University of Alberta

Identification of Data Requirements for Calibration of a Steady State ASM2d Model at GBWWTP

by

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ABSTRACT

An attempt was made to calibrate a steady state activated sludge model (ASM2d) for the biological nutrient removal process at the Gold bar wastewater treatment plant. This calibrated model could be used on a regular basis to test various operational strategies and predict effluent quality under different scenario. To achieve this historic data from the plant database was collected based on 24 composite samples. A trial and error method of wastewater characterization of the primary effluent was attempted using the influent advisor module of the GPS-[X] software. Sensitivity analysis of kinetic parameters was carried out and the most important ones identified were calibrated (default values were modified) based on literature. After calibration it was observed that the model was overestimating the concentrations of carbonaceous biological oxygen demand, total suspended solids and orthophosphate in the effluent, compared to the actual value measured at the plant. Similarly the effluent ammonia concentration was underestimated for most days along with the nitrate and nitrite concentration. This clearly indicated the need for a more accurate calibration based on experimental data to improve prediction capabilities and the reliability of the model.

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LIST OF ABBREVIATIONS

ASM	Activated Sludge Model
BNR	Biological Nutrient Removal
CBOD	Carbonaceous Biological Oxygen Demand
CBOD Model	Effluent CBOD predicted by the model
COD/ TCOD	Chemical Oxygen Demand
sCOD	Soluble Chemical Oxygen Demand
DO	Dissolved Oxygen
FE	Final Effluent
GBDATA	Data from Gold bar
HRT	Hydraulic Residence Time
IR	Internal Recycle
MLSS	Mixed Liquor Suspended Solids
MLVSS	Mixed Liquor Volatile Suspended Solids
NH_3	Ammonia Nitrogen
NH_3 Model	Effluent NH3 predicted by the model
NTOX	Total Oxidized Nitrogen
NTOX Model	Effluent NTOX predicted by the model
OPO_4	Soluble Orthophosphate
OPO_4 Model	Effluent OPO_4 predicted by the model
PAO	Phosphorus Accumulating Organisms
PE	Primary Effluent
RAS	Return Activated Sludge
rbCOD	Readily Biodegradable COD
SRT	Solids Residence Time
TKN	Total Kjeldahl Nitrogen
TN	Total Nitrogen
TP	Total Phosphorus
TS	Total Solids
TSS	Total Suspended Solids
TSS Model	Effluent TSS predicted by the model
UBOD	Ultimate Carbonaceous BOD
VFA	Volatile Fatty Acids
VSS	Volatile Suspended Solids
WAS	Waste Activated Sludge
WWTP	Wastewater Treatment Plant

CHAPTER 1

INTRODUCTION

Goldbar wastewater treatment plant (GBWWTP) was opened in 1956 as Canada's largest activated sludge treatment plant to treat domestic waste. It is located along the southwest shore of the North Saskatchewan River. Presently the plant serves a population of 700,000 and handles an average daily flow of 340 ML/D and a peak daily flow of 550 ML/D. Approximately 95% of sewer flow from Edmonton is treated by GBWWTP.

There were two major expansions at the plant during late 1960's and early 1980's to increase their treatment capacity. In 1996 secondary aeration tanks were converted to bioreactors for nutrient removal along with the installation of two new bioreactors and secondary clarifiers. In 2004 an additional bioreactor and secondary clarifier was installed and the plant presently has 11 bioreactors and secondary clarifiers numbered from 1 through 11. In 1998 U-V disinfection facility was also added for tertiary level treatment. In 2006 enhanced primary treatment was introduced to improve treatment during peak flow. The plant is currently owned by the city of Edmonton.

Wastewater entering the plant passes though various treatment stages before being discharged into the North Saskatchewan River. The various treatment stages include:

1) Pre-treatment: Raw effluent first enters aerated grit chambers. There are 7

grit chambers currently installed at the plant. In the grit chambers because of aeration, grit and other coarse material settle while the organics remain in suspension. Settled grit is removed using screw augers. The effluent then passes through bar screens. Materials trapped in the bar screens are removed using raker bars and are disposed along with the grit in landfills.

2) Primary treatment: After passing though mechanical screens, the effluent enters rectangular primary settling tanks/ primary clarifiers. There are currently 8 primary clarifiers installed at the plant. Dense solids settle under the influence of gravity in these large tanks and the lighter particles rise up and float on the surface forming scum. Mechanical scrappers operate at a slow speed of 2ft/ min (0.01 m/sec) gently scrapping off the settled sludge and scum. The sludge and scum are pumped to anaerobic digesters. Following anaerobic digestion, sludge is thickened in lagoons and then used as fertilizer. Around 55% of total suspended solids (TSS) and 45% of biological oxygen demand is removed during this stage of treatment. The effluent form the primary clarifier is referred to as the primary effluent and enters bioreactors for secondary treatment.

3) Secondary treatment: Primary effluent is distributed among the 11 bioreactors. Each bioreactor is divided in to 4 parallel passes. The dimensions of each pass are as shown in Table 1.A, Appendix 1. The BNR configuration operated at goldbar for nitrogen removal is single-sludge preanoxic (shown in Figure 1).

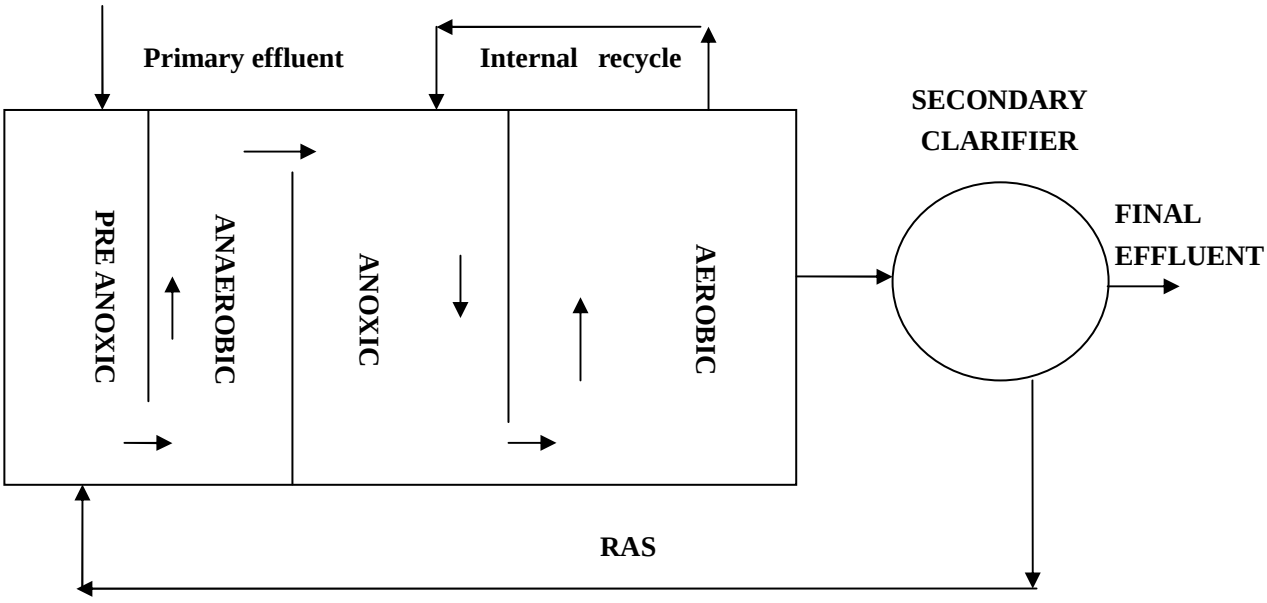

FIGURE 1: BNR configuration at GBWWTP.

Pass I: Pass I is divided in to three distinct zones, separated by baffles. Three zones in this pass are:

a) Pre-anoxic: Primary effluent enters this zone along with the return activated sludge (RAS) from the secondary clarifier. This zone is devoid of free oxygen. The only sources of oxygen for the microorganisms growing in this zone are the nitrates from the RAS and primary effluent. In this zone biological conversion of nitrates and nitrites to nitrogen gas (denitrification) occurs. Effluent from this zone enters the anaerobic zone. RAS flow is maintained at 100% the influent flow rate. RAS (sludge settled in the secondary clarifier) is rich in biomass and helps to maintain the microbial community for BNR process.

b) Anaerobic zone: The effluent stream stripped off nitrates and nitrites (inhibitors in this zone) enters the anaerobic zone. Here the phosphorus

accumulating organisms (PAO) uptake volatile fatty acids (supplemented externally from fermenter) and store them as poly-hydroxy-butarate. Energy requirement for this step comes from the hydrolysis of stored polyphosphate (in aerobic zone).

c) Anoxic zone: Effluent from the anaerobic zone along with the recycle from the aerobic zone (end of pass IV), called the internal recycle (IR) enters this zone. The IR stream is rich in nitrates and nitrites. Similar to the pre-anoxic zone denitrification occurs. IR flow is maintained as 2-3 times the influent flow rate.

Pass II, III and IV: The final three passes are aerobic zones where two major processes take place. One of them is the growth of PAOs and their uptake of phosphorous as polyphosphates. The second major process is the growth autotrophic organisms for the conversion of ammonia to nitrates and nitrites (nitrification). The hydraulic retention time at the aerobic zone is maximum, for the slow growing autotrophs and PAOs.

The BNR process configuration at GBWWTP is such that most of the CBOD is removed in the anoxic zone so as to reduce the oxygen demand in the aerobic zone. This saves cost and energy.

Effluent from the BNR (end of pass IV) enters the subsequent clarifier. Here the biomass is separated from the treated effluent. 90% of the settled sludge is recycled back to the pre-anoxic zone and 10% is wasted as waste activated sludge (WAS). The WAS is pumped in to anaerobic digesters. The effluent

from the clarifier enters U-V disinfection facility before being finally discharged into the river (Molla, 2008).

1.1 OBJECTIVE AND SCOPE OF PROJECT

The scope of this project was to evaluate the use of historic data available in the Gold Bar WWTP archives and information available in the literature to calibrate the ASM2d steady state model. The goal of this work was to identify data needs for the calibration of the ASM2d model and to catalogue parameter estimation methods.

CHAPTER 2

2.0 LITRATUTE REVIEW

2.1 NEED FOR WASTEWATER TREATMENT PLANT

Wastewater is generated from both industrial and domestic activities. Fresh water is often used for various domestic and industrial activities and the used water (wastewater) is discharged into water bodies. In order to protect the aquatic bodies from water pollution the waste stream has to be treated before being discharged. So the basic need for a wastewater treatment plant is to achieve a simple goal- protect nature's resources and maintain a balance in the ecosystem (USDE 1997).

Depending upon the source of wastewater the physical and chemical characteristics vary greatly. In general physical composition of wastewater is 0.1% solids and 99% water content. Of this about 30% is suspended solids and 70% dissolved solids. Chemically wastewater consists of organic compounds like proteins, fats, lipids, oil, phenols, carbohydrates and inorganic compounds like heavy metals, nutrients like nitrogen and phosphorus, sulphur compounds, chlorinated compounds, alkalinity, toxic compounds etc. Of these around 80-90% of the inorganic is dissolved and 55-60% of the organics are dissolved. Gases in wastewater include: hydrogen sulphide, methane, oxygen, carbon dioxide, and nitrogen. Biological composition includes microbes like bacteria, fungi, algae and protozoa. The coliform group of organisms are used as an

indicator of pathogenic organisms. Materials of plant and animal origin are also common. (http://www.atl.ec.gc.ca/epb/issues/wstewtr.html)

Factors like increasing awareness and consequences of water pollution, increasing demand for high water quality, diminishing water resources in contrast to increasing demand from rapid population growth and industrial development have resulted in the implementation of stringent regulations, imposed by agencies on effluent quality (Tabrizi et al., 2004).

2.2 PROCESSES IN A WASTEWATER TREATMENT PLANT

A typical wastewater treatment plant generally contains primary, secondary and an optional tertiary treatment stages. Primary stage is mainly to remove coarse suspended solids from the influent raw stream. Bar screens/ bar racks followed by grit chambers are employed for physical screening purposes. In case of enhanced primary treatment this is followed by chemical coagulation and flocculation to further remove fine solids from the waste stream. This treated water is referred to as primary effluent (PE). Following the primary treatment the PE enters the biological treatment stage where fixed or suspended cultures of microorganisms utilize the biodegradable organics and nutrients present in the PE for their growth and maintenance. This is referred to as the biological nutrient removal process. The effluent then enters secondary clarifiers where the flocs are allowed to settle and the final effluent is either directly discharged or enters a tertiary treatment stage depending on

the effluent regulations. Disinfection using UV, ozone or chemicals like chlorine is common treatment options in the tertiary stage.

2.3 BIOLOGICAL NUTRIENT REMOVAL

Presence of nutrients in waste stream poses disposal problems. Phosphorus and nitrogen are the major nutrients responsible for algal growth in most of the receiving streams. If wastewater is discharged untreated, eutrophication is a major problem. Eutrophication refers to excessive growth of algae and other aquatic plants which in turn prevents sunlight penetration into water body and depletes oxygen in the lower layers. As a result aquatic habitat is disturbed. Also the stream can no longer be used for domestic (because of odour problems), industrial or agricultural purposes (Vabolienė et al., 2007).

Use of Activated sludge process began as early as 1910 for biological removal of organic carbon. It was based on the principle of allowing the waste stream enter an aeration tank containing a suspension of microorganisms for a stipulated time period. Microorganisms use the organic carbon present in the waste stream as a substrate for growth and the treated effluent is sent to clarifier where the flocs settle down and the final effluent (treated waste) is discharged. The settled sludge is recycled back to the aeration tank and is called activated sludge. This is typically a single stage process. In case of two-stage process, two activated sludge plants operate in series. Sludge from the second plant is recycled to the first. This is generally used when the PE has

high concentrations of toxic substances and slowly biodegradable organics. (Jordening et al., 2005).

2.3.1 NITROGEN REMOVAL:

Nitrogen is a major nutrient that has to be almost completely removed for water reuse and to meet stringent effluent regulations for preventing problems like eutrophication and ammonia toxicity in the receiving bodies. Main sources of nitrogen include rainfall, runoffs from agricultural land (fertilizers), industrial and domestic waste, animal manure etc. (Reeves, 1972). Nitrogen is present in wastewater in various reduced forms such as urea, amino acids, urea, proteins, and ammonia. Nitrates and nitrites are generally present in negligible concentrations. Most of the organic nitrogen present in the waste stream is converted to ammonia by a process referred to as ammonification. Various mechanisms that result in the liberation of ammonia includes: hydrolytic, oxidative, reductive and desaturative deamination. (Jordening et al., 2005).

There are different methods of nitrogen removal. The commonly used ones are air stripping, ion exchange and biological nitrogen removal. Other processes include electrochemical treatment, demineralization (electrodialysis, reverse osmosis, and distillation), breakpoint chlorination, algae harvesting and land application.

All compounds of nitrogen are easily soluble in water. So chemical precipitation followed by sedimentation and flocculation is not applicable for

removal of nitrogen from wastewater. (Jordening et al., 2005).

Air Stripping: Ammonium ions exist in equilibrium with ammonia and hydrogen ions hydroxyl ions of water at neutral pH. In the presence of air and when the pH is elevated to 10, around 85% of ammonium is converted to ammonia liberated as gas. Generally air stripping is carried out in packed tray towers equipped with air blower. In wastewater around 90% of nitrogen is present as total ammonia (ammonium ion and ammonia) or compounds that can be converted to total ammonia. The optimum pH for stripping was found to be 11 (Reeves, 1972).

This method was well suited for industrial waste with high ammonia concentration. But in case of domestic waste because of low levels of ammonia this method did not provide satisfactory effluent quality. Other disadvantages of the method include high solubility of ammonia in water making the process difficult, high aeration requirement making the process expensive, and poor cold weather performance as solubility of ammonia in water increases with decrease in temperature (Reeves, 1972 and Cooper, 1994).

Ion Exchange: In the ion exchange unit process an ion exchange material is placed in a bed and the waste is passed through it. For demineralization of ground water or final effluent after nitrification, nitrate ions are removed using an anion exchange resin bed and ammonium using a cation bed. Once all the ions in the bed are replaced, and the bed is exhausted, it is regenerated using a

regeneration solution containing the anion or the cation. The main disadvantages of the method include complexity of the method, fouling of the bed because of dissolved organics in the waste stream. Also the regenerant has to be treated prior to disposal. This method is a good option for tertiary treatment. (Reeves, 1972 and Cooper, 1994)

Biological Nitrogen Removal: Microorganisms are capable of biologically transforming ammonia nitrogen to nitrogen gas by a two-step process of nitrification and denitrification. It is estimated that for the synthesis of 1g of bacterial biomass, approximately 0.08 g of ammonia nitrogen is required. The remaining ammonia that is not incorporated into the cells is transformed into molecular nitrogen and removed from the waste stream. (Jordening et al., 2005).

Nitrification:

Ammonia nitrogen present in wastewater is first converted to nitrite and then into nitrates by the process the process of nitrification (Cooper, 1994). Nitrification is generally carried out by a group of aerobic organisms referred as autotrophic nitrifiers. The first step in this is the conversion of ammonia nitrogen to nitrite.

$NH^+_4 \rightarrow NO^-_2 + 2H^+ + H_2O$

Organisms that are capable of catalyzing this reaction are: *Nitros*

Nitrosolobus sp, *Nitrosospira* sp, and *Nitrosovibrio sp*.

The second step is the conversion of nitrites to nitrates by *Nitrobacter sp*,

Nitrococcus sp and *Nitrospira sp*.

$NO^-_2 + 0.5\ O_2 \rightarrow NO_3^-$

Step two occurs at a faster rate. So the concentration of nitrites is generally very low.

Nitrification is an energy-yielding step for the autotrophic growth of the nitrifiers.

Heterotrophic organisms are also capable of nitrification. Some of the organisms include: *Arthobacter sp*, *Flavobacterium sp*, and *Thiosphaera sp*. In contrast to the autotrophs they are capable of utilizing only nitrogen containing organic compounds or require an organic substrate for growth. (Jordening et al., 2005).

The growth rate of autotrophs is much lower than the growth rate of the heterotrophs and thus there is tendency for the heterotrophs to out-compete the autotrophs and inhibit the nitrification process. Also the pH during nitrification fluctuates, becomes alkaline due to CO_2 consumption and acidic due to nitric acid production. In the absence of proper buffering, nitrification maybe inhibited (Jordening et al., 2005).

Denitrification

Denitrification is the process by which nitrate nitrogen is removed from wastewater under anoxic conditions. Denitrifying bacteria are heterotrophic organisms that require a carbon source as an electron donor. They are capable of utilizing nitrates as terminal electron acceptor for their growth. Since there

is no free oxygen, and only chemically bound oxygen in the form of nitrates is available for respiration it is referred to anoxic growth. Nitrates produced in the nitrification stage are reduced to nitrites followed by the conversion of nitrites to nitrous oxide and nitrogen gas, which is removed from the system and returned to the atmosphere.

Facultative heterotrophic bacteria require sufficient biodegradable source of carbon for growth. Waste stream is seldom devoid of free oxygen. So it is important sufficient carbon source should be supplied until it is respired and anoxic condition is achieved. This can be ensured either by supplementing sufficient amount of carbon source externally or by ensuring that the waste stream enters the anoxic zone of the reactor first (Cooper, 1994 and Jordening et al., 2005).

Another mechanism for ammonia oxidation is the anaerobic process referred as “Anammox” process. In this case a group of chemolithoautotrophic bacteria carries out the combined oxidation of ammonium and nitrite directly to dinitrogen gas under anaerobic conditions. This is suitable for waste streams with high ammonia and low carbon concentrations. A major disadvantage of this method is that the chemolithoautotrophs grow very slowly so it takes a long time for the process start, especially after breakdowns (Taylor et al., 2006).

2.3.2 PROCESS CONFIGURATIONS:

The following is a summary of information (of various process configurations available for biological nitrogen removal) available in Tchobanoglous et al., (2003).

1) **Ludzac- Ettinger and modified Ludzac- Ettinger**: This is a preanoxic configuration introduced as early as 1962. In this case the waste stream first enters the anoxic zone followed by the aerobic zone. The nitrate produced in the aerobic zone is recycled via RAS back into the anoxic zone. Denitrification greatly depends on the RAS recycle ratio. So this process was modified later in the 1970's by introducing an IR that enters the anoxic zone directly from the aerobic zone. The internal recycle ratio typically ranges from 2 to 4 and an effluent nitrate concentration of 4-7 mg/L can be achieved.
2) **Step-feed Denitrification:** In the step-feed denitrification configuration there are two to three Preanoxic/denitrification zones. The RAS from the secondary clarifier is allowed to enter the first anoxic zone. Influent stream is distributed into each of the anoxic units. IR from each aerobic zone enters the preceding anoxic zone for denitrification. A typical influent flow splitting in case of a 4-pass system is 15:35:30:20. Flow into the final pass is very critical as it determines the final nitrate concentration in the effluent.

3) **Bio-denitro**: The Bio-denitro process was developed in Denmark and a final effluent concentration as low as 8 mg/L was achieved. In this configuration at least two oxidation ditches operate in series. However the sequence and operation of the ditches as anoxic and aerobic zones are varied. Mixers are provided to ensure only mixing and no aeration in case of anoxic conditions.

4) **Nitrox:** Effluent nitrate nitrogen concentration less than 8 mg/L and ammonia nitrogen concentration as low as 1.0 to 1.5 mg/L can be achieved using the Nitrox process. Unlike Bio-denitro a single oxidation ditch is operated under alternatively aerobic and anoxic conditions by turning off aeration once nitrates are generated under aerobic conditions. Usually aeration is turned off twice a day.

5) **Postanoxic single-sludge:** In a postanoxic single sludge system the influent stream enters the aerobic zone first and then the anoxic zone for denitrification. In order to achieve high nitrogen removal efficiency detention time has to be longer in the anoxic tank.

   Preanoxic single sludge systems also exist. The only difference is that the influent stream enters the anoxic zone first.

6) **Bardenpho (4-stage):** Bardenpho configuration was developed in South Africa. It incorporates both pre and post-anoxic denitrification. It consists of alternating anoxic and aerobic tanks with the influent entering the first anoxic tank. The IR from the second tank (aerobic) and the RAS from the

clarifier enters the first anoxic tank. The effluent from the second aerobic tank enters the following anoxic and aerobic tanks and finally into the clarifier. Because of lack of readily biodegradable carbonaceous material in the second anoxic zone denitrification rate is low. So a carbon source is supplemented externally.

7) **Oxidation Ditch:** Different variations in an oxidation ditch can be created depending on the dissolved oxygen concentration along the ditch. Both aerobic and anoxic zones can exist in a single ditch. Ditches with suitable volume and length have also been designed for low rates of nitrification and denitrification under low dissolved oxygen concentration (below 0.5 mg/L). Typical example is the Sym-Bio^{TM} process.

8) **Orbal^{TM}:** In this process three channels operate in series. The dissolved oxygen in the first channel varies from 0-0.3 mg/L thus creating three distinct zones: aerobic, anoxic and anaerobic zones in the channel. In the subsequent channels the DO concentration increases from 0.5-1.5 mg/L in the second channel to 2-3 mg/L in the third channel. The IR and RAS from the third channel and the clarifier respectively, enter channel 1.

2.3.3 PHOSPHORUS REMOVAL:

Various technologies were introduced as early as 1950's for the removal of phosphorus from wastewater because of increasing surface eutrophication of the receiving streams. Different strategies include: chemical precipitation,

magnetic phosphorus removal and biological phosphorus removal

Chemical Precipitation: Divalent or trivalent metal salts like ferrous/ ferric chlorides or sulphates, aluminium sulphates are commonly used to precipitate phosphorus as metal phosphates. Lime was also used. However it produced a highly alkaline effluent. Anionic polymers were added to aid solids separation. Chemical precipitation could be applied to various stages of wastewater treatment, making it a very versatile process. It could be applied before primary clarification or during the activated sludge process to remove phosphorus in secondary clarifiers. The sludge wasted is then used as fertilizer (Cooper, 1994 and Morse et al., 1997).

A metal to phosphorus ratio of 1:1 has to be maintained to avoid competition from other ionic constituents in the waste stream, and achieve effective phosphorus precipitation. This ratio is also important to coagulate suspended solids and colloids. Although aeration cost and secondary sludge produced is reduced, expenses of chemical usage and associated primary sludge produced are high. Also, this process cannot precipitate organically bound phosphates (Cooper, 1994).

Magnetic Phosphorus Removal: This process is relatively new and has been used for the last ten years. This process has been mostly used in the tertiary stages of water treatment. In this case phosphorus is first precipitated as metal phosphates as in case of chemical precipitation. Magnetite is then added to induce magnetic properties to the precipitate. Polyelectrolyte is added to

enhance attachment of magnetite to the precipitates. This mixture is then passed through a large magnet where the precipitate is removed. Magnet is then cleansed by backwashing and the precipitate is disposed (Cooper, 1994 and Morse et al 1997).

Biological Phosphorus Removal: Biological P removal is brought about by a group of microorganisms called "Phosphorus accumulating organisms", PAOs. They are capable of accumulating polyphosphates intracellularly. When they are subjected to varying aerobic and anaerobic conditions phosphorus accumulation and release occurs accordingly.

When bacteria are subjected to anaerobic conditions, uptake of volatile fatty acids that are naturally available or supplemented externally occurs. The volatile fatty acids are stored as poly hydroxyl butyrate. Energy required for this step is obtained from the hydrolysis of the polyphosphates stored in the cells during the aerobic phase (Taylor, et al 2006). Under aerobic conditions, uptake of soluble phosphates by the selected strain of bacteria occurs. These are stored intracellularly as polyphosphates. Poly hydroxyl butyrate stored in the cells under the anaerobic conditions is used in this phase for the synthesis of new biomass. Various process designs for biological phosphorus removal includes:

1) **Photostrip Process**: It is one of the oldest designs that can be added to an existing plant without modifying the existing plant design (Cooper, 1994). Here a portion of the activated sludge from the secondary clarifier and the

influent enters the anaerobic zone, with a residence time of 8-12 hour. The PAO release phosphate under anaerobic conditions. The supernatant is separated from the sludge and is lime-treated to precipitate phosphorus. The sludge is sent to the aerobic zone of the reactor for further phosphorus uptake from the influent stream (Tchobanoglous et al., 2003).

2) **A^2/O Process:** This refers to Anaerobic/ Anoxic/ Aerobic process. This is similar to A/O process, except that the anoxic tank is added for denitrification. Oxygen in the form of nitrate is provided through an IR stream that enters the anoxic zone from the aerobic zone. The detention time in the anoxic zone is approximately one hour. This offers an advantage of minimizing the amount of nitrate entering the anaerobic zone through the RAS line (Tchobanoglous et al., 2003).

3) **Modified Bardenpho Process/ Phoredox**: In case of modified Bardenpho process, phosphorus removal is achieved by adding an anaerobic zone to the existing Bardenpho process (used for nitrogen removal) thereby combining nitrogen removal and phosphorus removal. To ensure that the concentration of nitrates and nitrites entering the anaerobic zone is minimal, the RAS is mixed with the influent and an IR stream enters the anoxic zone for denitrification to minimize nitrates in the RAS line (Cooper, 1994).

4) **University of Cape Town (UCT)**: The UCT process was introduced to resolve the problem of nitrates and dissolved oxygen entering the anaerobic zone as in the case of phoredox process. To achieve this RAS is combined

with an IR stream from the aerobic zone, and is sent to the anoxic zone to enhance nitrate removal. An IR from the anoxic zone then enters the anaerobic zone.

In the case of modified the UCT process, there are two anoxic zones. The RAS enters the first anoxic zone and an IR from anoxic tanks after denitrification, enters the anaerobic zone. The second IR enters the second anoxic tank from the aerobic tank (Tchobanoglous et al., 2003).

5) **Virginia Initiative Plant (VIP):** The main objective of the Virginia Initiative Plant process is to achieve enhanced phosphate removal with short retention time. It operates similarly to the A^2/O and UCT processes except that the zones are staged such that at least two completely mixed cells are in series. IR from the end of the anoxic zone enters the anaerobic zone along with the influent and IR from the end of aerobic zone enters the anoxic zone inlet along with the RAS (Tchobanoglous et al., 2003).

6) **Johannesburg Process:** This was another strategy to minimize nitrate concentration entering the anaerobic zone. The zones are arranged in the following sequence: preanoxic-anaerobic-anoxic-aerobic. The influent enters the anaerobic zone along with the effluent from the preanoxic tank. The RAS enters the preanoxic zone preceding the anaerobic zone. IR stream from the aerobic zone enters the anoxic zone along with the effluent form the anaerobic pass. The anaerobic zone has a detention time of about an hour (Tchobanoglous et al., 2003).

2.3.4 ADVANTAGES OF BNR TEATMENT

In the recent past more importance has been given to the concept of:"green engineering". This refers to application of technology that is eco-friendly. Biological nutrient removal process fits this for the following reasons (Randall, 1998 and Sharma et al., 2005):

1) The effluent discharged after BNR treatment has acceptably low concentrations of nutrients like N and P, organics and suspended solids. The quality of the effluent produced is better than chemical treatment (Cooper, 1994). This reduces chances of eutropification and depletion of oxygen in the receiving water bodies
2) Reduction in amount of nutrients also reduces the chances of microbial re-growth in the distribution systems
3) Reduces usage of chemicals and eliminates further problems of sludge handling and disposal making it more economical by lowering capital and operating cost relative to chemical methods.
4) Biological transformation of hazardous components like benzenes, ethyl benzene to other less harmful end–products has also been observed**.**
5) With the introduction of various configurations with anoxic and anaerobic zones, oxygen requirements have reduced significantly making BNR processes economically more feasible and reduce dependence on energy. Also the amount of sludge produced in these zones is significantly less

when compared to the amount of sludge produced by aerobic processes

6) The waste activated sludge is rich in nutrients like P making it a good fertilizer.

