in the project is based on the Fuzzy Logic Toolbox which bundled with the software.

# CHAPTER 4
# RESULTS AND DISCUSSIONS

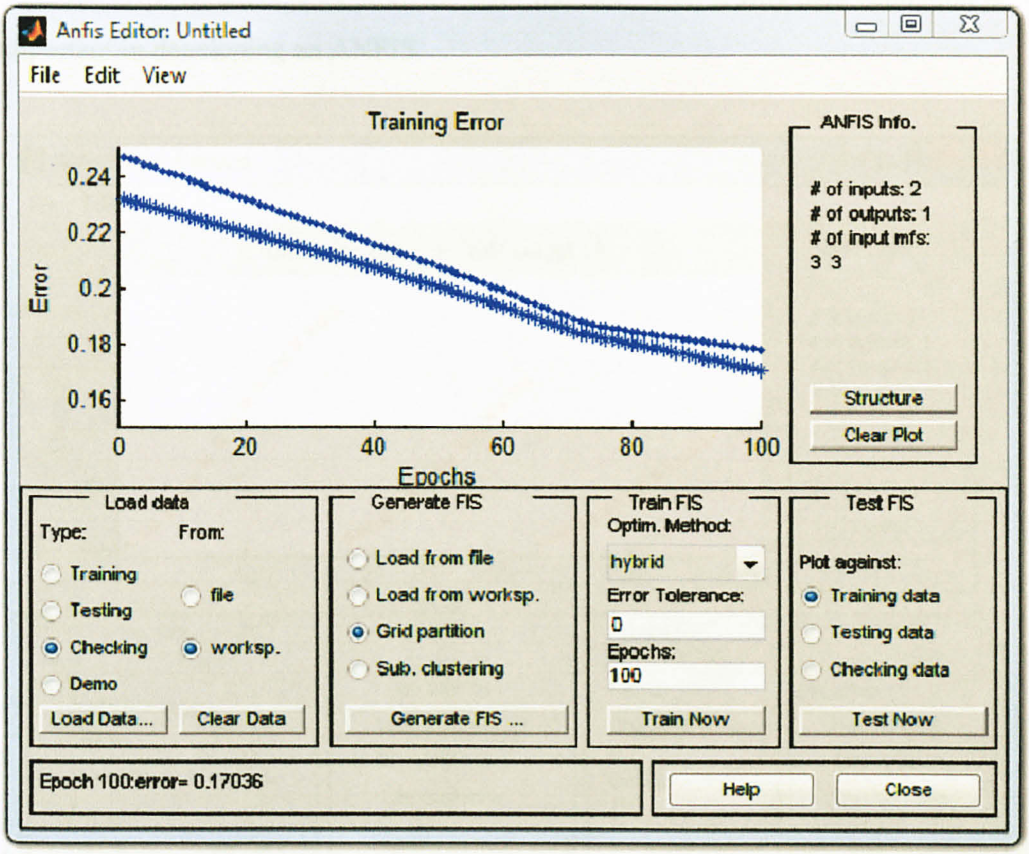


Figure 11: Training result

The plot in Figure 10 shows both checking error and training error. Checking error is the line on the top while training error is on the bottom. From the plot, we can see that the checking error is decreasing until a certain point where it starts to increase again.

This increase represents model overfitting. Overfitting occurs when a model describes random error or noise instead of the underlying relationship. A model which has been overfit will generally have poor predictive performance, as it can exaggerate minor fluctuations in the data.

In order to avoid overfitting, additional techniques such as early stopping, cross-validation, regularization, or model comparison can be used. In this project, the author use model comparison which is the checking data in order to avoid overfitting. ANFIS chooses the model parameters associated with the minimum checking error which is just before the error increase. That is why data validation is important in developing an ANFIS.

