CERTIFICATION OF APPROVAL

Effect of Dissolved Oxygen Concentration on BOD Decay

by

MUHAMAD FIRDAUS BIN AMRIZAL (2632)

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Approved by,

(MISS NG TZE LING)
Research Supervisor

Universiti Teknologi PETRONAS, Bandar Seri Iskandar, 31750, Bandar Seri Iskandar, Tronoh, Perak Darul Ridzuan

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 thereferences and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

Firdaus

MUHAMAD FIRDAUS BIN AMRIZAL
Author,
Final Year Research Project,
Universiti Teknologi Petronas

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TABLE OF CONTENTS

NOMENCLATURE

L	Concentration of BOD, maybe defined as L_t or L_r depnding on the condition (mg/L)
L_r	Concentration of BOD remaining at time t (mg/L)
L_o	Concentration of ultimate BOD or the initial concentration of the BOD at time $t=0$ (mg/L)
L_t	Concentration of BOD being degraded at time t, $L_o - L_r$ (mg/L)
O_2	Concentration of dissolved oxygen (mg/L)
k_1	First Order rate constant (day^{-1})
k_2	Reaeration rate constant (day^{-1})
k_3	Second Order rate constant (L/mg.day)
A_x	Area of mass transfer at direction x (m)
D_L	Diffusion or dispersion coefficient (m^2/s)
$\bar{u}$	Mean velocity of the water system (m/s or ft/s)
K	Dispersion constant
n	Manning's roughness coefficient
d	Depth of water river or channel (ft or m)

LIST OF FIGURE AND TABLES

CHAPTER 1

ABSTRACT

The Biochemical Oxygen Demand (BOD) is a quantity of the dissolved oxygen being utilized by the aquatic microorganisms in metabolizing the organic matter, oxidize reduced nitrogen, and oxidize reduced minerals such as ferrous iron. BOD is also an indirect measure of the substrate itself.

For this project, the main objective is to identify the relationship between BOD decay and the dissolved oxygen concentration. Dissolved oxygen concentration is one of the major factors affecting the BOD decay.

Basically, the scope of study for this project is to relate the dissolved oxygen concentration term into the BOD decay rate models, either in the First Order or Second Order Model and then relate the effect of the order of the models itself to the BOD decay rate.

The methods used in this project are to apply the models into a software application to see the graphical presentation of the BOD decay rate for the model. This is done by assuming the First-Order BOD decay rate constant or k_1 according to other researchers' works and journals and then applied into the models which further integrated into the mass transport equation. From the mathematical approach and computer modeling works, the main findings of the project is that when the dissolved oxygen concentration is increased, the rate of BOD decay will increase but this only come up until certain value of dissolved oxygen concentration due to the saturation factor of the oxygen. This applies to both models that are used in this project. It is also found that, the Second-Order Model exhibit a bit faster reaction than the First-Order Model but this difference only applies in the earlier stage of the decaying. Other than that, there are no significant differences between First-Order Model and Second-Order Model.

In conclusion, the BOD decay rate increases as the dissolved oxygen concentration increases until the saturation point of the oxygen and the Second-Order Model decay rate is slower in the BOD removal comparing to the First-Order Model but this does not mean that First-Order Model is better than the Second Order Model but only highlighting the importance of different approaches by researchers in interpreting the BOD decay in order to obtain more accurate interpretation of the BOD decay rate in water.

CHAPTER 2

INTRODUCTION

2.1 Background of Study

Biochemical Oxygen Demand (BOD) is a parameter that is used generally to describe the pollution level of a water system, usually the wastewater system. Basically, the definition of BOD is the quantity of the dissolved oxygen being utilized by the aquatic microorganisms in metabolizing the organic matter, oxidize reduced nitrogen, and oxidize reduced minerals such as ferrous iron. BOD also applied to the substrate itself (EPA, 1985).

Normally the BOD value for certain water system is measured in term of BOD_5, where the test for the BOD is done for water sample which has been in incubation period of five days. There are other methods in measuring the value of BOD either by varying the number of days for the incubation period or just by converting the BOD value for these tests to an ultimate BOD value.

The BOD is divided into two main fractions which are the carbonaceous BOD and the nitrogenous BOD. For this project, the focus is the carbonaceous BOD which is the degradation of carbonaceous matter which either can be in dissolved or suspended matter.

The BOD is actually regarded as one of the major pollutant factors in water as it consumes a lot of oxygen which is vital to the aquatic life. There are many factors which affecting the value of the BOD decay rate, such as the temperature, flow rate of the water, the number of microorganisms and also the dissolved oxygen concentration in the water. Regarding the BOD is one of the major pollutants, is important to study on how to optimize the BOD decay rate and this can be done by manipulating the factors that have been stated before. For this project, the factor that is being analyzed is the dissolved oxygen concentration.

2.3 Objectives and Scope of Study

Generally, the main objective of the project is to identify the relationship between the BOD decay and dissolved oxygen concentration. Basically, the study of the BOD decay rate can be determined using the first-order model. Nevertheless, other mathematical models are taken into account to compare between the models in analyzing the BOD decay. The models can be obtained from existing models which have been developed by other people through mathematical method or using experimental work for a certain water sample. These models including the first-order models include a constant usually denoted by k, as a function of oxygen. This constant can be determined by interpreting the experimental data and theories that have been produced by other researchers.

Basically, the scope of this project is to analyze and to study the first-order model with other different models which could have the constant, k as a function of oxygen with different order models. Secondly, is to make a computer-based modeling in order to compare these models in determining the relationship between the BOD decay and dissolved oxygen concentration. The interpretation of the constant k should include the dissolved oxygen variables as to relate the effect of oxygen to the BOD decay rates. The value of k can be assumed as any values obtained by experiments done in any case studies of any water system and justifications have to be included on why the value is chosen.

CHAPTER 3

LITERATURE REVIEW

Basically, the BOD decay is usually regarded by the water quality models as first-order kinetics as proposed by Phelps (1909), where the oxygen consumption is proportional to the concentration of the remaining BOD, L_T. It is expressed mathematically as shown below:

$$\frac{dL}{dt} = -k_1 L_r \qquad (2)$$

and after integration and substitution of $(L_o$-$L_t)$ for L_r gives:

$$L_t = L_0(1 - e^{-k_1 t}) \qquad (3)$$

Where L_t is the oxygen consumed (BOD) at time t, in mg/l, L_o is the ultimate BOD in mg/l or also known as the initial concentration of BOD, t is time in days and k_1 is a reaction rate constant in 1/days.

