Fuzzy Logic Model of Nitrate Release from Polymer-Coated Fertilizers

by

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CERTIFICATION OF APPROVAL

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Approved by,

____

(Dr Radzuan Razali)

UNIVERSITI TEKNOLOGI PETRONAS
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January 2015

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.

TIONG YAN XIANG

ABSTRACT

In real world, mathematical model is commonly used to explain complicated system so that people can understand the system or the behavior of the system easily. Biopolymer is very useful and beneficial in various fields such as medical, agriculture, bioengineering and so on. However, the complexity of the process of biodegradation makes it difficult to optimize the design of polymers application. Chemical reactions such as degradation of biopolymer usually take years and it costs a lot of money due to the numerous experiments sets used. Therefore, the objectives of this project are to apply fuzzy logic theory on modelling to find the effect of temperature on polymers biodegradation, and to use the Matlab simulation to show the biopolymer degradation behavior. In order to perform the fuzzy logic modelling, the scope of study involves the basic knowledge on the fuzzy logic theory and fuzzy rules. Simple mathematical modelling equations on degradation are used for simulation and performed in Matlab to obtain the results for polymer biodegradation. Modelling can quickly predict the nitrogen release profile for the biodegradation process and this becomes very helpful in optimizing the design of polymer in many applications such as tissue engineering, bone fixation, drug delivery, etc.

ACKNOWLEDGEMENTS

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

In Science field, various systems are being provided verbal descriptions and explanations by human observers. However, a proper mathematical model is very important in analyzing a system. This is where fuzzy logic model comes into place. Fuzzy logic model is a simple and direct tool used to transform oral descriptions into mathematical models. Fuzzy logic is very useful because it is able to interpret the information based on what human perceived rather than equations. Besides, this model represents the real system which is close to human perception. This is why this model is easier to understand if compared to others artificial intelligence techniques such as artificial neural network (ANN), adaptive-neuro-fuzzy- interference system (ANFIS) and radial basis function (RBF) [1].

Polymer coated fertilizers are also known as the controlled release fertilizers. The percentage of the nitrogen released into the environment can be controlled based on the need of the plant at different period of time. If excessive nitrate is loss to the environment without controlled, this can cause severe environmental pollution. These fertilizers are widely used in the plant production in the container as they maximize the efficiency use of the nutrient, increase the crop yields of the plant, reduce the labor needs and control the fertilizer runoff pollution. Since few years ago, biodegradation has caught the attention of the world regardless agriculture or medical field. Biodegradation is defined as a bioactive decomposition process. There are many types of biodegradation such as mechanical degradation, thermal degradation, light degradation, oxidation degradation and hydrolysis degradation. Due to the complicated mechanism of biodegradation which include hydrolysis reaction, simultaneous crystallization and diffusions, this entire field would benefits from the fuzzy logic model which is capable of predicting the degradation and any device property changes.

Temperature is one of the most significant factor which affects the release of nitrogen of a controlled-release fertilizer. Most of the literature papers agree that the release rate almost doubled when the temperature increased from 10 ℃ to 20 ℃. Temperature-induced coating characteristics made a significantly increase to the release rate of the nitrogen through the polymer coating to the environment. The nutrient release is found to increase with the increase in the temperature and the release of nutrient decreases with time after the beginning of the high release levels. Besides the temperature, there are others factors which affect the biopolymer degradation such as the soil pH, soil moisture, reacting agent, coating thickness and so on. On the other hand, the bacterial activity and concentration of external salt do not have a significant effect on the nitrogen release profile of controlled-release fertilizers [2].

1.1.1 Fuzzy set theory

The basic theory of classical theory focus on “set”. The individual of a set either belongs or does not belong to the set. However in probability and statistics, many people concern about the probability of this individual, but the classical theory can only define the individual in a way that either “it is” or “it is not” a member of the set. It is either false symbolized by a logic ‘0’ or it is true symbolized by a logic ‘1’. There is no partial membership of the individual. The individual cannot be partially in a set or partially not in the set. This causes difficulties in describing many real-life applications problems, mainly those with partial membership. For example, the height of a person. If the person is 160 cm tall, the fuzzy logic will define the height as 0.6 short and 0.4 tall while the traditional logic can only define that person as either tall or short. In spite of this, the fuzzy set theory can be said help to solve this partiality membership problem which in another words it makes the classical set theory more general. Fuzzy set theory is associated with fuzzy membership function (FMF). In general, FMF can have various shapes, as shown in three figures below, which is chosen by the user based on the different applications in different natures [3].

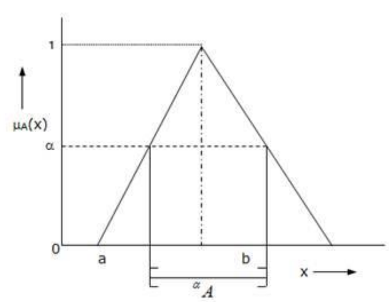


Figure 1.1 Triangular MF

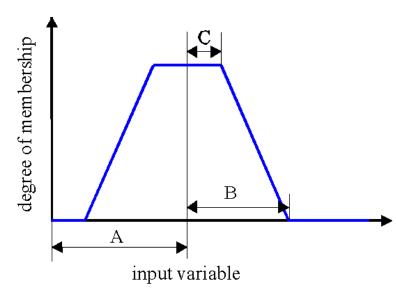


Figure 1.2 Trapezoidal MF

1.1.2 Fuzzy Modelling

Modelling generally means describing a physical system by explaining the relationship between the input and output in the form of mathematics. Fuzzy system modeling is using the fuzzy logic theory and fuzzy membership function for computation of logical linguistic form, where this modelling usually involves IF-THEN rule as shown below [1].

If the input is x1 and… input xn,
then the output is y1 and …output ym.

One of the initial steps when designing a model is setting the range for the input variables. Once the reasonable range of the input variables has been determined, different descriptive linguistic terms are considered to each range. Then the membership functions are used to represent the input. For example, the universal space is divided into n numbers of triangular fuzzy sets. The linguistically significant name will be assigned to the n membership functions. Like the input, the range of the output variable will be divided up into numerous membership functions. One thing that should be aware of when naming the membership functions is that the names used must be distinct. After the inputs and outputs have been defined, a set of rules are specified to produce a model. The fuzzy rules being set are based on experimental data or merely through observations.

1.2 Problem Statement

In real life, biodegradation process is very complicated due to many reactions involved. The complexity of this mechanism makes it difficult to optimize the design of the polymers applications. Furthermore, the biodegradation process takes a very long period of time. For example, the complete degradation of poly (L-lactide) (PLA) interference screws in human body has been found to take up to four years [4]. Huge efforts made by many researchers in order to understand the complexity of the polymer biodegradations. In this project, fuzzy logic modelling is introduced to solve the complexity of biodegradation process by using the mathematical equations to represent the real system. Not only that, the project will only focus on temperature factor that affect the biodegradation of polymer despite there are many others factors which affect biodegradation such as enzymatic reactions, soil pH, diffusion coefficient, coat thickness, granule radius and so on [5]. The significance of this project is that fuzzy logic provides an easier and understandable way to clearly analyze the degradation behavior of polymers due to temperature effects where we highly agree that the degradation of biopolymer is bringing great impact to the society such as in tissue engineering, drugs delivery, bone fixing and etc.