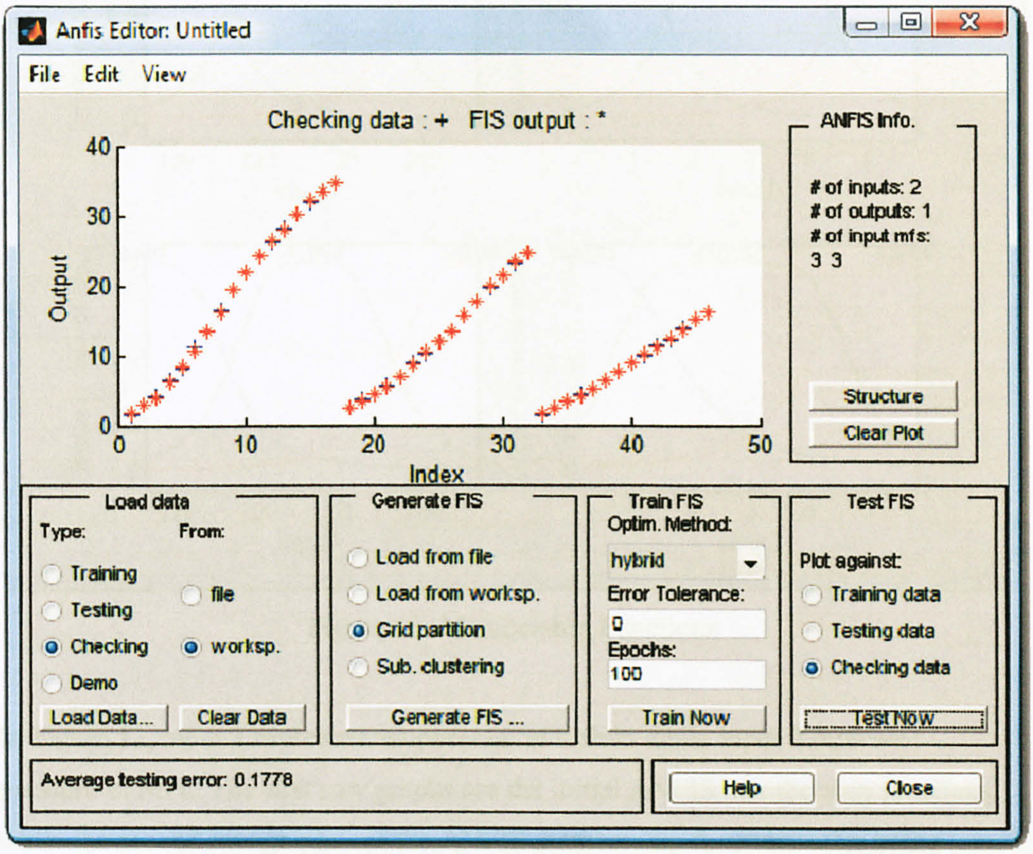


Figure 12: Plot of Checking data & FIS output

The red '*' in Figure 11 shows the Fuzzy Inference System (FIS) output which is the predicted adsorption at temperature 173K, 213K and 253K while the blue '+' is the checking data. From the plot, it is found out that the FIS is able to predict the data as intended for temperature 173K, 213K and 253K.

From the figure, it is found that the FIS is ready to be used. However, further verification is required in order to make sure that the future prediction data are reliable.