One way to relate it with the effect of dissolved oxygen, some modification has been made into the equation by coupling it with the stream dissolved oxygen kinetics;

$$O_t = \frac{k_1 L_0}{k_2 - k_1}[\exp(-k_1 t) - \exp(-k_2 t)] + O_0 \exp(-k_2 t)] \qquad (4)$$

where

O_t = Dissolved oxygen deficit at time t (mg/L)

O_0 = Dissolved oxygen deficit at time zero (mg/L)

k_1 = BOD reaction rate constant (First-Order) (1/day)

k_2 = reaeration constant (1/day)

L_o = ultimate BOD (mg/L)

t = time (day)

In this project, the concerned part is the BOD decay, thus other correlations have to be implied into the BOD reaction rate, *(dL/dt)* so it would be depending on the dissolved oxygen concentration.

Thus, the dissolved oxygen effect can also be applied into the reaction rate constant of First Order, k_1 directly as a way of describing the consumption of oxygen as a function of water column BOD decay.

Such correlation can be described as below:

$$L_r = -k_1 L \frac{O_2}{k_{O_2} + O_2} \qquad \text{(Di Toro and Connolly, 1980)} \quad (5)$$

where

k_1 = BOD reaction rate constant (1/day)

L_r = remaining BOD concentration (mg/L)

k_{O_2} =half saturation constant for oxygen (mg/L)

The above correlation can be put into the First-Order Model equation as shown below:

$$\frac{dL}{dt} = -k_1 L \frac{O_2}{k_{O_2} + O_2} \qquad (6)$$

Then this equation can be put back into the mass transport equation (Brown and Barnwell, 1987)

$$\frac{\partial M}{\partial t} = \frac{\partial (A_x D_L \frac{\partial L}{\partial x})}{\partial x} dx - \frac{\partial (A_x \bar{u} L\ )}{\partial x} dx + (A_x dx) \frac{dL}{dt} + s \qquad (7)$$

where the variable “s” is replaced with the BOD decay equation. This is to model the BOD concentration in a mass transport condition. The first term $\frac{\partial M}{\partial t}$ is the mass transfer rate which we assumed zero for this simulation. The second term $\frac{\partial (A_x D_L \frac{\partial L_r}{\partial x})}{\partial x} dx$ is representing the effects of dispersion while the third term $\frac{\partial (A_x \bar{u} L_r)}{\partial x} dx$ is representing the effects of convection for this whole equation.

The fourth term is also cancelled out from the equation for the modeling purpose as the relation of the concentration against time is not considered. Thus the equation become

$$0 = \frac{\partial (A_x D_L \frac{\partial L_r}{\partial x})}{\partial x} dx - \frac{\partial (A_x \bar{u} L_r)}{\partial x} dx + \frac{dL_r}{dt} \qquad (7a)$$

For the purpose of the modeling, some of the variables value have to assume accordingly to the findings of researchers in this field, especially which come out from experiments. As for instance, the value of k_1, which is the rate constant have to be assumed as a specified values. This value can be taken either from Lake Eerie Model (Di Toro and Connolly, 1980). This k_1 value can also be assumed as an average value of various experimental values from numerous reports as it usually around the 0.2 to 0.6. This is the normal range of the k_1 value.

Up until this point, the only way to interpret this project is using first order model. But a few researchers had proposed new approaches for interpreting the BOD decay rate. One of them is such as Adrian and Sanders (1997) who proposed a second order BOD decay equation. This is an extension of research which has been initiated by Young and Clark (1965) which has proposed an equation of the second order BOD decay as below:

$$\frac{dL_r}{dt} = -k_3 {L_r}^2 \qquad (8)$$

where

L_r = BOD remaining (mg/l)

k_3 =Second-Order rate constant (l/mg-day)

The above equation can then be integrated to become

$$\frac{1}{L_0} - \frac{1}{L_r} = -k_3 t \qquad (9)$$

where L_o is the ultimate first stage BOD.

This equation can be further expressed in term y as in the amount of oxygen consumed by a sample as a function of time, just like in the BOD bottle test by using the relationship L_o-L_t = L_r and $k_3 = k_1/L_0$ to obtain

$$\frac{dL_t}{dt} = \frac{k_1}{L_0}(L_0 - L_t)^2 \quad (10)$$

After substitution of L_o-L_t = L_r, the equation can be further expressed as

$$L_t = \frac{k_3 L_0^2 t}{1 + k_3 L_0 t} \qquad (11)$$

where L_t is equal to the BOD being consumed at time t.

This is where the value of k_3 and L_o can be determined from using the best fit in the least square sense and the measured values of y versus t. To relate with the oxygen concentration, the value of k_1/Lo can be just be used as the same method used in the first order decay rate. This is because the value of k_1/L_o is the same as k_3, looking at the derivation of the equations above.

The value of k_1 and the usage of first-order or second order equation can be assumed as in ranges shown by Marske and Polkowski (1972) which shows that when k_1 <0.34day^{-1}, it is best to use the first order model, while when 0.34day^{-1}< k_1 <0.45day^{-1}, both fist order and second order models show the same result and when k_1 >0.45 day^{-1}, the second order model gives the best result.

CHAPTER 4

METHODOLOGY

4.1 Procedures

There are *four* main procedures for this project which are:

1. *Analyzing the constant k*

   Basically, this is to analyze the way to assess the value of constant *k* (BOD decay rate) or how to interpret the *k*, from other people's theory or experimental work. This is done so that to relate the value of *k* with the dissolved oxygen concentration and justifying the value of *k* before being plugged into the mathematical models.

   The correlation between the rate constant, *k* finally found from the Lake Eerie model (Di Toro and Connolly, 1980) which is

   $$L_r = -k_1 L \frac{O_2}{k_{O_2} + O_2} \quad (5)$$

   and combined up with the reaction rate of the First-Order Model or the Second-Order Model to become

   $$\frac{dL}{dt} = -k_1 L \frac{O_2}{k_{O_2} + O_2} \qquad \text{First-Order Model} \quad (6)$$

   $$\frac{dL}{dt} = -k_3 L^2 \frac{O_2}{k_{O_2} + O_2} \qquad \text{Second-Order Model} \quad (12)$$

2. *Analyzing the First-Order Model*

Basically, this is to analyze and to study the first-order decay model with the dissolved oxygen concentration from the equation given in the QUAL2E manual and other journals.

From the literature studies, it is found out that the First-Order Model is interpreted differently in terms of the BOD concentration, L. Some journals defined it as BOD that to be degraded at time *t*, while some defined it as the ultimate BOD. For the modeling purposes, it is defined as BOD concentration remaining along the timeframe.

Since its introduction in studying the BOD decay, the First-Order Model has been accepted widely as it simpler, thus giving convenience for researchers to interpret the BOD decay either mathematical or including modeling or simulation.