1.3 Objectives

The main purpose of the research is to develop a fuzzy logic modelling to determine the degradation behavior of polymers due to temperature effects. This research aims to achieve the following at the end of the project:

1. Use mathematical modelling to simulate results for biodegradation related equations.
2. Use fuzzy logic to model the release profile of nitrogen of the polymer-coated fertilizers based on temperature changes.

1.4 Scope of Study

This project requires a lot of knowledge on the fuzzy logic theory and fuzzy modelling. It also requires a lot of researches on how the modelling takes place using MATLAB simulation and also studying about the temperature effect on biodegradation. Since biodegradation mechanism itself is affected by so many external factors, due to limitation time of FYP 1 and FYP 2, we will be focusing on temperature factors for the time being in this project. This project is highly achievable within the time frame because the standard mathematical equations for biodegradation is already ready, so in this project only the mathematical modelling using MATLAB will be highlighted.

1.5 Relevancy of the project

This project is highly relevant because biodegradation is extremely useful in applied science, agriculture field and also medical field. Since the biodegradation of polymers usually takes longer time in human body at 37˚C, by applying the same behavior of polymer biodegradation on slow controlled released fertilizers in plants can help in reducing the time needed for biodegradation of polymers with elevated temperature.

1.6 Feasibility of the project

The scope of the study of this project is designed based on consideration on FYP1 and FYP2. This project is feasible as we just need to come out with the mathematical model using fuzzy logic model by putting in the given mathematical equations and formulas which are related to biodegradation of polymers with respect to temperature. As the design and system analysis will be done based on MATLAB simulation, this can reduce the lengthy process of natural biodegradation of polymers in real life.

CHAPTER 2

LITERATURE REVIEW

In this literature review, both the biodegradation process and fuzzy logic modelling are being covered. Besides, the comparison between different artificial intelligence techniques are meant to explain why fuzzy logic model is a better way to be chosen for this project. This is to ensure the understanding of the basic on how the biodegradation of polymers is performed and how fuzzy logic is applied for modelling.

2.1 Process of Biodegradation

Biodegradation of polymers is defined as bioactive decomposition process where microorganisms and enzymes are used to degrade polymers. In fact, even though there is not much changes in chemical structures of polymers, the biodegradability is greatly affected by the molecular properties and the crystallinity. When the molecular weight increases, the biodegradability reduces. In biodegradation of polymers, two categories of enzymes are involved which are extracellular and intracellular depolymerases. During the initial process, depolymerization takes place. The exoenzymes from the microorganism breakdown the long complex polymers chains into short chains. The chains are small enough and can diffuse through the cell walls and used for carbon and energy sources. After that, mineralization takes place where the end products produced are carbon dioxide, water or methane. In fact, end products produced will be different depending on their variations of degradation pathway [6].

2.2 Comparison of Different Artificial Intelligence Techniques

Forrester cooperates with his team did a modelling of the complex systems dynamic behaviors using system dynamics method. They come out with fundamental brainstorming ideas which use different polarity feedback loops to represent the system. The graphical is transformed into differential equations and this method was later applied widely in industrial sciences, social, economic and etc. In spite of this, this method has ignored the verbal description. Later the qualitative reasoning (QR) is being introduced to model the physical systems because it is much more logical. This reasoning is explained in a way such that the differential equations are generalized. QR was able to do simulation and analyzing various actual physical systems. Despite its advantages, it also has a drawback such that its application seems to be incomplete in knowledge if compared with a verbal description of the system [1]. In the past three decades, artificial intelligence techniques has been developed to solve complicated practical problems, for examples artificial neural network (ANN), adaptive-neuro-fuzzy-interference system (ANFIS) and radial basis function (RBF). ANN approach is a good mathematical tool but for that particular process, the parameters relationship is vague. To overcome the problem, fuzzy modeling is applied together with ANN method in order to explicate the relationships among the parameters. Fuzzy interference system (FIS) modeling consists of fuzzifier, fuzzy rule base, fuzzy inference engine (FIE) and defuzzifier. Input is being transformed into useful fuzzy facts. Moreover, fuzzy rule uses the concept of input and output relationship to solve the real-world application problems [7]. The defuzzifier will convert the fuzzy facts from FIS to the expected results or performances. Table 2.1 shows the summary of the related work of different founders who used different modeling techniques to represent a system.

Table 2.1 Related work

Paper Published	Techniques	Founders	Descriptions
1950	System Dynamics	Forrester & colleagues	Use elementary structures to represent the system
1994	Qualitative reasoning (QR)	-	A more logical modeling method for systems
1973	Fuzzy sets & fuzzy logic foundation	Zadeh	Linked to human linguistics
1974	Design first fuzzy controller	Mamdani	The design is based on verbal control protocol.
1981	Verbal models	Wenstop	Analyzing verbal information and process it
2002	Fuzzy Cognitive Maps (FCMS)	Kosko	Method used to describe the relationship between different linguistic concepts

2.3 Critical and gap analysis

From the literature review, we can see that very few people focusing on the biodegradation behavior of polymers with respect to effects of elevated temperature using fuzzy logic. Besides, the fuzzy logic model is found to be a more direct and simpler method which is easier to understand. Therefore, among so many artificial intelligence techniques, fuzzy logic is being chosen in this project as the technique used for modelling to find the degradation behavior of the polymers with elevated temperature as the main factor.

CHAPTER 3

METHODOLOGY

In the beginning, use verbal descriptions to analyze the system. The process of degradation of controlled-release fertilizers when temperature changes are studied in order to understand thoroughly. Next, determine the variables corresponding to the system. The variables can be more than one and those are the variables which will affect the biodegradation process. In real systems, the variables are normally measurable physical quantities. In this project, there is only one input and output variable which is the temperature and nitrogen diffusion rate respectively. The verbal descriptions are later being transformed into the fuzzy rules to state the relationship between the variables. Five fuzzy rules are applied during the fuzzy modeling. After that, the fuzzy terms are described with suitable fuzzy membership functions and they are connected using the Boolean operators such as AND, OR and NOT. Before the simulation is carried out, fuzzy inferencing takes place where fuzzy rule base is being transformed into a mathematical model. The users can choose any kinds of membership functions, logical operators, inferencing method and different parameters values based on the need of the physical system. The simpler the mathematical model, the better it is [1]. System analysis and simulation will be done using Matlab software and compared with the fuzzy result. A flowchart which shows each step of fuzzy modeling is shown in figure 3.1 below.