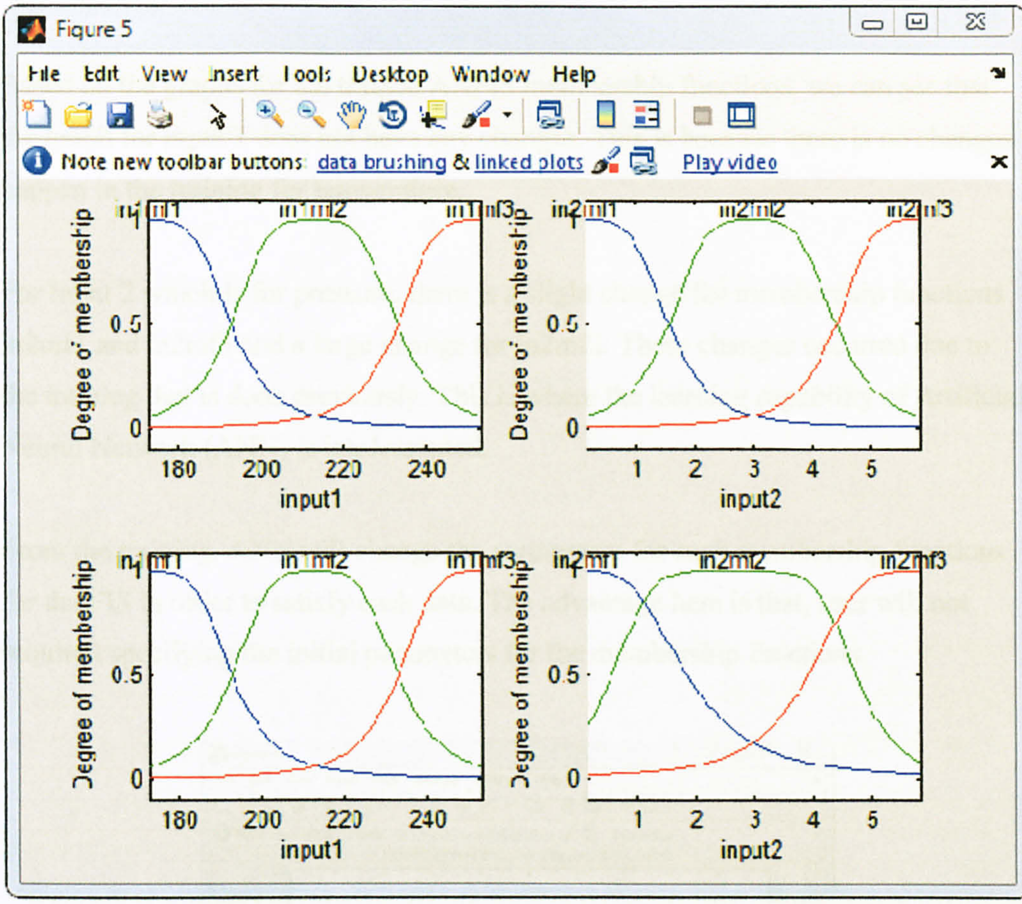


Figure 13: Membership Functions

In Figure 12, input 1 represent temperature in Kelvin while input 2 represent pressure in MPa. The first row graphs are the initial ANFIS membership functions while the second row graphs are the ANFIS membership functions after being trained. The graphs consist of three Gaussian bell membership functions. The three membership functions for both inputs are evenly distributed so that they will cover from the minimum to maximum data for each input. This is to make sure that none of the data given for the input will be left out in developing the ANFIS.

| Type | Min | Max |
|---|---|---|
| Temperature (K) | 173 | 253 |
| Pressure (MPa) | 0.1232 | 5.828 |

Table 4: Minimum & Maximum for Temperature & Pressure

Based on the graphs for the trained ANFIS membership functions, we can see that the graph for input 1 does not have any changes. This is because there is no changes happen in the training for temperature.

For input 2 which is for pressure, there is a slight change for membership functions in2mf1 and in2mf3 and a large change for in2mf2. These changes occurred due to the training that is done previously. This is where the learning capability of Artificial Neural Network (ANN) is implemented.

From the training, ANN will change the parameters for each membership functions for the FIS in order to satisfy each data. The advantage here is that, user will not required specifying the initial parameters for the membership functions.

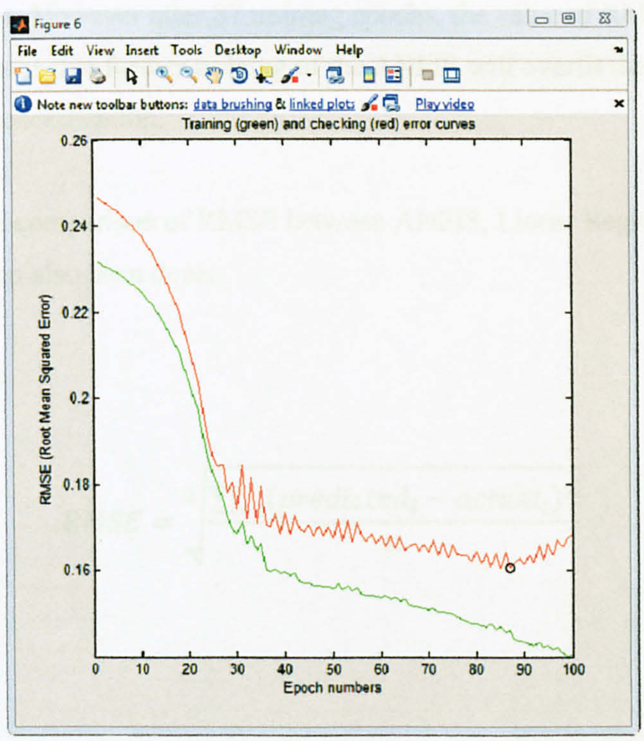


Figure 14: RMSE curve

In Figure 13, the Root Mean Squared Error (RMSE) for both training and checking data are given. The main focus here is the RMSE error for the checking data. RMSE calculation is very important because it is used to calculate the average magnitude of the error.