The validity of the First-Order Model is also depending on rate constant itself, k_1, which depends entirely to the conditions of the water system itself. This is because the conditions of the water system itself is different for various types, such as between rivers and lakes. Such conditions that contribute to different value of k_1 are the dispersion constant of the water systems and the half-saturation constant of the oxygen.

3. *Analyzing the Second-Order Model*

Besides the first order model, other mathematical models which relating to the BOD decay are taken into account. For the time being, the other model being studied is the Second-Order Model.

Although a lot of researchers has urged for the study of Second-Order Model (Thomas, 1957; Young and Clark,1965; Adrian and Sanders,1992-93), there are certain other researchers' works have shown that the First-Order Model is valid for most of the water systems. Such research was done by Butts and Kothandaraman (1970) who had analyzed the Illinois River to determine whether the samples taken from the river was better described by First-Order Model or Second-Order Model. They found out that, from 23 of 28 samples they took were best described by the First-Order Model. (Adrian and Sanders, 1998).

Nevertheless, for this project, both First-Order Model and Second-Order Model are analyzed and programmed into our modeling for comparison purposes.

4. *Computer Modeling*

The analyzed models are put into computer modeling tool to produce graphs in order to make comparisons among them.

The computer softwares used are FEMLAB and Microsoft Excel.

Microsoft Excel is used to study mainly on the effect of dissolved oxygen concentration on BOD decay and to compare between First-Order Model and Second-Order Model. To achieve this, the modified models equation:

$$\frac{dL}{dt} = -k_1 L \frac{O_2}{k_{O_2} + O_2} \qquad \text{(First-Order Model)}$$

$$\frac{dL}{dt} = -k_3 L^2 \frac{O_2}{k_{O_2} + O_2} \qquad \text{(Second-Order Model)}$$

For the equation of the First Order Model, it is integrated against *dL* and at boundaries:

$t = 0, L = L_0$

$t = t, L = L_t$

L_0 is the ultimate BOD concentration and L_t is the concentration of BOD being degraded at that time equals to t.

Thus the equation (6) becomes:

$$L_t = L_0(\exp[(-k_1 \frac{O_2}{k_{O_2} + O_2})t]) \qquad (13)$$

For the modeling purposes, the term L_t is replaced with L_r as $L_r = L_0 - L_t$. L_r is the concentration of BOD remaining in the system at time *t*. Thus the equation (13) becomes:

$$L_r = L_0 - L_0(\exp[(-k_1 \frac{O_2}{k_{O_2} + O_2})t]) \quad (14)$$

For the equation of the Second Order Model, it is integrated against *dL* and at boundaries:

$t = 0, L = L_0$

$t = t, L = L_r$

Thus the equation (12) becomes:

$$L_r = \frac{L_0}{1+(k_3 L_0 \frac{O_2}{k_{O_2}+O_2})t} \qquad (15)$$

As the Second-Order rate constant, k_3 is equal to k_1/L_o (Adrian and Sanders, 1998), the integration of Second-Order Model is equal to:

$$L_r = \frac{L_0}{1+(k_1 \frac{O_2}{k_{O_2}+O_2})t} \qquad (16)$$

For the simulation purposes, the equation (14) and (16) is put into Excel sheets as in condition of batch reactor where there in flow out or into the system. This is purposely to show the decaying of BOD according to the equation given. From the equations above, four different graphs can be plotted, which are the graph of BOD decay against time with for First-Order Model and Second-Order Model, two graphs of BOD decay against time for different dissolved oxygen concentration, one for First-Order Model and followed by Second-Order Model. Meanwhile, another graph which is the comparison of BOD decay between rate constant dependent of oxygen which is represented by equation (14),

$$L_r = L_0 - L_0(\exp[(-k_1 \frac{O_2}{k_{O_2}+O_2})t]) \qquad (14)$$

with rate constant independent of oxygen, that is the integrated original version decay equation ,

$$L_r = L_0 - L_0(\exp[-k_1 t]) \qquad (17)$$

Another graph is also obtained using Excel, which is the comparison effect of dissolved oxygen concentration on rate of BOD decay. This is obtained by using equation (5)

$$L_r = -k_1 L \ \frac{O_2}{k_{O_2} + O_2} \quad (5)$$

where the definition of L is changed as the concentration BOD being degraded, L_t and plug in into an Excel sheet in the same condition as above simulation. For this simulation, the negative sign is cancelled out as it is intended to see the incremental of the decay rate.

FEMLAB is used to model a water system e.g., river to look at the BOD decay against the range of the water system. This is mainly to look at the effect of dissolved oxygen towards the BOD decay with the inclusion of dispersion process.

FEMLAB is modeling and simulation software designed to simulate especially engineering studies and cases. It is derived from the MATLAB, another modeling application which basically can be done for the same purposes. Nevertheless, FEMLAB has been enhanced and upgraded with more engineering specifications.

For example, for the modeling of this project, it would fall under the "Mass Balance". Then, it would have to be specified what are the mechanisms for the mass balance condition. The FEMLAB has its own series of modeling or simulation conditions such as mass balance, diffusion, or temperature control analysis. After the condition has been chosen, the software will show the work area of the intended simulation work. Geometry of the simulation work would have to be chosen, whether rectangular, square or circle depending to the need of the case being studied. Then, the sub domain conditions and the boundary conditions of the geometry have to be determined such as the variables value in the equations. After that, the simulation can be run to develop the graph needed, depending on what is being analyzed for the case study such as the concentration or temperature. The FEMLAB has given the equation being specified for each simulation conditions.

Thus, the equation being studied must be correlated with the equation given and other than that, the simulation condition is chosen accordingly to the case being studied.

For this project, the condition used in the modeling is steady-state mass transfer in convection and diffusion, or dispersion mechanism. This condition uses the equation which derived from the Fick's Law

$\nabla.(-D\nabla c) = R - u.\nabla c$

where

D = dispersion or diffusion coefficient (m^2/s)

R = reaction rate (mg/L.s)

u = velocity (m/s)

c = concentration of BOD being studied (mg/L)

This equation is actually same with the previous equation, equation (7a)

$$\frac{\partial(A_x D_L \frac{\partial L_r}{\partial x})}{\partial x} dx = \frac{dL_r}{dt} - \frac{\partial(A_x \bar{u} L_r)}{\partial x} dx$$

where the D is actually the D_L, u is equal to $\bar{u}$ and R for the model is the BOD decay rate which is $\frac{dL}{dt}$.