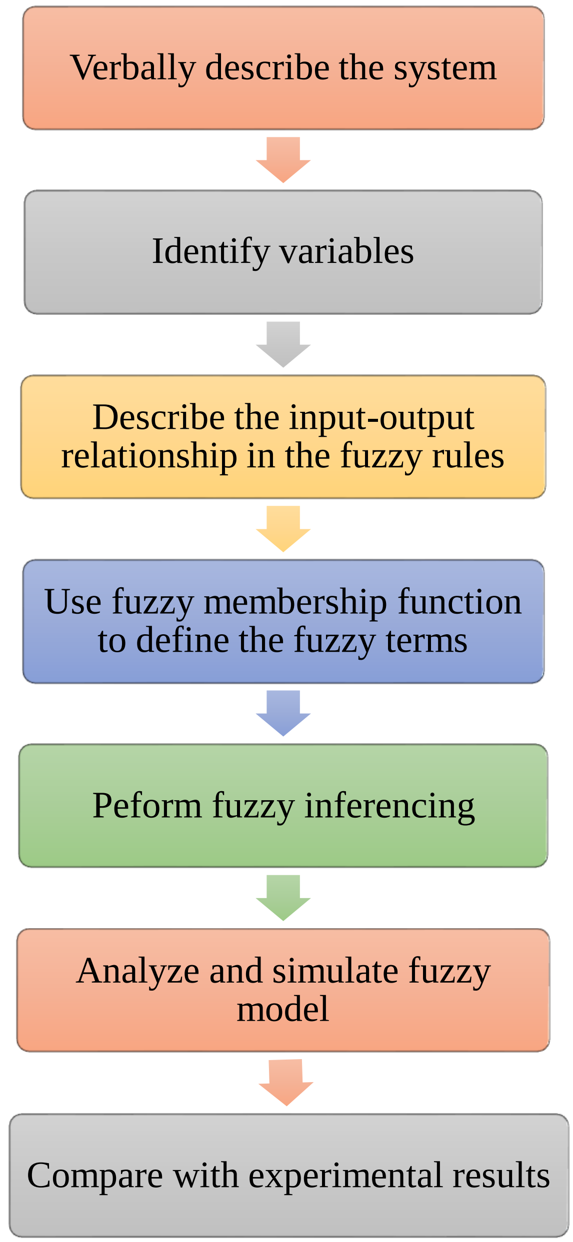


Figure 3.1 Flowchart

CHAPTER 4

RESULTS AND DISCUSSION

The fundamental rate equation of the degradation is as shown below [6]:

$$\frac{d\propto}{dt} = Kf(\propto) \qquad (1)$$

$\frac{d\propto}{dt}$ = Conversion rate;

f (α) = Temperature-independent function of the conversion;

K = Temperature-dependent constant rate of reaction.

K is expressed in terms of Arrhenius equation as shown below [6]:

$$K = A \exp\left(\frac{-E_a}{RT}\right) \qquad (2)$$

A = Frequency factor corresponding to the incidence of molecular collisions that should be obtained to produce a chemical reaction;

E_a = Activation Energy;

R = Gas constant;

T = Absolute Temperature.

f (α) assumes the rate of conversion is proportional to the nth order of the material concentration. The formula is as shown below [6], where n is the order of reaction.

$$f(\alpha) = (1 - \alpha)^n \qquad (3)$$

By inserting equation (2) and (3) into equation (1), rearranging and taking logarithms, the resulting equation is expressed as below [6]:

$$\ln \left(\frac{d\alpha}{dt}\right) = \ln A + n \ln (1 - \alpha) - \frac{E_a}{RT} \quad (4)$$

As shown from the Figure 4.1, it shows the relationship between rate of reaction, K (in $cm^3 mol^{-1} s^{-1}$) and temperature, T (in Kelvin). The result is as expected as the graph is increasing exponentially due to the logarithm mathematical equation will always give an exponential graph. As seen from the graph in the first simulation, the rate of reaction, K increase with the increase of T. However, if the graph is a plot of ln K against 1/T, then the result of the graph will shows a decreasing linear graph. Arrhenius plots are often used to analyze the effect of temperature on the rate of chemical reactions. The simulation is done in Matlab based on equation (2), where this shows the simulation for simple mathematical equation of a biodegradation process. The reason of performing the simulation based on this mathematical equation is to see the effect of temperature on the temperature-dependence constant rate of reaction. The parameters such as the frequency factor is kept constant, and the optimum value of the activation energy and the universal gas constant are being chosen to be put into the mathematical equation.

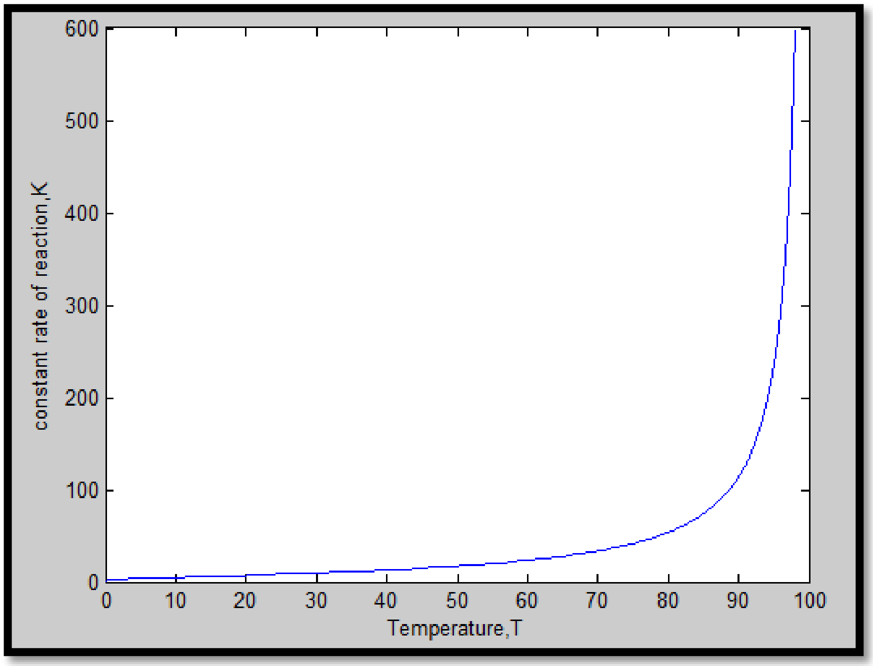


Figure 4.1 Graph of K against T

According to [8], the mathematical equation below involves variables which will affect the mass diffused over time:

$$\frac{Mt}{M\infty} = 6(1+\propto)(\frac{tD}{\pi R^2})^{0.5} \quad , \text{ where} \tag{5}$$

$$\alpha = \frac{C_\infty}{C_o - C_\infty} \tag{6}$$

Mt = Mass diffused up to time t;

M∞ = Mass diffused after infinite time;

D = Diffusion coefficient of the fertilizer;

R = Radius of the spherical particle;

C_o = Initial concentration of the fertilizer;

C_∞ = Concentration inside the sphere at the infinite time

The mathematical formula basically describes the quantity of dissolved active agent diffused through the polymer membrane released at any given time per total amount of active agent initially for a spherical particle, M_t/M_∞. The fertilizer used in the laboratory experiment is controlled-release fertilizers coated in urea as polymeric membrane. This modelling keeps the parameters such as diffusion coefficient, D and radius values, R as constant. Modeling is done using Matlab and the values of α are changed with values 0.001, 0.01, 0.1, 1 and 10 respectively to see the relationship between alpha and its mass diffusivity. The simulation of the Matlab result is shown below in figure 4.2 below. The graph is plotted based on mass diffusion versus time based on different values of alpha. In this calculation, variables such as diffusion coefficient and radius are kept constant. Based on the graph, when alpha value is increased by ten times, the mass diffusion rate also increases. From the graph, it is shown that when alpha value is 10, the mass diffusion is the highest. Each output data of the graph drawn from different alpha values is represented by different colors on the graph. The alpha values are calculated based on equation 6.