2.3.5 LIMITATIONS OF BNR TREATMENT

1. Long sludge age is required to achieve sufficient population of nitrifiers for nitrification. This is mainly due to the slow growth of autotrophs. If the sludge age is reduced it was observed that the plant capacity could actually be increased by about 40% (Ekama, et al., 1999).
2. Influent composition of the waste stream is very important. High concentrations of certain constituents or even the mere presence of certain compounds can be toxic to the microorganisms involved in the BNR process. It was noted that BNR process:

   (i) Cannot be used to treat waste stream with high concentration of ammonia (500mg/L) as this inhibits the process of nitrification (Carrera, et al., 2003 and Ekama, et al., 1999).

   (ii) Cannot be used to treat waste stream with high concentration of iron (over 10mg/L). In case of iron oxidation the microbe first absorbs iron and intracellular and extracellular enzymes further catalyze the oxidation reaction. Since the rate of rate of absorption is low, waste stream with high iron concentration is not treated effectively (Sharma et al., 2005).

3) Another important constraint of BNR process is that not all compounds

can be subjected to the process of biodegradation. Some compounds depending on their chemical structure (size and presence of reactive sites) can be bio-recalcitrant. These compounds have to subjected to pre-treatment or post treatment methods that defeat the advantage of BNR as the most economic alternative. Most recent is the use of advanced oxidation process using chemical and photochemical methods (Tabrizi., et al 2004 and Scott., et al 1995).

There are also specific problems associated with the activated sludge process. They are:

1) Problems of sludge disposal: Waste sludge generated poses great disposal problems and affects effluent quality. To effectively settle, the individual microbes must flocculate and aggregate into units large enough to settle out of suspension. If the biomass does not flocculate well, some biosolids will end up in the final effluent and affect effluent quality (Peeters et al., 2007).

Dewatering (water should be reduced to below 80%) is commonly done, as it will reduce sludge volume and the subsequent treatment and the disposal operations. Many elements, such as particle size, floc structure and composition have been found to control activated sludge dewaterability **(**Sheintuch et al., 1986).

A survey on bulking of sludge on biological wastewater treatment plant was conducted and it was estimated that at least 25% of them suffered bulking problem (Wilen et al., 2004). Factors that might affect the rate of flocculation

may include:

i) Alteration in the physicochemical conditions of the sludge taking place without bacterial influence;

ii) Alteration in the local physico-chemical conditions indirectly mediated by bacterial activity (e.g. pH changes); or

iii) Changes in the bacterial metabolism directly affecting the stability, e.g. extracellular polymeric substances (EPS) production;

iv) Negative influence of filamentous microorganisms on sludge settling as they cause filamentous bulking. Their control is still very difficult to achieve because of the diversity of species.

Studies have been carried out to study the importance of aerobic microbial activity on the strength of activated sludge flocs. It was identified that extra cellular polymeric substances play an important role in the structural and functional integrity of the flocs. (Chen et al., 2001)

2.4 PROCESS CONTROL

Because of the variability in influent quality and flow rates WWTP process parameters have to be constantly monitored to ensure effluent quality criteria are not violated. Control tests are recommended for this reason. Both physiochemical and microbiological parameters are used. Physiochemical parameters include: TSS, BOD_5, TN, TP, TS, COD, conductivity, pH, and temperature. Frequently used microbiological parameters include: Total

coliforms, fecal coliforms (FC), fecal streptococci (FS), sulphite reducing clostridia, somatic coliphages, and bacteriophages of *Bacteroides flagilis* **(**TCEQ regulatory guidance**,** 2000 and Howard et al., 2004).

However the use of physical or chemical parameters as indicators of toxicity to aquatic species has disadvantages. They are:

1) Large number of toxic compounds exists at varying concentrations
2) Numerous interaction effects exist that are difficult to study.
3) Results from lab may not be a reliable source
4) Results from the lab may not be applicable to field because of various environmental factors.
5) Highly treated effluent stream can also cause pollution in the receiving stream because of the chemicals used.
6) Concentration of certain toxic chemicals can be below detectable levels

In such cases biological parameters such as changes in the structure of a community are better indicators to assess water quality (Howard et al., 2004).

State, federal and local government to deal with increasing water pollution and as a new approach to water quality management has passed new stricter laws. As a result online monitoring of water quality along with the concept of instrumentation, control and automation (ICA) is gaining importance with increasing pressure on wastewater treatment plant to comply with discharge requirements. Main aim behind these new technologies is to improve the efficiency of WWTP, help in the implementation of new solutions by lowering

operational and capital costs.

Important characteristics of online analysers are: Rapid and automatic data transmission, reliable data in terms of sensitivity, availability and ability to reproduce measured data. The most important aspect is the design, operational and maintenance cost associated with the sensors and suitable recording equipment for recording all online data measurements (Schlegel et al., 1996). Monitoring activities are broadly classified as: Data acquisition and data utilization. Data acquisition refers to the sample collection from different locations, sample analysis using laboratory techniques or automated sensors. Once relevant data is collected it is saved in appropriate databases using data acquisition software. Data utilization includes the process of data handling, data analysis, data interpretation and information utilization for decision making (Bourgeois et al., 2001**, W**ard, 1979 and Jeppsson et al., 2002).

For successful monitoring and control at a WWTP **(**Vanrolleghem et al., 2003):

1) Clear understanding of the processes occurring at the plant is important.
2) Accurate sensors that provide reliable online data is required.
3) Proper control strategies depending on controller output must be implemented.

2.5 MODELLING AND SIMULATION

Models are generally defined as:" mathematical representation of real systems". They serve as an important tool that helps researchers, designers, and operators to optimize and better understand processes occurring in a wastewater treatment plant. A model that is well calibrated is capable of providing valuable information about the following aspects of a WWTP(GPS-[X] user guide, 2006 and Pena-Tijerina, 2007):

1) Variable flow conditions that can affect performance of the plant

2) Equipment requirements

3) Pre-treatment requirements

4) Chemical usage for treatment

5) Identify bottleneck situations

6) Cost and energy savings associated with new technologies by predicting the outcome of implementing a new technology

7) Effects of upgrades to meet stringent effluent guidelines

Because of the above advantages, large efforts have been taken to promote user-friendly computer tools that create model frameworks depending on the needs. (GPS- [X] user guide, 2006 and Pena-Tijerina, 2007)

Models are broadly classified as being mechanistic or empirical.

1) **Mechanistic Models**: These models are based on fundamental laws of physics, chemistry and biology. So a thorough understanding of the processes

is essential. The model framework is constructed based on the processes. In case of mechanistic models, data are collected from the plant and used as a basis to modify the parameters (rate constants, stoichiometric coefficients, and physical dimensions) contained in the model.

Generally a bottom-up approach is adopted in the construction of mechanistic models. This means that the model is first constructed based on fundamental laws and the parameters in the equations used to construct the model are then modified according to the data collected.

2) **Empirical Models**: In the case of empirical models, more importance is given to data in the sense that the model is constructed based on data collected. This approach to modelling is considered as top-down approach. This means that the equations used to construct the model are selected from basic candidate equations based on goodness of fit to the data collected at the plant. Although these models are simpler than the mechanistic models they are less reliable that the mechanistic models. These models are useful in cases where there is limited knowledge about the systems being modelled (GPS- [X] user guide, 2006).

Non- mechanistic models are also referred to as black-box models. These models are generally used for prediction purposes or in cases when mechanistic models fail. An artificial neural network is an example of non- mechanistic model where online or offline data from the present or past are used for prediction purposes (Matas, 2000).

2.5.1 STEPS IN MODELLING

1) Goals in modelling: The first step in any modelling process is to define the goal. It is essential to identify the reason for modelling, the expected results from modelling and the acceptable limitations of modelling. Prior to data collection a model is selected so that the modeller gets an idea about the data requirements.
2) Data collection: Data are collected for calibration purposes. Data are collected from the plant through sampling or historic data available can be used. The amount of data collected depends on model requirements, data reliability and plant stability. Sampling is generally done in cases where the following parameters are not monitored at the plant on a daily basis: TSS, VSS, COD, BOD TP. Soluble P compounds, NTOX and TKN. Generally, 24-hour composite samples are collected from the major streams at the plant for calibration of a steady-state model. A well planned and carefully conducted sampling programme can provide good information for reliable calibration.
3) Data Analysis: Data analysis is essential to screen data that can be used in the model calibration stage. This is done by means of mass balances, flow balances to input data, comparing data from sampling to the historic data available at the plant, and by solids mass balances on clarifier data
4) Model Calibration: Models generally comprise state variables, composite variables (calculated from state variables), and kinetic and stoichiometric

constants. State variables are defined as “basic wastewater components like nitrates, ammonia, biomass that are continuously integrated over time” (GPS- [X] user guide, 2006). State variables are organized into different libraries in GPS-[X].

Common composite variables include TSS, VSS, COD, BOD TP, soluble P compounds, NTOX and TKN and are calculated from state variables. Values for kinetic constants is initially assumed and then calibrated / modified until a good fit is obtained between the values predicted by the model and the actual measured value.

During this stage “sensitivity analysis” is performed. The sensitivity of model output to changes in each of the model parameters is measured. This is done systematically or in most cases is done based on the modellers experience and knowledge. This is the most important step as it decides the reliability of a model.

5) Model Simulations: Once the model is calibrated, simulations can be performed. Simulations are the process of testing a plant against “What if” scenarios. It helps the operators to get an answer to questions such as responses to upgrades, problems at the plant during varying flow conditions and so on. Some of the common simulations performed include: Feasibility assessment, aeration analysis, solids management, and biological nutrient removal (Pena-Tijerina, 2007).

2.5.2 IMPORTANCE OF MODELLING

WWTP involve a series of complex treatment processes to address a variety of problems. However introduction of advanced technology to improve the performance of WWTP is difficult because of lack of reliable instrumentation. Reasons for constantly improving the performance of WWTP include: stringent legislation for the discharge of pollutants, cost effectiveness, concerns about partially treated waste and untreated waste on receiving water quality. At most existing WWTP, control strategies depend on operator's experience, technology available at the plant and the monitoring of a few common process parameters (Gamal El-Din, 2002).

WWTP are subjected to large variations in and uncertainties with respect to flow, composition of influent and loading. Complexity increases, as BNR facility is included. Various control strategies have been proposed. However, comparing different strategies and implementing the most effective one is limited because of cost and time. Modelling plays an important role in the optimization of existing facilities and in the design and development of new facilities.

Different software like GPS-[X] has been developed to test the various control strategies and implant the most effective one. This is done by subjecting the plant input to varying influent composition; flow and loadings as in the case with a real plant and using the predicted results to study plant performance (Alex et al., 1999 and Makinia [a] et al., 2006).

2.5.3 REQURIEMENTS FOR MODEL CALIBRATION

Major steps involved in model calibration include (Petersen et al., 2002 and Alex et al., 1999):

1) Information collection: Design data about tank volume, dimensions ; operational information including flow rate of internal recycle, return activated sludge, influent stream, effluent stream, temperature, pH; plant hydraulics including residence time and loading; settler model characteristics like settling velocity.
2) Organizing intensive sampling campaigns
3) Lab analysis for- characterization of wastewater in terms of BOD, COD, TKN, TP etc depending on model requirements; estimation of kinetic parameters like growth rates, decay rates; estimation of stoichiometric parameters like yield coefficient
4) Defining model structure followed by parameter adjustment to obtain a good fit between predicted value and measured value

   Requirements vary depending upon the purpose of modeling. If the requirement is only to understand processes at a plant, compare process design or during modeling situation where only qualitative information is required, then the default values, for example recommended by the international water association task group for ASM can be used and the laboratory estimation of kinetic and stoichiometric parameters can be minimized.

However for performance evaluation and optimization purpose more elaborate description of the processes are required. In such cases extensive sampling campaigns to collect average or dynamic data, performing mass balance and online data collection is recommended. (Petersen et al., 2002 and Alex et al., 1999).

2.5.4 SENSITIVITY ANALYSIS

Sensitivity analysis is used to determine the sensitivity of a model output to changes in parameter value and structure of the model.

In case of parameter sensitivity a modeller changes values of a parameter and tests how different parameter values affect the behaviour of a model. This type of analysis helps to study uncertainties associated with parameter that are sometimes difficult to measure in reality. Reliable models can be built by estimating values of a few important parameters with greater precision than others. Also testing a wide range of values can provide a good insight into the dynamic behaviour of a system under varying conditions. (http://sysdyn.clexchange.org/sdep/Roadmaps/RM8/D-4526-2.pdf)

2.6 MONOD KINETICS

The kinetics of microbial growth under substrate limited condition is clearly explained by Monod kinetics based on the following equation (Tchobanoglous et al., 2003):

$$r_{su} = \frac{\mu_m XS}{Y(K_s + S)}$$

where r_{su} = rate of substrate utilization ($g/m^3.d$)

μ_m = maximum specific bacterial growth rate (g new cells /g cells. d)

Y = true yield coefficient (g/g)

X = biomass concentration (g/m^3)

S = growth limiting substrate concentration (g/m^3)

K_s= half saturation or velocity constant, substrate concentration at half maximum specific substrate utilization rate (g/m^3)

Efficiency of any biological wastewater treatment process depends on the dynamics of substrate utilization and microbial growth. The term substrate utilization is used to indicate the depletion of electron donors (organic substances, ammonia, nitrites etc) for the production of biomass. Monod kinetics explains that the rate of substrate utilization is maximum at high substrate concentration and decreases almost linearly with decrease in the substrate concentration.

All rate equations used in ASM is based on Monod kinetics. Table 2.7.1 contains the rate expressions used in ASM2d along with the kinetic constants that are all in the form of Monod kinetic equation. Any model in which the rate equations are not limited by Monod terms, simulations are difficult and less reliable (Tchobanoglous et al., 2003 and Henze et al., 2000).

2.7 ACTIVATED SLUDGE MODEL PLATFORMS

Realising the importance of mathematical modelling for design, control and optimization, the IAWQ (International Association on water quality) group in 1987 introduced a common platform for model development (Gujer et al., 1995). It was called as the Activated Sludge model (ASM 1). Following this a series of similar models was developed.

It is very important to judiciously develop a mathematical model and ensure that a good balance is achieved by incorporating all major processes essential to describe the system being modeled at the same time the model equation involved must be solvable.

ASM-1: This was the first model developed by the IWA task group. It involves major processes such as carbon oxidation, nitrification and denitrification. All the kinetic and stoichiometric coefficients required to describe these processes are written in matrix format for easy understanding and to clearly indicate the interaction between the variables. Major components involved are first identified. Particulate and soluble components are distinguished using X and S subscripts, respectively. Subscripts were also used to specify individual components: B for biomass, O for oxygen, S for substrates and so on. Once the major components are identified, an index i is assigned to them. For ASM1, the index i range from 1 to 13 (for each of the 13 components) and these components are represented across the matrix. Similarly, major processes are

identified by an index j. For ASM1, j ranges from 1 to 8 to represent each of the 8 major processes. These are listed on the leftmost column of the matrix and the corresponding process rate for each of the process is listed on the rightmost column of the matrix. Process rates are represented as ρ_j. The elements within the matrix system are stoichiometric coefficients that establish mass relationships and interaction between components of individual processes (Henze et al., 2000). A simple example of matrix representation for heterotrophic growth rate is presented in Table 2.7.1.

The main advantage of using matrix representation is that fate of each component involved can be studied and mass balance equations can be prepared easily. Continuity checks can also be performed easily by ensuring that the sum of stoichiometric coefficients across the matrix is zero when the units are consistent (Henze et al., 2000).

To maintain consistency in the measurement of organics in wastewater, COD was chosen as it provides a link between organic substrate, biomass and oxygen utilized. Mass balance equations can also be prepared based on COD. So all organics, including biomass are expressed as COD units in all ASM models (Henze et al., 2000).

Components included in this model: Particulate- Autotrophic and heterotrophic biomass, inert organics, biodegradable organic nitrogen, product of biomass decay.

2.7.1 PROCESS EQUATION FOR AEROBIC HETEROTROPHIC GROWTH RATE (Henze et al., 2000)

Component (i)	1	2	3	Process rate,
Process (j)	X_B	S_S	S_O	(ρ_j)
1.Growth	1	$\frac{-1}{Y}$	$-\frac{1-Y}{Y}$	$\frac{\mu S_S}{K_S + S_S} X_B$
2.Decay	-1		-1	bX_B

Soluble: Inert organics, readily biodegradable substrate, dissolved oxygen, nitrate and nitrites, ammonia nitrogen, alkalinity, organic nitrogen.

Constraints of ASM1 (Henze et al., 2000):

1) System operates at constant temperature
2) pH is assumed to be constant near neutral
3) Changes in wastewater characteristics with respect to nature of organic matter cannot be modeled
4) Limitation of nutrients like nitrogen, phosphorus on the cell growth and removal of organics are not considered.
5) Changes to correction factors of denitrification with changes in system configuration are not considered.
6) Hydrolysis of organic matter and organic nitrogen is assumed to occur simultaneously with equal rates.
7) Factors affecting sludge settleability are not considered The entire process of nitrification and denitrification can be modelled using the

activated sludge model ASM1 or the improved version ASM3 developed by the international water association task group (IWA) (Henze et al., 2000).

ASM2: ASM2 is an extension of ASM1. In addition to the processes included in ASM1, biological and chemical phosphorus removal can be modeled using ASM2. Hence major component- internal cell storage is included in this model. However only the basics of bio-p removal are included and the model is a base for further development. Unlike ASM1 units in this model are not entirely based on COD. TSS was included to model poly-phosphate component that is important for bio-p removal. Compared to ASM1 this model is more complex because of the number of components included. However to simplify the model to the greatest possible extent those components that do not affect the kinetics of the processes were excluded from the matrix. Another important fact about ASM2 model is that the kinetic expression used are non-linear in nature and are based on average properties of cell population and not on unique cell properties **(**Gujer et al., 1995 and Henze et al., 2000).

Notations for matrix representation are similar to ASM1.

Components included in this model are:

Particulate: Nitrifying organisms, heterotrophic organisms, inert organics, metal hydroxides, metal phosphates, PAO, cell internal storage of PAO, polyphosphates, slowly biodegradable substrates, and TSS.

Soluble: Fermentation products (acetates), alkalinity of wastewater,

fermentable readily biodegradable organics, inert soluble organics, dinitrogen, ammonium and ammonia, nitrate and nitrite, dissolved oxygen, inorganic soluble phosphates and readily biodegradable substrates.

Constraints of ASM2 (Henze et al., 2000):

The exact role of PAO in phosphorus removal is yet to be studied. So assumptions made include:

1) PAOs can utilize only fermentation products such as acetate for their growth
2) PAO can grow aerobically only on stored PHA and not utilize fermentation products directly for their growth.
3) PAO cannot denitrify
4) PAO are capable of storing glycogen and carbohydrates as carbon storage material. However due to lack of sufficient information they have not been included as a model parameter.
5) Similar assumptions as in ASM1 with respect to pH and coefficient values.
6) Like ASM1 hydrolysis of organic matter, organic nitrogen and organic phosphate are coupled.
7) Growth limitations at low inorganic nutrient concentrations were not considered. So it is essential to assume that sufficient nutrients are provided
8) Reduced poly-phosphate uptake by PAO in the absence of cations like magnesium and potassium was not considered.

9) Inhibitory effect of nitrite and nitrogen monoxide was not considered

10) The model was applicable only for domestic wastewater and at temperatures rages of 10- 25^{o}C as the behavior of PAO beyond this temperature was not studied.

ASM2d: ASM2d was developed to resolve the assumption that PAOs cannot denitrify by considering both aerobic and anoxic growth of PAOs unlike ASM2 where only aerobic growth was considered. Hence it is only a “minor extension” of ASM2.

Components included in this model are:

Particulate: Nitrifying organisms, heterotrophic organisms, inert organics, metal hydroxides, metal phosphates, PAO, cell internal storage of PAO, polyphosphates, slowly biodegradable substrates, TSS.

Soluble: Fermentation products (acetates), alkalinity of wastewater, fermentable readily biodegradable organics, inert soluble organics, dinitrogen, ammonium and ammonia, nitrate and nitrite, dissolved oxygen, inorganic soluble phosphates and readily biodegradable substrates.

Like ASM2 this model is applicable only for municipal wastewater containing sufficient magnesium and potassium ions, at neutral pH and temperature range of 10-25 ^{o}C (Henze et al., 2000).

The process equations to represent the entire BNR process using ASM2d is as shown in Table 2.7.2 and the definitions of model components is as shown in Table 2.7.3

2.7.2 ASM 2d MODEL PROCESS EQUATIONS:

PROCESS	EQUATION	CONSTANTS				
		HYDROLYSIS				UNITS
Aerobic Hydrolysis	$K_h \cdot \frac{S_{O_2}}{K_{O_2}+S_{O_2}} \cdot \frac{X_S/X_H}{K_X + X_s/X_H} \cdot X_H$	K_h	Hydrolysis Rate Constant	3.00	2.00	d^{-1}
		η_{NO_3}	Anoxic Hydrolysis Reduction factor	0.60	0.60	-
Anoxic Hydrolysis	$K_h \cdot \eta_{NO_3} \cdot \frac{K_{O_2}}{K_{O_2}+S_{O_2}} \cdot \frac{S_{NO_3}}{S_{NO_3}+K_{NO_3}} \cdot \frac{X_S/X_H}{K_X + X_s/X_H} \cdot X_H$	η_{fe}	Anaerobic hydrolysis reduction factor	0.40	0.40	-
		K_{O_2}	Saturation/Inhibition coefficient for Oxygen	0.20	0.20	$g\ O_2\ m^{-3}$
		K_{NO_3}	Saturation/Inhibition coefficient for nitrate	0.50	0.50	$g\ N\ m^{-3}$
Anaerobic Hydrolysis	$K_h \quad \eta_{fe} \quad \frac{K_{O_2}}{K_{O_2}+S_{O_2}} \quad \frac{K_{NO_3}}{S_{NO_3}+K_{NO_3}} \quad \cdot \quad \frac{X_S/X_H}{K_X + X_s/X_H} \cdot X_H$	K_X	Saturation coefficient of particulate COD	0.10	0.10	$g\ X_s\ g^{-1}\ X_H$

HETEROTROPHIC ORGANISMS							
Growth on fermentable substrates, S_F	$\mu_H \frac{S_{O_2}}{K_{O_2}+S_{O_2}} \frac{S_F}{K_F+S_F} \frac{S_F}{S_F+S_A} \frac{S_{NH_4}}{S_{NH_4}+K_{NH_4}} \frac{S_{PO_4}}{S_{PO_4}+K_P} \frac{S_{ALK}}{S_{ALK}+K_{ALK}} X_H$	μ_H	Maximum Growth Rate on substrate	6.00	3.00	g X_s $g^{-1}X_H$ d^{-1}
		η_{fe}	Maximum rate for frementation	3.00	1.50	g S_F $G^{-1}X_H$ d^{-1}
		η_{NO_3}	Reduction factor for denitirification	0.80	0.80	-
Growth on fermentation products, S_A	$\mu_H \frac{S_{O_2}}{K_{O_2}+S_{O_2}} \frac{S_A}{S_A+K_A} \frac{S_A}{S_F+S_A} \frac{S_{NH_4}}{S_{NH_4}+K_{NH_4}} \frac{S_{PO_4}}{S_{PO_4}+K_P} \frac{S_{ALK}}{S_{ALK}+K_{ALK}} X_H$	b_H	Rate constant for lysis and decay	0.40	0.20	d^{-1}
		K_{O_2}	Saturation/inhibition coefficient for oxygen	0.20	0.20	g O_2 m^{-3}
		K_F	Saturation coefficient for growth on S_f	4.00	4.00	g COD m^{-3}
Denitrification with fermentable substrates S_F	$\mu_H \eta_{NO_3} \frac{K_{O_2}}{K_{O_2}+S_{O_2}} \frac{S_F}{K_F+S_F} \frac{S_F}{S_F+S_A} \frac{S_{NH_4}}{S_{NH_4}+K_{NH_4}} \frac{S_{NO_3}}{S_{NO_3}+K_{NO_3}} \frac{S_{ALK}}{S_{ALK}+K_{ALK}} \frac{S_{PO_4}}{S_{PO_4}+K_P} X_H$	K_{fe}	Saturation coefficient for fermentation of S_f	4.00	4.00	g COD m^{-3}
		K_A	Saturation coefficient for growth on acetate S_A	4.00	4.00	g COD m^{-3}
		K_{NO_3}	Saturation/inhibition coefficient for nitrate	0.50	0.50	g N m^{-3}
		K_{NH_4}	Saturation coefficient for ammonium (nutrient)	0.05	0.05	g N m^{-3}

Denitrification with fermentation products S_A	$\mu_H \quad \eta_{NO_3} \quad \frac{K_{O_2}}{K_{O_2}+S_{O_2}} \quad \frac{S_A}{S_A+K_A} \quad \frac{S_A}{S_F+S_A}$ $\frac{S_{NH_4}}{S_{NH_4}+K_{NH_4}} \quad \frac{S_{NO_3}}{S_{NO_3}+K_{NO_3}} \quad \frac{S_{ALK}}{S_{ALK}+K_{ALK}}$ $\frac{S_{PO_4}}{S_{PO_4}+K_P} X_H$	K_P K_{ALK}	Saturation coefficient for phosphate (nutrient) Saturation coefficient for alkalinity (HCO_3)	0.01 0.10	0.01 0.10	g P m^{-3} moleHCO_3^{-1} m^{-3}
Fermentation	$q_{fe} \quad \frac{K_{O_2}}{K_{O_2}+S_{O_2}} \quad \frac{K_{NO_3}}{S_{NO_3}+K_{NO_3}} \quad \frac{S_F}{K_{fe}+S_F}$ $\frac{S_{ALK}}{S_{ALK}+K_{ALK}} X_H$					
Lysis	$b_H X_H$					

PAO						
Storage of X_{PHA}	$q_{PHA} \cdot \frac{S_{ALK}}{S_{ALK}+K_{ALK}} \cdot \frac{S_A}{S_A+K_A} \cdot \frac{X_{PP}/X_{PAO}}{K_{PP}+X_{PP}/X_{PAO}} \cdot X_{PAO}$	q_{PHA}	Rate constant for Storage of X_{PHA}	3.00	2.00	g X_{PHA} g^{-1} X_{PAO} d^{-1}
		q_{pp}	Rate constant for Storage of X_{PP}	1.50	1.00	g X_{PP} g^{-1} X_{PAO} d^{-1}
		μ_{PAO}	Maximum growth rate of PAO	1.00	0.67	d^{-1}
Aerobic Storage of Xpp	$q_{pp} \cdot \frac{S_{O_2}}{K_{O_2}+S_{O_2}} \cdot \frac{S_{PO_4}}{S_{PO_4}+K_{Ps}} \cdot \frac{S_{ALK}}{S_{ALK}+K_{ALK}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA}+X_{PHA}/X_{PAO}} \cdot \frac{K_{MAX}-X_{PP}/X_{PAO}}{K_{IPP}+K_{MAX}-X_{PP}/X_{PAO}} \cdot X_{PAO}$	η_{NO_3}	Reduction factor for anoxic activity	0.60	0.60	-
		b_{PAO}	Rate for lysis of X_{PAO}	0.20	0.10	d^{-1}
		b_{PP}	Rate for lysis of X_{PP}	0.20	0.10	d^{-1}
		b_{PHA}	Rate for lysis of X_{PHA}	0.20	0.10	d^{-1}
Aerobic growth on X_{PHA}	$\mu_{PAO} \cdot \frac{S_{O_2}}{K_{O_2}+S_{O_2}} \cdot \frac{S_{NH_4}}{S_{NH_4}+K_{NH_4}} \cdot \frac{S_{ALK}}{S_{ALK}+K_{ALK}} \cdot \frac{S_{PO_4}}{S_{PO_4}+K_P} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA}+X_{PHA}/X_{PAO}} \cdot X_{PAO}$	K_{O_2}	Saturation/inhibition coefficient for oxygen	0.20	0.20	g O_2 m^{-3}
		K_{NO_3}	Saturation/inhibition coefficient for nitrate	0.50	0.50	g N m^{-3}
		K_A	Saturation coefficient for growth on acetate S_A	4.00	4.00	g COD m^{-3}

Anoxic storage of Xpp	$\rho_{12} = \rho_{11}.\eta_{NO_3} \frac{K_{O_2}}{S_{O_2}} . \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}$	K_{NH_4}	Saturation coefficient for ammonium (nutrient)	0.05	0.05	g N m^{-3}
		K_{PS}	Saturation coefficient for phosphorus in storage of PP	0.20	0.20	g P m^{-3}
Anoxic storage of Xpp	$\rho_{14} = \rho_{13}.\eta_{NO_3} \frac{K_{O_2}}{S_{O_2}} . \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}}$			0.01	0.01	g P m^{-3}
Lysis of X_{PAO}	$b_{PAO} . X_{PAO} . \frac{S_{ALK}}{S_{ALK} + K_{ALK}}$	K_P	Saturation coefficient for phosphate (nutrient)			
		K_{ALK}	Saturation coefficient for alkalinity	0.10	0.10	moleHCO_3^{-1} m^{-3}
Lysis of Xpp	$b_{PP} . X_{pp} . \frac{S_{ALK}}{S_{ALK} + K_{ALK}}$	K_{PP}	Saturation coefficient for polyphosphate	0.01	0.01	g X_{PP} g^{-1} X_{PAO}
		K_{max}	Maximum ratio of X_{pp}/X_{PAO}	0.34	0.34	g X_{PP} g^{-1} X_{PAO}
Lysis of X_{PHA}	$b_{PHA} . X_{PHA} \frac{S_{ALK}}{S_{ALK} + K_{ALK}}$	K_{IPP}	Inhibition coefficient for PP storage	0.02	0.02	g X_{PP} g^{-1} X_{PAO}
		K_{PHA}	Saturation coefficient for PHA	0.01	0.01	g X_{PHA} g^{-1} X_{PAO}

AUTOTROPHIC BIOMASS						
Aerobic growth of X_{AUT}	$\mu_{AUT} \cdot \frac{S_{O_2}}{K_{O_2}+S_{O_2}} \frac{S_{NH_4}}{S_{NH_4}+K_{NH_4}} \frac{S_{PO_4}}{S_{PO_4}+K_P}$ $\frac{S_{ALK}}{S_{ALK}+K_{ALK}} X_{AUT}$	μ_{AUT}	Maximum growth rate of X_{AUT}	1.00	0.35	d^{-1}
		b_{AUT}	Decay rate of X_{AUT}	0.15	0.05	d^{-1}
		K_{O_2}	Saturation coefficient for oxygen	0.50	0.50	g O_2 m^{-3}
Lysis of X_{AUT}	$b_{AUT} X_{AUT} S_{PO_4}$	K_{NH_4}	Saturation coefficient for ammonium (substrate)	1.00	1.00	g N m^{-3}
		K_{ALK}	Saturation coefficient for alkalinity	0.50	0.50	moleHCO_3^{-1} m^{-3}
		K_P	Saturation coefficient for phosphorus	0.01	0.01	g P m^{-3}

SIMULTANEOUS PRECIPITATION OF P WITH FERRIC CHLORIDE						
Precipitation	$K_{PRE} X_{MeOH}$	K_{PRE}	Rate constant for P precipitation	1.00	1.00	m^3 g^{-1} $Fe(OH)_3$ d^{-1}
Redissolution	$K_{RED} X_{MeP} \frac{S_{ALK}}{S_{ALK}+K_{ALK}}$	K_{RED}	Rate constant for Redissolution	0.60	0.60	d^{-1}
		K_{ALK}	Saturation coefficient for alkalinity	0.50	0.50	moleHCO_3^{-1} m^{-3}

2.7.3 DEFINITION OF MODEL COMPONENTS:

SOLUBLE COMPONENT		UNITS
S_{O_2}	Dissolved oxygen	g O_2 m^{-3}
S_F	Readily biodegradable substrate	g COD m^{-3}
S_A	Fermentation product (acetate)	g COD m^{-3}
S_{NH_4}	Ammonium	g N m^{-3}
S_{NO_3}	Nitrate + nitrite	g N m^{-3}
S_{PO_4}	Phosphate	g P m^{-3}
S_I	Inert non- biodegradable organics	g COD m^{-3}
S_{ALK}	Bicarbonate alkalinity	mole HCO_3^{-1} m^{-3}
PARTICULATE COMPONENTS		**UNITS**
X_I	Inert non- biodegradable organics	g COD m^{-3}
X_S	Slowly biodegradable substrate	g COD m^{-3}
X_H	Heterotrophic biomass	g COD m^{-3}
X_{PAO}	Phosphorus-accumulating organisms	g COD m^{-3}
X_{PP}	Stored poly-phosphate of PAO	g P m^{-3}
X_{PHA}	Organic storage products of PAO	g COD m^{-3}
X_{AUT}	Autotrophic biomass	g COD m^{-3}
X_{MeOH}	Ferric-hydroxide	g $Fe(OH)_3$ m^{-3}
X_{MeP}	Ferric-phosphate	g $FePO_4$ m^{-3}
X_{TSS}	Particulate material as model component	g TSS m^{-3}

ASM 3: Similar to ASM1, ASM3 was developed to describe removal of organic compounds and nitrogen from municipal wastewater. It is now used as a standard model as number of defects in ASM1 was corrected in this model. The main differences between ASM1 and ASM3 are(Gernaey et al., 2004):

1) ASM3 assumes that all rbCOD is initially stored as internal cell components before it is used for growth. So ASM3 includes storage components similar to biological-p removal models. On the other hand ASM1 assumes the direct use of rbCOD for growth
2) ASM3 is easier to calibrate as it is based on growth- endogenous respiration model, unlike ASM1, which is based on growth –decay model.