For the simulation purposes, the values of constants are taken from the journals of other researchers' work as these constants are totally depending on the environment of the system itself. The dispersion or the diffusion coefficient, D is a constant which depend on many other variables of different water system, such as the velocity of the water, the depth of the water system, and the roughness coefficient of the water system. It is also different according on how the researchers interpret it. For instance, in QUAL2E manual, the D or D_L value is obtained from the equation

$$D_L = 3.82Knd^{\frac{5}{6}}\bar{u}$$

where

K = Dispersion constant

n = Manning's roughness coefficient

d = Diameter of water river or channel (ft)

$\bar{u}$ = Mean velocity (ft/s)

The resulting D_L from the above equation is in ft^2/s and has to be converted into m^2/s.Meanwhile, the First-Order reaction constant, k_1 has to be assumed as standardize value for the entire simulation, in FEMLAB and Excel. Thus an optimum value of 0.04mg/L is chosen as the value of the k_1 as it is suitable to be used in either the First-Order or Second-Order model. This value is chosen based on the values that are commonly used by the researchers in their modeling work for the checking certain water system parameters, such as used by the Singaporean researchers for their work in looking at the water quality of certain part of Tebrau Strait.

The domain is set as a rectangle which represents a portion of the water system in term of specific length and depth as shown in Figure 1.

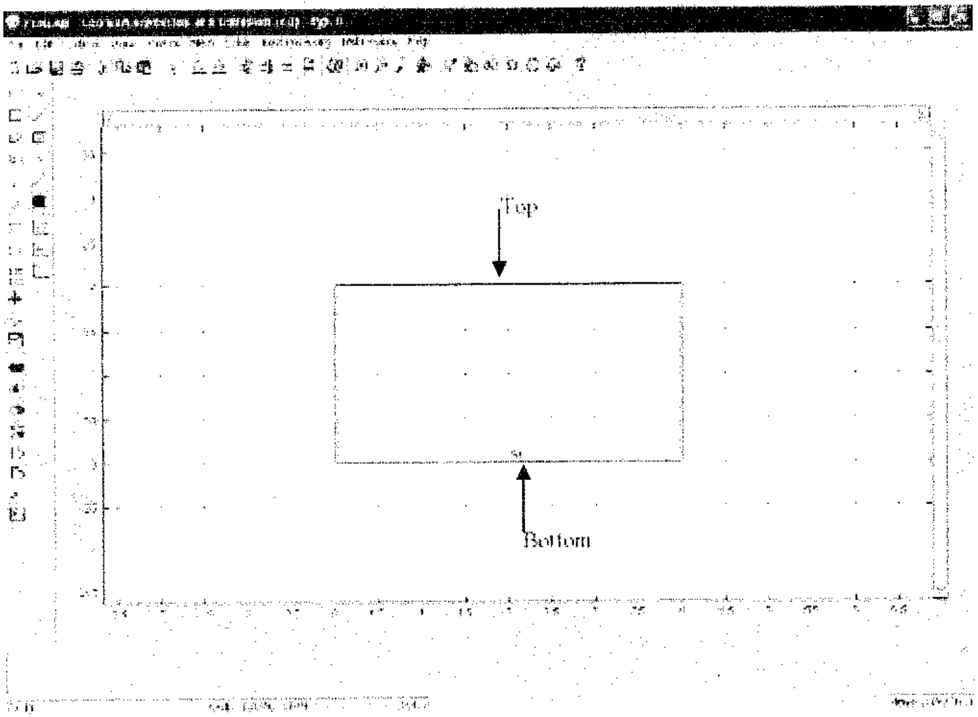
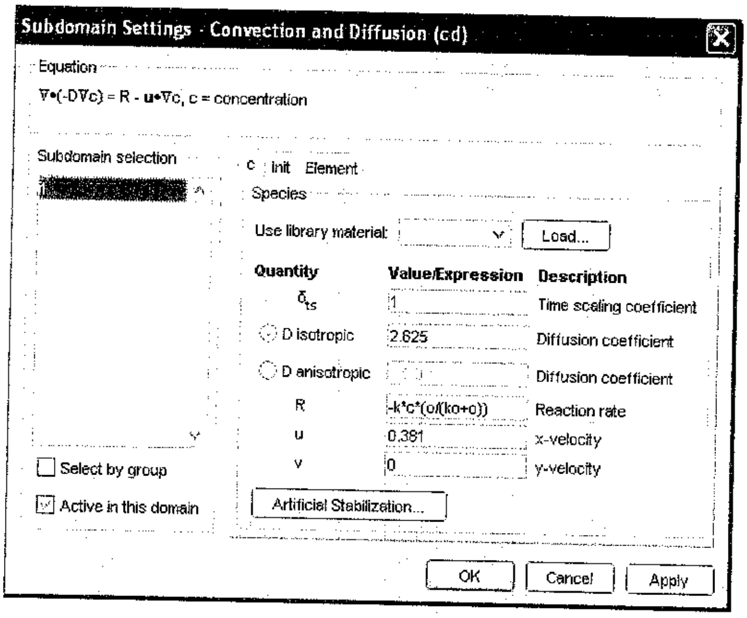


Figure 1: Domain specification in FEMLAB

Then, the sub domain settings are set according to the above equation as shown in Figure 2.


Subdomain Settings - Convection and Diffusion (cd)

Equation

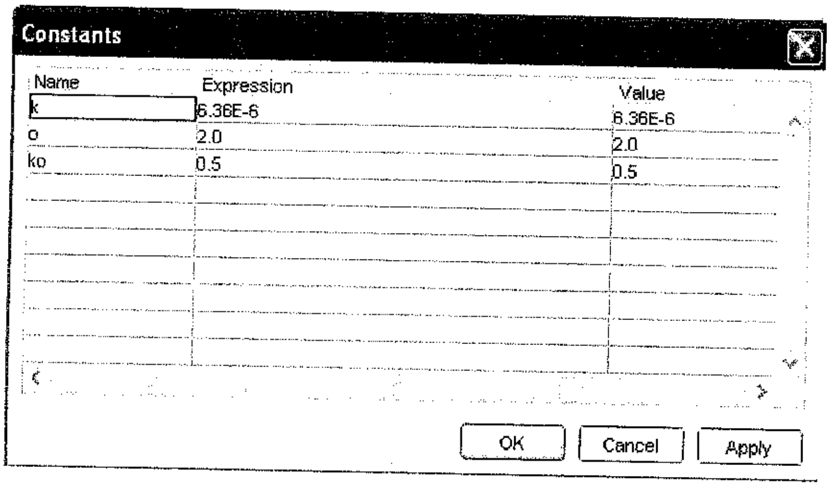
$\nabla \bullet (-D\nabla c) = R - \mathbf{u} \bullet \nabla c$, c = concentration

Quantity	Value/Expression	Description
δ_{ts}	1	Time scaling coefficient
○ D isotropic	2.625	Diffusion coefficient
○ D anisotropic		Diffusion coefficient
R	-k*c*(o/(ko+o))	Reaction rate
u	0.381	x-velocity
v	0	y-velocity

Figure 2: Subdomain setting in FEMLAB

From Figure 2, the D_L is specified as 2.625 m^2/s, and the mean velocity is specified as 0.381m/s. These values are different for every different water system. Thus these values are just expressed to represent one water system only. The reaction rate dL/dt is represented by *-k*c*(o/ (ko+o))* which is actually the model representation of$[-k_1 L \frac{O_2}{k_{O_2}+O_2}]$..