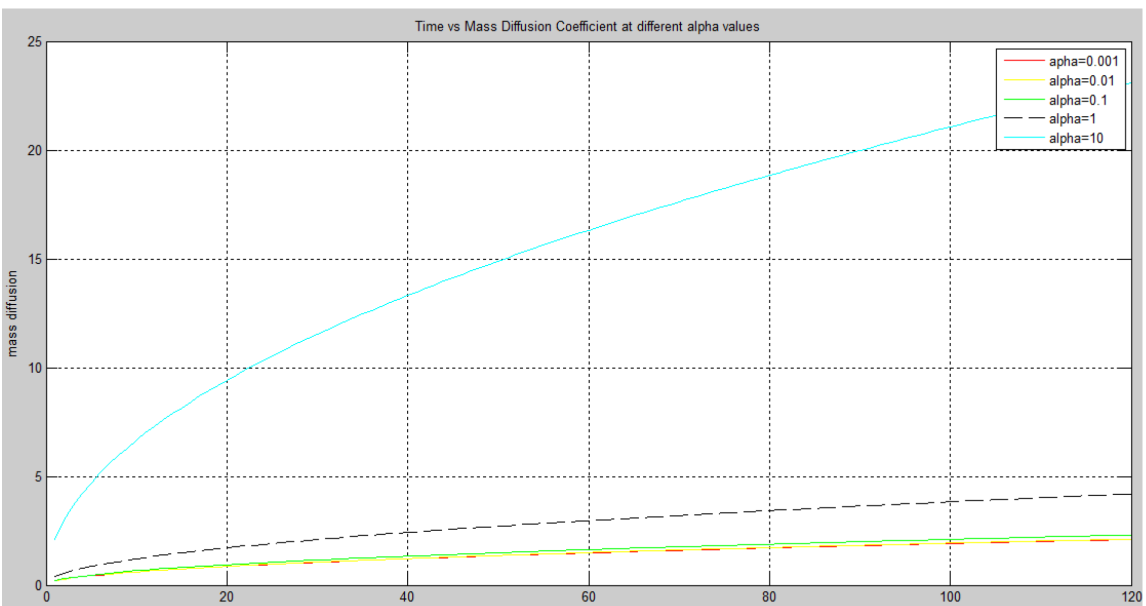


Figure 4.2 Graph of mass diffusion versus time

4.1 Using the Fuzzy Modeling

Fuzzy modeling is easier for everyone to understand especially for users who want to understand a complicated behavior of the system but not a mathematical expert. They can simply understand the behavior of the system by verbal description of the fuzzy rules. In Matlab, the Fuzzy toolbox enables fuzzy modeling to be designed. In this project, users can understand the behavior pattern of mass diffusivity of urea by giving the desired input and see the output of the results. The behavior pattern of the nitrogen released with time is computed using the Fuzzy modeling.

Firstly, the number and type of inputs and output are being set. The two inputs are alpha and time respectively while the one and only output set is set which is the mass diffused. Calculations are done based on equation 5 stated previously, which is the mass diffusivity equation. The values of α varied from 0.001, 0.01, 0.1, 1 and 10. The results are tabulated as shown in table 4.1 below.

Table 4.1 Table of mass diffused with time based on different values of $\propto$

$\propto$	Mass diffused, $M_t/M_\propto$			
	t=20	t=40	t=60	t=80
0.001	0.86	1.21	1.48	1.71
0.01	0.86	1.22	1.50	1.73
0.1	0.94	1.33	1.63	1.88
1	1.71	2.42	2.97	3.43

In the Fuzzy toolbox, the range of values are set for input and output variables. Membership functions are chosen for each variable. The range of parameters are set based on the results obtained from the calculations tabulated above. A fuzzy set is thoroughly characterized by its membership function (MF). MF is defined to express it as a mathematical formula. The membership function must fulfil the condition that it is between 0 and 1. The shape can be defined that suits us for simplicity and efficiency.