RMSE is the difference between forecast and corresponding observed values are each squared and then averaged over the sample. Then the square root of the average is taken. Since the errors are squared before they are averaged, the RMSE gives a relatively high weight to large errors. This means the RMSE is most useful when large errors are particularly undesirable in which is happening in this project.

From the curve, it is found out that the lowest RMSE is 0.1605 at 87 training epoch. Lower RMSE is preferable. After this point, RMSE start to increase. This is due to model overfitting. As explained before, ANFIS will choose the model parameters that go with the lowest RMSE.

From this curve, it also shown that a large number of training epochs is important. This is because a good amount of training epoch will help the ANFIS to find the best model parameters. However after 87 training epochs, the value of RMSE starting to increase, this means that further training of the ANFIS will overfit the data and produce worse generalization.

In this modeling, comparison of RMSE between ANFIS, Linear Regression and Non Linear Regression also been done.

RMSE equation:

$$RMSE = \sqrt[2]{\frac{\sum_{i=1}^{n}(predicted_i - actual_i)^2}{n}}$$

## 1. LINEAR REGRESSION ANALYSIS

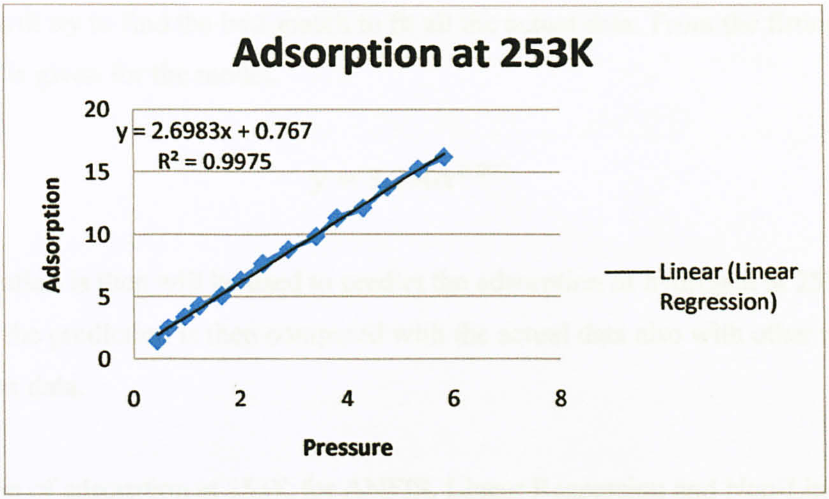


Figure 15: Linear regression analysis for adsorption at 253K

In Figure 14, the actual data is modeled using Linear Regression method. An equation is given to give the best fitting for the actual data which is:

$$y = 2.698x + 0.767$$

From this equation, the prediction of adsorption at 253K is done and compared with other models.

## 2. NON-LINEAR REGRESSION ANALYSIS

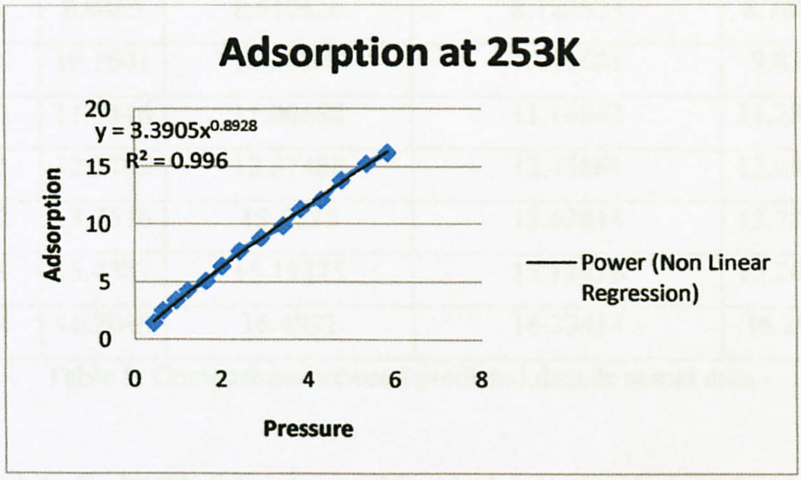


Figure 16: Non-Linear Regression analysis for adsorption at 253K

In Figure 15, the actual data is model is using Non-Linear Regression method. This method will try to find the best match to fit all the actual data. From the fitting, an equation is given for the model.