The value of the terms in the reaction rate is determined in the "Constants" window which is applicable throughout the simulation, as shown in Figure 3.


Constants

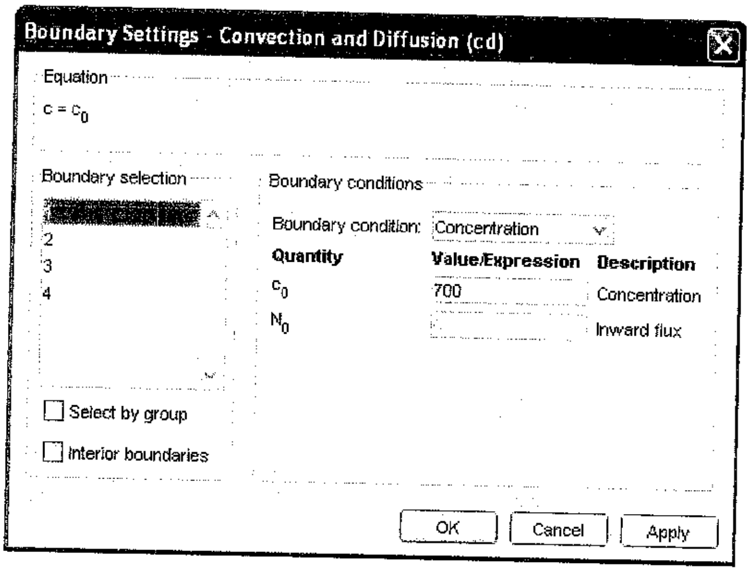
Name	Expression	Value
k	6.36E-6	6.36E-6
o	2.0	2.0
ko	0.5	0.5

Figure 3: Constant specifications in FEMLAB

From Figure 3, the First-Order rate constant,k_1 is represented in the model by *k* which is set as $6.36 \times 10^{-6}\ s^{-1}$ which is actually equal to $0.4 day^{-1}$. The dissolved oxygen concentration, O_2 is represented by *o* and is set at 2 mg/L while the half saturation constant, k_{O_2} is represented as *ko* and is set as 0.5 mg/L.

Then, the boundary settings for the sub domain are specified. Both the top and bottom boundary is assumed as insulation as the top part is assumed to be the surface of the water and bottom part is assumed to be the bed of the water. Therefore, there is no BOD coming in or out from both parts. The first boundary, which is the left part, is the inlet flow while the fourth boundary, which is the right part, is the outlet flow.

The condition at the inlet flow is set as initial concentration of the BOD value (L_0) in the water and at the outlet flow, the condition is set as 0, as we assume all BOD is fully decayed. This can be shown in Figure 4 where in this model, the L_0 is represented as c_0 and is set as 700 mg/L.



Equation

$c = c_0$

Boundary selection: 1, 2, 3, 4

☐ Select by group

☐ Interior boundaries

Boundary condition: Concentration

Quantity	Value/Expression	Description
c_0	700	Concentration
N_0		Inward flux

Figure 4: Boundary settings in FEMLAB

The value of the constants and variables are different according to different FEMLAB simulation models which are ran for the project, except for the value of the First Order rate constant, k_1 which is set at $6.36 \times 10^{-6}\ s^{-1}$ (or $0.4 day^{-1}$) for all the models, including Excel models.

After all the settings are done and confirmed, the model is run and at the end of the simulation, a graph showing the decay of the BOD against the range of the sub domain can be obtained.

4.2 Project Gantt chart

ACTIVITIES	WEEK NO / DATE													
	1	2	3	4	5	6	7	8	9	10	11	12	13	14
	Jan 24-30	Jan31-Feb6	Feb7-13	Feb14-20	Feb21-27	Feb28-Mac6	Mac7-13	Mac14-20	Mac21-27	Mac28-Apr3	Apr4-10	Apr11-17	Apr18-24	Apr25-May1
Topic Selection	▨													
Preliminary Research Work		▨	▨											
Literature review • Study of the constant k • Research of the first model • Research of other models			▨	▨	▨	▨	▨	▨						
Engineering Analysis • Analyzing of the k constant • Analyzing of the first order model and other models						▨	▨	▨	▨					
Data interpretations and comparisons • Modeling and simulation								▨	▨	▨	▨	▨		
Final Report											▨	▨	▨	▨

Figure 5

CHAPTER 5

RESULTS AND DISCUSSION

5.1 Results from Excel

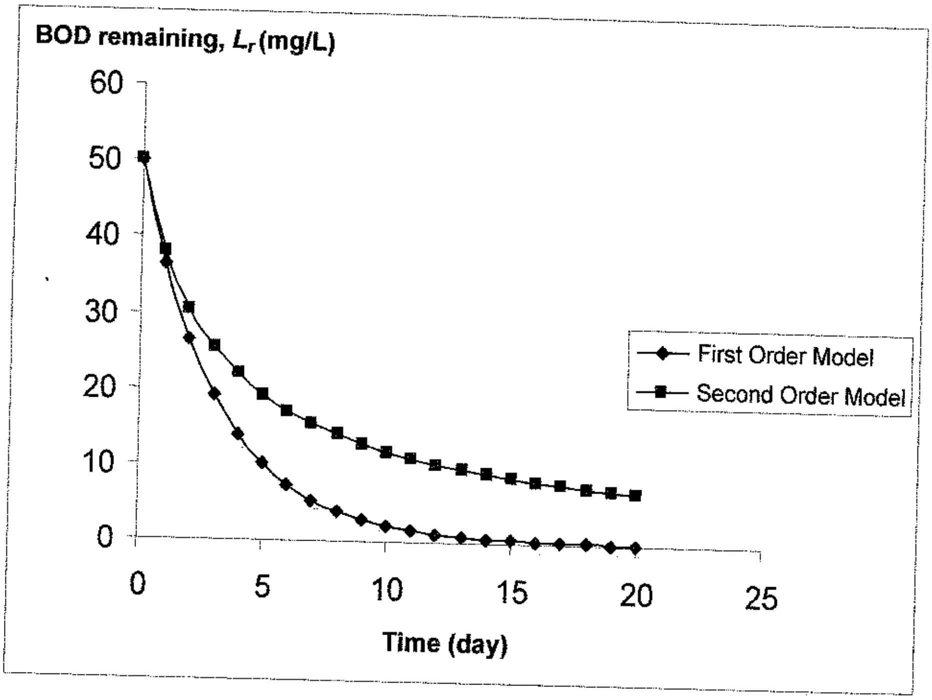


Figure 6: Graph of comparison of BOD remaining, L_r against time between First Order Model and Second Order Model at dissolved oxygen (DO) concentration of 2 mg/L.