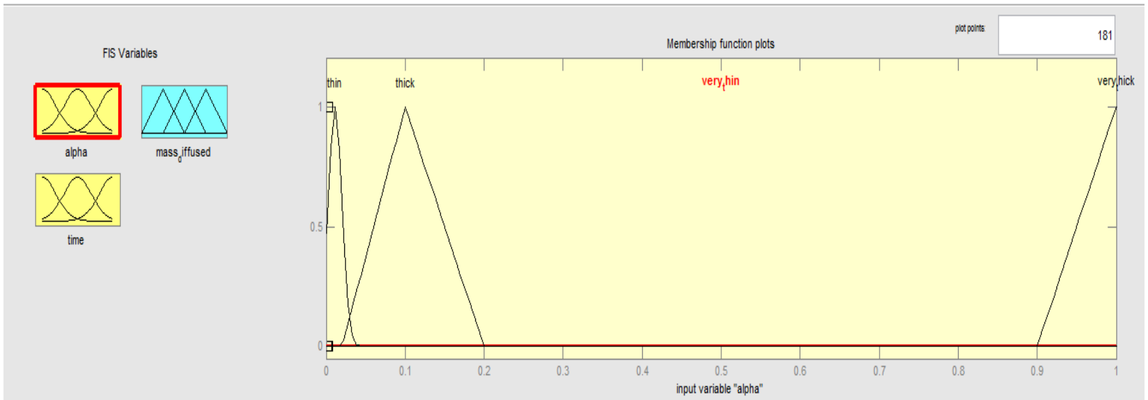


Figure 4.3 Membership functions of alpha

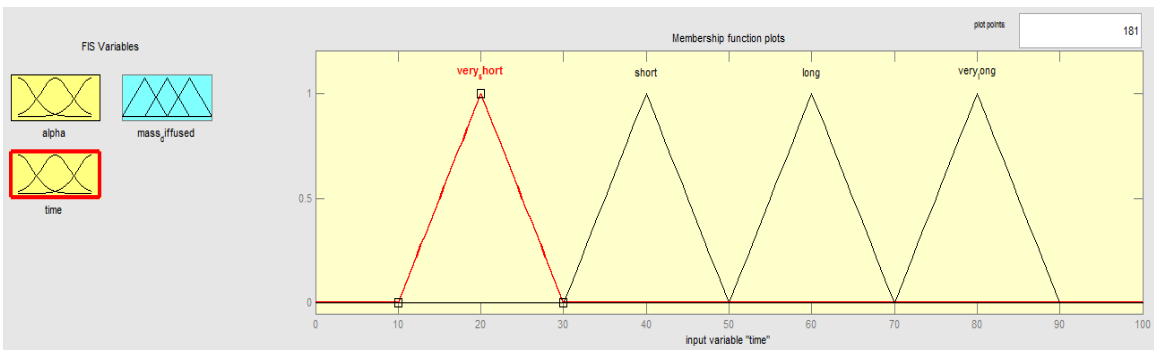


Figure 4.4 Membership functions of time

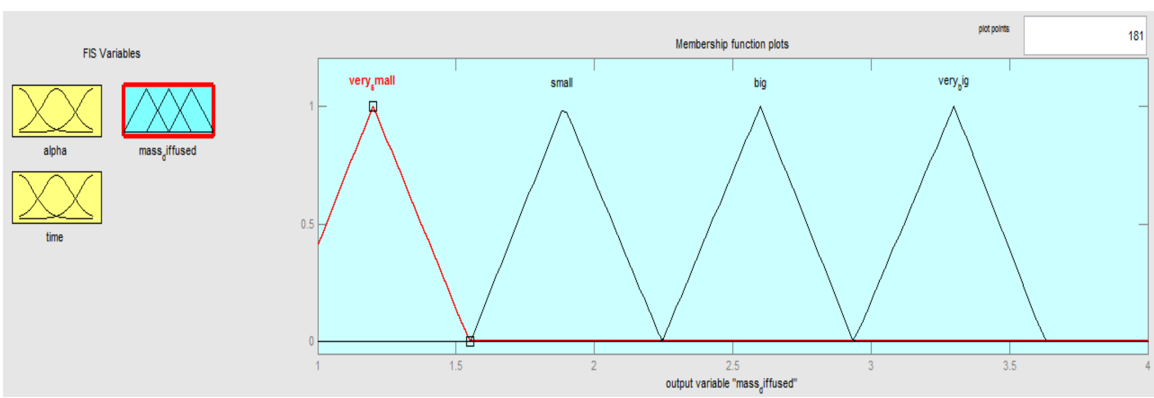
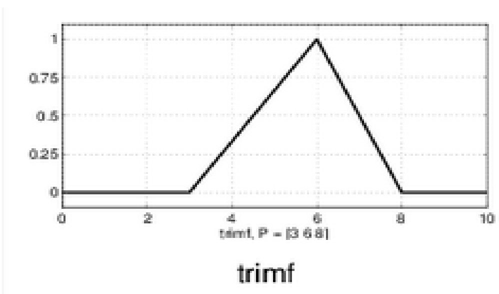


Figure 4.5 Membership functions of mass diffused

As shown in figures above, for each parameters (both inputs and output), four membership functions are set. In this case, among others membership function such as trapezoidal MFs (trapmmf), Gaussian MFs (gaussmf), Generalised bell MFs (gauss2mf), and etc., the triangular membership function (trimf) is chosen as the type of membership function as it is known as the simplest membership function (Figure 4.6). The simplest membership functions are formed using straight lines. This function is formed by a collection of three points to form a triangle. Triangular MFs is identified by parameters a, b, and c as shown in figure 4.7. Ranges of input and output are labelled with different membership functions as tabulated in table 4.2.



$$\text{triangle}(x; a, b, c) = \begin{cases} 0, & x \le a. \\ \dfrac{x-a}{b-a}, & a \le x \le b. \\ \dfrac{c-x}{c-b}, & b \le x \le c. \\ 0, & c \le x. \end{cases}$$

Figure 4.6 Triangular membership function

Figure 4.7 range of parameters

Table 4.2 Descriptions of membership functions of input and output

∝	MFs		Time, t	MFs		Mass diffused	MFs
0.001	v. thin		20	v. short		0.86-1.55	v. small
0.01	Thin		40	Short		1.55-2.25	Small
0.1	Thick		60	Long		2.25-2.94	big
1	v. thick		80	v. long		2.94-3.63	v. big

Sixteen If-Then rule statements which are also known as fuzzy rules are used to formulate the conditional statements that comprise fuzzy logic. Fuzzy operator is applied to multiple part antecedents and implication method is applied. As seen from figure 4.8, the fuzzy rules matched the relationship between the two inputs to produce the output.