ASM1 growth of heterotrophs is correlated to decay of nitrifiers. It is assumed that autotrophic biomass decays to form particulate inert and particulate slowly biodegradable substrates. The particulate slowly biodegradable substrates then contribute to the growth of heterotrophic biomass. On the other hand ASM3 clearly separates the growth of autotrophs and heterotrophs, and assumes no flow substrate from one to another (Henze et al., 2000).

3) State variables in ASM1 are very sensitive to changes in the value of parameters during modelling, unlike ASM3 (Gernaey et al., 2004).

Components in ASM3 include: Soluble: Inert organics, readily biodegradable substrate, dissolved oxygen, nitrate and nitrites, ammonia nitrogen, alkalinity, and dinitrogen. Particulate: Inert organic material, slowly biodegradable

substrates, heterotrophic biomass, cell storage product of heterotrophs, nitrifying organisms, suspended solids.

Limitations of ASM3 (Henze et al., 2000):

1) Applicable only for domestic wastewater and not for industrial waste
2) Like ASM1 it is applicable only within a temperature range of 8-23^{o}C and a pH range of 6.5-7.5.
3) Does not describe the growth of biomass in an anaerobic environment.
4) ASM3 is not applicable to waste stream with very high concentration of nitrites
5) Like ASM1 it is not suitable if SRT is less than 1 day, when flocculation is limited.
6) ASM3 does not provide an absolute value of model parameters, users have to identify applicable parameters.

ASM3 C: It is an extension of ASM3 and is a carbon based model. Dichromate method for COD determination (COD-Cr) is greatly inhibited in the presence of heavy metals like Hg, Ar, and Cr. The permanganate method (COD-Mn) underestimates theoretical oxygen demand (ThOD) and hence is not valid for use in ASM3. To rectify this ASM3C was introduced where all of the organic state variables were measured in terms of total organic carbon (TOC). Rest of the processes and parameters are similar to the ones in ASM3. (Henze et al., 2000).

A3DX: Technological University of Delft developed a new mathematical

model similar to ASM3 called A3DX to model carbon, nitrogen and biological phosphorus removal. This new model was a modification of ASM3 by including processes for chemical and biological phosphorus removal using GPS-[X] and Mathlab software. A special Monod based kinetics was also included to account for Magnesium limitation. Apart from the variables included in ASM3, soluble phosphorus, polyhydroxyalkonoates, polyphosphates, glycogen and PAO is also included **(**R.C. Ky et al., 2001).

Different simulation platforms include AQUASIM (Switzerland), BioWin (Canada), GPS-[X] (Canada), SIMBA (Germany), STOAT (UK), and WEST (Belgium) (Makinia, 2010).

2.8 PARAMETER ESTIMATION

No single estimation procedure is capable of identifying all of the model parameters because ASM variables that are measured do not help in the identification of all model parameters. Also the quality and quantity of data obtained are seldom sufficient for modeling all parameters. Search algorithms can be used to estimate model parameters. The main disadvantage of this method is that it is very complex, time consuming, tedious and enormous simulations have to be performed before model parameters are estimated. Some of the commonly used search algorithms include Nelder and Mead‘s simplex algorithm, genetic algorithms, simulated annealing and Monte Carlo simulation (Sin et al., 2008).

Structural identifiability and practical identifiability are two commonly used approaches for parameter identification. Structural identifiability is used to identify distinct values of parameters once model structure and measurements to be performed are identified. Practical identifiability gives an estimate of the accuracy of the parameters estimated. Fisher information matrix, parameter estimation covariance matrix or its inverse are commonly used for practical identifiability (De Pauw et al., 2004).

2.9 WASTEWATER CHARACTERIZATION

Wastewater characterization is used to estimate all the components in wastewater according to the requirements of the model chosen. It can be done using physical, chemical and biological methods. Characterization includes the biodegradable organic fractions, nitrogen fractions and phosphorus fractions present in wastewater. Important readily biodegradable organics include volatile fatty acids, ethanol, methanol and glucose (Henze et al., 2000).

Organic Fractions: The total organic content of wastewater is calculated as COD. IWA recommends all measurements and mass balances be made based on COD units because COD provides a link between organic substrate, biomass and oxygen utilized in terms of electron equivalence. To ensure accurate mass balance calculations, it is generally recommended to use the dichromate method of COD estimation instead of the permanganate method (Henze et al., 2000). For ASM 2 and ASM2d:

1) Organic fractions include: VFA/ Fermentation products (S_A), readily biodegradable substrate (S_F), inert non-biodegradable organics (dissolved and soluble) (S_I, X_I), slowly biodegradable organics (X_S), Heterotrophic, autotrophic and phosphorus accumulating biomass (X_H, X_{AUT}, X_{PAO}) and stored poly-hydroxy-alkanoate (X_{PHA}).

i) Inert non-biodegradable organics (dissolved) S_I: Generally the effluent concentration of S_I is higher than the influent concentration because S_I is produced from the hydrolysis of X_S. Since there is no direct method to estimate the concentration of S_I analysis of effluent soluble COD gives a good estimate of S_I.

ii) Slowly biodegradable organics (X_S): This component is generally measured using oxygen uptake rates (OUR) or Nitrogen uptake rate (NUR).

iii) Inert non-biodegradable organics (Particulate) X_I : Since there is no direct method to determine this component, it is obtained through model calibration

iv) X_H Heterotrophic biomass fraction is either included along with X_S component or is neglected as it does not affect modelling significantly

v) VFA/ Fermentation products (S_A), readily biodegradable substrate (S_F): These components are measured using OUR and plotting calibration curves. The VFA portion is also measured using titrimetric measurements.

vi) The other biomass components (autotrophic and phosphorus accumulating organisms) and poly-hydroxy-alkanoate (X_{PHA}) components is present in negligible quantities in the wastewater and hence is neglected (Petersen, 2000, Henze, 1992, Henze et al., 2000 and Xu et al., 1996).

2) Nitrogen Fractions:

Nitrogen fractions include: Dinitrogen, Ammonia nitrogen, Nitrate and Nitrite nitrogen. The major portion of nitrogen in the waste stream is present in the form of ammonia which can be measured using conventional chemical analytical techniques. The ammonia and organic portion can be measured with the TKN analysis. Similarly there are standard chemical procedures to measure the nitrate and the nitrite portions (Petersen, 2000, Henze, 1992, Henze et al., 2000 and Xu et al., 1996).

3) Phosphorus Fraction: It is not necessary to characterize the phosphorus fraction in detail similar to the organic fractions. The most important is the soluble orthophosphate component and standard analytical procedures are available. The stored polyphosphate and the metal phosphate concentration are generally negligible (Petersen, 2000, Henze, 1992, Henze et al., 2000 and Xu et al., 1996).

2.10 ESTIMATION OF KINETIC AND STOICHIOMETRIC COEFFICIENTS

It is generally difficult to set up lab scale experiments for the estimation of most of the kinetic constants of the process equations. Also, using data obtained through lab scale experiments may not be a reliable source to calibrate full-scale plants. So in most of the cases using recommended default values followed by model calibration to adjust the constants accordingly is recommended. Nevertheless, lab scale experiments can be performed to obtain values for a few constants.

Respirometric lab scale experiments using samples of wastewater and activated sludge are commonly performed for the estimation of various constants. Other experiments like titrimetry, nitrate utilization rates and ammonium uptake rates are also used. Respirometric measurements help in the calculation of oxygen uptake rate and oxygen transfer coefficient (Petersen, 2000, Petersen et al., 2002).

Maximum specific growth rates of autotrophic and heterotrophic bacteria are commonly measured using the exogenous oxygen uptake rate, $R_{o,ex,}$ that is caused by wastewater COD and ammonium addition during the respirometric experiments. On the other hand the decay rates are measured from the endogenous oxygen uptake rate $R_{o,end.}$). No reliable lab scale experiments to determine kinetic parameters of phosphorus accumulating organisms are presently available (Petersen, 2000, Petersen et al., 2002. A few guidelines

were recommended by the IWA task group for the calibration of ASM2 using non-dynamic data.

For the calibration of heterotrophic organisms: Results from respirometric experiments can be used to calibrate b_h (rate of lysis of heterotrophs). If the observed S_A (soluble products of fermentation, acetate) value is lower than the simulated one then it is recommended to decrease the K_A (saturation coefficient for growth on acetate) value to increase the value of the Monod term. Typical range of K_A varies between 3 and 5 g COD m^{-3} and is affected by diffusion limitation in the floc. K_{O_2} (oxygen saturation coefficient) is modified only if experiments have been carried out in a DO range where oxygen is process rate limiting (0 to 2 mg/L) (Henze et al., 2000).

Autotrophic calibration: Calibration of terms related to autotrophic metabolism is very similar to the calibration for processes carried out by heterotrophic organisms. Effluent ammonia concentration is considered in this case instead of soluble biodegradable COD. Similar to the K_A value, K_{NH_4} depends on turbulence and floc size distribution. The default growth rate is modified only if it is impossible to fit the effluent ammonia value by changing ammonia saturation coefficient value (Henze et al., 2000).

Denitrification Calibration: Once the μ_H value has been calibrated using respirometric measurement it should not be altered. η_{NO_3} is calibrated based on the effluent nitrate level from the anoxic tank. Typical values of η_{NO_3} ranges between 0.6 and 0.9. K_{NO_3} is calibrated similarly to K_A (Henze et al., 2000).

Calibration of phosphorus removal: Y_{PO_4} can be calibrated using effluent phosphate concentration from the anaerobic tank. If the S_F value is high, then model is calibrated by modifying the q_{fe} value. Otherwise K_{fe} is used. For aerobic growth of PAOs, it is recommended not to modify μ_{PAO} until respirometric data are available or if modifying K_P does not give good fit (Henze et al., 2000).

CHAPTER 3

3.0 METHODS AND MATERIALS

3.1 MODEL DEVELOPMENT AND CALIBRATION

Modelling was attempted using the General Purpose Simulator version 5.0 (GPS-[X]) developed by Hydromantis Inc. GPS-[X] allows both dynamic and steady-state modelling of both industrial and municipal wastewater treatment plants. It has 50 pre-compiled layouts and allows user to create/ add new layouts. Modelling carbon removal, nitrogen and phosphorus removal is possible using the GPS-[X] software. GPS-[X] includes several modules and utility tools. The modules include: simulator, builder, optimizer, analyzer, dynamic parameter estimator, advanced control and multi-instance licences. Utility tools include: influent advisor to characterize the influent and MOUSE to GPS-[X] link tool to link GPS-[X] to MOUSE simulation software package.

One of the most important features of GPS-[X] is that any dynamic system can be represented on a drawing board without a need to develop complex computer code for modelling and simulations. GPS-[X] writes “error- free simulation code” which saves the user from the tedious task of “program coding and debugging”. As a result of this the modeller can devote much time in understanding the processes of the system rather than programming and debugging. Another feature of this software is that it offers an “extensive library of process models” ranging from pre-treatment units to biological

nutrient removal processes.

In 1994, a study of plant flow measurements was conducted in Goldbar and modelling was conducted using GPS-[X]. So it was decided to continue using the same software for this project too (Report for flow improvement study for GBWWTP, 1994).

To begin with, a suitable library (containing all the state and composite variables) along with appropriate ASM model has to chosen. In this work, ASM2d and the carbon-nitrogen-phosphorus library was chosen to model carbon, nitrogen and phosphorus removal processes. The various processes (shown in Table 2.7.2) modelled using ASM2d include (Henze et al., 2000):

1. Hydrolysis: This is a process where high molecular weight organics (slowly biodegradable substrate- X_S) are converted to readily biodegradable substrates by hydrolytic enzymes. This process can occur under aerobic, anoxic and anaerobic conditions. This process is slow under anoxic and anaerobic conditions and is accounted for in the model by using reduction factors.
2. Aerobic growth of heterotrophs: Growth occurs on both fermentable substrates and fermentation products (S_F and S_A). Both the processes are modelled parallel with identical growth rate and yield coefficents. These processes require oxygen and nutrients like ammonia and phosphorus that are included in the process equations.
3. Anoxic growth of heterotrophs: This is similar to the aerobic growth.

However instead of oxygen S_{NO_3} is included in the process equation. A reduction factor (η_{NO_3}) is also included to compensate for a reduction in the growth rate under anoxic conditions.

4. Fermentation : This process in carried out by heterotrophs under anaerobic conditions where S_F is transformed to S_A
5. Lysis of heterotrophs: This includes all processes like endogenous respiration, lysis, predation etc and is indicated by the term b_H .
6. Storage of poly-hydroxy-alkanoates: This process is an anaerobic process and occurs along with the release of phosphates from poly-phosphates (S_{PO_4} from X_{PP}).
7. Aerobic and anoxic storage of poly-phosphates: This is essentially the storage of orthophosphate as cell internal poly-phosphate (S_{PO_4} as X_{PP}). This process occurs at a reduced rate under anoxic condition by a factor of η_{NO_3}
8. Aerobic and anoxic growth of PAOs: PAOs grow by using stored poly-hydroxy-alkanoates (X_{PHA}). This is reduced under anoxic conditions and is accounted for by the reduction factor.
9. Lysis of PAO: This is modelled as 3 processes- lysis of PAOs, lysis of X_{PP} and lysis of X_{PHA} .
10. Growth of autotrophs: This process is modelled as an aerobic process where ammonium is consumed as nutrient.
11. Lysis of autotrophs: This process is modelled similar to the lysis of

heterotrophs and the product of lysis X_S (converted to S_F by hydrolysis reactions) is used by heterotrophs for growth.

A model of the GBWWTP (the BNR system along with the secondary clarifier) was created. The physical and operational parameters required as input were obtained from Gold Bar personnel. Physical dimensions of the bioreactor are tabulated in the Appendix 1 (Table 1.A). The method to build a model and conduct simulations is clearly indicated in the user guide manual of the software (GPS- [X] user guide, 2006).

Data collected from the plant database were first validated by calculating SRT based on MLSS concentration and WAS flow rate monitored at the plant. Data for days when the calculated SRT exceeded 6 days was not used for modeling. For the remaining days, influent was characterized based on a trial and error approach using the influent advisor utility tool. Input to the model along with wastewater characterization is as shown in Table 1.B.1 in Appendix 1. The goal of this work was to attempt model calibration based solely on historic data available in the GBWWTP archives and information available in the literature.

This calibration process involved the following phases: (1) The use of default values (values suggested by the IWA task group); (2) A sensitivity analysis of important kinetic parameters (identified from the literature) in which the value of a parameter was varied by ±50% relative to its default value and the influence of the change on the model output was observed; and

(3) Based on the results of the sensitivity analysis, the kinetic parameters were modified (from default value) based on literature.

A steady state simulation was conducted and the predicted model output was compared to values measured at the plant. Since a BNR system was being modelled, the following output parameters were considered: final effluent CBOD, TSS, OPO_4, NH_3 and NTOX.

Steady state simulations were conducted a number of times until a reasonable fit between the predicted and measured value was obtained.

3.2 SAMPLE COLLECTION

A sampling program was also begun to provide data for use in the next phase of the plant model calibration project. Two intense 24 hour sampling programs were conducted during the month of August and November, 2008. During the first sampling campaign discreet samples were collected every hour for 24 hours (24 samples from each sampling location). Samples were collected from different locations at the plant. The sampling points include: raw influent, primary effluent, effluent at the end of Pass I (BNR), effluent at the end of Pass IV (BNR) and RAS. All samples were collected using auto samplers provided at the GBWWTP.

During the second 24 hour sampling campaign conducted in November, 24 hour composite samples were collected from raw influent, primary effluent, effluent at the end of Pass I (BNR), effluent at the end of Pass IV (BNR). Auto

samplers provided at the GBWWTP were used for sample collection.

Apart from the sampling campaigns historic data from the plant database (collected at the plant) based on 24 hour composite samples was also collected.

3.3 SAMPLE ANALYSIS

The samples collected were analyzed for various parameters based on model requirement. The samples from the first campaign were analyzed for the following parameters:

1 Raw influent: Ammonia nitrogen, TKN, nitrate and nitrite, total phosphorus, orthophosphate, total and soluble COD, total and soluble BOD, TSS and VSS

2 Primary Effluent : Ammonia nitrogen, TKN, nitrate and nitrite, total phosphorus, orthophosphate, total and soluble COD, TSS and VSS

3 Effluent from Pass I : MLSS, MLVSS, nitrates and nitrites

4 Effluent from Pass IV : Ammonia nitrogen, TKN, nitrate and nitrite, total phosphorus, orthophosphate, total and soluble COD, MLSS and ML VSS

5 RAS : Alkalinity, MLSS and MLVSS

Samples from the second campaign were analyzed for the following parameters:

1 Raw influent: Ammonia nitrogen, TKN, total and soluble COD, total and soluble BOD.

2 Primary Effluent: Ammonia nitrogen, TKN, total and soluble COD, total and soluble BOD.

3 Effluent from Pass I: MLSS and MLVSS

4 Effluent from Pass IV : Ammonia nitrogen, TKN, total phosphorus,

orthophosphate, total and soluble COD, MLSS and ML VSS

All analysis was performed in the Gold bar wastewater laboratory based on standard methods.

CHAPTER 4

4. RESULTS AND DISCUSSION

The main scope of the project was to calibrate an ASM2d model (GPS-[X]software) for GBWWTP using historic plant data and parameter values available in the literature. The parameters modelled include: final effluent CBOD, NH_3, OPO_4, TSS and NTOX. Characteristics of the influent stream (PE) are shown in Table 1.B.1 in Appendix 1.B. Historic data collected at the plant (from 2007-2009) for PE and final effluent (for the parameters mentioned above) was used for modelling purposes.

4.1 DEFAULT MODEL VALUES

4.1.1 CBOD Modelling

Figure 4.1.1 presents a comparison of the CBOD values predicted by the model to the actual CBOD values measured at GBWWTP. Default values of the all kinetic parameters indicated in Table 4.1 were used during the first run of calibration. It is evident from Figure 4.1.1 that the model was overestimating the CBOD concentration as compared to the CBOD concentration measured at the plant for most of the days. The mean square error calculated was 1.728.

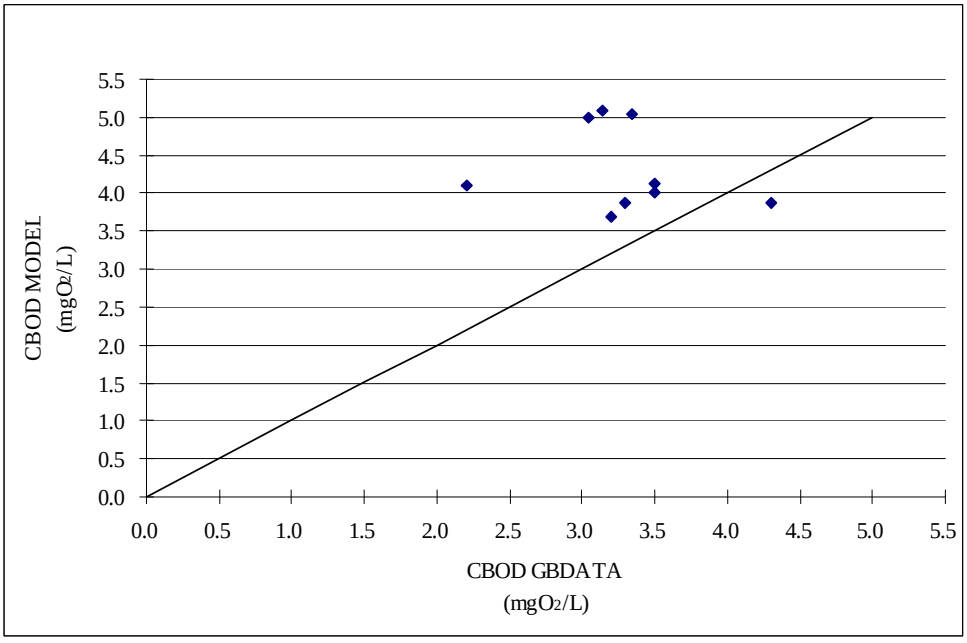

FIGURE 4.1.1: Comparison of measured and predicted CBOD concentration using default values of model kinetic parameter. Symbols lying on the 45^{o} line would indicate perfect agreement between modelled and observed values.

4.1.2 NTOX Modelling

Figure 4.1.2 presents a comparison of NTOX values predicted by the model to the NTOX values measured at GBWWTP. Default values of the all the kinetic parameters were used during the first run of the calibration. It is evident from the figure that the model was underestimating the concentration as compared to the actual NTOX concentration measured at the plant. The mean square error calculated was 29.302

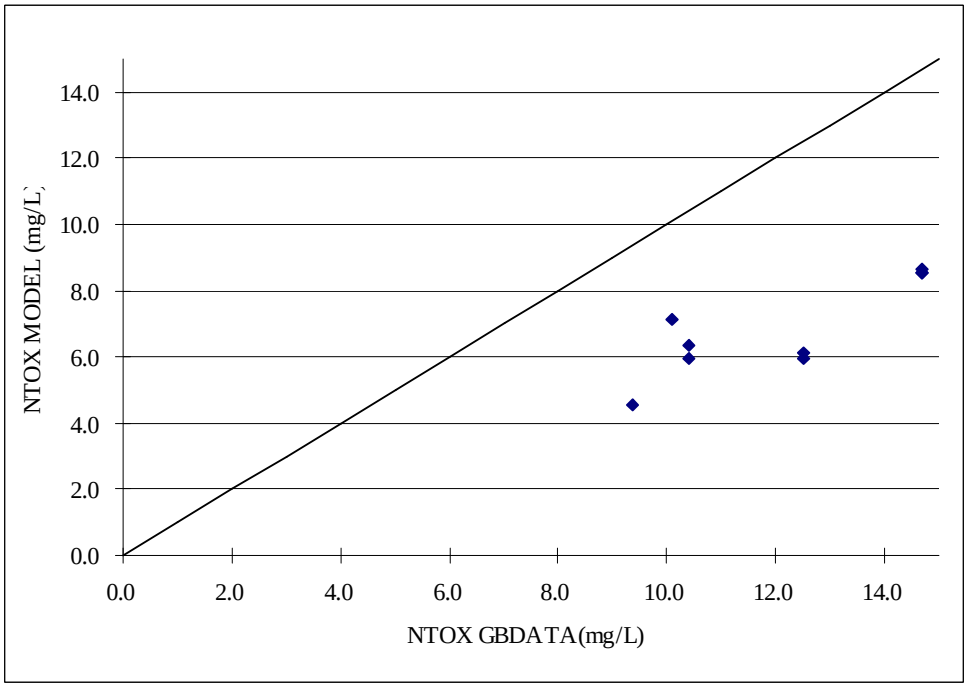

FIGURE 4.1.2: Comparison of measured and predicted NTOX concentration using default values of model kinetic parameter. Symbols lying on the 45^{o} line would indicate perfect agreement between modelled and observed values

4.1.3 TSS Modelling

Figure 4.1.3 presents a comparison of TSS values predicted by the model to the TSS values measured at GBWWTP. Default values of the all the kinetic parameters were used during the first run of calibration. It is evident from the figure that the model was overestimating the concentration as compared to the TSS concentration measured at the plant. The mean square error calculated was 14.11.

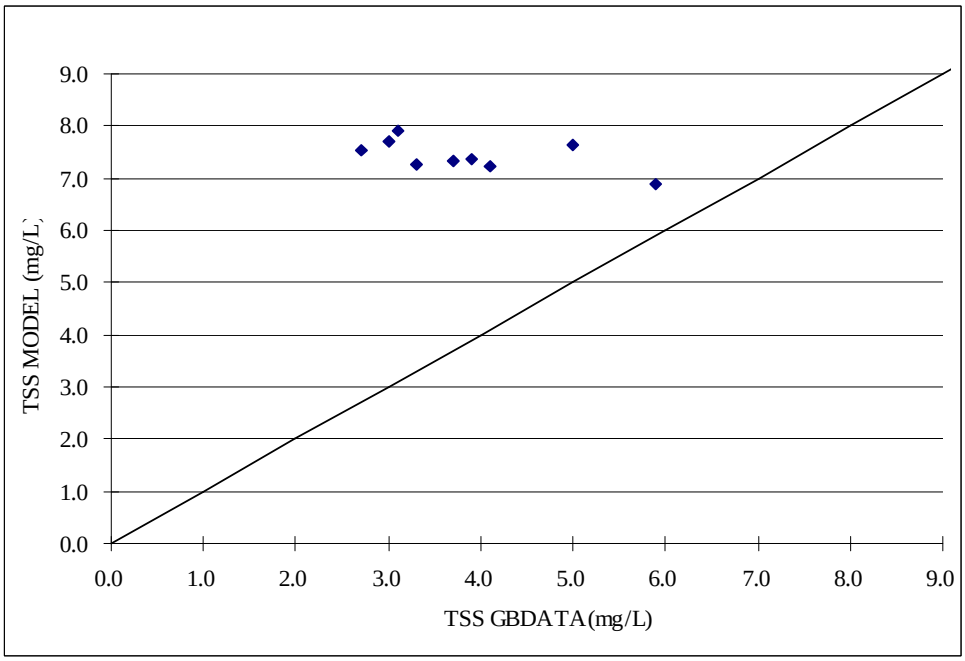

FIGURE 4.1.3: Comparison of measured and predicted TSS concentration using default values of model kinetic parameter. Symbols lying on the 45^{o} line would indicate perfect agreement between modelled and observed values.