$$y = 3.390x^{0.892}$$

This equation is then will be used to predict the adsorption of hydrogen at 253K. The result of the prediction is then compared with the actual data also with other models prediction data.

Prediction of adsorption at 253K for ANFIS, Linear Regression and Non-Linear Regression are given in the table below:

| Point | Prediction | | | Actual |
|---|---|---|---|---|
| | ANFIS | Linear Regression | Non-Linear Regression | |
| 1 | 1.5980 | 1.945486 | 1.619317 | 1.4508 |
| 2 | 2.3188 | 2.519621 | 2.307172 | 2.4986 |
| 3 | 3.3471 | 3.335496 | 3.244471 | 3.3852 |
| 4 | 4.1046 | 4.069352 | 4.059763 | 4.2718 |
| 5 | 5.2058 | 5.217621 | 5.297872 | 5.0806 |
| 6 | 6.3017 | 6.193218 | 6.322397 | 6.3702 |
| 7 | 7.6151 | 7.311269 | 7.472371 | 7.6598 |
| 8 | 8.9465 | 8.610626 | 8.782523 | 8.7882 |
| 9 | 10.1601 | 10.00927 | 10.16681 | 9.836 |
| 10 | 11.0446 | 11.06688 | 11.19842 | 11.2896 |
| 11 | 12.2765 | 12.37488 | 12.45861 | 12.0956 |
| 12 | 13.7576 | 13.6138 | 13.63814 | 13.7882 |
| 13 | 15.4387 | 15.19375 | 15.12476 | 15.2418 |
| 14 | 16.2040 | 16.4931 | 16.33414 | 16.209 |

Table 5: Comparison between predicted data & actual data

From this data, the RMSE for each model is calculated using the RMSE equation as stated above. Calculated RMSE for each model is shown in Table 5.

| RMSE | | |
|---|---|---|
| ANFIS model | Linear Regression model | Non-Linear Regression model |
| 0.161 | 0.233 | 0.192 |

Table 6: RMSE comparison between ANFIS, Linear & Non-Linear Regression

From the comparison, it is found out that ANFIS model outperforms Linear Regression model and also Non-Linear Regression model.

The drawback of using Linear & Non-Linear Regression is that the equation for the model is only for a particular set of data which is adsorption at 253K. If the user wants to predict the data for adsorption at 213K and 253K, the prediction will give a huge error. This is because the adsorption isotherm between 173K, 213K and 253K a significant different.

However, for ANFIS, this problem is reduced since ANFIS will try to adapt to each data in the given training. From various training, ANFIS will be able to give a generalized prediction for the adsorption. This is because ANFIS operate base on rules and membership function. The membership functions are the main factors that deciding the prediction.