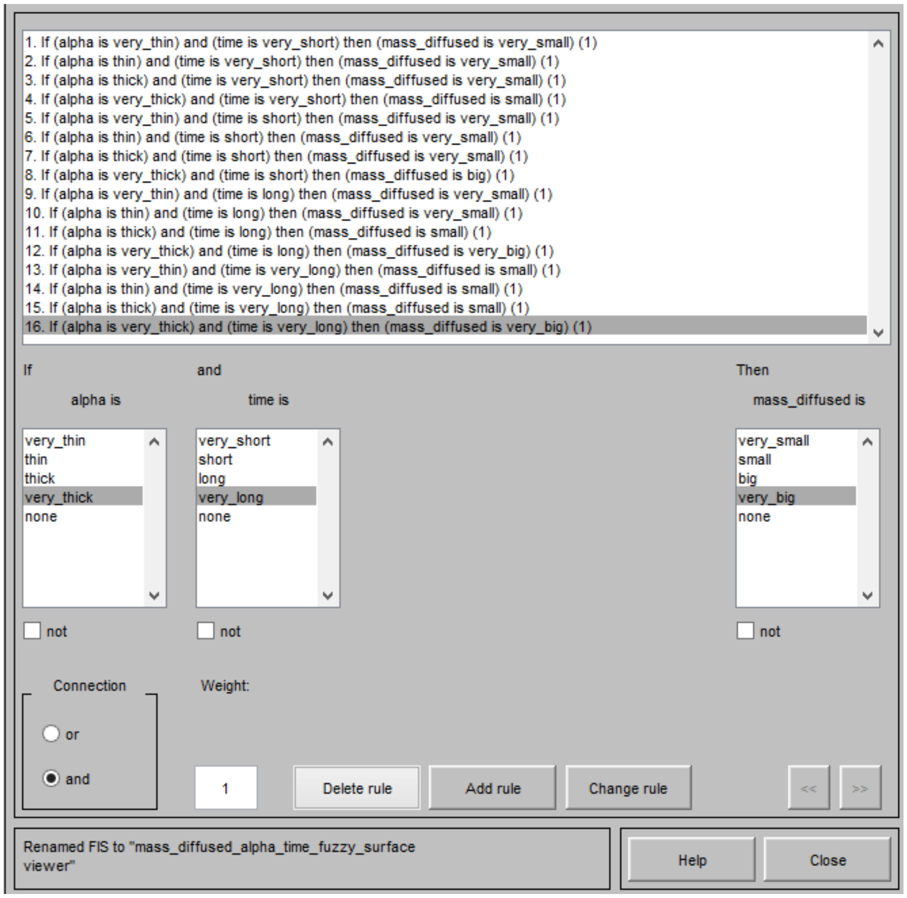


Figure 4.8 Fuzzy rules : alpha versus mass dffusion

Figure 4.9 shows that as the values of alpha and time are being input, there will be output value computed based on the fuzzy modeling. User can input any values for the two input variables and see what are the output value obtained based on the Fuzzy rules and membership functions being set. Based on the trial on the modeling, it is observed that the values computed has 0.02 small deviation compared to the results computed by Matlab simulation. There are some differences in the output values which results in the percentage error possibly because in fuzzy, the natural behavior of the system is involved and this is one of the advantages of the fuzzy logic modelling. Usually when involves a natural phenomenon, a traditional logic is insufficient and fuzzy logic is a better way to describe the complicated system.

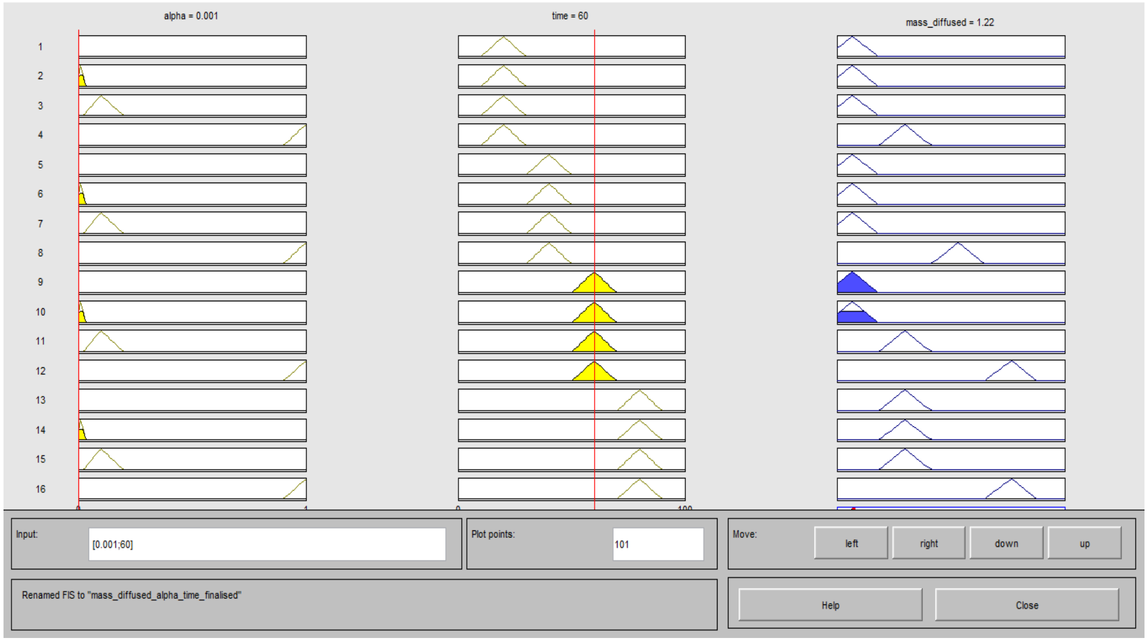


Figure 4.9 Computational of output based on the values being input

As can be seen from the Matlab surface view in the figure 4.11, mass diffused increases with time with the increase of alpha values. It is very obvious that when the alpha=1, the mass diffused is the biggest whereas when the alpha=0.001, 0.01 and 0.1, there is no significant difference in the mass diffusivity. The significance of the difference of mass diffusivity will be even bigger when the alpha values are increased by ten times. For examples, alpha=10, 100, and 1000 respectively.

However, there is limitation of the fuzzy toolbox when comes to set the range of parameters. If the difference between the variable parameter is too big, normally this occurs when the multiple of the difference is ten. For example, if the first input variable is 0.001 and the last input variable is 100, the range is extremely big and the membership function shown becomes insignificant. The results pattern of the surface viewer of the fuzzy modeling has been compared with the graph simulated with Matlab. It is proven that the fuzzy modeling is working correctly because the pattern of output is similar to that of simulated graph in Matlab.

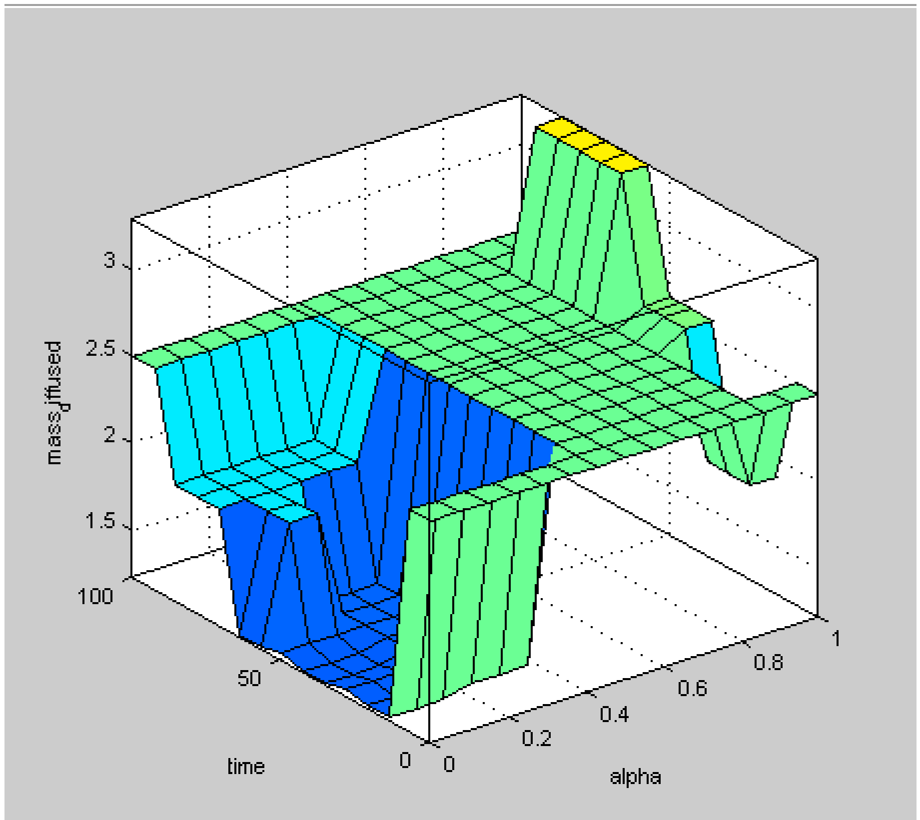


Figure 4.10 Surface view of Fuzzy result in Matlab

The mathematical equation below is important in describing the variations in the rates of linear release, R_{lin} and the lag periods of the controlled-released fertilizers affected by different factors such as temperature and water content [9].

$$R_{lin} \propto C^0{}_{sat} \text{ x } P_s{}^0{}_{sat} \exp\left(-\frac{EA_{ps+EA_c}}{RT}\right) \qquad (7)$$

From this Arrhenius type relation equation, the release is dependence on the temperature changes, T and the overall activation energy of the coated granule release during the linear period of release can be estimated. The permeability Ps and the saturation concentration Csat are the two parameters which are temperature dependent. The reference solubility and permeability are represented by $C^0{}_{sat}$ and $P_s{}^0{}_{sat}$ respectively.