4.1.4 OPO_4 Modelling

Figure 4.1.4 presents a comparison of OPO_4 values predicted by the model to the OPO_4 concentration measured at the GBWWTP. Default values of the all the kinetic parameters were used during the first run of calibration. It is evident from the figure that the model was overestimating the concentration as compared to the OPO_4 concentration measured at the plant for all days. The mean square error calculated was 52.42

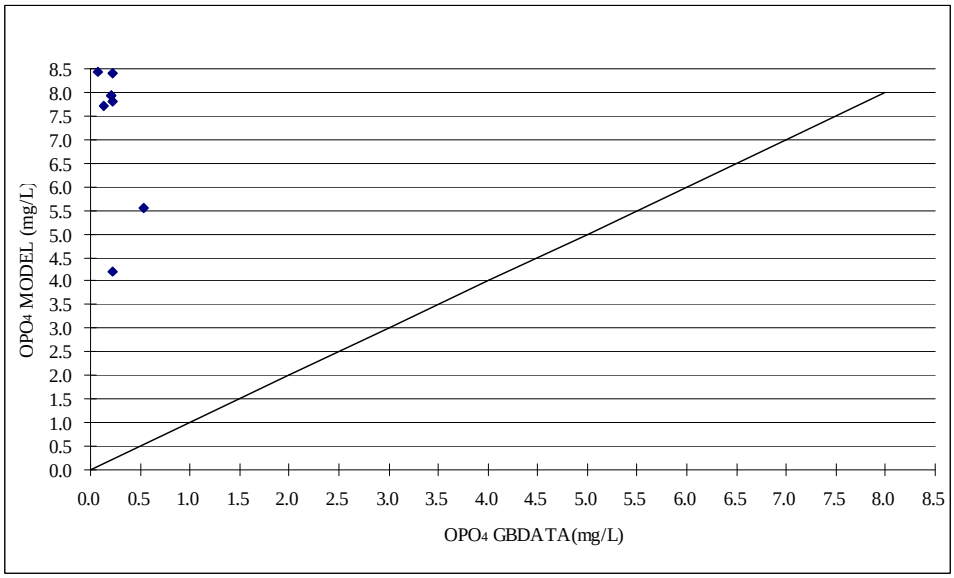

FIGURE 4.1.4: Comparison of measured and predicted OPO_4 concentration using default values of model kinetic parameter. Symbols lying on the 45^o line would indicate perfect agreement between modelled and observed values

4.1.5 NH_3 Modelling

Figure 4.5.1 presents a comparison of NH_3 values predicted by the model to the NH_3 values measured at the GBWWTP. Default values of the all the kinetic parameters were used during the first run of the calibration. It is evident from the figure that the model was underestimating the concentration as compared to the NH_3 concentration measured at the plant for most of the days. The mean square error calculated was 3.915

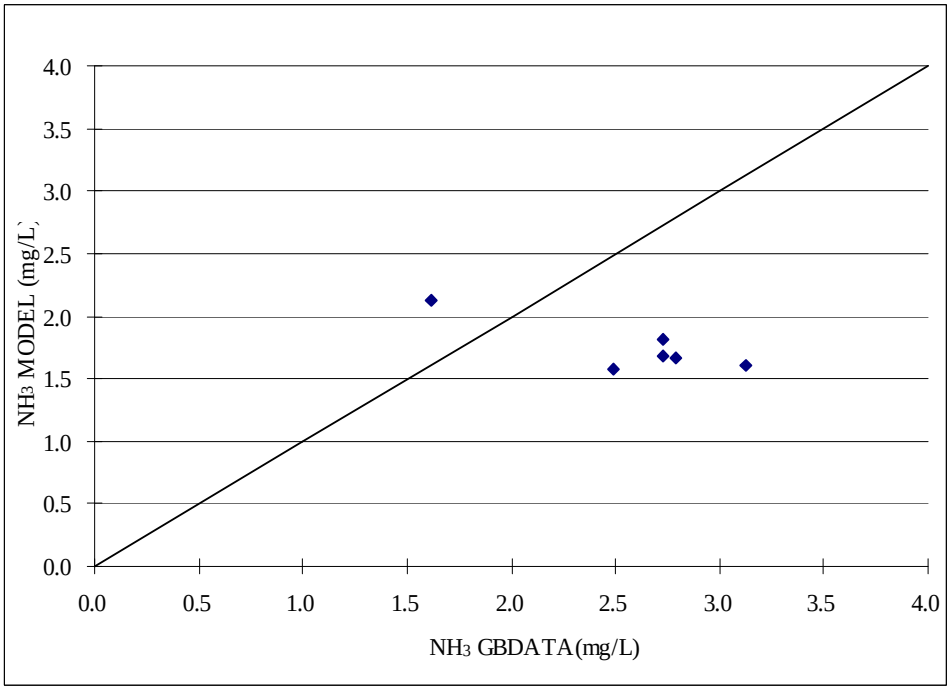

FIGURE 4.1.5: Comparison of measured and predicted NH_3 concentration using default values of model kinetic parameter. Symbols lying on the 45^o line would indicate perfect agreement between modelled and observed values

4.2 SENSITIVITY ANALYSIS

Sensitivity analysis is used to identify the degree of model output sensitivity to changes in input parameters. In this type of analysis the input variable value is sequentially increased then decreased by a certain percentage and the effect of these changes on the output variables is observed.

Sensitivity analysis was carried out on the kinetic parameters as indicated in Table 4.1. For all the parameters, 100% is the default value set in model. The default value was decreased by 50% initially and its effect on the output variables like CBOD, ammonia, TSS and orthophosphate was monitored and plotted in the graph as shown in Appendix 1. During the second run of the sensitivity analysis the default value was increased by a factor of 50% and the effect was observed on the same set of output variables. All sensitivity analysis results are shown graphically in Appendix 1.

Table 4.1: List of kinetic parameters calibrated after sensitivity analysis.
Default value = 100%, 50% = 50% reduction in the default value, 150% = 50% increase in the default value. *calibrated value = 100%, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value.

Name	**Units**	**Default (100%)**	**150%**	**50%**	**Calibrated Value(**Makinia [b] et al., 2006)	**150 %**	**50 %**
Hydrolysis rate constant (K_H)	d^{-1}	3	4.5	1.5	4		
Anoxic hydrolysis reduction factor (η_{NO3})	-	0.6	0.9	0.3	0.8		
Rate constant for storage of X_{PHA} (q_{PHA})	g X_{PHA} $g^{-1}X_{PAO}$ d^{-1}	3	4.5	1.5	10		
Rate constant for storage of X_{PP} (q_{PP})*	g X_{PP} $g^{-1}X_{PAO}$ d^{-1}	1.5	2.25	0.75	8	12	4
Rate of lysis for X_{PAO} (b_{PAO})	d^{-1}	0.2	0.3	0.1	0.14		
Rate of lysis for X_{PP} (b_{PP})	d^{-1}	0.2	0.3	0.1	0.14		
Rate of lysis for X_{PHA} (b_{PHA})	d^{-1}	0.2	0.3	0.1	0.14		
Saturation coefficient for growth on acetate (K_A)	g COD m^{-3}	4	6	2	1		
Inhibition coefficient for PP storage (K_{IPP})*	g X_{PP} $g^{-1}X_{PAO}$	0.02	0.03	0.01	0.3	0.45	0.15
Maximum growth rate of autotrophs- X_{AUT} (μ_{AUT})	d^{-1}	1	1.5	0.5	1.2		

It is evident from the sensitivity analysis that the model output was more sensitive to the following parameters:

1) Lysis of PAO: From the sensitivity analysis (Figure 4.2.1) it is evident that when the rate of lysis was increased from the default value, the orthophosphate concentration in effluent also increased and decreased with the subsequent decrease in the value of the kinetic parameter. So during model calibration the rate of lysis was decreased from a value of 0.2 d^{-1} (default value) to 0.14 d^{-1} (Makinia [b] et al., 2006) to improve the rate of orthophosphate removal.

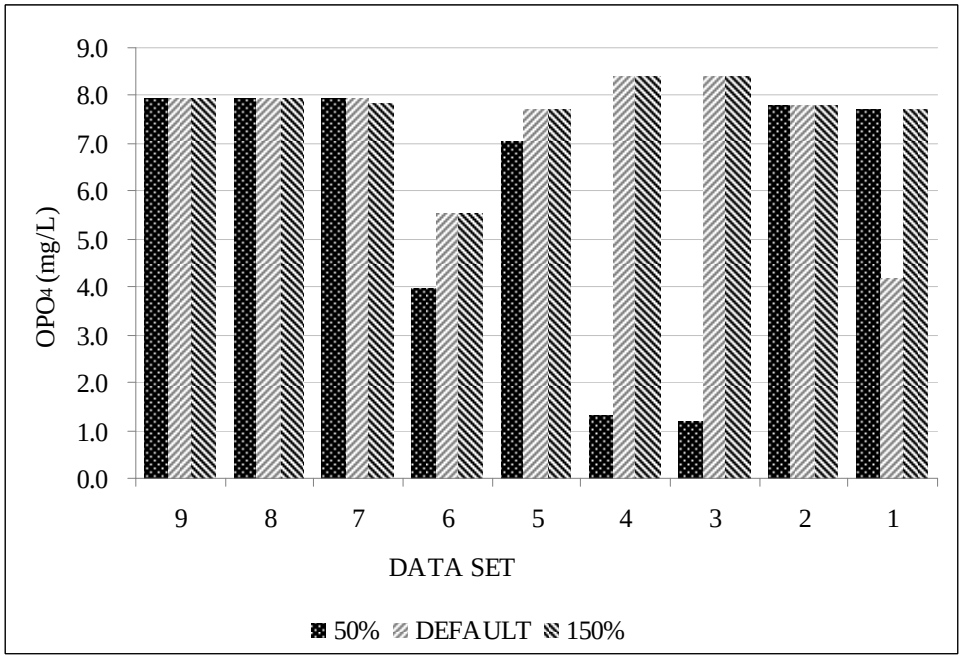

FIGURE 4.2.1: Effect of rate of lysis of PAO on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

2) Rate constant for storage of $X_{PHA:}$ From Figure 4.2.2 it can be clearly observed that the orthophosphate concentration in the effluent decreased

with the increase in the value of the rate constant. Based on this result it was decided to increase the value from 3 g X_{PHA} $g^{-1}X_{PAO}$ d^{-1} (default value) to 8 g X_{PHA} $g^{-1}X_{PAO}$ d^{-1} (Makinia [b] et al., 2006). Even though the calibrated value of 8 g X_{PHA} $g^{-1}X_{PAO}$ d^{-1} was outside the range of the sensitivity analysis values, the effect of X_{PHA} on the effluent OPO_4 concentration was evident within the range used.

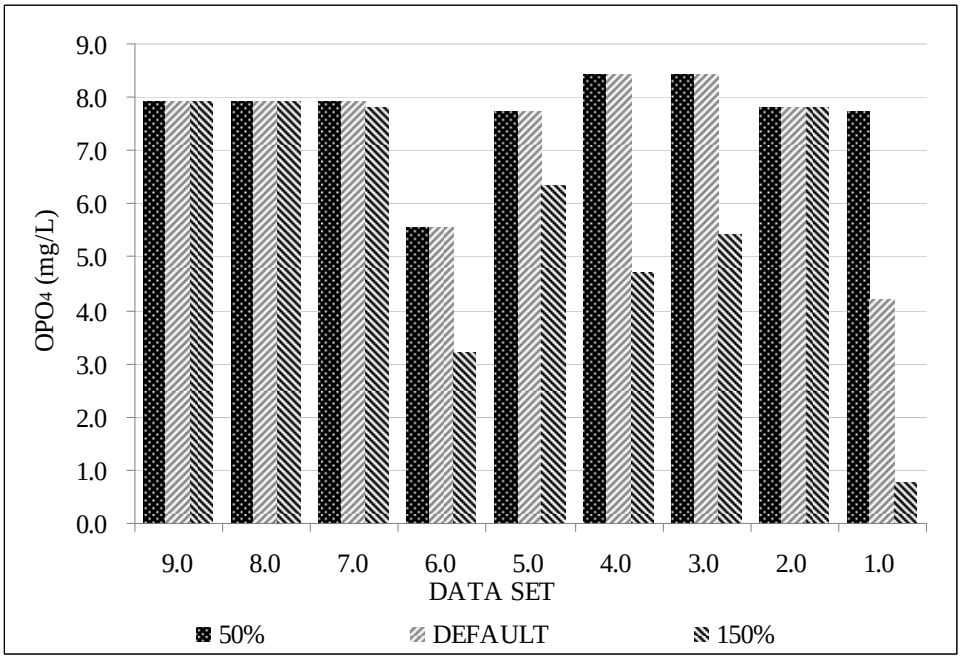

FIGURE 4.2.2: Effect of rate constant for storage of X_{PHA} on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

3) Saturation coefficient for growth on acetate for PAOs: From Figure 4.2.3 it is evident that orthophosphate concentration in the effluent decreased with the decrease in the value of the saturation coefficient. So the default value of 4 $gCODm^{-3}$ was decreased to 1 $gCODm^{-3}$ (Makinia [b] et al., 2006).

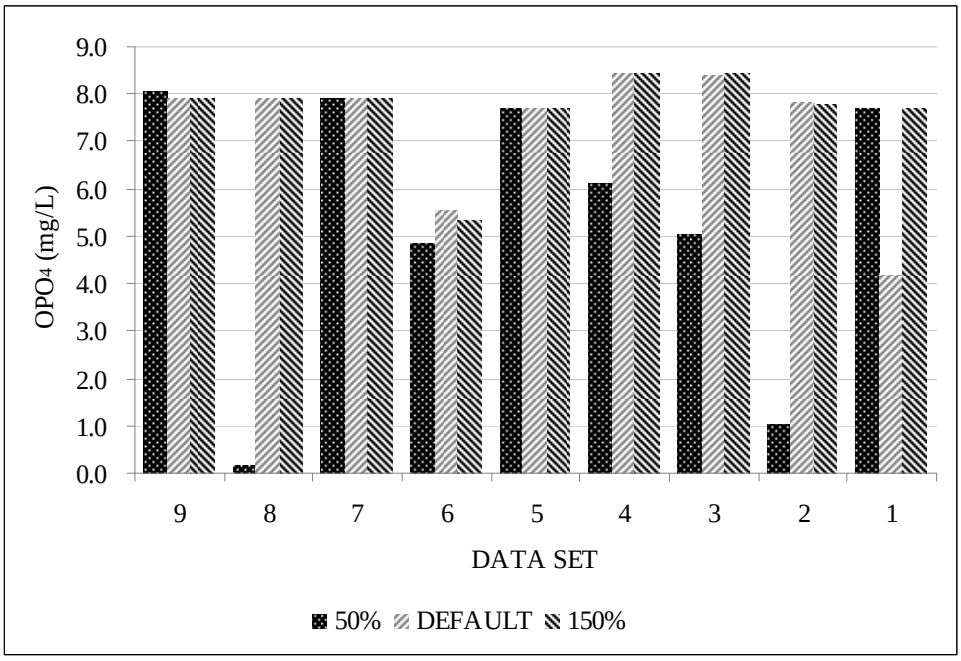

FIGURE 4.2.3: Effect of saturation coefficient for growth on acetate for PAOs on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

4) Autotrophic maximum growth rate: From Figure 4.2.4, it is evident that it is one of the most important parameter as it controls the growth of the aerobic autotrophs. Autotrophs are generally slow growing and face competition from the heterotrophs and PAOs for CBOD. Sensitivity analysis indicates that when their growth rate was reduced by 50% of the default value there was almost no nitrogen removal (because of lack of nitrification). On increasing the value 50% from the default value significant nitrogen removal was observed. So during calibration the default value of 1 d^{-1} was increased to 1.2 d^{-1} (Makinia [b] et al., 2006).

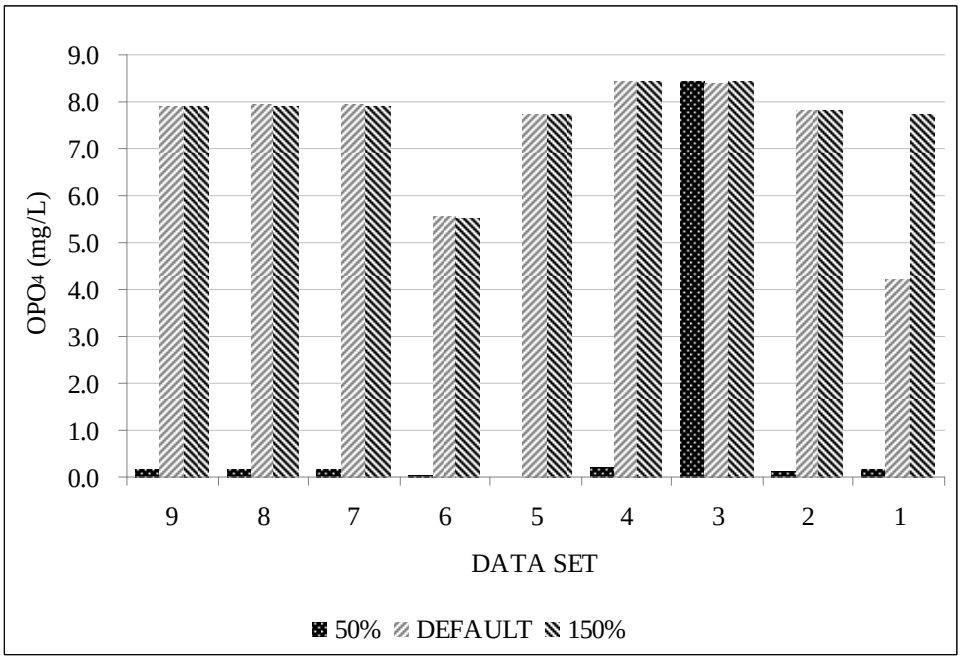

FIGURE 4.2.4: Effect of maximum growth rate of autotrophs on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

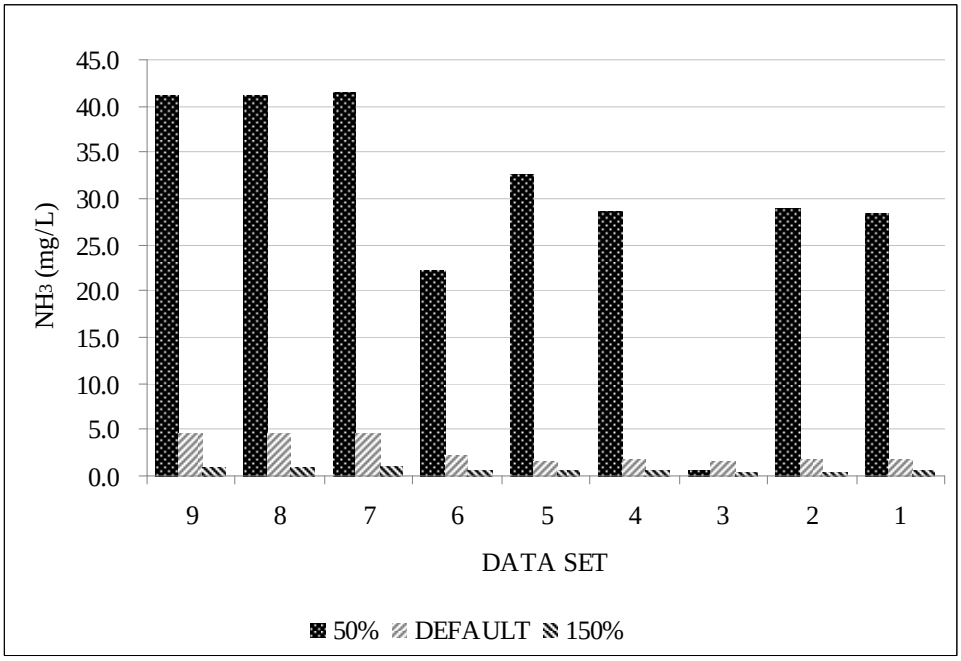

FIGURE 4.2.5: Effect of autotrophic maximum growth rate on the effluent NH_3 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

The effect was also observed in the effluent nitrate concentration (graph attached in Appendix 1) which was zero when the growth rate was reduced by 50 % of the default value. The effect was also observed in the effluent nitrate concentration which was almost zero (Figure 1.C.18, Appendix 1) indicating that there was no nitrification and denitrification.

The other variables that were calibrated include hydrolysis rate constant, anoxic hydrolysis reduction factor, rate constant for storage of X_{PP}, lysis rate of X_{PP} and X_{PHA}, and inhibition coefficient for PP storage did not have an independent impact during the sensitivity analysis on the model output. However the combined effect of all the kinetic parameters had improved the overall prediction of the model in terms of CBOD, OPO_4 and NH_3 concentrations. A final run to study the combined effect of the kinetic parameters was carried out by using default values for those parameters whose impact was not observed through the sensitivity analysis and the results are presented in the Appendix 1 (Figures 1.D.1- 1.D.5). It was evident that in the absence of calibration of these parameters model prediction results were poor.

4.3 MODEL CALIBRATION

Selected model parameters were calibrated to values available in the literature (Makinia [b] et al., 2006) based on the results of the sensitivity analysis.

4.3.1 CBOD modelling

Figure 4.3.1 presents a comparison of the CBOD values predicted by the model to the CBOD values measured at GBWWTP. Kinetic parameters used were modified (Table 4.2) as explained in section 4.2, to improve the fit during the second run of calibration. It is evident from the figure that the model was overestimating the CBOD. However the mean square error after model calibration had decreased to 0.936.

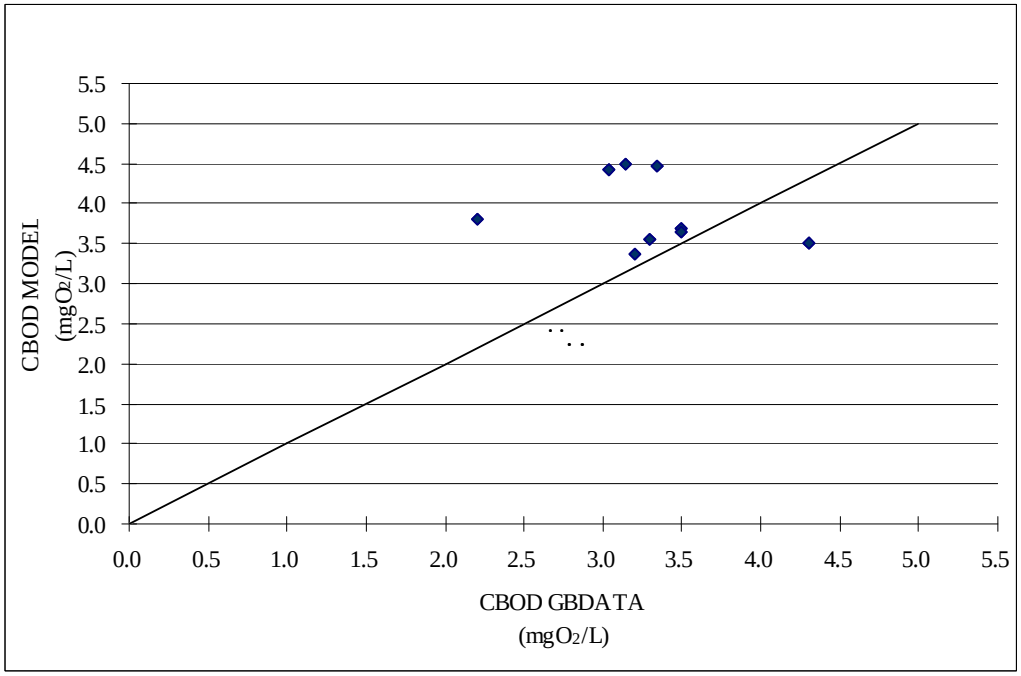

FIGURE 4.3.1: **Comparison of measured and predicted CBOD concentration using calibrated values of model kinetic parameter. Symbols lying on the 45^{o} line would indicate perfect agreement between modelled and observed values.**

4.3.2 NTOX Modelling

Figure 4.3.2 presents a comparison of the NTOX values predicted by the model to the NTOX values measured at the GBWWTP. Kinetic parameters used were modified (Table 4.2) to improve the fit during the second run of the calibration. It is evident from the figure that the model was underestimating the NTOX concentration as compared to the actual NTOX concentration measured at the plant. However the mean square error after model calibration had reduced to 13.941.

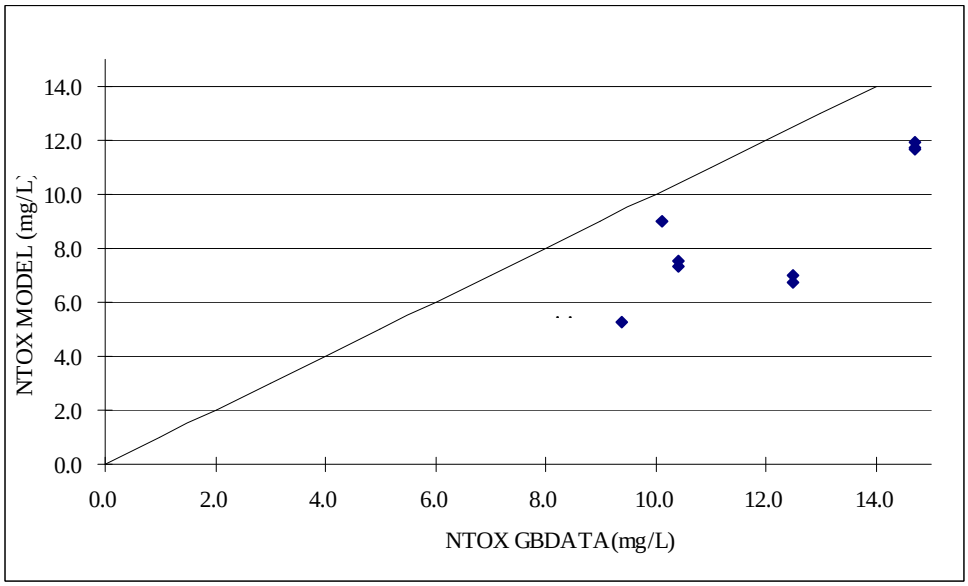

FIGURE 4.3.2: Comparison of measured and predicted NTOX concentration using calibrated values of model kinetic parameter. Symbols lying on the 45^{o} line would indicate perfect agreement between modelled and observed values

4.3.3 TSS Modelling

Figure 4.3.3 presents a comparison of TSS values predicted by the model to the TSS values measured at the GBWWTP. Kinetic parameters used were modified (Table 4.2) to improve the fit during the second run of the calibration. It is evident from the figure that calibration had very little impact on the effluent TSS concentration and the model continued to overestimate the TSS concentration as compared to the TSS concentration measured at the plant. The mean square error was 15.66.

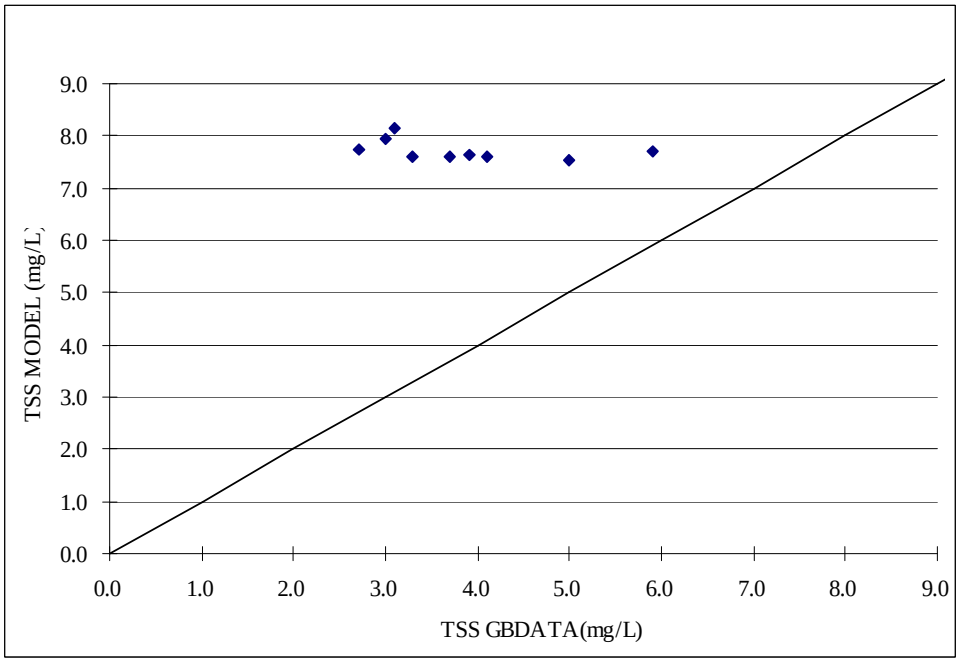

FIGURE 4.3.3: Comparison of measured and predicted TSS concentration using calibrated values of model kinetic parameter. Symbols lying on the 45^{o} line would indicate perfect agreement between modelled and observed values.

4.3.4 OPO_4 Modelling

Figure 4.3.4 presents a comparison of OPO_4 values predicted by the model to the OPO_4 values measured at the GBWWTP. Kinetic parameters used were modified (Table 4.2) to improve the fit during the second run of the calibration. It is evident from the figure that the model was overestimating the concentration as compared to the actual OPO_4 concentration measured at the plant for most of the days. However the mean square error had reduced considerably to 0.1803 due to model calibration.