From the graph above, it is plotted from data tabulated in Table 1 and Table 2 which produced from equation (14) for the First Order Model and equation (16) for the Second Order Model. The L_0 is set as 50 mg/L and the dissolved oxygen concentration is set at 2 mg/L for both models. The two models are projecting the concentration of BOD remaining in the water system, which is represented as L_r at certain days with the conditions of batch reactor where there is no flow into or out from the system. Both models are run up until 20 days.

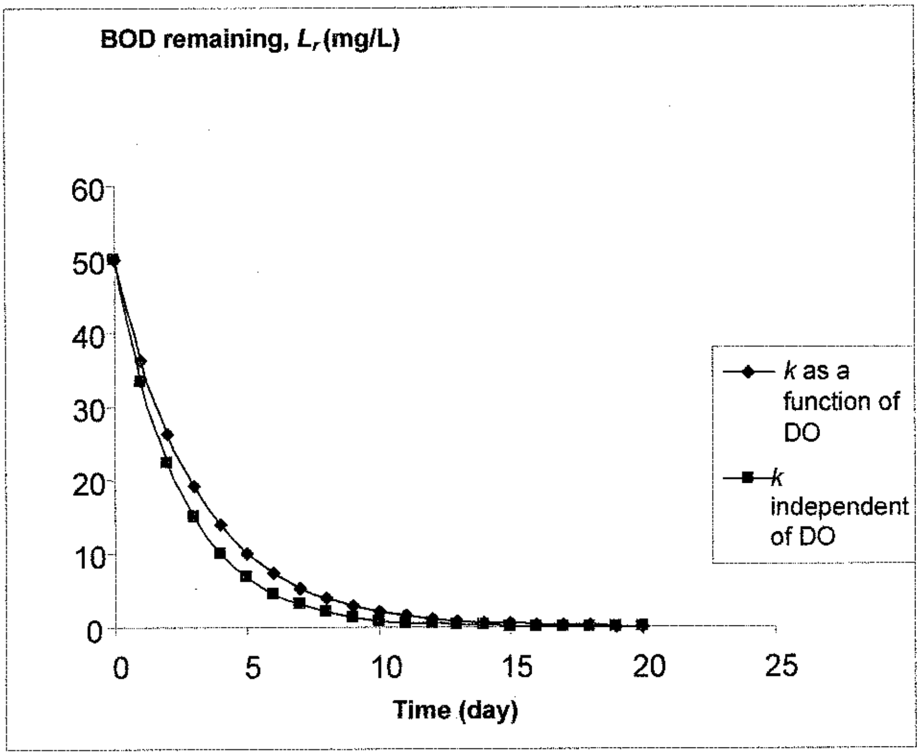


Figure 11: Comparison BOD remaining for First Order Model between rate constant, *k* as a function of Dissolved Oxygen (DO) and *k* independent of Dissolved Oxygen (DO).

For Figure 11, the graph is plotted based on data generated from the equation (14) for the curve of *k* as a function of DO and equation (17) for the curve of *k* independent of DO. For the BOD remaining curve against time with rate constant, *k* as a function of dissolved oxygen, the dissolved oxygen concentration is set as 2 mg/L. Basically, it is observed that the BOD decay rate with *k* as a function of dissolved oxygen is a little slower than the BOD decay rate with *k* independent of dissolved oxygen as the time increases. But this trend only happens momentarily after during the steep part of both curves and then gradually both curves show quite same behavior towards the complete degradation of the remaining BOD. Thus the effect of dissolved oxygen has some impact on the BOD decay rate.

5.2 Results from FEMLAB

FEMLAB Simulation No.1

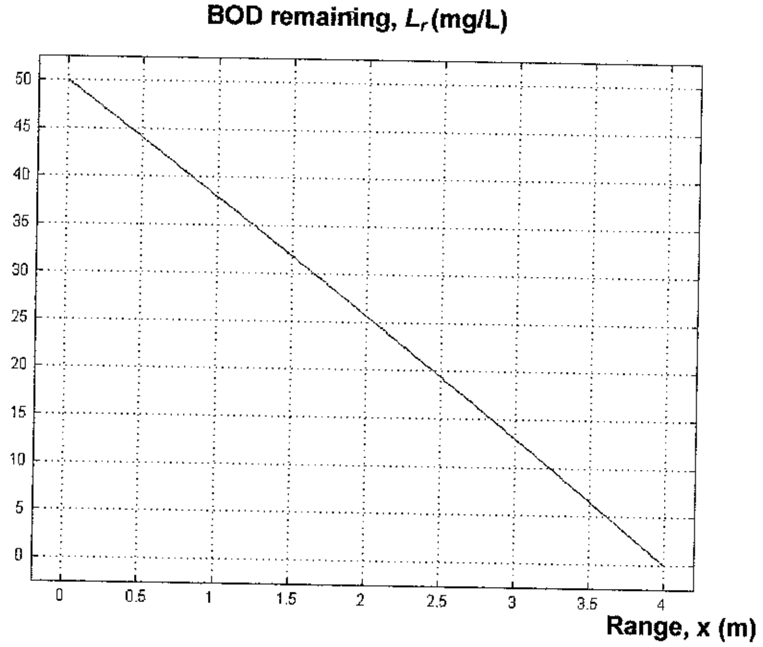


Figure 12: Graph showing the remaining BOD concentration against range of water system for First-Order Model with dissolved oxygen concentration of 2 mg/L and high value of diffusion coefficient, D_L.

Graph from Figure 12 is developed by using FEMLAB simulation using the value of constants and variables as shown in Table 4 below:

Constants/Variables	Value
Diffusion coefficient, D_L	5.715 m^2/s
Mean velocity, u	0.15m/s
First-Order rate constant, k_1	6.36 x 10^{-6} s^{-1}
Dissolved oxygen concentration, O_2	2 mg/L
Half-saturation constant for oxygen, k_{O_2}	0.5 mg/L
Initial BOD concentration, L_0	50 mg/L