Figure 4.11 shows the result of how is the rate of release of nitrogen during the linear period when temperature changes from 20℃ to 100℃. During the lag period, when the plant is still at the initial growing stage, particularly when the temperature is low, the supply of nutrient maybe too slow. Therefore, the thickness of coating can be reduced to ensure fast release of nitrogen. The lag period is affected by the temperature which the lag period is reduced when the temperature increased. The simulation result also goes parallel with the theory which says that the controlled-release fertilizers are most suitable to be used in the paddy fields compared to others fields. This is because most of the time the paddy fields are occupied by water everywhere, so the temperature is lower. If the controlled-release fertilizers are put in the saturated soil, then the temperature soil will slowly increase in the temperature and increase the release of the amount of nitrate. The bulk increase in the rate of nitrate is not good as it can bring pollution to the environment. The plot of the graph in figure 4.11 shows that when the temperature increases, the rate during linear period also increases gradually. From the graph, the overall energy of activation of the release $EA_{rel} = EA_c + EA_{ps}$ can be estimated. The overall estimation of energy is a vital factor as it indicates how sensible the nutrients release rate is to the temperature.

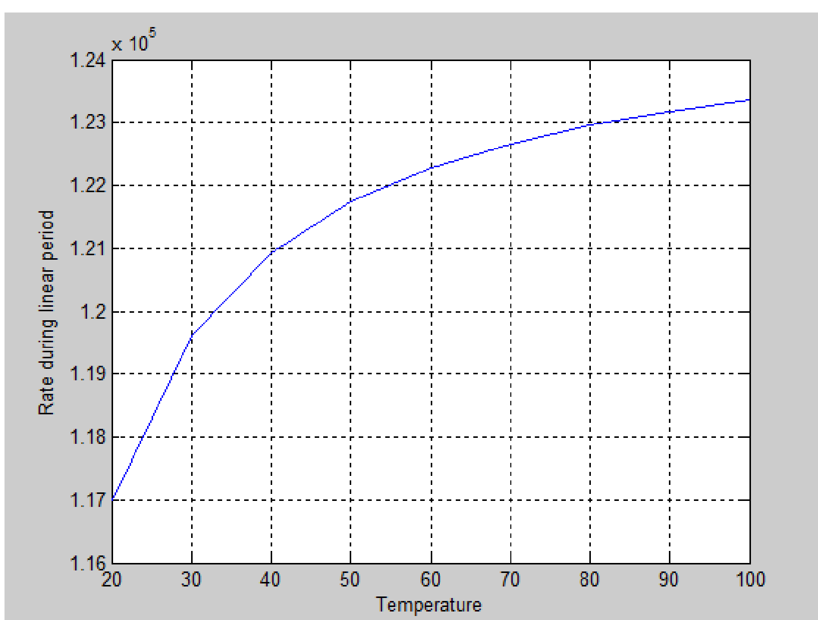


Figure 4.11 Matlab simulation of rate during linear period when temperature changes

Fuzzy Logic is used to model the equation (7) to obtain the relationship between the rate of release during the linear period and the temperature changes. Figure 4.12 shows the fuzzy rules which are used in the fuzzy logic modeling. The fuzzy rules make use of "IF-Then" rules to relate the input to the output. In this case, the temperature becomes the input of the rule while the rate of diffusion becomes the output. The input parameter is described as very low, low, moderate, high and very high whereas the output is described as very slow, slow, middle, fast and very fast. The result of the fuzzy modelling is shown in figure 4.13. The result shows that when there is a change in temperature, the rate of diffusion will also increase. The diffusion coefficient is most highly affected by the temperature and the thickness of coated membrane. A lower diffusion coefficient of coated membrane is due to lower temperature and thicker coated membrane which slowed down the release rate of the nutrients. The graph simulated by the fuzzy logic is not as smooth as the one simulate in Matlab most probably because fuzzy involves the natural behavior of the system, in this case is the biopolymer degradation. This is actually an advantage of fuzzy logic modelling because traditional logic is insufficient to describe a complicated behavior as there is no a specific true or false for a particular natural behavior.