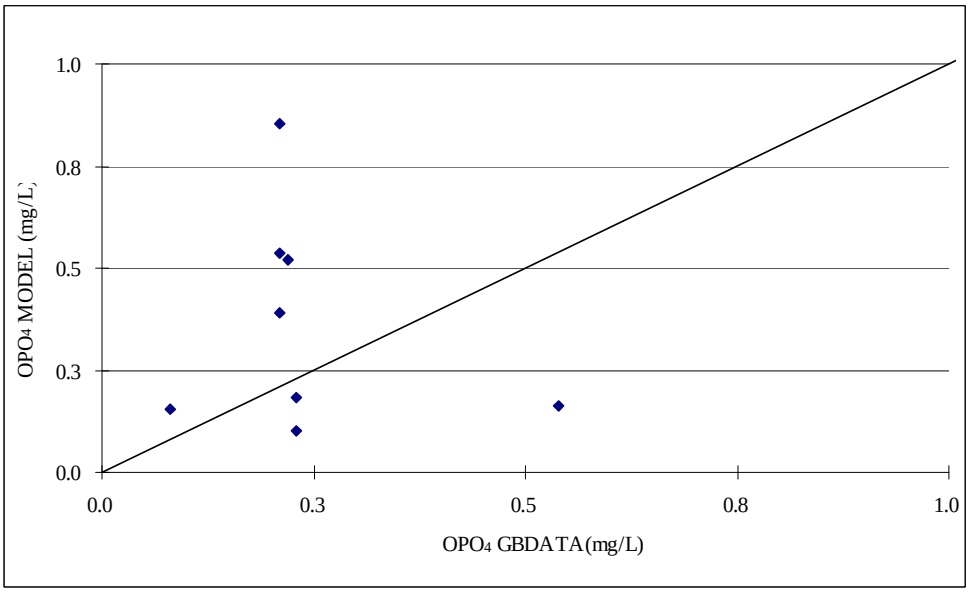

FIGURE 4.3.4: Comparison of measured and predicted OPO_4 concentration using calibrated values of model kinetic parameter. Symbols lying on the 45^o line would indicate perfect agreement between modelled and observed values.

4.3.5 NH_3 Modelling

Figure 4.3.5 presents a comparison of NH_3 values predicted by the model to the NH_3 values measured at the GBWWTP. Kinetic parameters used were modified (Table 4.2) to improve the fit during the second run of the calibration. It is evident from the figure that the model was underestimating the concentration as compared to the NH_3 concentration measured at the plant for most of the days and overestimating for three days. However the mean square error had reduced to 1.95 after calibration.

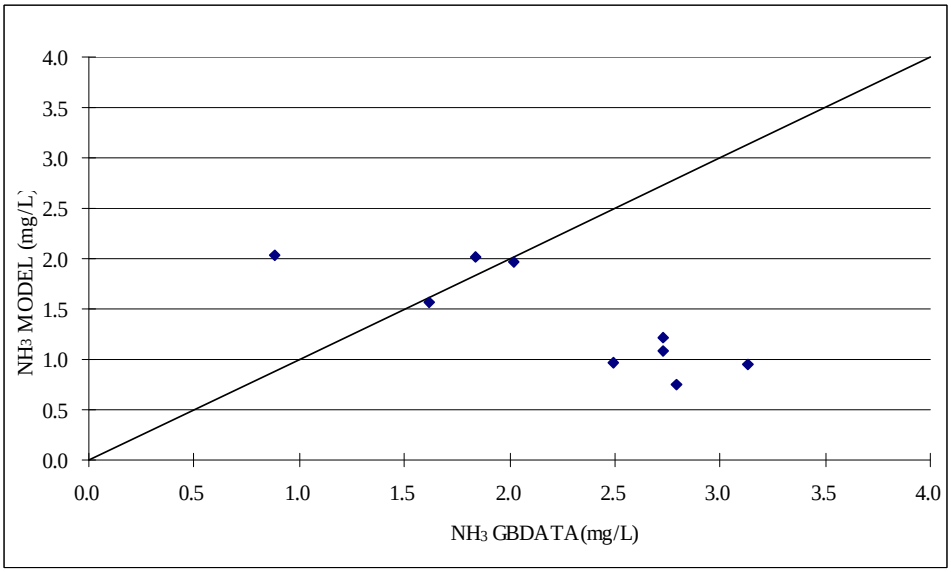

FIGURE 4.3.5: Comparison of measured and predicted NH_3 concentration using calibrated value of model kinetic parameter. Symbols lying on the 45^o line would indicate perfect agreement between modelled and observed values.

4.4 DISCUSSION

From most of the graphs in sections 4.1 and 4.3, it is evident that model was either overestimating or underestimating the concentration of all the parameters when compared to the actual data collected from the plant. The main reason for an inaccurate calibration (from the mean square error) could be attributed to wastewater characterization. Characterization of the influent waste stream is an essential step that affects the quality of any modelling process. The COD fraction especially the biodegradable and inert fractions have to be estimated using various analytical methods as this greatly affects the performance of any wastewater treatment system. The basic theory behind a BNR system is that a group of microorganisms use the biodegradable fraction in the input stream as a substrate and the nutrients like nitrogen and phosphorus for their growth and maintenance.

The scope of the project was to use historic data available at the plant for calibration purposes. However during the course of modelling it was identified that the wastewater characteristics was an important part of the input to the model. In the absence of experimental data, characterization of the wastewater was attempted using the influent advisor module of the GPS-[X] software and successful characterization based on a trial and error approach was possible for nine days during the months of November, January and February. Lack of experimental data for accurate influent characterization could be one of the major contributing factors to the inaccuracy in the calibration of the model. The soluble fraction of total COD and the inert fraction of

soluble COD were modified based on a trial and error approach as shown in Table 1.B.1 in Appendix 1. The VSS/ TSS ratio was calculated from plant historic data. For the other stoichiometric coefficients, default values were used as shown in Table 1.B.2 in Appendix 1.

CBOD removal: From Figures 4.1.1 and 4.3.1 it is evident that the model was predicting higher CBOD concentration, with reduced error (mean square error reduced from 1.728 to 0.9361) after calibration. As discussed, the main reason could be due to the errors in the influent wastewater characterization. This is evident from the differences in the influent CBOD concentrations measured at the plant and calculated by the model based on the influent COD values, shown in Table 4.2. Figure 1.E.1 attached in Appendix 1 gives a comparison of the effluent CBOD concentration measured at the plant to the effluent concentration predicted by the model before (using default values of kinetic constants) and after calibration.

Table 4.2: CBOD concentration of primary effluent measured at the plant and predicted by the model.

DATA SET	INFLUENT CBOD MEASURED AT PLANT (mgO_2/l)	INFLUENT CBOD PREDICTED BY MODEL(mgO_2/l)
1	142	203.4
2	170	220.2
3	149	201.5
4	164	205.9
5	140	188.8
6	136	163.6
7	192	226.7
8	206	219.2
9	190	224.2

Nitrogen removal: Nitrogen removal is a two step process of nitrification under aerobic conditions followed by denitrification under anoxic conditions. It is evident from the Figures 4.1.2 and 4.3.2 that the nitrate concentration was underestimated by the model even after calibration. The main reason could be that in GBWWTP the BNR design is such that the influent stream rich in biodegradable organics comes in contact with the anoxic zone first followed by the anaerobic zone where the heterotrophs and the PAOs respectively, consume most of the CBOD. These organisms especially the heterotrophs are fast growing and compete with the relatively slow growing autotrophs. For ASM2d, the default growth rates for heterotrophs, autotrophs and PAOs are 6 d^{-1}, 1 d^{-1} and 1 d^{-1}, respectively. This clearly explains that the rate of denitrification occurring at the plant was less when compared to the rate predicted by the model resulting in the underestimation of NTOX concentration. To compensate for this and to improve nitrification the autotrophic growth rate was increased from the default value to the value reported in Makinia [b] et al. (2006). From Figures 4.1.5 and 4.3.5 it is evident that after calibration, the mean square error in predicting ammonia removal had reduced from 3.915 to 1.95. Influence of autotrophic growth rate can be seen from the results of sensitivity analysis, Figures 1.C.16-1.C.17 in Appendix 1.

Phosphorus removal: Orthophosphate removal is achieved by group of organisms called PAOs. These organisms are slow growing and face competition for biodegradable organics from the heterotrophs. So VFA‘s are supplemented externally. From Figures 4.1.4 and 4.3.4 it is evident that the model is underestimating

orthophosphate removal. Using default value for the kinetic parameters there was little or no removal owing to the high competition from the heterotrophs. To compensate for this kinetic parameters like: rate constant for storage of X_{PHA} , rate constant for storage of X_{PP}, rate of lysis for X_{PAO}, rate of lysis for X_{PP}, rate of lysis for X_{PHA}, saturation coefficient for growth on acetate, inhibition coefficient for PP storage was calibrated (as shown in the Table 4.2). After calibration there was a significant improvement in the removal as the mean square error had reduced from 52.42 to 0.1803. Results of sensitivity analysis for the above mentioned parameters are shown in Appendix 1.

Another reason for the noted discrepancy could be that the soluble orthophosphate concentration which is an important input parameter to the model is not measured for the primary effluent from the clarifier at the plant. A default value of (90% of total phosphate) as suggested by the influent advisor tool of the GPS-[X] software was used. Although OPO_4 was measured during the first sampling program, it was not used for modelling purposes because it was not reliable to make an estimate based on limited data (one sampling campaign).

Total Suspended Solids removal: From Figures 4.1.3 and 4.3.3 it is evident that the model was overestimating the value of TSS. Calibration did not seem to have a great impact on the TSS value. This could be because the main objective of the project was to calibrate a model for the BNR system. So information required to model the secondary clarifier where the settling and removal of total suspended solids occurs was not collected. To improve TSS calibration, sampling at of the secondary clarifier

is recommended.

Other major observations:

1. All the kinetic constants calibrated were based on literature. After sensitivity analysis if lab experiments are carried out to determine the values of the most important parameters (discussed under sensitivity analysis section) then a more accurate calibration could be achieved.
2. The data collected at the plant are the combined post disinfection final effluent, from all the secondary clarifiers and was compared to the model output from the secondary clarifier specific to the BNR modelled. This could be the other reason for the observed discrepancies between the models predicted and observed value at the plant.
3. Differences were also seen in the SRT calculated using plant data and the SRT predicted by the model as shown in Figure 1.E.6 in Appendix 1. A reason for this difference could be attributed to the fact that the SRT was calculated using MLSS concentration monitored at the end of pass 4 of the BNR system at the plant. However SRT is predicted by the model from the MLSS concentration observed at the end of each pass of the modelled BNR system.
4. Parameter values adopted from the literature were evaluated at 19.6^{o}C and validated for a temperature of 14.1^{o}C (Makinia[b] et al., 2006). The effluent temperature measured at Gold bar was within the range of 14 to 17^{o}C. However to improve the overall prediction capabilities and reliability of the model it is important to study the temperature sensitivity of the kinetic parameters. Due to

limited time frame and scope of the project, the effect of temperature on the kinetic parameters was not included in the modelling.

CHAPTER 5

5.0 CONCLUSIONS:

An attempt was made to calibrate a steady state model to predict final effluent water quality at GBWWTP. Historic data collected from the plant supplemented by information from the literature were used to calibrate the ASM2d model using the Hydromatis GPS-[X] software. ASM2d was chosen to model the entire BNR process (nitrogen and phosphorus removal) occurring at the plant. Several observations were made during the course of model calibration:

- A complete characterization of the wastewater (primary effluent from the clarifier) is very important to determine the biodegradable organic fractions required for the BNR process. Characterizing wastewater to monitor seasonal variations would be ideal especially for modelling BNR process.
- Trial and error approach for characterizing wastewater during the months of November, January and February was used in the absence of experimental data. Since the differences in the wastewater characteristics observed was minimal during these months seasonal characterization maybe sufficient (Table 1.B.1 in Appendix 1).
- Only the soluble fraction of total COD and inert fraction of soluble COD were modified from the default value used in the influent advisor module.
- Difference was observed in the CBOD of the influent (primary effluent from the primary clarifier) calculated by the model and the actual value measured at the

plant indicating discrepancies in the influent wastewater characterization (Table 4.1).

- Exact orthophosphate concentration of the primary effluent at the plant was unknown as this parameter is not measured for the primary effluent at the plant.
- The nitrate and nitrites and dinitrogen concentration of the primary effluent were assumed to be 0.03 and 0.00 gN/m^{-3} respectively.
- The most important parameters recognized and calibrated after sensitivity analysis include: hydrolysis rate constant (K_H), anoxic hydrolysis reduction factor (η_{NO3}), rate constant for storage of X_{PHA} (q_{PHA}), rate constant for storage of X_{PP} (q_{PP}),rate of lysis for X_{PAO} (b_{PAO}), rate of lysis for X_{PP} (b_{PP}), rate of lysis for X_{PHA} (b_{PHA}), saturation coefficient for growth on acetate (K_A), inhibition coefficient for PP storage (K_{IPP}), maximum growth rate of X_{AUT} (μ_{AUT}). Laboratory experiments to determine the value for these constants can be conducted for a more accurate calibration.
- Calibration results indicate that the CBOD concentration in the final effluent was overestimated for all days by the model. However the mean square error in prediction had reduced from 1.728 to 0.936 after calibration.
- Ammonia removal was overestimated for most days except for two days when a higher concentration than observed at the plant was predicted. Similarly nitrate and nitrite concentration predicted by the model after calibration is lower than the concentration observed at the plant.
- The TSS concentration did not seem to vary much even after calibration and was

overestimated for all days. A separate modelling of the secondary clarifier would be required for accurate calibration.

- The mean square error in the prediction of orthophosphate concentration has reduced considerably after calibration from 52.42 to 0.1803 although the concentration predicted for most of the days was higher than the actual concentration observed at the plant.
- Competition for CBOD between the fast growing heterotrophs, and the relatively slow growing PAOs was clearly seen. Hence, a higher rate of denitrification and lower rate of phosphorus removal was predicted than observed at the plant.
- The mean square error for nitrate removal was reduced from 29.302 to 13.941. More accurate calibration of the denitrification process is required to improve the overall prediction capabilities of the model.
- Difference in the SRT predicted by the model and calculated using plant MLSS data was also observed (Figure 1.E.6, Appendix 1).
- Values predicted by the model were for the effluent from the secondary clarifier specific to the BNR system being modelled and this was compared to the final effluent (combined effluent from all the clarifiers) data collected at the plant which could add to the differences observed between the measured and predicted values.

5.1 RECOMMENDATIONS

A well calibrated steady state model can be used to study the outcome of operational changes under different scenario. One of the important requirements of a reliable model is good wastewater characterization. So an important recommendation is to perform laboratory experiments to determine the COD fractions of the influent. The COD fractions would include: readily biodegradable COD (S_F), volatile fatty acids (S_A), inert soluble COD (S_I), heterotrophic biomass fraction (X_H), autotrophic biomass fraction (X_{AUT}), phosphorus accumulating biomass fraction (X_{PAO}), inert particulate COD (X_I) and slowly biodegradable particulate COD (X_S) (Roeleveld.et al., 2002 and Garcı´a-Usach et al., 2006). Since a there is a difference in the influent BOD calculated by the model and measured at the plant it is recommended to measure the BOD_5 to UBOD ratio.

Seasonal characterization of the primary effluent may be sufficient to model BNR system, as differences in the wastewater characteristics observed during the months of November, January and February (trial and error approach for characterization was used) were minimal. Seasonal characterization is also important to study the temperature sensitivity of kinetic parameters.

From the sensitivity analysis, around ten kinetic parameters were identified to have an impact on the model output. The most important ones of these are: rate of lysis of PAO (b_{PAO}), rate constant for storage of X_{PHA} (q_{PHA}), maximum growth rate of X_{AUT} (μ_{AUT}), and saturation coefficient for growth on acetate (K_A). Respirometric

measurements can be used to estimate the value of these constants.

Apart from using historic data from the plant, 24-hour composite samples can be collected from the end of primary clarifier, end of preanoxic, anoxic, anaerobic and aerobic zone and the effluent from the secondary clarifier. Samples collected at the end of primary and secondary clarifiers can be analysed for: total COD, total TKN, total phosphorus, DO, soluble OPO_4, free and ionized ammonia, nitrite and nitrates, dinitrogen, alkalinity, TSS and VSS. Nitrates and nitrites, ammonia, alkalinity and orthophosphates at the end of each zone can be analysed to characterize activated sludge. For SRT calculation MLSS at end of each zone and RAS can be measured.

Temperature sensitivity of the kinetic parameters has to be studied to improve the overall prediction capabilities of the model. This can be done by including temperature correction factors in the modelling process.

Characterization of effluent from the secondary clarifier is necessary because at present no historic data are available. Only the final combined effluent from the clarifiers post disinfection is sampled and analysed at the plant.

The above recommendations are based on the requirements to calibrate ASM2d steady state model using GPS-[X] software.

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APPENDIX 1:

1.A Physical dimensions of the bioreactor at GBWWTP:

CELL NUMBER	LENGTH (m)	WIDTH (m)	DEPTH (m)
1	18.50	6.17	4.6
2	23.00	6.17	4.6
3	56.02	6.17	4.6
4	97.52	6.17	4.6
5	48.76	6.17	4.6
6	48.76	6.17	4.6
7	48.76	6.17	4.6
8	48.76	6.17	4.6

1. B. WASTERWATER CHARACTERIZATION USING INFLUENT ADVISOR

TABLE 1.B.1: Wastewater characterization using influent advisor module of GPS-[X]

Data Set	COD (mg/L)	TKN (mg/L)	TP (mg/L)	OPO_4 (mg/L)	NH_3 (mg/L)	TSS (mg/L)	VSS (mg/L)	VSS/TSS	Soluble fraction of TCOD	Inert fraction sCOD
1	327	33.7	8.46	7.614	24	96	80	0.833	0.31	0.03
2	354	33.7	8.46	7.614	24	128	102	0.797	0.31	0.03
3	324	35.7	9.16	8.244	25	107	82	0.766	0.31	0.03
4	331	35.7	9.16	8.244	24	98	82	0.837	0.31	0.03
5	303	38.6	8.56	7.704	28	108	88	0.815	0.35	0.03
6	263	24.4	6.15	5.535	19	100	80	0.8	0.31	0.03
7	363	51.1	9.49	8.541	38	98	84	0.857	0.41	0.03
8	351	51.1	9.49	8.541	38	110	94	0.855	0.41	0.03
9	359	51.1	9.49	8.541	38	94	78	0.83	0.41	0.03

TABLE 1.B.2: Default values of influent stoichiometric coefficients used in GPS-[X].

S.NO	PARAMETER	DEFAULT VALUE
1	VFA fraction of sCOD	0.00
2	Substrate fraction of pCOD	0.75
3	Unbiodegradable fraction of pCOD	0.00
4	Heterotrophic biomass fraction of pCOD	0.18
5	Autotrophic biomass fraction of pCOD	0.00
6	PAO biomass fraction of pCOD	0.00
7	PolyP fraction of pCOD	0.00
8	PHA fraction of pCOD	0.00
9	Stored fraction of pCOD	0.00
10	Glycogen fraction of pCOD	0.00
11	OPO_4 fraction of soluble phosphorus	0.90
12	X_{PP} fraction of particulate phosphorus	0.00
13	X_{PPr} fraction of particulate phosphorus	0.00
14	Ammonium fraction of soluble fraction	0.90
15	Inert fraction of soluble TKN	0.00
16	Metal- hydroxide fraction of inorganic suspended solids	0.00
17	Metal- phosphate fraction of inorganic suspended solids	0.00
18	XCOD/VSS ratio	1.50
19	BOD_5/UBOD ratio	0.66

1. C. RESULTS OF SENSITIVITY ANALYSIS:

1) Lysis of PAO (b_{PAO}):

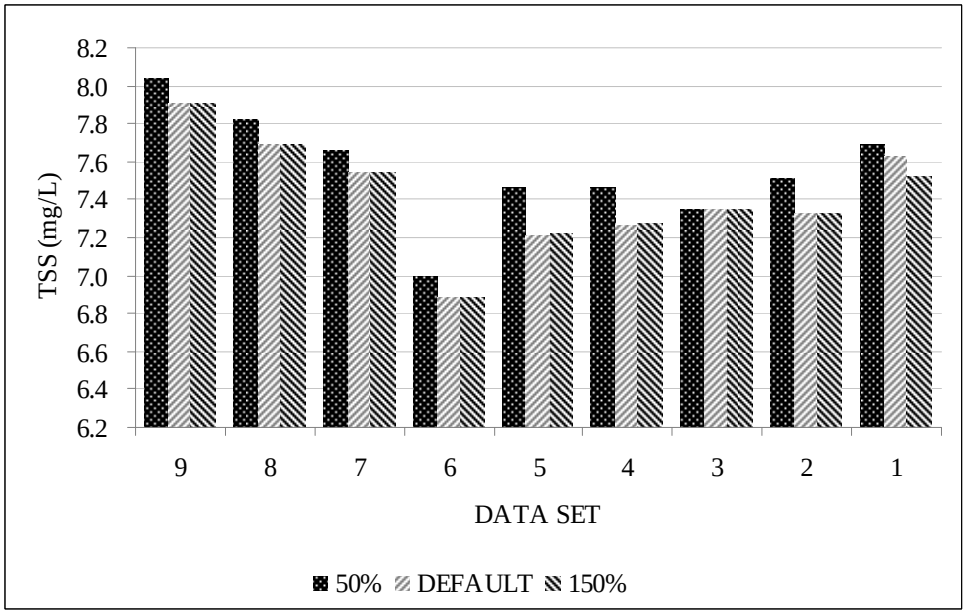

FIGURE 1.C.1: Effect of lysis of PAO on the effluent TSS concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

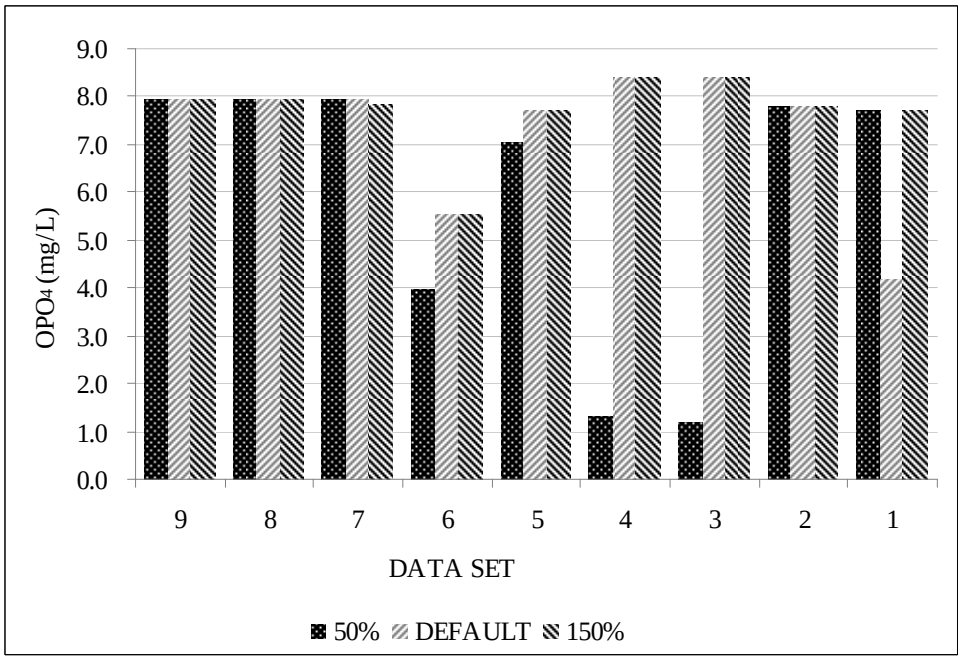

FIGURE 1.C.2: Effect of lysis of PAO on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

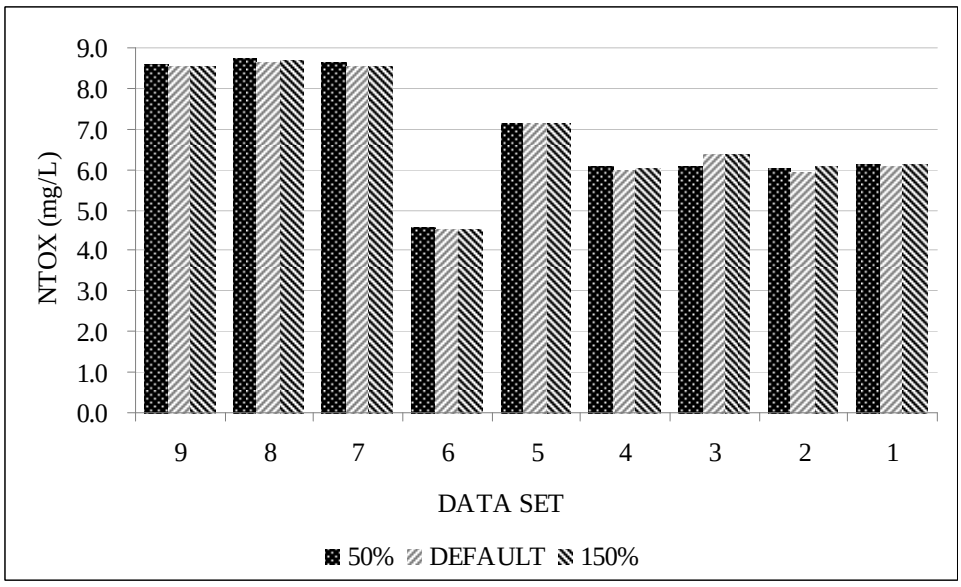

FIGURE 1.C.3: Effect of lysis of PAO on the effluent NTOX concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

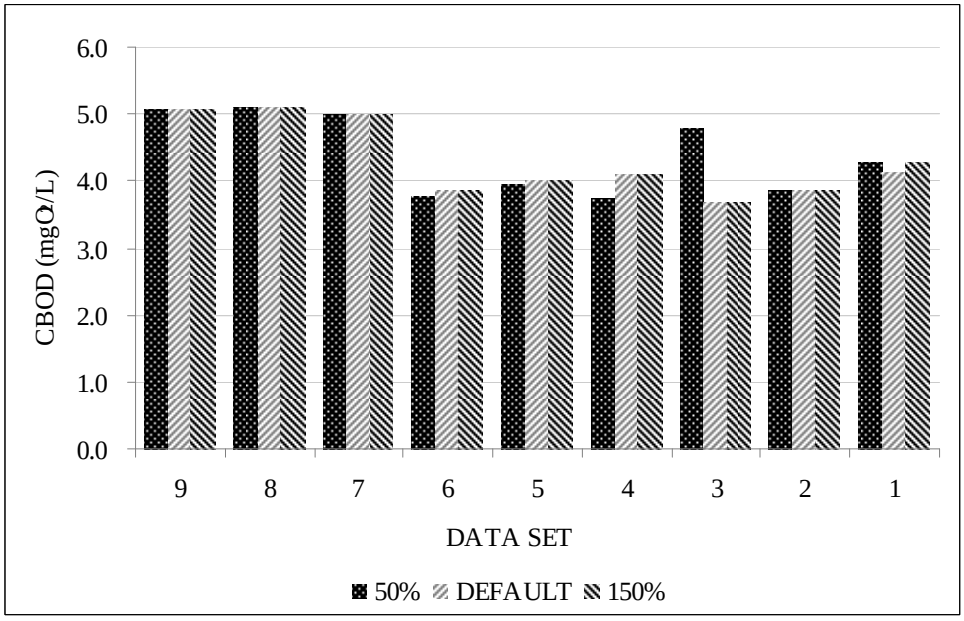

FIGURE 1.C.4: Effect of lysis of PAO on the effluent CBOD concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

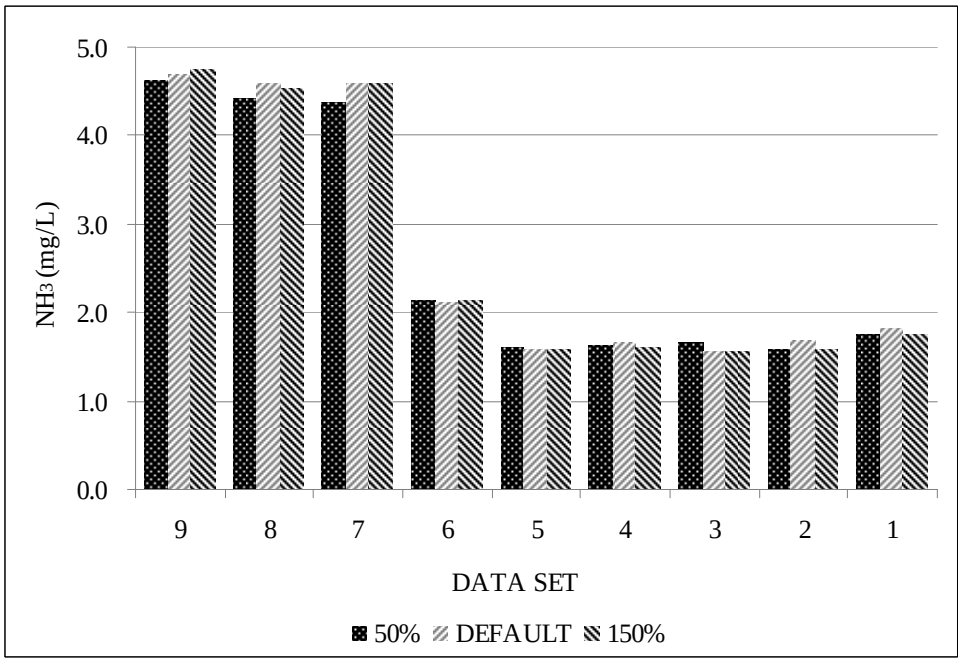

FIGURE 1.C.5: Effect of lysis of PAO on the effluent NH_3 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

2) Rate constant for storage of X_{PHA} (q_{PHA}):