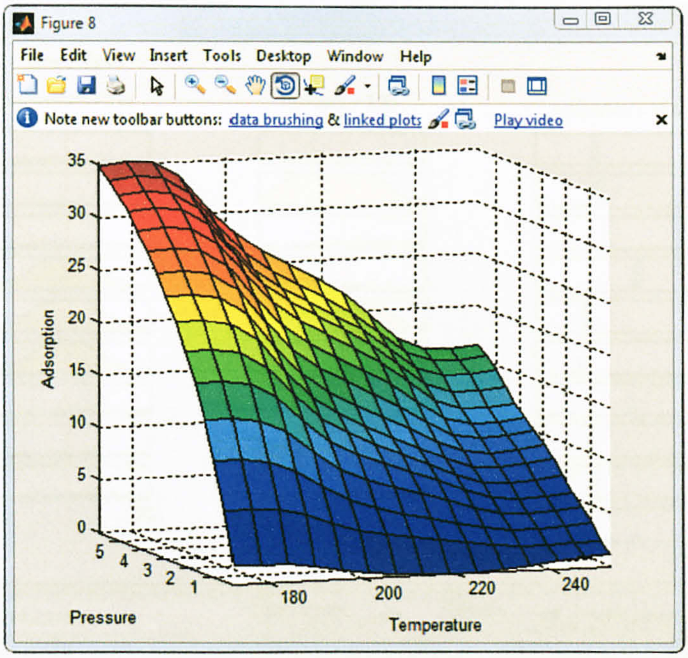


Figure 17: Surface view

Figure 16 shows the surface view of the predicted adsorption data based on the training from the literature data. In the figure, it is shown that as pressure increase and temperature decrease, adsorption will increase. The surface view also shows the generalized prediction at each temperate between 173K and 253K.

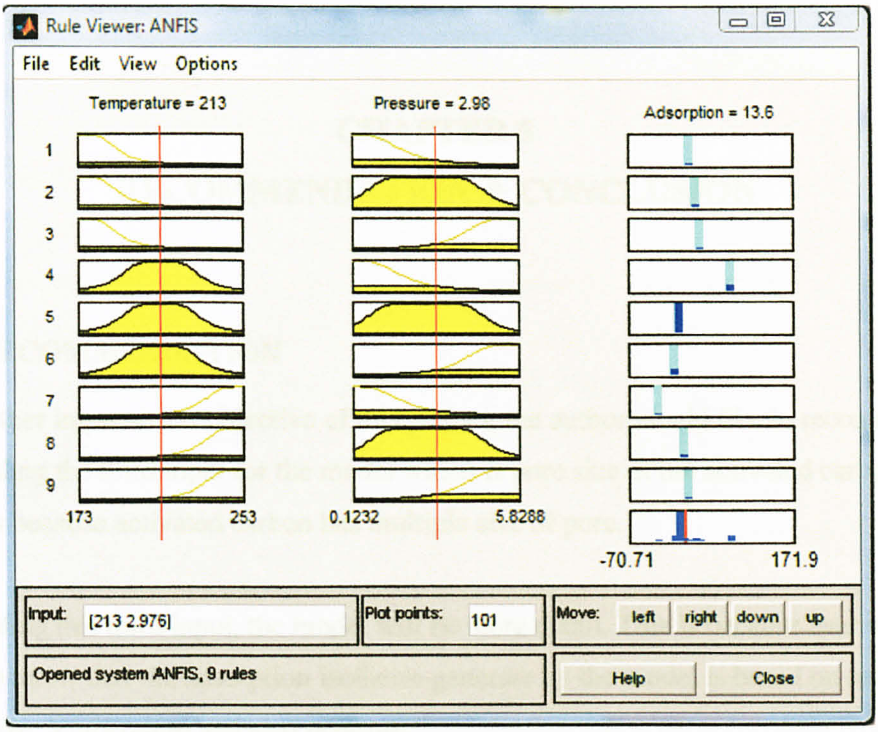


Figure 18: Rules view

Figure 17 shows the rules applied in ANFIS. As mentioned above, this ANFIS employed three membership functions for each input. By calculating the degree of each membership functions in each input, ANFIS will be able to predict the adsorption amount.

In this figure, it shows the prediction of adsorption at temperature of 213K and pressure of 2.98 bar. The yellow color shows how much each membership functions affect the prediction of the data.

# CHAPTER 5
# RECOMMENDATION & CONCLUSION

## 1. RECOMMENDATION

To further improve the objective of this project, the author would like to recommend for adding the third input for the model which is pore size of the activated carbon. This is because activated carbon has multiple size of pore.

By adding this third input, the model will be more detail. This is because user will be able to know that the adsorption isotherm generate by the model is based on specific pore size, temperature and also pressure.