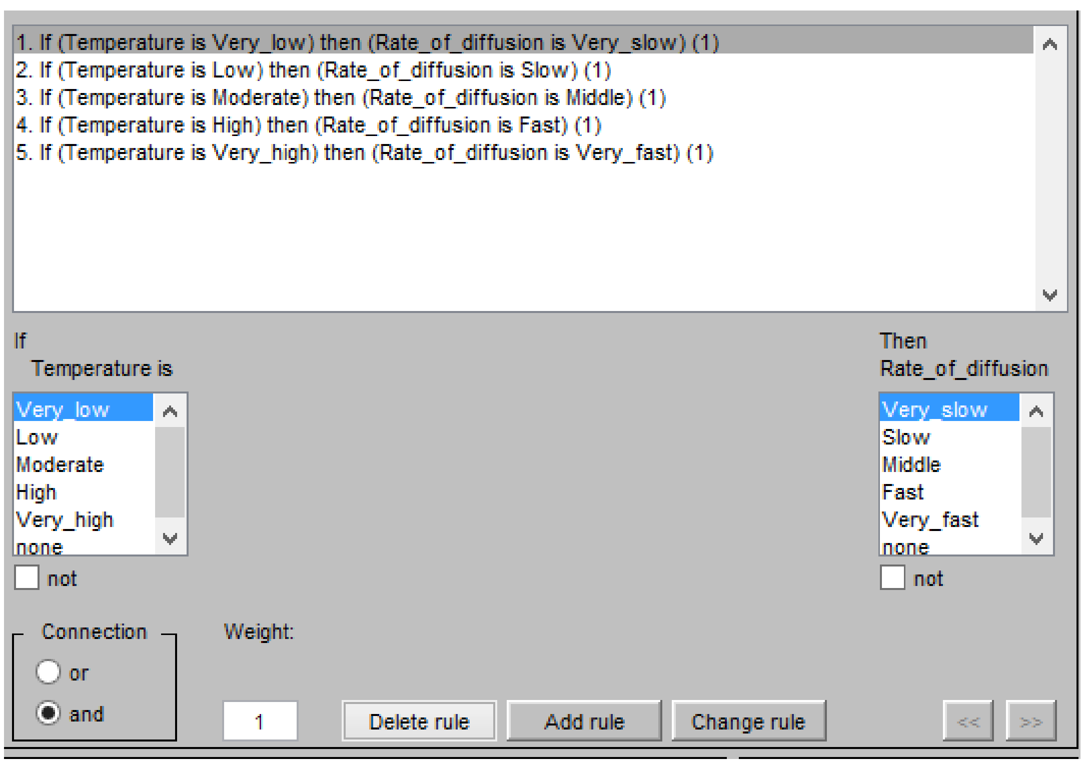


Figure 4.12 Fuzzy rules: Temperature vs Rate of Diffusion

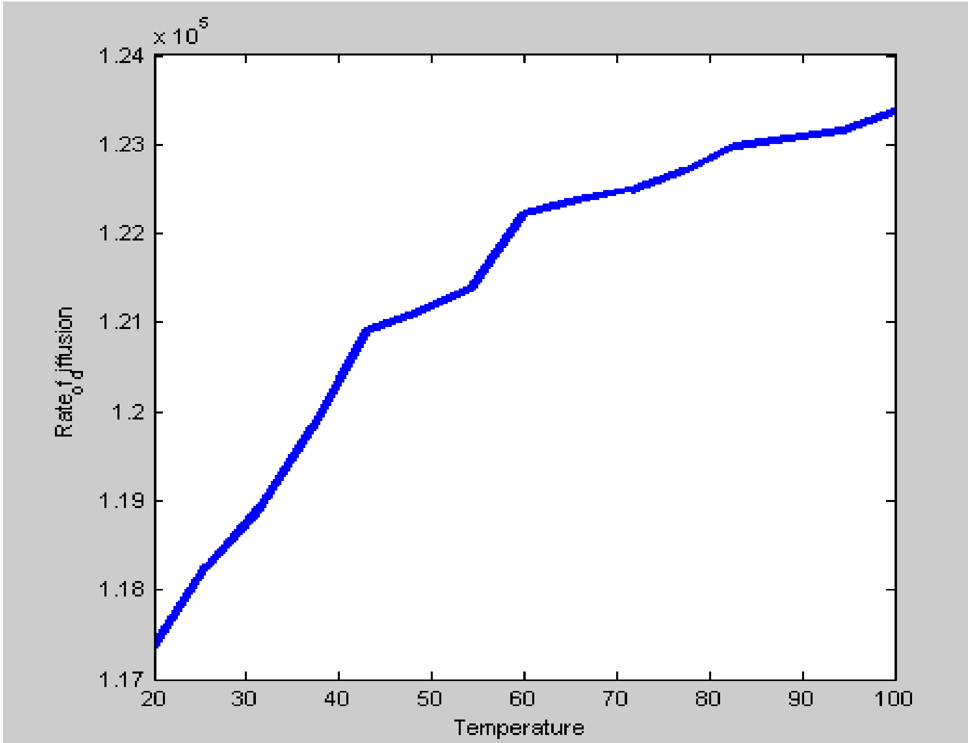


Figure 4.13 Fuzzy result of rate during linear period when temperature changes

CHAPTER 5
CONCLUSION AND RECOMMENDATIONS

Matlab is a good software tool used for mathematical modeling simulation and is user-friendly. The simulation enables user to study and understand the behavior of a complicated system such as the degradation process of fertilizer. In this project, fuzzy modeling has been applied to study the behavior of degradation of biopolymer such as slow-released fertilizers with respect to temperature.

The mathematical equations are simulated in Matlab and the data is integrated with fuzzy rules to perform Fuzzy Inference System (FIS) modeling. In FIS, four interconnected segments such as fuzzifier, fuzzy rule base, fuzzy inference engine (FIE) and defuzzifier are involved. Furthermore, it involves fuzzy rule base which applies certain rules and knowledge required to solve related input-output relationship problems. The FIS is the core of fuzzy system which simulates thinking and decision-making models of humans via suitable reasoning or fuzzy inference, while in the mean time finding solutions to existing problems [6]. The Fuzzy modeling is very user-friendly and enables the polymer applications to be expanded widely for multi-purposes.

As a conclusion, the objectives of this project have been achieved. Mass diffusivity of the polymer with respect to time and rate of release during the linear period based on different alphas are being simulated using Matlab and fuzzy modeling.

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APPENDICES

APPENDIX 1 Matlab code to plot constant rate of reaction versus temperature.

```
a= 100; %frequency factor
Ea=100;
r=8.314;
t=1:600;
b=exp(-Ea./(r.*t));
k=a.*b;%temperature dependent constant rate of reaction

grid;
plot(k,t);
xlabel('Temperature,1/T');
ylabel('constant rate of reaction,K');
```

APPENDIX 2 Matlab code to plot conversion rate versus time.

```
A=100; %constant value
Ea=100;%activation energy
R=8.314;%universal gas constant
n=1;%the order of reaction
t=1:1:3000; time in seconds
T=20; %Temperature as input variables

syms a; %symbolic math to define variable
q=dsolve (Da = exp (log A+ n*log(1-a)-Ea /R*T), ‘t’); %differentiation of da/dt

plot(q,t);
xlabel('time,t');
ylabel('conversion rate,da/dt');
```

APPENDIX 3 Matlab code to plot mass of diffusion vs time (different alpha values with radius kept constant)

```
alpha=0.001
t=1:1:120
D=3.2*10^-7
R=0.01
Mass_diffusion=6*(1+alpha)*sqrt(t*D/(pi*R^2))
plot(t,Mass_diffusion,'r')
xlabel('time')
ylabel('mass diffusion')
title ('Time vs Mass Diffusion Coefficient at different alpha values')
grid on
hold on

alpha=0.01
t=1:1:120
D=3.2*10^-7
R=0.01
Mass_diffusion=6*(1+alpha)*sqrt(t*D/(pi*R^2))
plot(t,Mass_diffusion,'y')
xlabel('time')
ylabel('mass diffusion')
hold on

alpha=0.1
t=1:1:120
D=3.2*10^-7
R=0.01
Mass_diffusion=6*(1+alpha)*sqrt(t*D/(pi*R^2))
plot(t,Mass_diffusion,'g')
xlabel('time')
ylabel('mass diffusion')
hold on
```

```
alpha=1
t=1:1:120
D=3.2*10^-7
R=0.01
Mass_diffusion=6*(1+alpha)*sqrt(t*D/(pi*R^2))
plot(t,Mass_diffusion,'k--')
xlabel('time')
ylabel('mass diffusion')
hold on



alpha=10
t=1:1:120
D=3.2*10^-7
R=0.01
Mass_diffusion=6*(1+alpha)*sqrt(t*D/(pi*R^2))
plot(t,Mass_diffusion,'c')
xlabel('time')
ylabel('mass diffusion')
legend('apha=0.001','alpha=0.01','alpha=0.1','alpha=1','alpha=10')
hold off
```