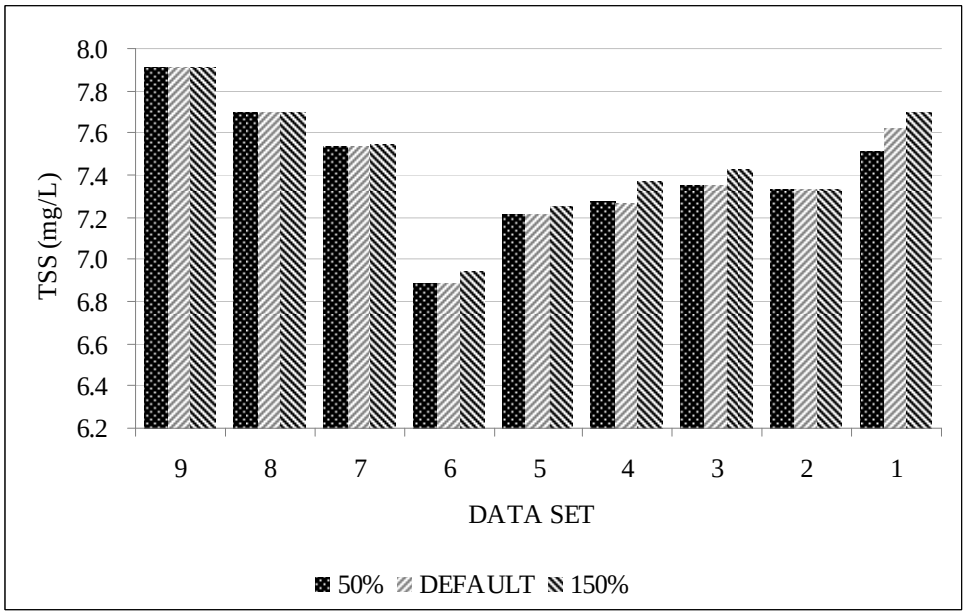

FIGURE 1.C.6: Effect of rate constant for storage of X_{PHA} on the effluent TSS concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

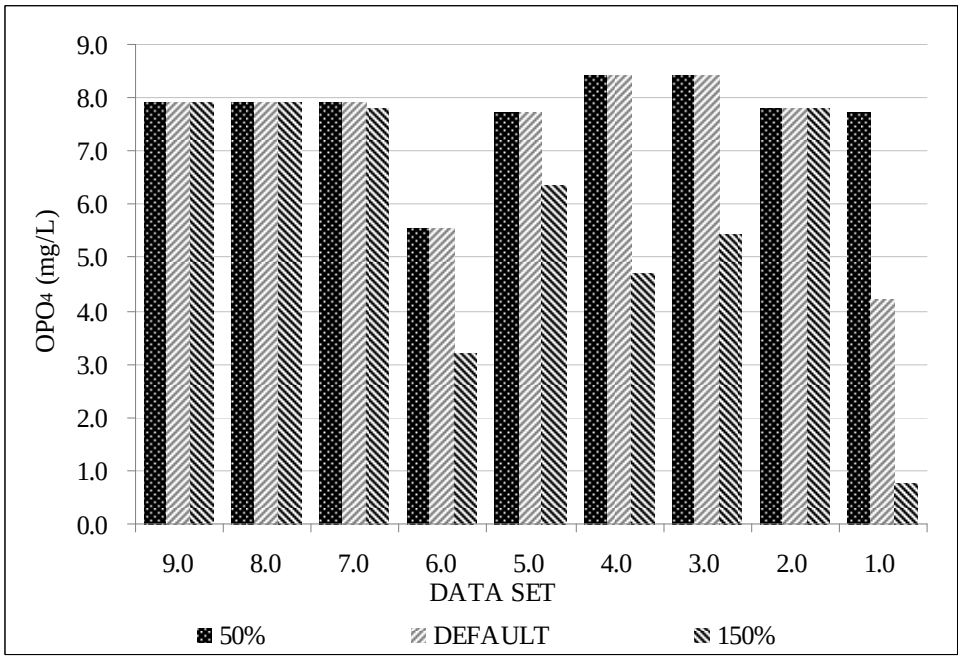

FIGURE 1.C.7: Effect of rate constant for storage of X_{PHA} on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

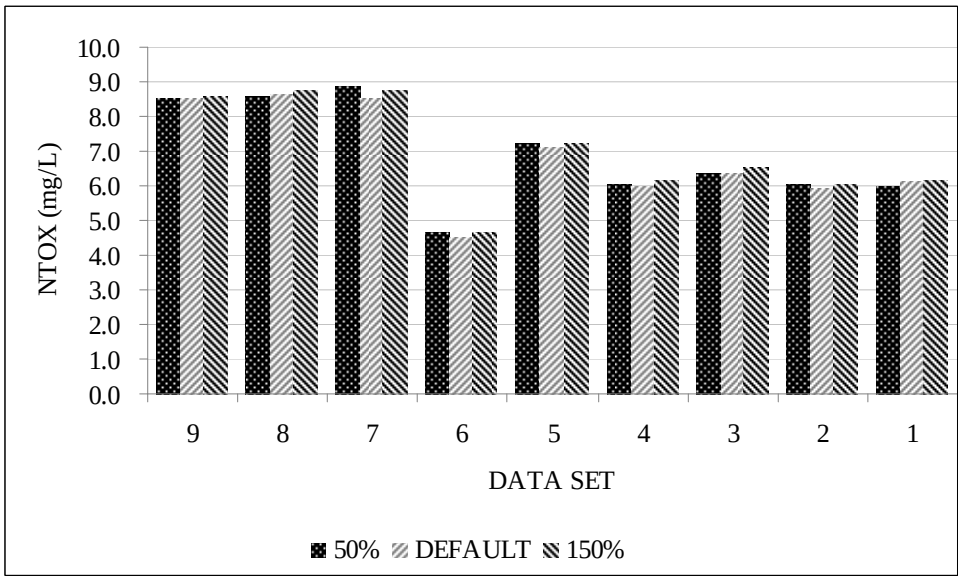

FIGURE 1.C.8: Effect of rate constant for storage OF X_{PHA} on the effluent NTOX concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

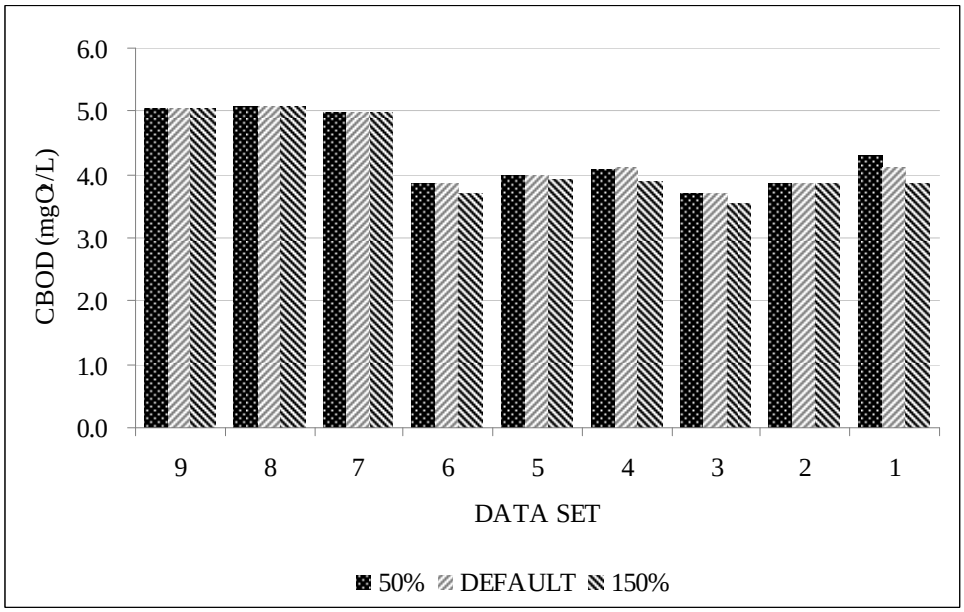

FIGURE 1.C.9: Effect of rate constant for storage of X_{PHA} on the effluent CBOD concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

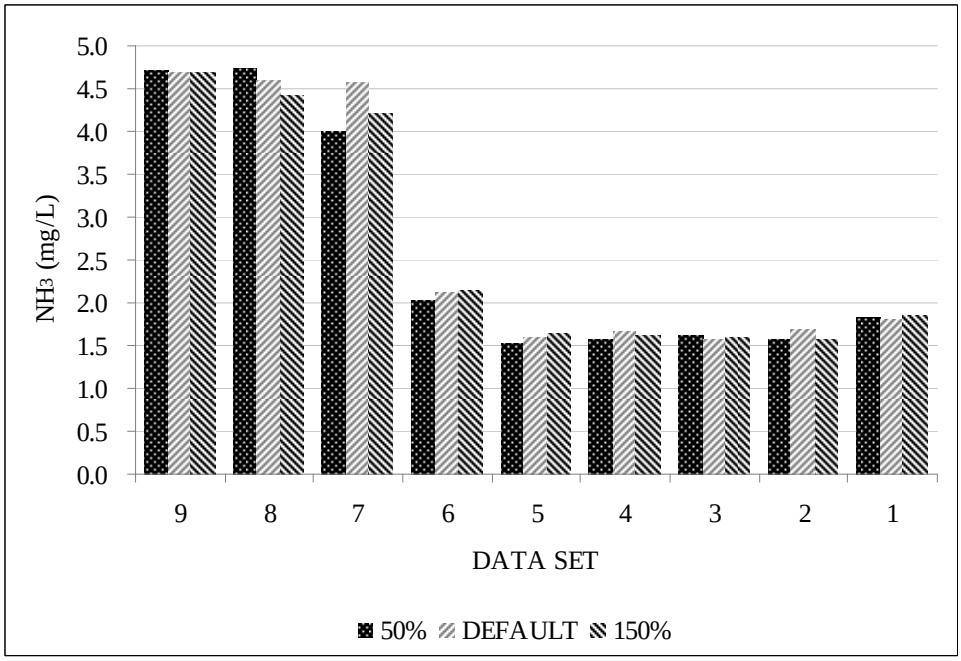

FIGURE 1.C.10: Effect of rate constant for storage of X_{PHA} on the effluent NH_3 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

3) Saturation coefficient for growth on acetate (K_A):

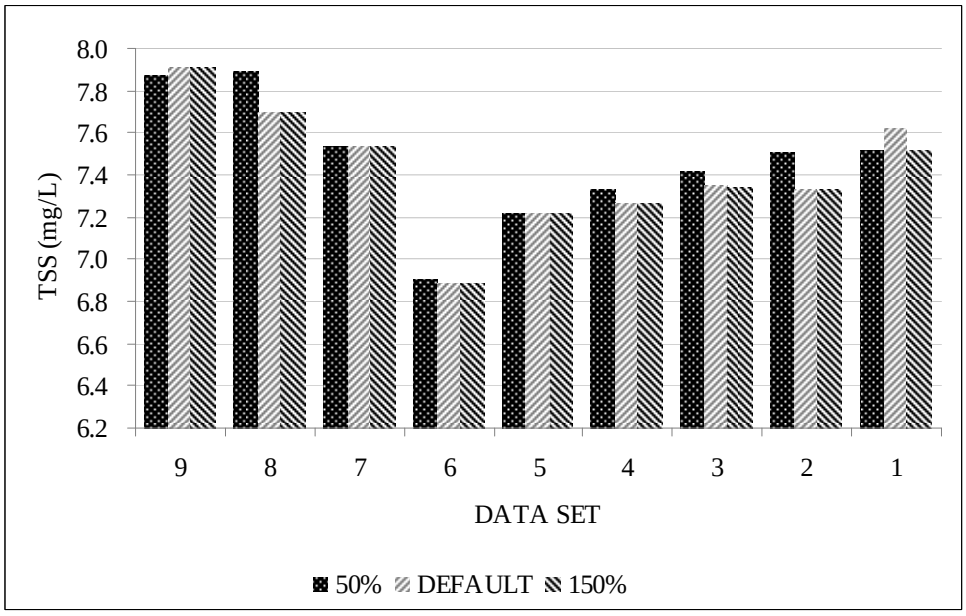

FIGURE 1.C.11: Effect of saturation coefficient for growth on acetate on the effluent TSS concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

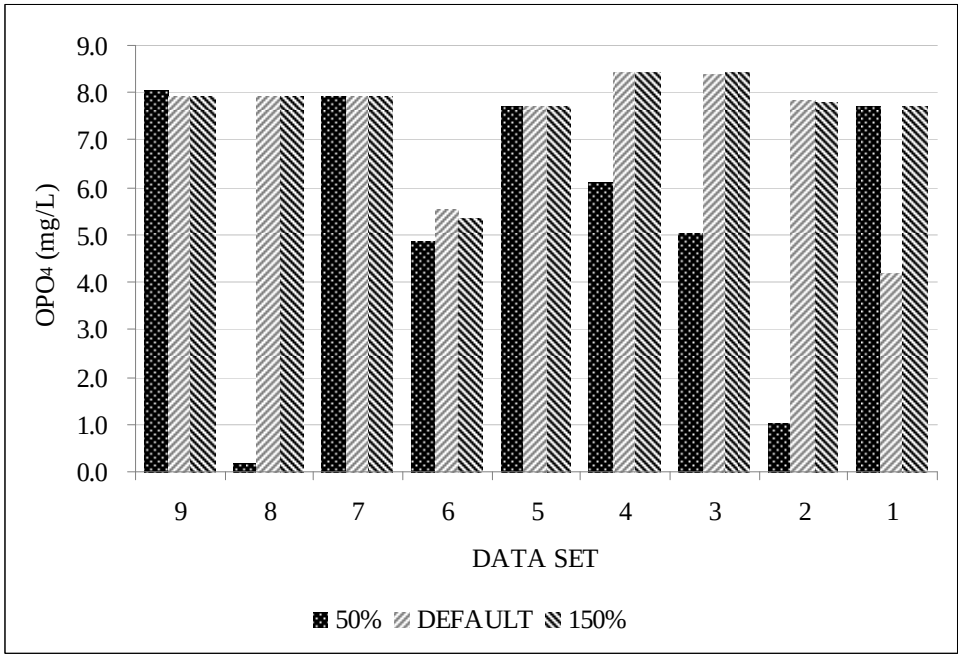

FIGURE 1.C.12: Effect of saturation coefficient for growth on acetate on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

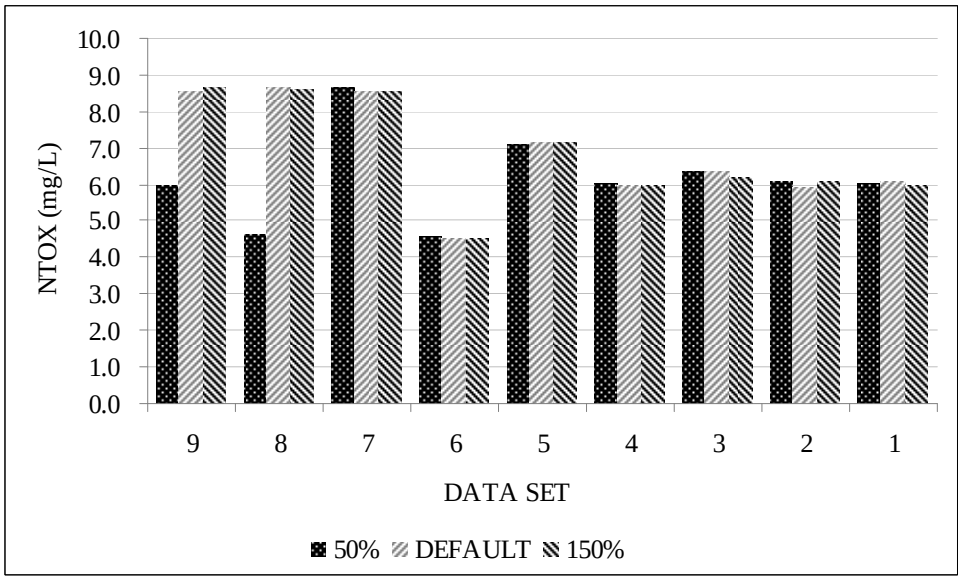

FIGURE 1.C.13: Effect of saturation coefficient for growth on acetate on the effluent NTOX concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

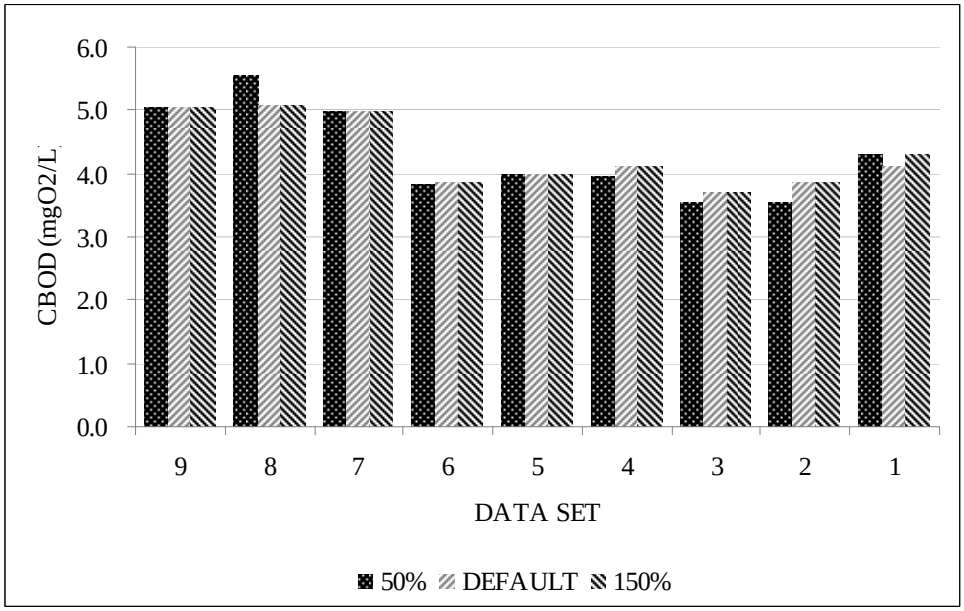

FIGURE 1.C.14: Effect of saturation coefficient for growth on acetate on the effluent CBOD concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

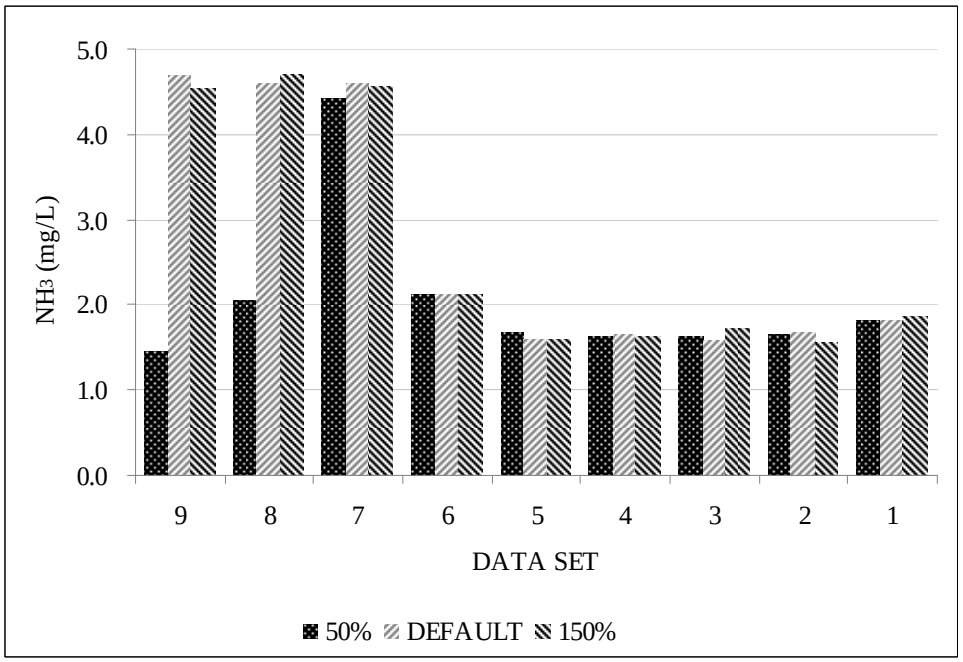

FIGURE 1.C.15: Effect of saturation coefficient for growth on acetate on the effluent NH_3 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

4) Maximum growth rate of autotrophs X_{AUT} (μ_{AUT}):

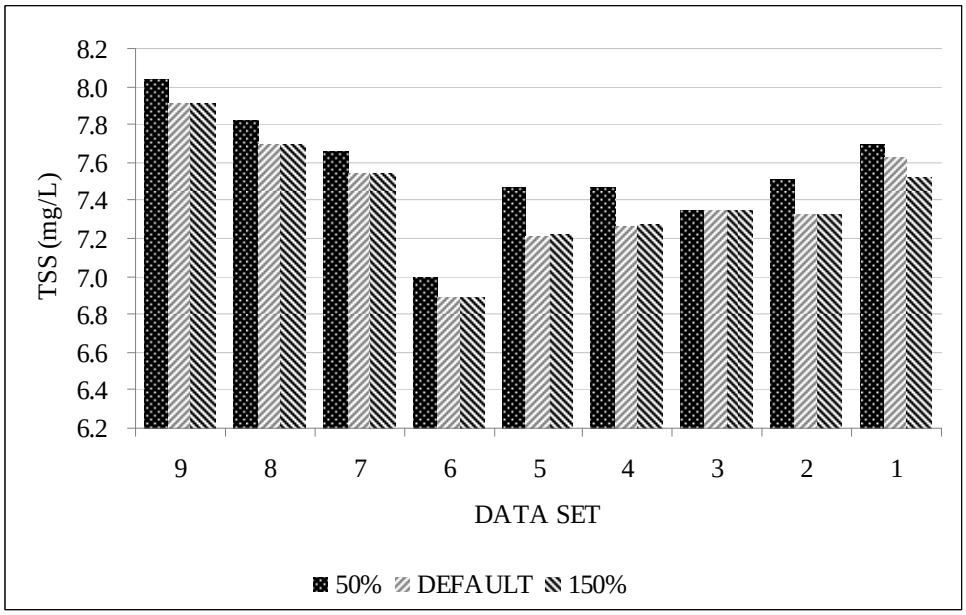

FIGURE 1.C.16: Effect of maximum growth rate of autotrophs on the effluent TSS concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

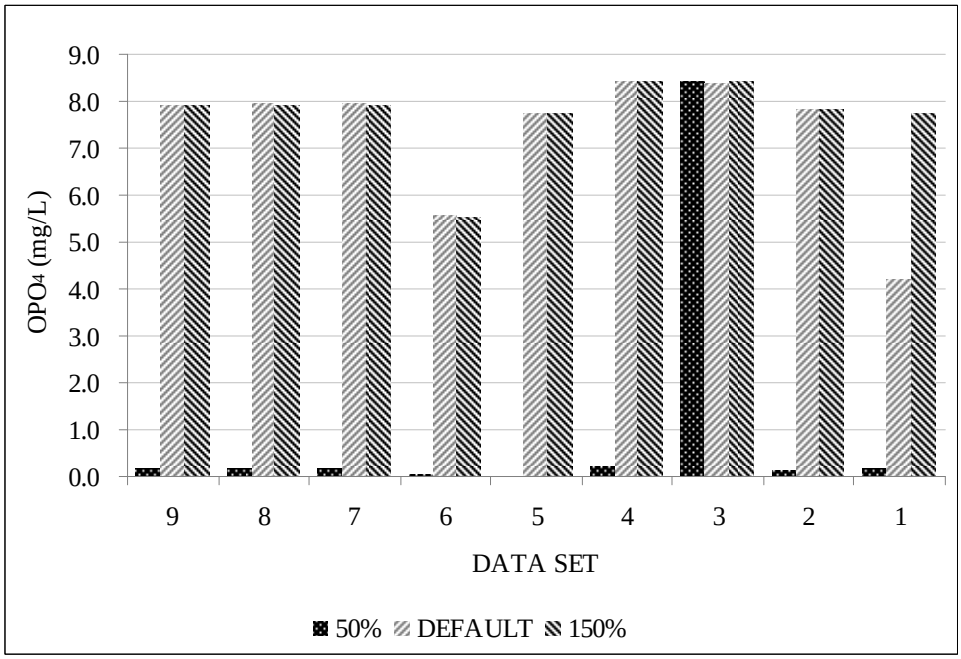

FIGURE 1.C.17: Effect of maximum growth rate of autotrophs on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

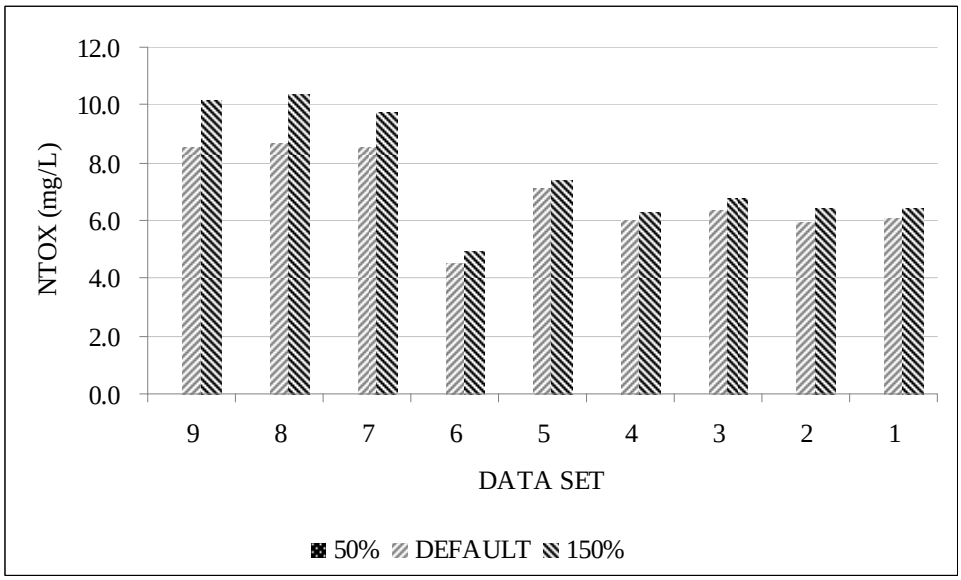

FIGURE 1.C.18: Effect of maximum growth rate of autotrophs on the effluent NTOX concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

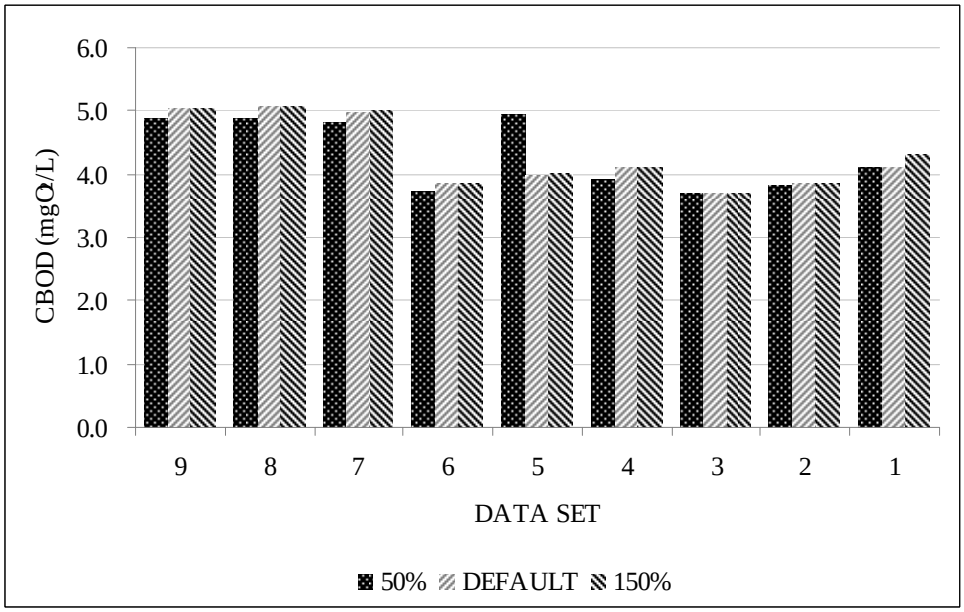

FIGURE 1.C.19: Effect of maximum growth rate of autotrophs on the effluent CBOD concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

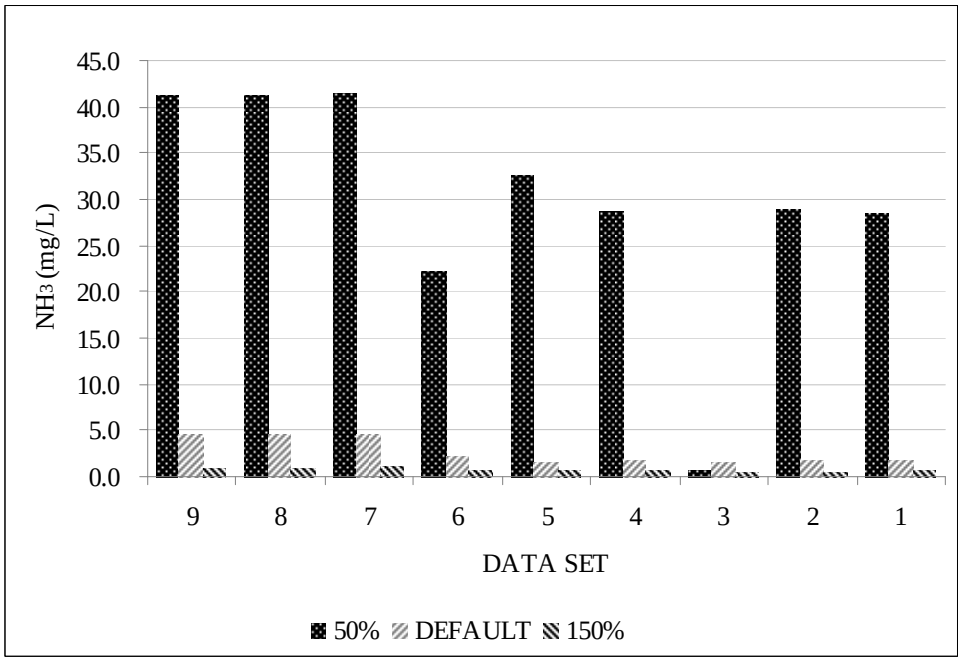

FIGURE 1.C.20: Effect of maximum growth rate of autotrophs on the effluent NH_3 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

5) Hydrolysis rate constant (K_H):