The structure of the ANFIS should be developed as the figure below:

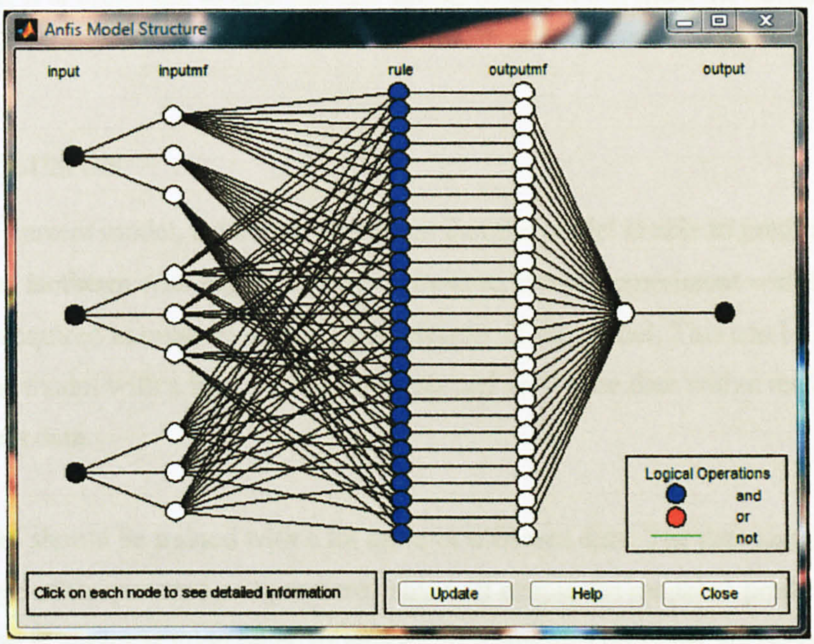


Figure 19: Three Input ANFIS structure

This structure of three inputs is using 3 membership functions for each input. As previously stated before, choice of data is very important because by adding the third input, the model will require more training.

Another method to improve the model is by adding the membership functions. This is because the membership functions are used to determine the output of the model. Therefore, by adding more membership functions, the ANFIS will be able to divide the data it received for training to a smaller range. Less membership functions means wider range and a more generalize output. Since the objective of this project is to develop a high accuracy model, increasing the number of membership functions will enable the model to increase its accuracy. However, adding too much of membership functions are not favorable since it will consume a lot of computing power. Therefore, a suitable choice should be made base on the range of the input.

ANFIS also can be used not only for hydrogen adsorption but also for other types of material. This is because it still using the same concept as the model for hydrogen adsorption. However, the membership functions should be tuned differently. This is because different type of material will give different type of adsorption isotherm. Therefore, it is important to tune the new model so that it can meet the desired output.

## 2. CONCLUSION

From the current model, the author found out that the model is able to predict the adsorption isotherm with high accuracy. However, further experiment with the model is required in order to increase the integrity of the model. This can be done by testing the model with a few more sets of data and verify the data with a real experiment data.

The model should be trained with a lot more of different data. The data should be in wide range of temperature and pressure. This will enable the model to predict the adsorption isotherm at wide range of temperature and also pressure. By doing this, the model will be truly useful to researcher in the future.

Comparison with other models created by others also should be done in the near future. This should be done in order to compare the efficiency with the model. An optimization also should be done in order to get the best model for the prediction.

In this project, the author employs a Sugeno Fuzzy Inference System which has a lot of advantages such as:

- It is computationally efficient.
- It works well with linear techniques.
- It works well with optimization and adaptive techniques
- It has guaranteed continuity of the output surface
- It is well suited to mathematical analysis

ANFIS is really useful in modeling. Its capability in prediction will help reducing the cost and time for a real experiment. However, ANFIS also has its own weaknesses. If the training data given to the ANFIS has high level of noise, the ANFIS might learn and model the parameters correctly. This will results in the ANFIS given wrong prediction in the futures.