Table 4: Constants and Variables value for FEMLAB Simulation No.1

FEMLAB Simulation No.2

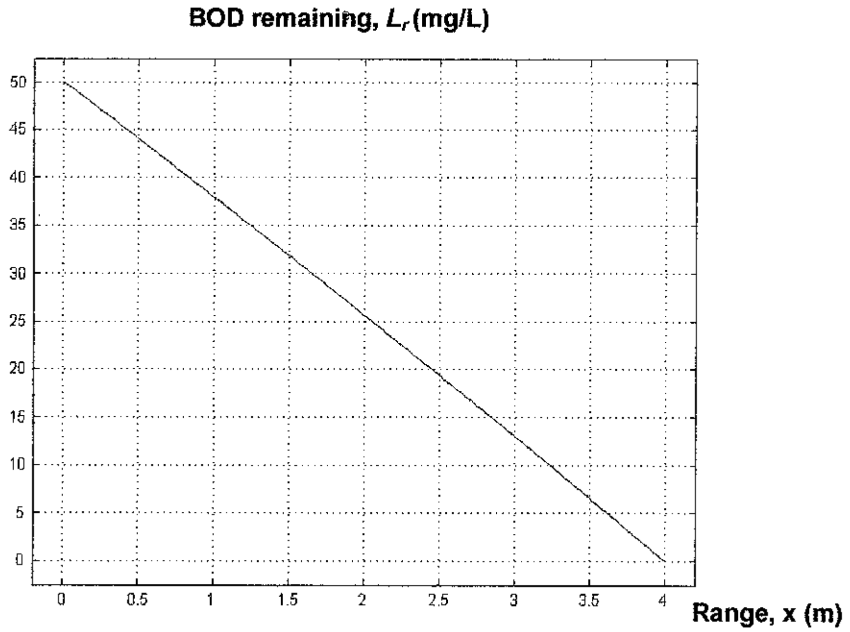


Figure 13: Graph showing the remaining BOD concentration against range of water system for First-Order Model with dissolved oxygen concentration of 5 mg/L and high value of diffusion coefficient, D_L.

Graph from Figure 13 is developed by using FEMLAB simulation using the value of constants and variables as shown in Table 5 below:

Constants/Variables	Value
Diffusion coefficient, D_L	5.715 m^2/s
Mean velocity, u	0.15m/s
First-Order rate constant, k_1	$6.36 \times 10^{-6} s^{-1}$
Dissolved oxygen concentration, O_2	5 mg/L
Half-saturation constant for oxygen, k_{O_2}	0.5 mg/L
Initial BOD concentration, L_0	50 mg/L

Table 5: Constants and Variables value for FEMLAB Simulation No.2

Both graphs from Figure 12 and 13 show the same characteristic of the remaining BOD concentration, L_r against the range of the water system although with different dissolved oxygen concentrations.

FEMLAB Simulation No.3

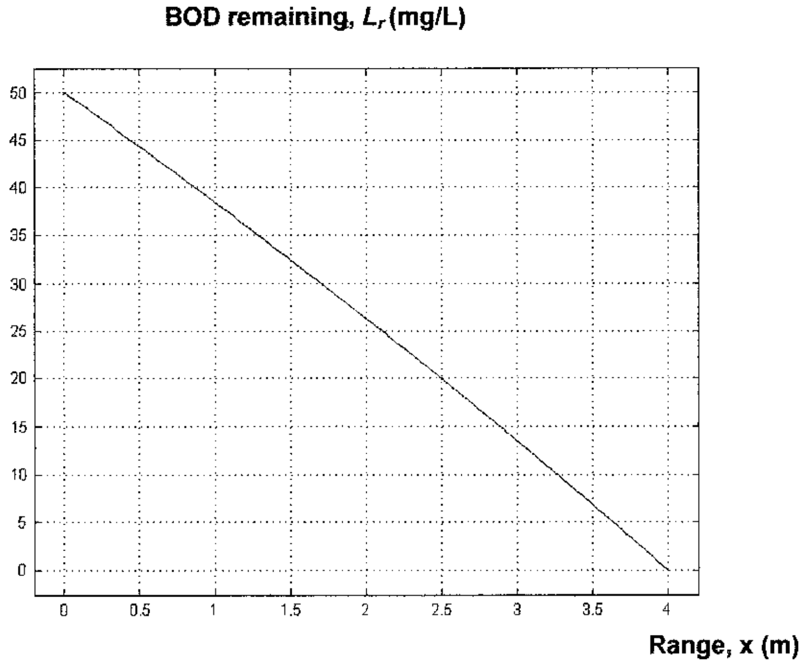


Figure 14: Graph showing the BOD decay rate against range of water system for First-Order Model with dissolve oxygen concentration of 2 mg/L and low value of diffusion coefficient, D_L.

Graph from Figure 14 is developed by using FEMLAB simulation using the value of constants and variables as shown in Table 6 below:

Constants/Variables	**Value**
Diffusion coefficient, D_L	0.04 m^2/s
Mean velocity, u	0.0021m/s
First-Order rate constant, k_1	$6.36 \times 10^{-6}\ s^{-1}$
Dissolved oxygen concentration, O_2	2 mg/L
Half-saturation constant for oxygen, k_{O_2}	0.5 mg/L
Initial BOD concentration, L_0	50 mg/L

Table 6: Constants and Variables value for FEMLAB Simulation No.3

FEMLAB Simulation No.4

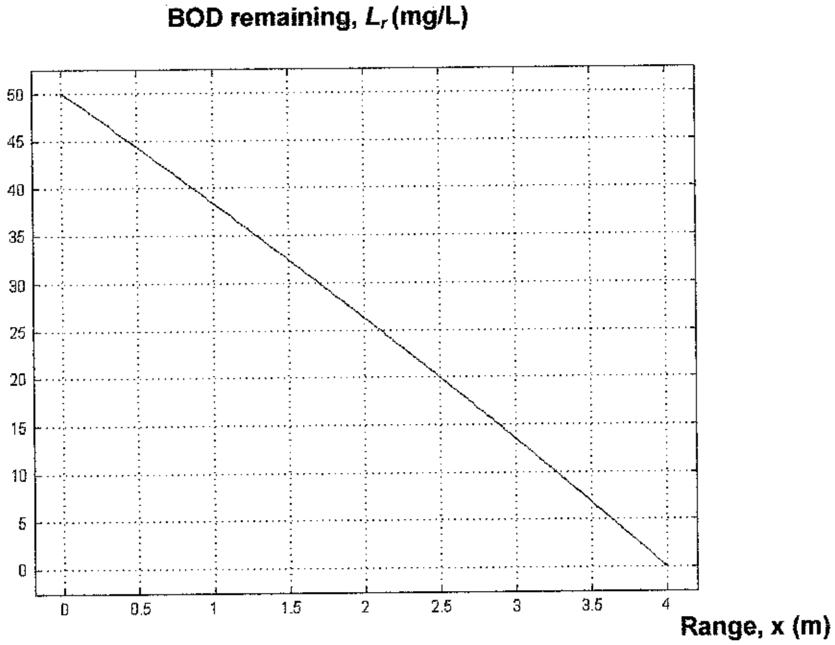


Figure 15: Graph showing the BOD decay rate against range of water system for First-Order Model with dissolve oxygen concentration of 5 mg/L and low value of diffusion coefficient, D_L.