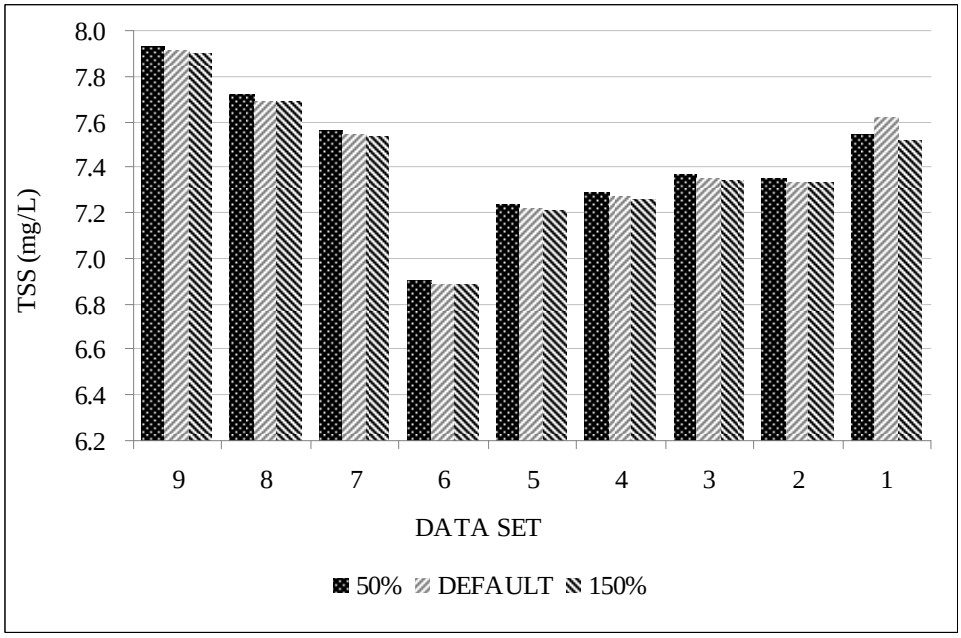

FIGURE 1.C.21: Effect of hydrolysis rate constant on the effluent TSS concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

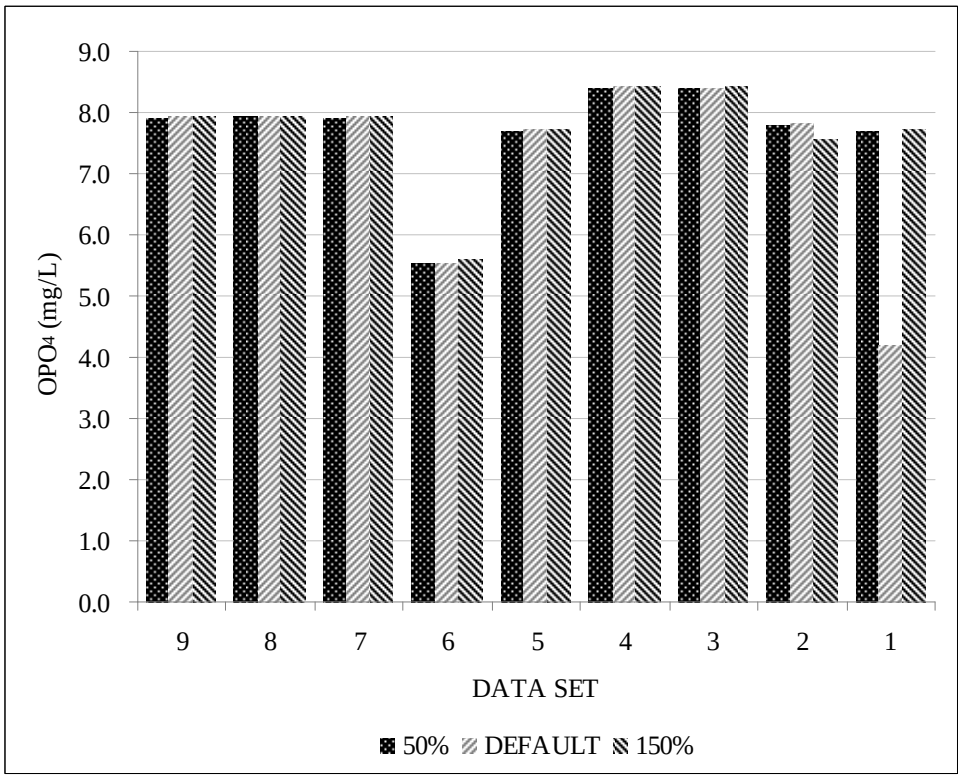

FIGURE 1.C.22: Effect of hydrolysis rate constant on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

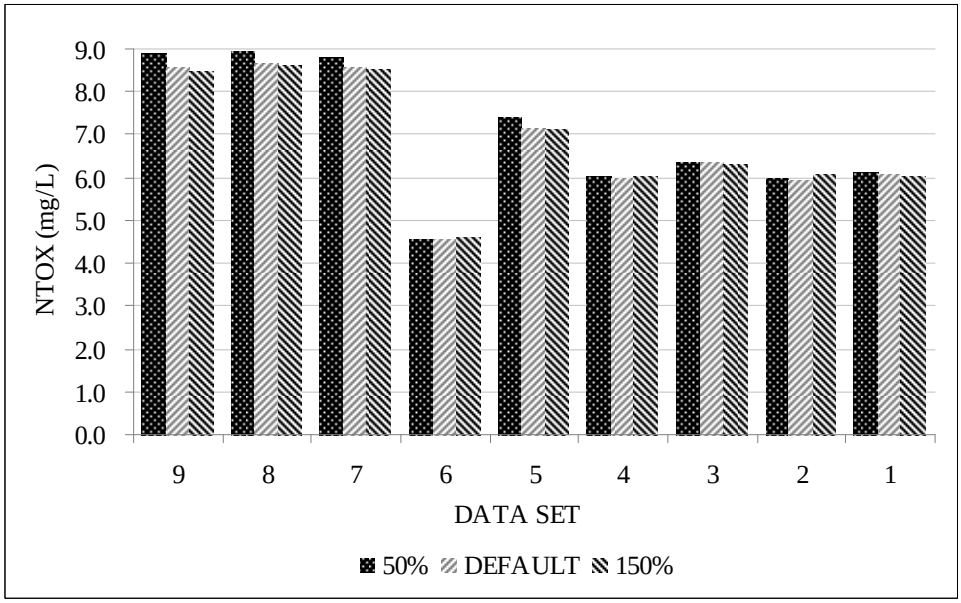

FIGURE 1.C.23: Effect of hydrolysis rate constant on the effluent NTOX concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

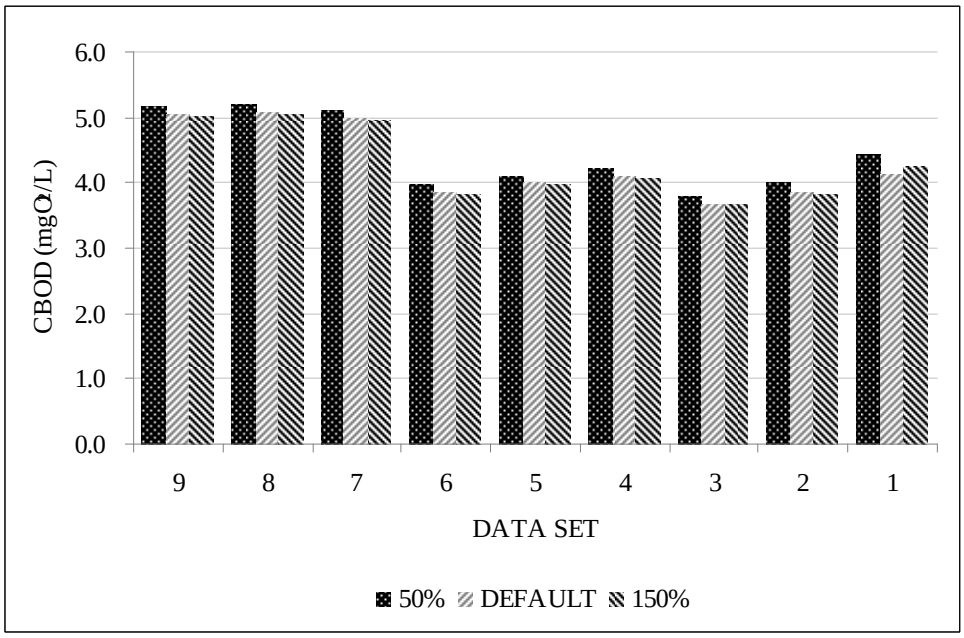

FIGURE 1.C.24: Effect of hydrolysis rate constant on the effluent CBOD concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

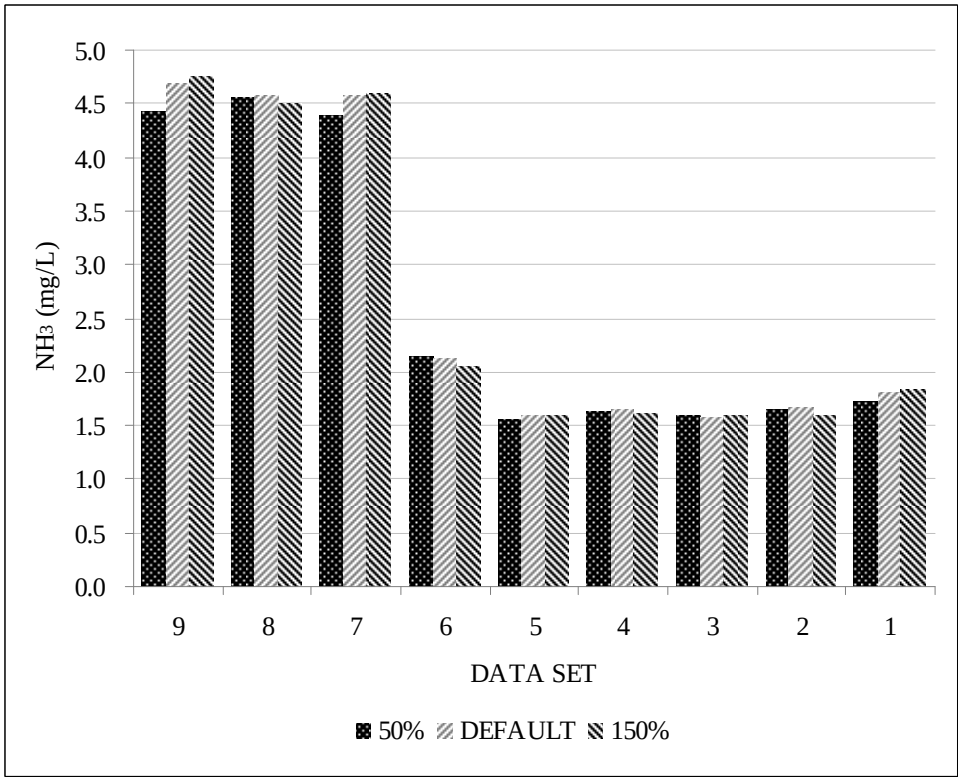

FIGURE 1.C.25: Effect of hydrolysis rate constant on the effluent NH_3 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

6) Anoxic hydrolysis reduction factor (η_{NO3}):

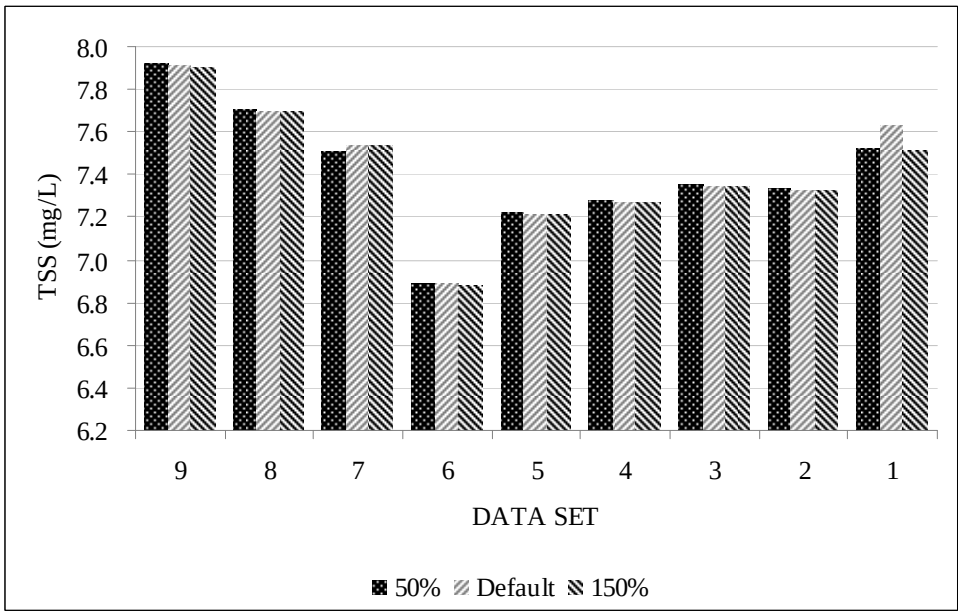

FIGURE 1.C.26: Effect of hydrolysis rate constant on the effluent TSS concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

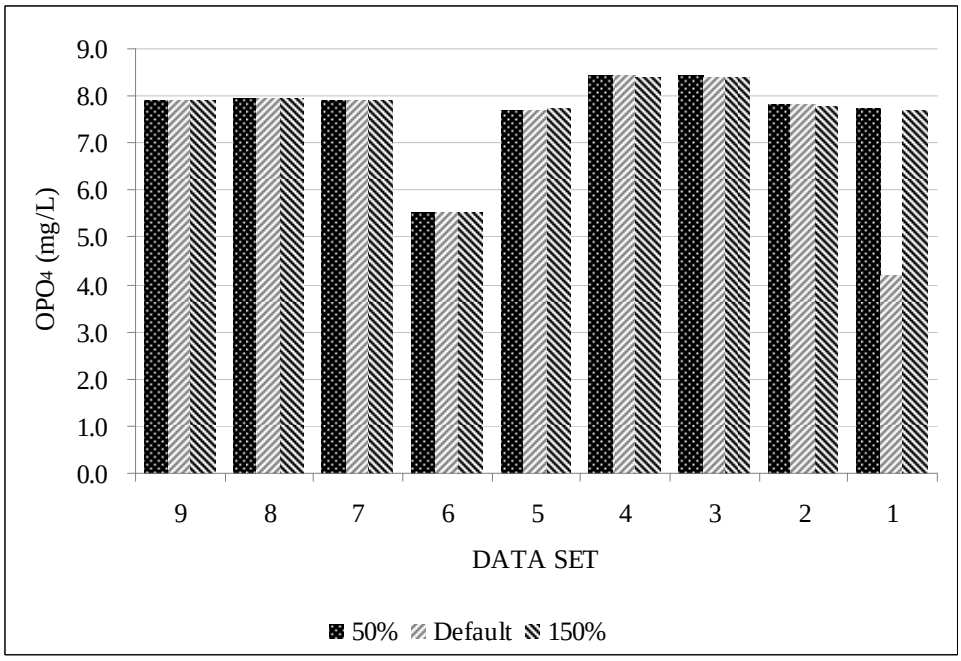

FIGURE 1.C.27: Effect of hydrolysis rate constant on the effluent OPO_4 concentration, Where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

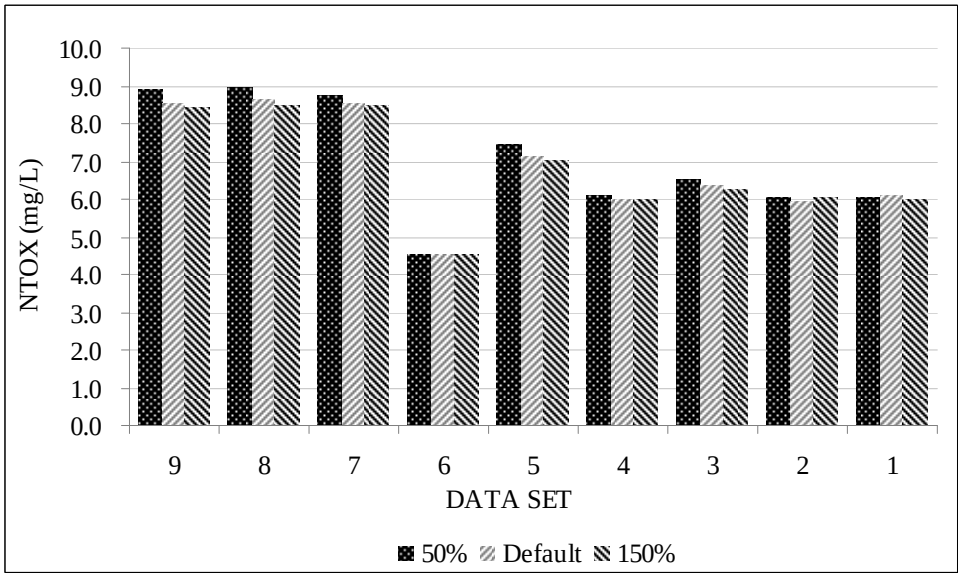

FIGURE 1.C.28: Effect of hydrolysis rate constant on the effluent NTOX concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value.

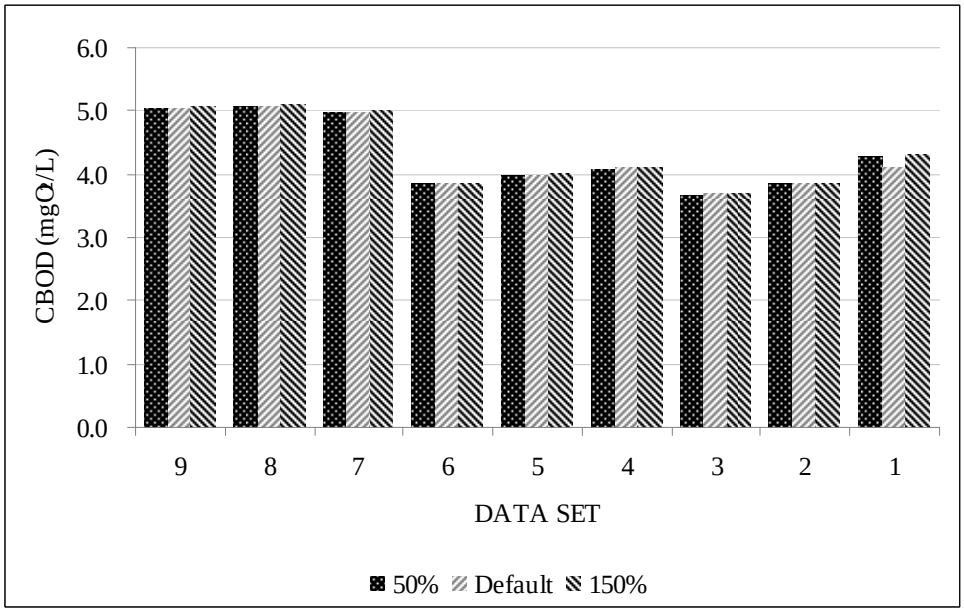

FIGURE 1.C.29: Effect of hydrolysis rate constant on the effluent CBOD concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

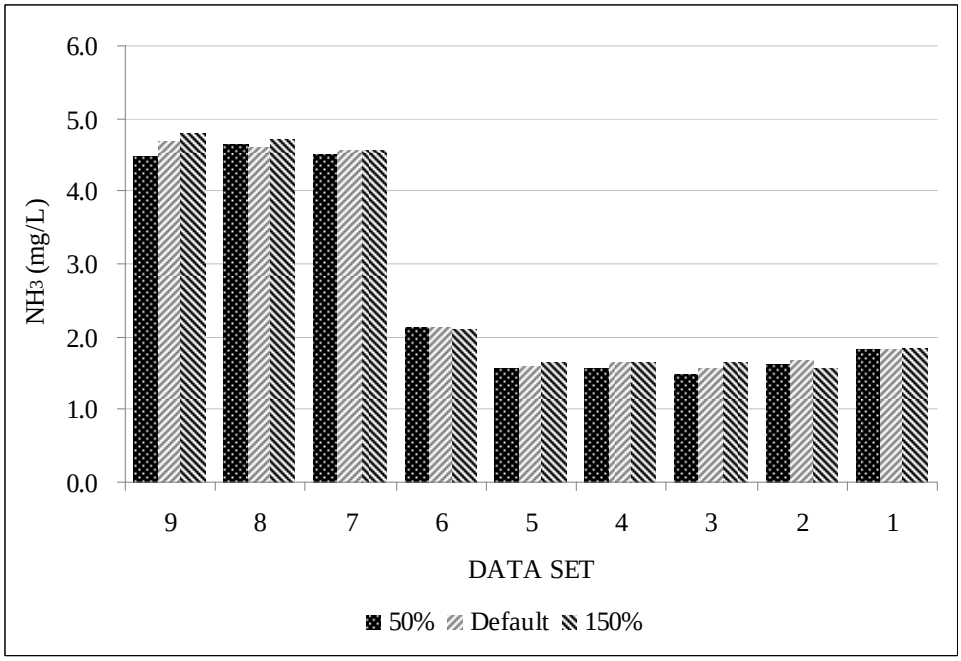

FIGURE 1.C.30: Effect of hydrolysis rate constant on the effluent NH_3 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

7) Rate of lysis for X_{PP} (b_{PP}) :

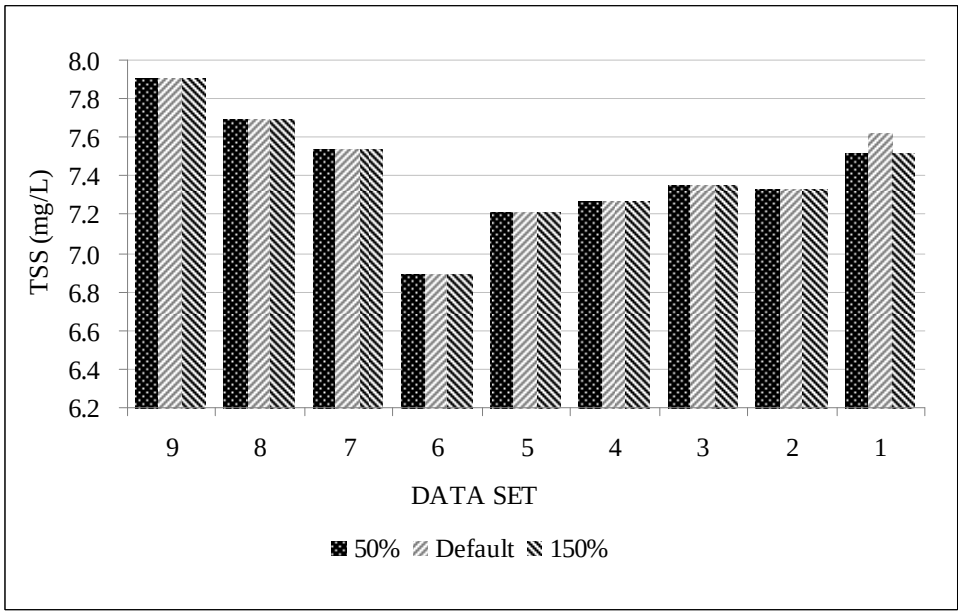

FIGURE 1.C.31: Effect of rate of lysis for x_{pp} on the effluent TSS concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

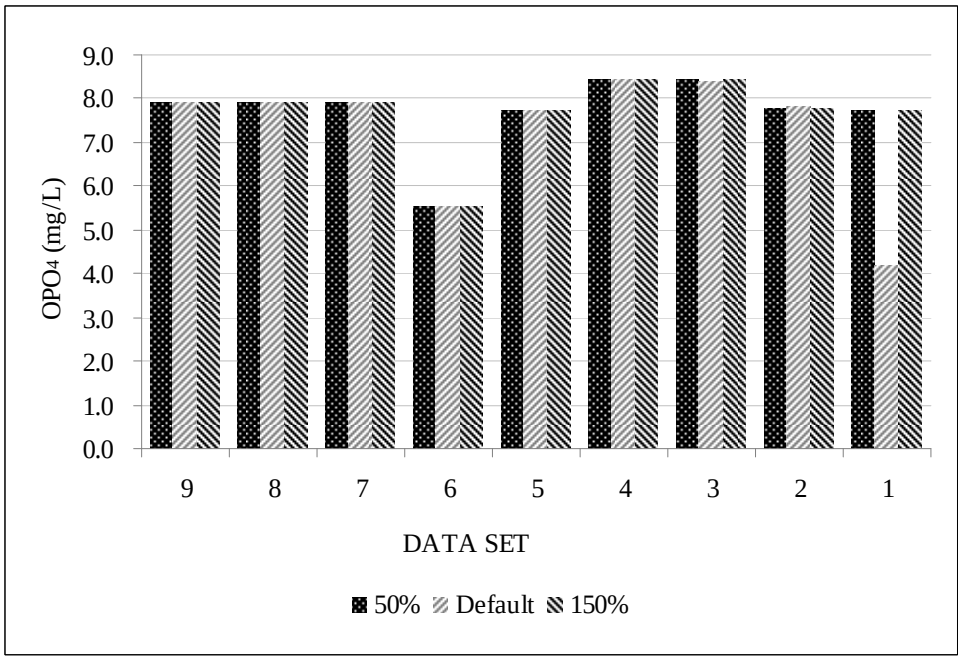

FIGURE 1.C.32: Effect of rate of lysis for X_{PP} on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

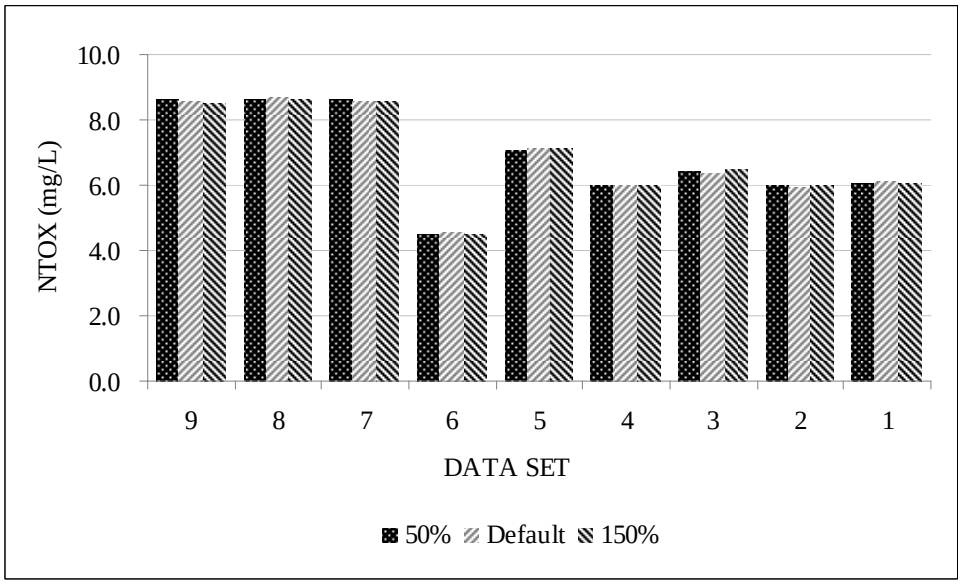

FIGURE 1.C.33: Effect of rate of lysis for X_{PP} on the effluent NTOX concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

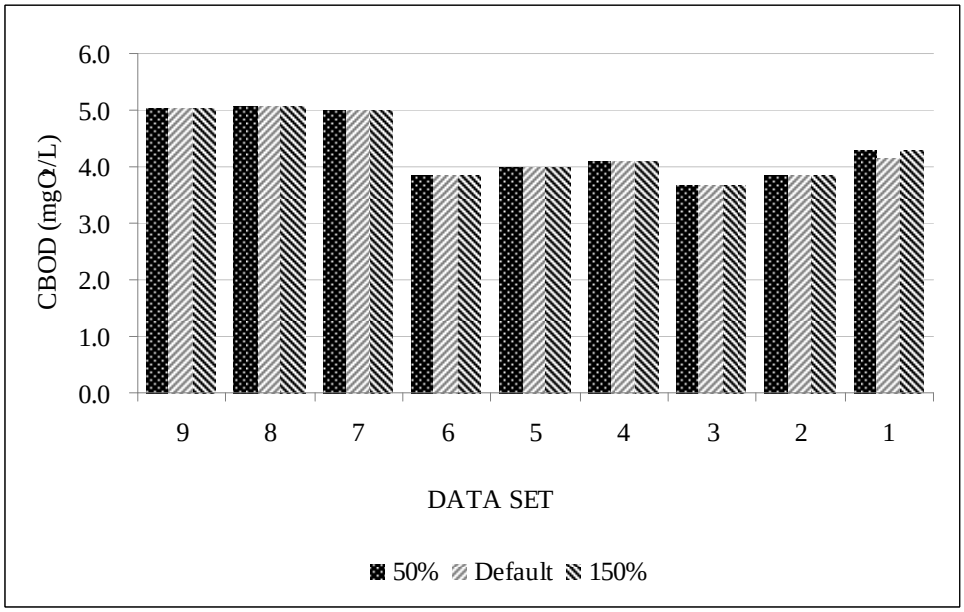

FIGURE 1.C.34: Effect of rate of lysis for X_{PP} on the effluent CBOD concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