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# APPENDICES

```
clear all;
clc;

%data reading for full data
comp_data=xlsread ('chk_complete');

%173K
ad_173comp=comp_data(1:17,3);
pr_173comp=comp_data(1:17,2);

%213K
ad_213comp=comp_data(18:32,3);
pr_213comp=comp_data(18:32,2);

%253
ad_253comp=comp_data(33:46,3);
pr_253comp=comp_data(33:46,2);

%Plotting graph for complete literature data
figure(1)
plot(pr_173comp,ad_173comp,'bo',pr_213comp,ad_213comp,'go',pr_253com
p,ad_253comp,'ro');
legend('173K','213K','253K','Location','NorthEastOutside');
title('Checking data for Hydrogen adsorption isotherm at different
temperature (Literature)');
xlabel('Pressure (MPa)');
ylabel('Capacity(mmol/g)');

%data reading for training data
trn_data=xlsread ('trn_complete');

%173K
ad_173trn=trn_data(1:14,3);
pr_173trn=trn_data(1:14,2);

%213K
ad_213trn=trn_data(15:27,3);
pr_213trn=trn_data(15:27,2);

%253
ad_253trn=trn_data(28:38,3);
pr_253trn=trn_data(28:38,2);

%Plotting graph for complete literature data
figure(2)
plot(pr_173trn,ad_173trn,'bo',pr_213trn,ad_213trn,'go',pr_253trn,ad_
253trn,'ro');
legend('173K','213K','253K','Location','NorthEastOutside');
title('Training data for Hydrogen adsorption isotherm at different
temperature (Literature)');
xlabel('Pressure (MPa)');
```

```
ylabel('Capacity(mmol/g)');

%Generating initial ANFIS
in_fismat=genfis1(trn_data, 3, 'gbellmf');

%Initial ANFIS membership function
figure(3)
subplot(2,2,1);
plotmf(in_fismat, 'input', 1);
subplot(2,2,2);
plotmf(in_fismat, 'input', 2);

%Starting ANFIS training
[trn_out_fismat trn_error step_size chk_out_fismat chk_error] = ...
    anfis(trn_data, in_fismat, [100 nan 0.01 0.5 1.5], 1, comp_data,
1);

%Trained ANFIS
figure(4)
subplot(2,2,1);
plotmf(chk_out_fismat, 'input', 1);
subplot(2,2,2);
plotmf(chk_out_fismat, 'input', 2);

%Membership comparison
figure(5)
subplot(2,2,1);
plotmf(in_fismat, 'input', 1);
subplot(2,2,2);
plotmf(in_fismat, 'input', 2);
subplot(2,2,3);
plotmf(chk_out_fismat, 'input', 1);
subplot(2,2,4);
plotmf(chk_out_fismat, 'input', 2);



%Training results
figure(6)
[m, n] = min(chk_error);
plot(1:100, trn_error, 'g-', 1:100, chk_error, 'r-', n, m, 'ko');
title('Training (green) and checking (red) error curves');
xlabel('Epoch numbers');
ylabel('RMSE (Root Mean Squared Error)');

%Linear Regression Calculation
%data
LGA=xlsread ('trn');
LGB=xlsread ('chk');

%multiple linear regression
X=[ones(size(LGA,1),1) LGA(:,1:2)];
y=LGA(:,3);
[b,bint,r,rint,stats]=regress(y,X);
stats;

%y prediction
xte=[ones(size(LGB,1),1) LGB(:,1:2)];
```

```
ypr=xte*b;

%graph
a=transpose (ypr);
yac= LGB(:,3);
c=transpose (yac);
figure(7)
[slope5,intercept5,R5]=postreg(a,c);
ylabel('Predicted Hydrogen Adsorption Isotherm '),xlabel('Actual
Hydrogen Adsorptiom Isotherm'),...
    title([ ' Predicted vs. Actual, y=(', num2str(slope5),') x+
(',num2str(intercept5),')    R squared=',num2str(R5*R5)]);

%RMSE comparison between ANFIS & Linear Regression
%Data for Linear Regression RMSE calculation

A=trn_data(28:38,:);
B=comp_data(33:46,:);

N=size(A,1);
C=[A(:,1:2) ones(N,1)];
D=A(:,3);
coef=C\D;

Nc=size(B,1);
C_ck=[B(:,1:2) ones(Nc,1)];
D_ck=B(:,3);
lr_rmse = norm(C_ck*coef-D_ck)/sqrt(Nc);

%Results
fprintf('\nRMSE against checking data\nANFIS : %1.3f\tLinear
Regression : %1.3f\n', m, lr_rmse);

%Surface view on the ANFIS model
chk_out_fismat = setfis(chk_out_fismat, 'input', 1, 'name',
'Temperature');
chk_out_fismat = setfis(chk_out_fismat, 'input', 2, 'name',
'Pressure');
chk_out_fismat = setfis(chk_out_fismat, 'output', 1, 'name',
'Adsorption');

%Generating the FIS output surface plot
figure(8)
gensurf(chk_out_fismat);
```