Graph from Figure 15 is developed by using FEMLAB simulation using the value of constants and variables as shown in Table 7 below:

Constants/Variables	**Value**
Diffusion coefficient, D_L	0.04 m^2/s
Mean velocity, u	0.0021m/s
First-Order rate constant, k_1	6.36 x 10^{-6} s^{-1}
Dissolved oxygen concentration, O_2	5 mg/L
Half-saturation constant for oxygen, k_{O_2}	0.5 mg/L
Initial BOD concentration, L_0	50 mg/L

Table 7: Constants and Variables value for FEMLAB Simulation No.4

Graphs from Figure 14 and Figure 15 also do not show any differences in term of the concentration of BOD remaining against the range of water system although with different dissolved oxygen levels.

5.3 Discussion of Results

Basically, from the Figures 6 to Figure 10, all the graphs, which are obtained from the Excel spreadsheet, show that when the dissolved oxygen concentration in a water system is increased, the rate of BOD decay will increase gradually until the BOD is fully degraded. For all the figures mentioned above, the system is simulated as a batch reactor where there is no water coming into the system or flowing out of the system. Thus, the BOD decay happens as according to the reaction rate, which depends on time without any outer, factors such diffusion or dispersion or benthic factor. As mentioned earlier, the dissolved oxygen factor become insignificant when it reaches higher value of concentration. This is caused by the saturation factor of the oxygen itself in the water where there are only certain limits of oxygen level which can be dissolved in the water. The saturation factor of the oxygen is represented in the BOD decay rate as the half-saturation constant, k_{O_2} which is actually an experimental value which is different from other system to another system. The saturation factor depends on the several conditions of the water such as the salinity of water, the temperature of the water and the partial pressure variations due to elevation from sea level. Basically, when the salinity levels together with the temperature, of the water are high, less oxygen can be held by the water. (Gray N.F. 2004)

For Figure 11, the graph shows the comparison of the BOD concentration remaining as the time increases, between reaction rate with rate constant as a function of dissolved oxygen levels and reaction rate with a rate constant independent of dissolved oxygen concentration. Same assumptions are made for this graph like the other graphs in previous figures. Although there is slight different of characteristic between the curves, this differences maybe significant for designing wastewater treatment plants which handle large amount of BOD loadings. Errors such as actual time taken for degrading the BOD to the specified limit is more than the calculated time, could happen if the dissolved oxygen factor is not taken into account.

Generally, it can be concluded that the First-Order Model for the BOD decay is showing faster removal of BOD than the Second-Order Model. But this does not mean that the First-Order model is better than the Second-Order Model.

This is because it is not certain whether the BOD decay rate in the water is really following the rule of First-Order characteristic or not. The First-Order Model is widely used in the interpretation of the BOD decay as for convenience purposes. Thus, researches have done a lot of experimental and simulation works to determine the exact characteristic of the BOD decay rate in the water.

For Figure 12 until Figure 15, the graphs were obtained from the FEMLAB simulations which more advanced and can been specified to follow the convection and diffusion mass transfer condition. The assumption that is made for all the simulations is that all of them are done in a steady state condition. There is no increment in concentration of BOD due to growth factor and the concentration of BOD is decreasing with the increasing of range is only due to the diffusion or dispersion effect together with the BOD decay reaction rate with the rate constant as a function of dissolved oxygen. The first two graphs, from Figure 12 and Figure 13 has high diffusion coefficient representing the simulation of a portion of a river. Both graphs show exact characteristic of curves for the remaining BOD concentration as the range of the river increases. This show that the BOD decay rates of in both river systems are the same although has different levels of dissolved oxygen. The rate of the BOD decay between rivers which have different levels of dissolved oxygen should be different.

The latter Figure 14 and Figure 15 shows the graphs of system with smaller value of diffusion coefficient which represent a portion of a lake, due to low velocity of water and also specified at different level of dissolved oxygen levels. Again, both graphs from the figures show exact characteristic of curves for the remaining BOD concentration as the range of the lake increases which concluded that, BOD decay rates of in both portion of lake systems are the same although has different levels of dissolved oxygen. This exact characteristic shown by the graphs from Figure 13 and Figure 14 are quite contrasting to the results from the Excel model spreadsheets as the water system for both modeling works are nearly the same. The models from the Excel spreadsheets are nearly similar to a lake system except that the lake has inlet flow into the system, but nevertheless, the batch reactor system has velocity of zero while the lake system has velocity of nearly zero.

Thus, the graph in Figure 15 should show increment in BOD decay rate with the increasing of range as the dissolved oxygen level increase, due the retention period is quite long due to low mobility. For the river, the differences might be too small even for different dissolved oxygen levels due to low retention time caused by the high mobility of water.

Apart from that, there is a misunderstanding between the dispersion term and diffusion term where the diffusion term is due to the random motion in the water whereas for dispersion, is actually due to differential movement of water in the space of the system. Thus, in rivers, dispersion usually predominates due to strong shears developed by the large mean velocity flows which are due to gravity flow and tide, while diffusion is usually predominates in the lake and other stagnant, wide body water as the wind is the primary agent which creates random motion to the water.

Thus for better simulation purposes especially for the study for BOD decay rate against the water system range either rivers or lakes, other factors which affecting BOD removal rates should be taken into account such as the temperature effect on the rate constant, the settling effect, and also the bed effects as it would conclude the whole equation into a complete equation. Apart from that, suitable and more specified software application should be used other than FEMLAB as FEMLAB is more suitable for simple convection and diffusion mass balance. For this BOD decay rate simulation, it is more suitable for three dimensional model where as in this project, it is only done in two dimensional model as for normal computer cannot bare the load of three dimensional processing for the FEMLAB simulation. Thus, other more appropriate simulation tool should be used such as the QUAL2E application.

CHAPTER 6

CONCLUSION

The value of the BOD decay rate constant of First-Order, k_1 is can be represented with the dissolved oxygen term as to show the effect of dissolved oxygen onto the decay rates of BOD while the rate constant of Second-Order, k_3 can be represented as First-Order rate constant, k_1 divided with the ultimate BOD concentration, L_0.

From the Excel spreadsheets modeling result, it is found that, the rate of BOD decay increases when the dissolved oxygen concentration increases but only up to a certain value of concentration, which is when the saturation of oxygen occurs. This general conclusion stands although the simulation works from FEMLAB fails to support the result from the Excel modeling.

The Second-Order Model decay rate is slower in the BOD removal comparing to the First-Order Model but this does not mean that First-Order Model is better than the Second Order Model but only highlighting the importance of difference of approach by researchers in interpreting the BOD decay in order to obtain more accurate interpretation of the BOD decay rate in water.

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