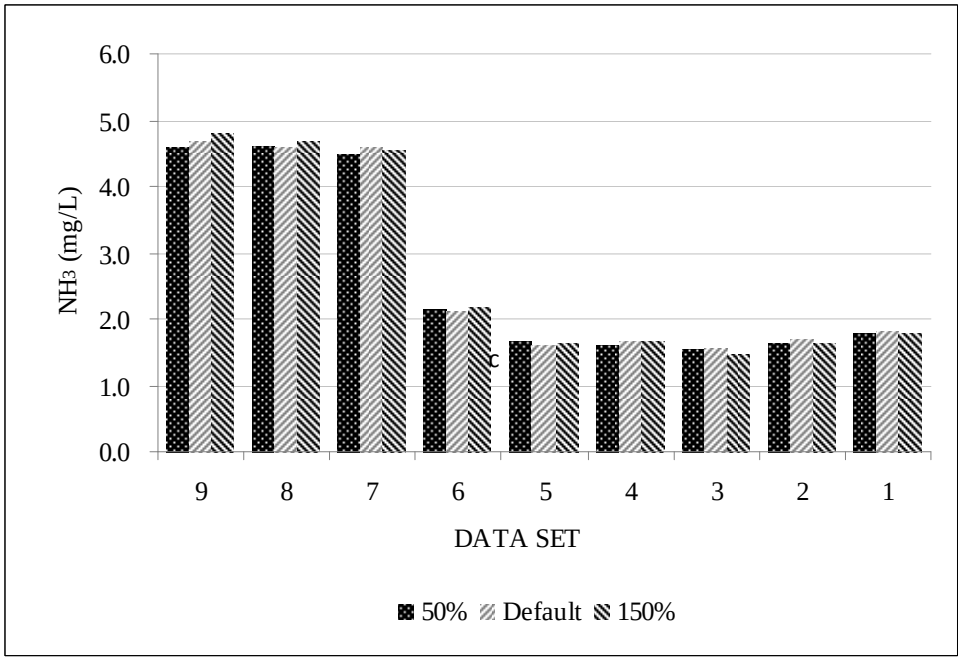

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FIGURE 1.C.35: Effect of rate of lysis for X_{PP} on the effluent NH_3 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

8) Rate of lysis for X_{PHA} (b_{PHA}) :

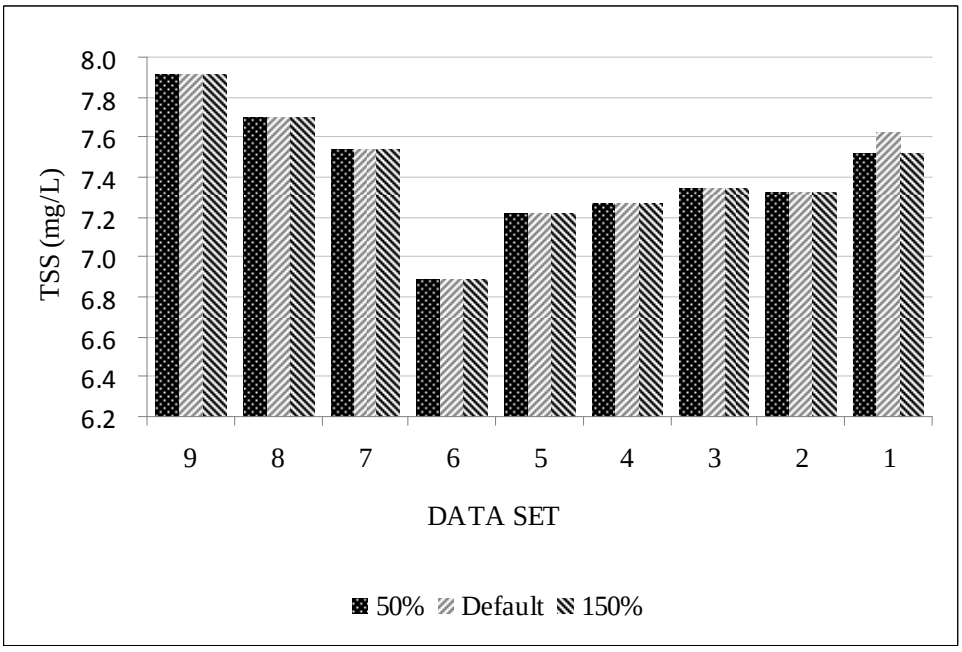

FIGURE 1.C.36: Effect of rate of lysis for X_{PHA} on the effluent TSS concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

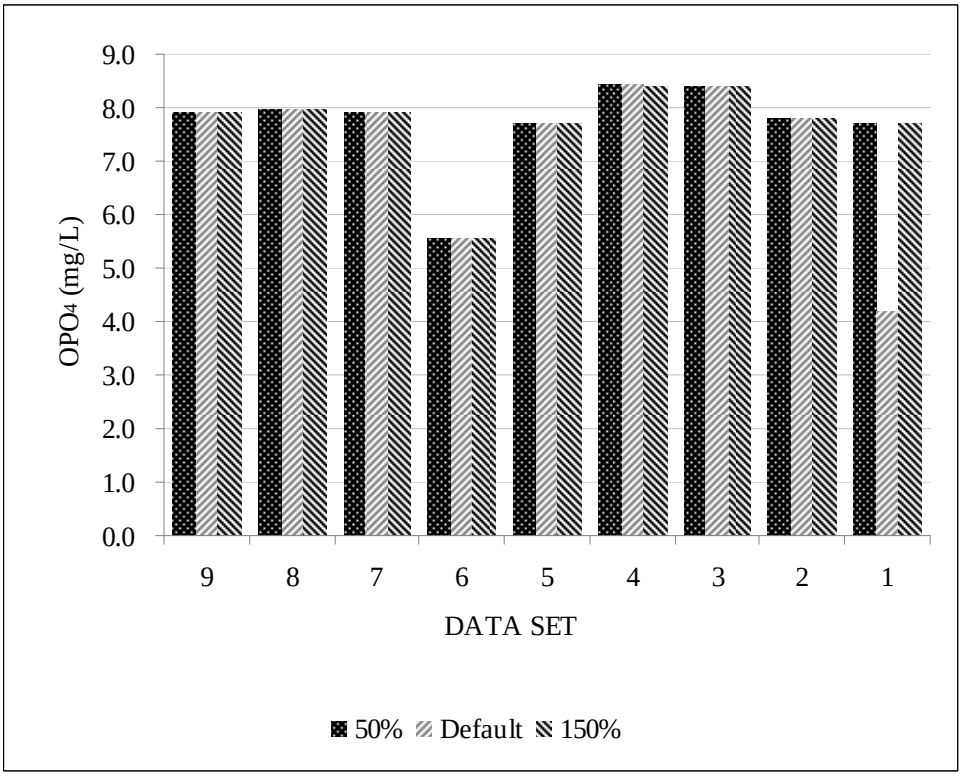

FIGURE 1.C.37: Effect of rate of lysis for X_{PHA} on the effluent OPO_4 concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

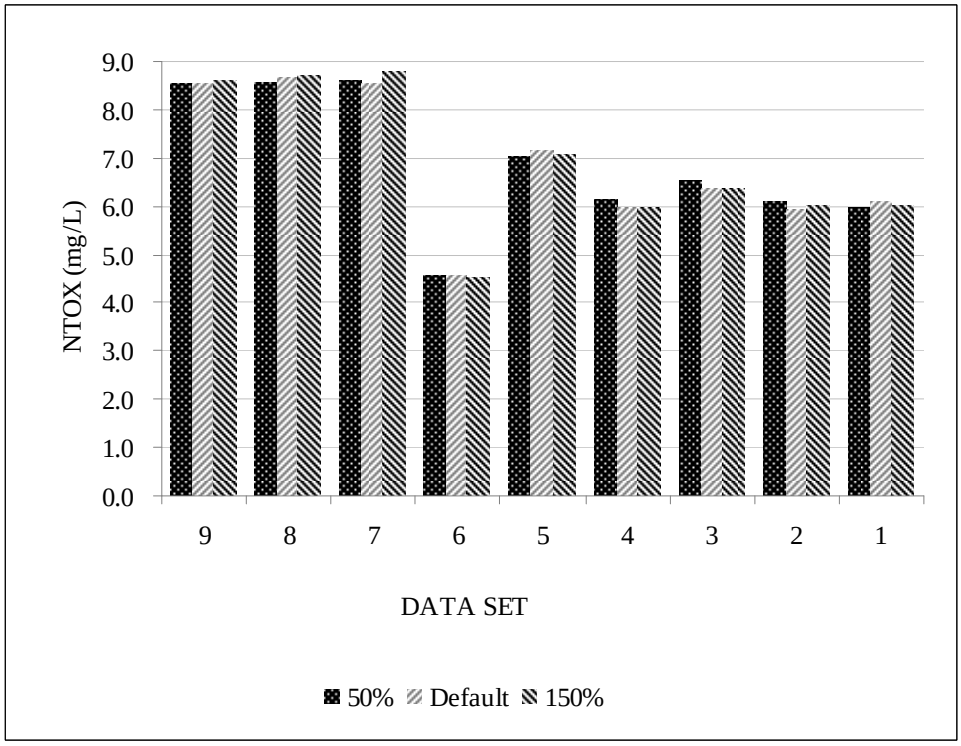

FIGURE 1.C.38: Effect of rate of lysis for X_{PHA} on the effluent NTOX concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

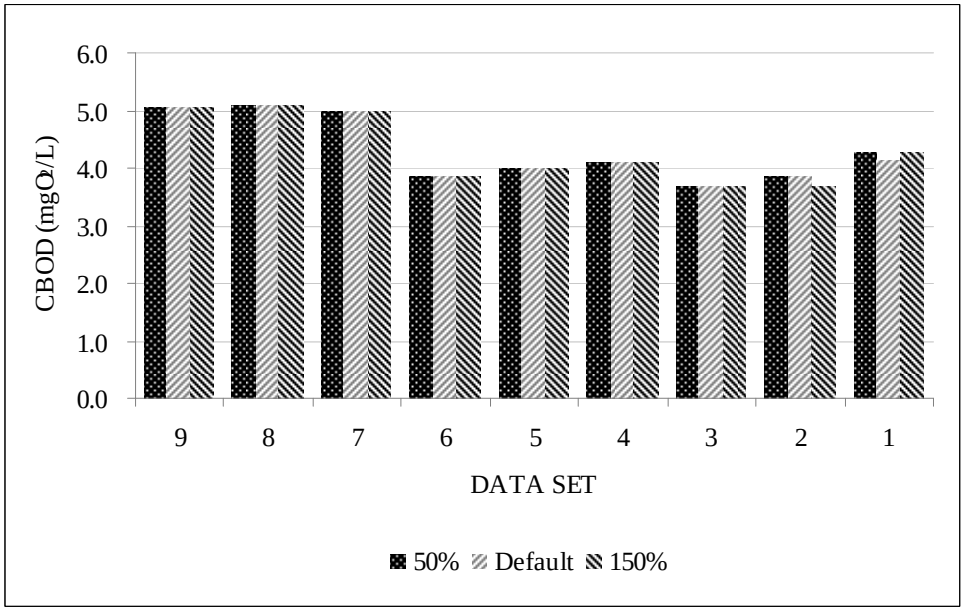

FIGURE 1.C.39: Effect of rate of lysis for X_{PHA} on the effluent CBOD concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

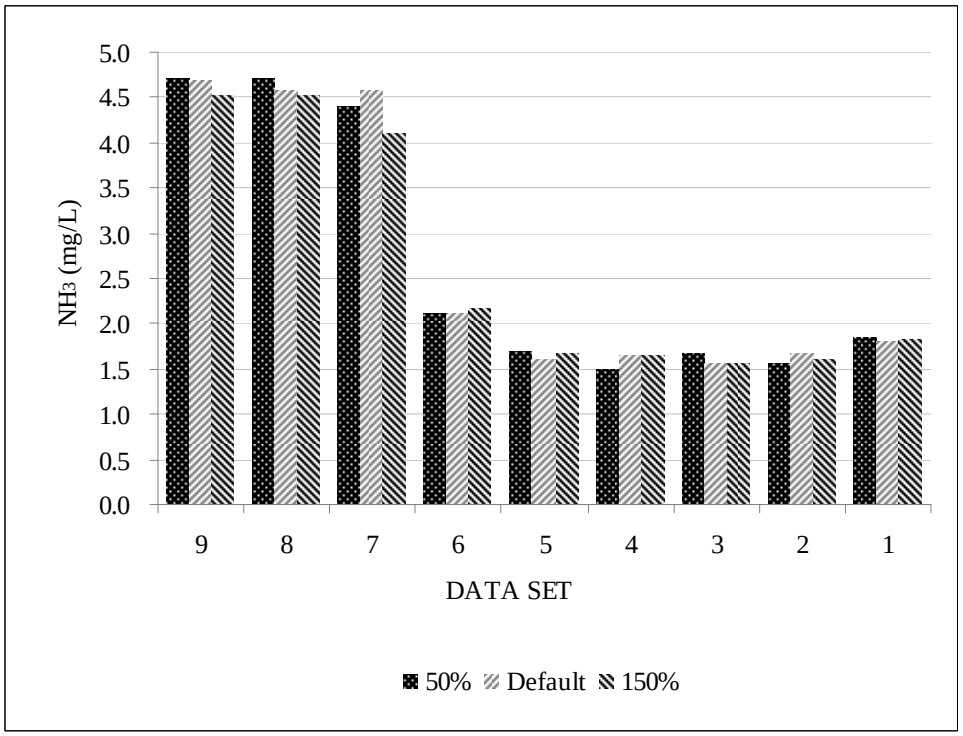

FIGURE 1.C.40: Effect of rate of lysis for X_{PHA} on the effluent NH_3concentration, where 100% = default value, 50% = 50% reduction in the default value, 150% = 50% increase in the default value

9) Inhibition coefficient for PP storage (K_{IPP}):

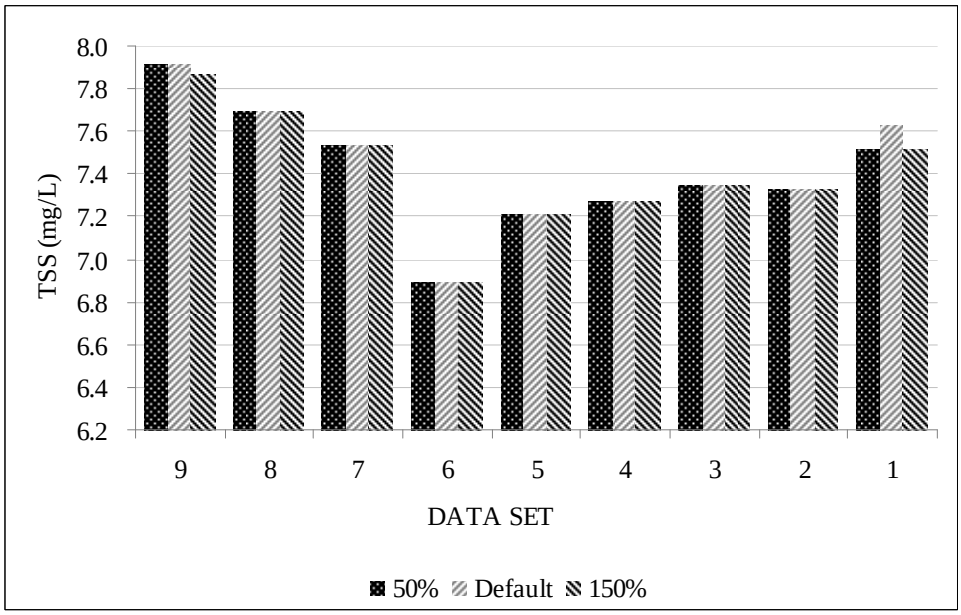

FIGURE 1.C.41: Effect of inhibition coefficient for PP storage on the effluent TSS concentration, where 100% =calibrated value, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value

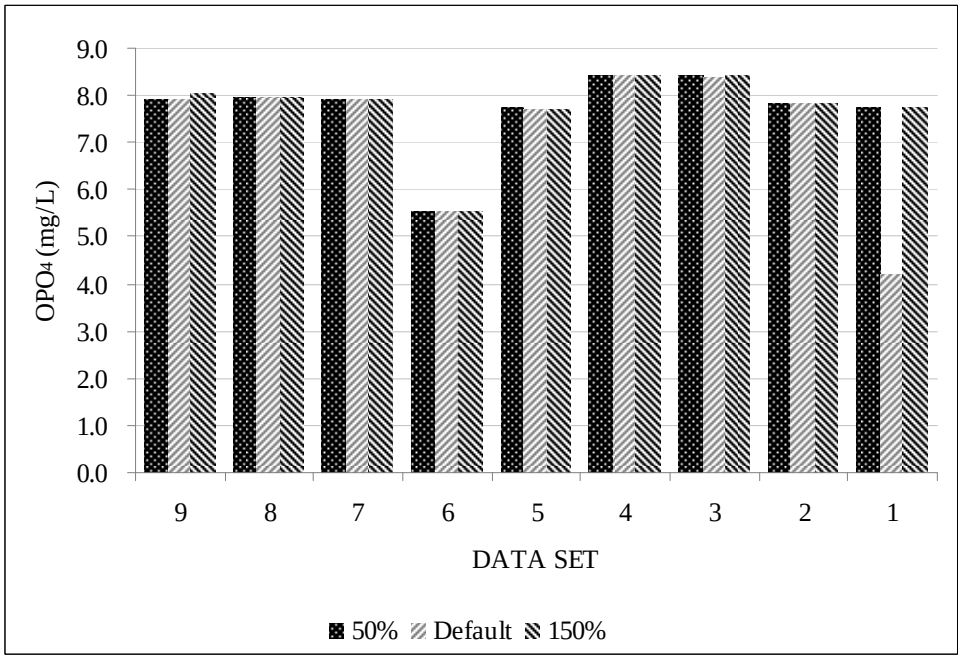

FIGURE 1.C.42: Effect of inhibition coefficient for PP storage on the effluent OPO_4 concentration, where 100% =calibrated value, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value

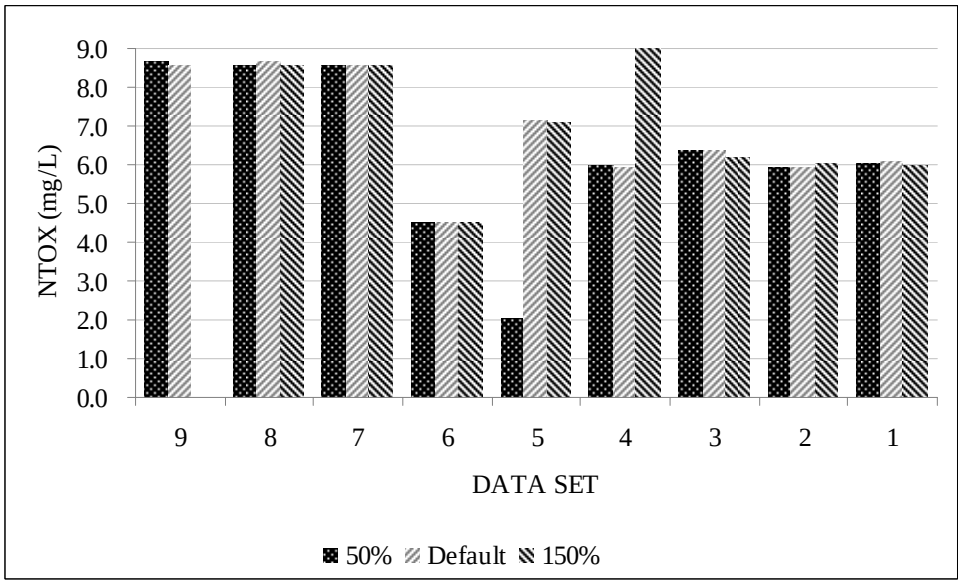

FIGURE 1.C.43: Effect of inhibition coefficient for PP storage on the effluent NTOX Concentration, where 100% =calibrated value, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value

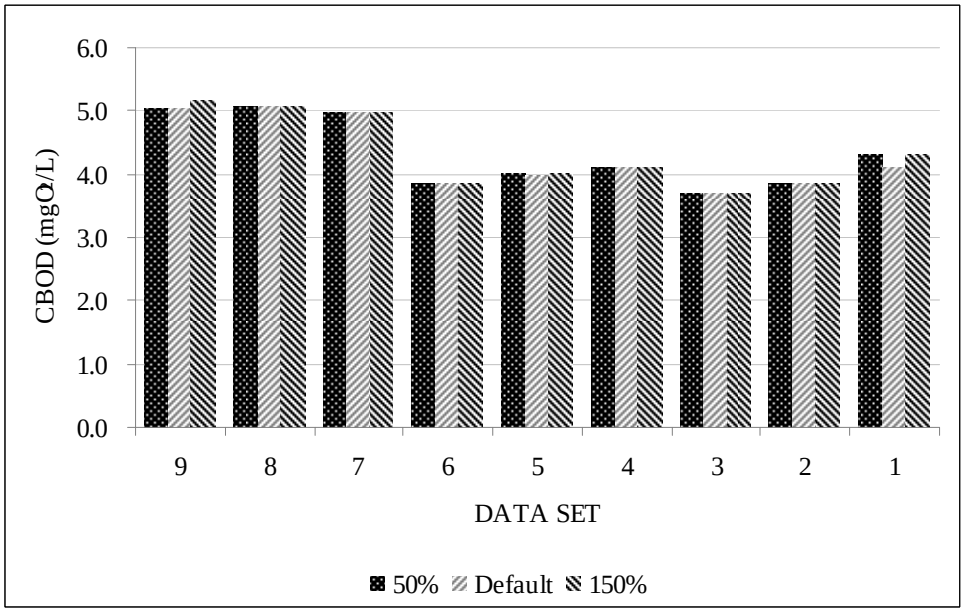

FIGURE 1.C.44: Effect of inhibition coefficient for PP storage on the effluent CBOD concentration, where 100% =calibrated value, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value

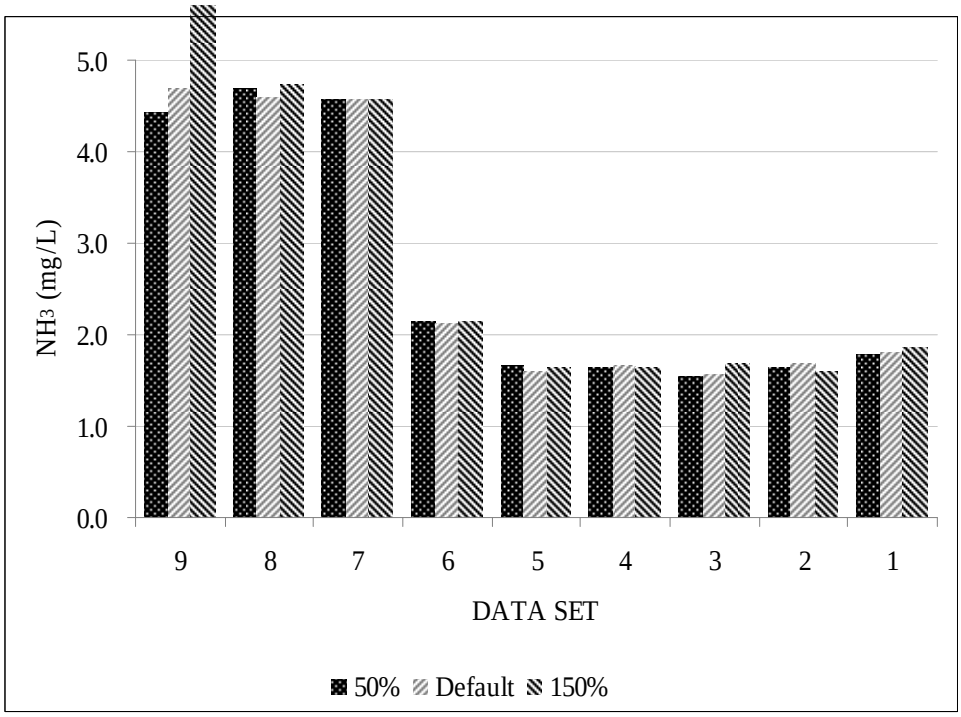

FIGURE 1.C.45: Effect of inhibition coefficient for PP storage on the effluent NH_3 concentration, where 100% =calibrated value, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value

10) Rate constant for storage of X_{PP} :

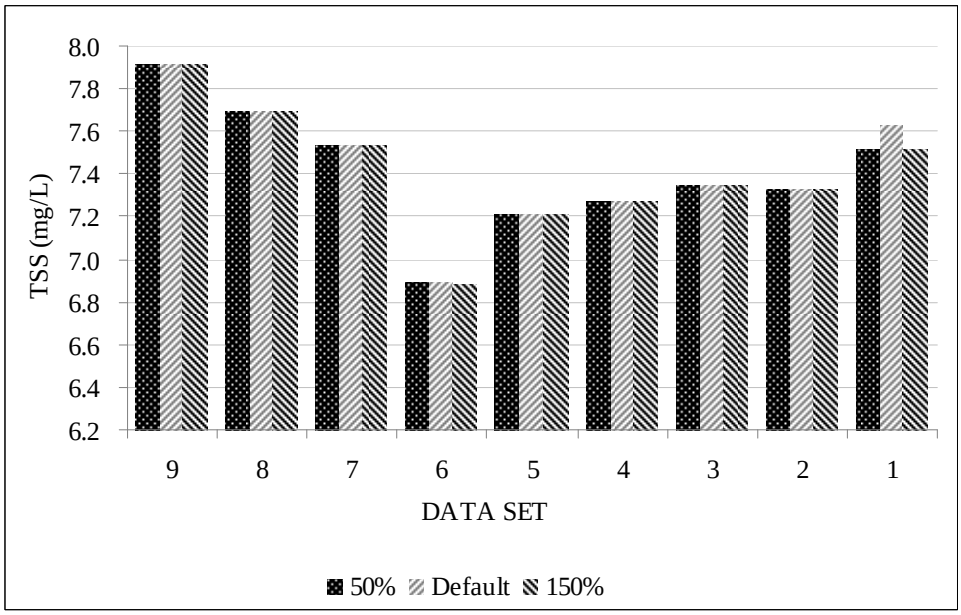

FIGURE 1.C.46: Effect of rate constant for storage of X_{PP} on the effluent TSS concentration, where 100% =calibrated value, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value

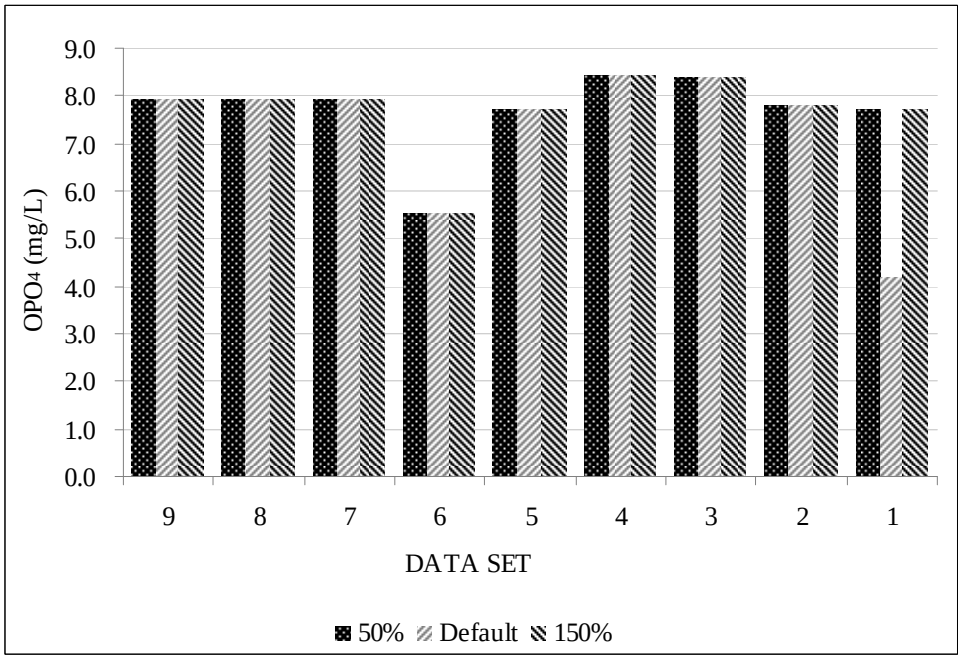

FIGURE 1.C.47: Effect of rate constant for storage of X_{PP} on the effluent OPO_4 concentration, where 100% =calibrated value, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value

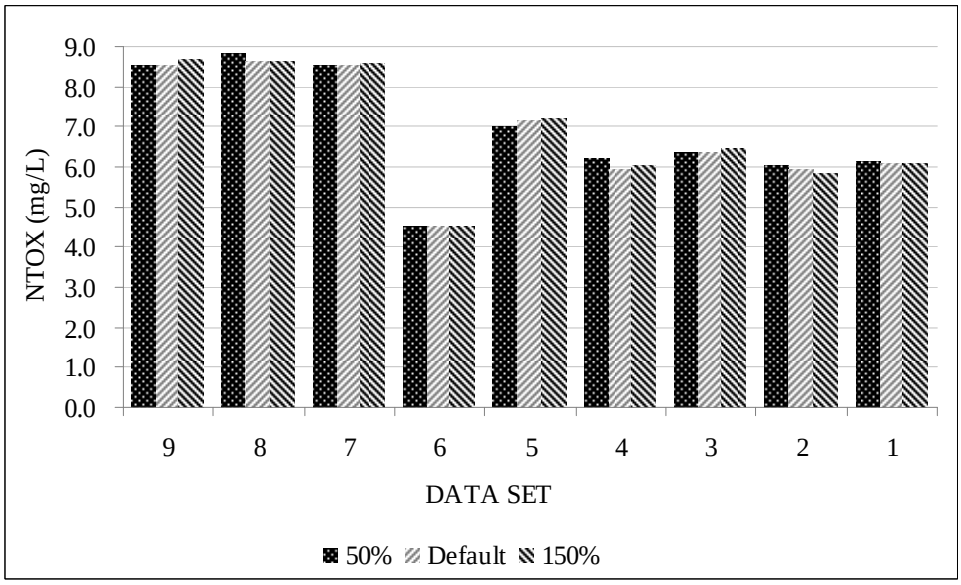

FIGURE 1.C.48: Effect of rate constant for storage of X_{PP} on the effluent NTOX concentration, where 100% =calibrated value, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value

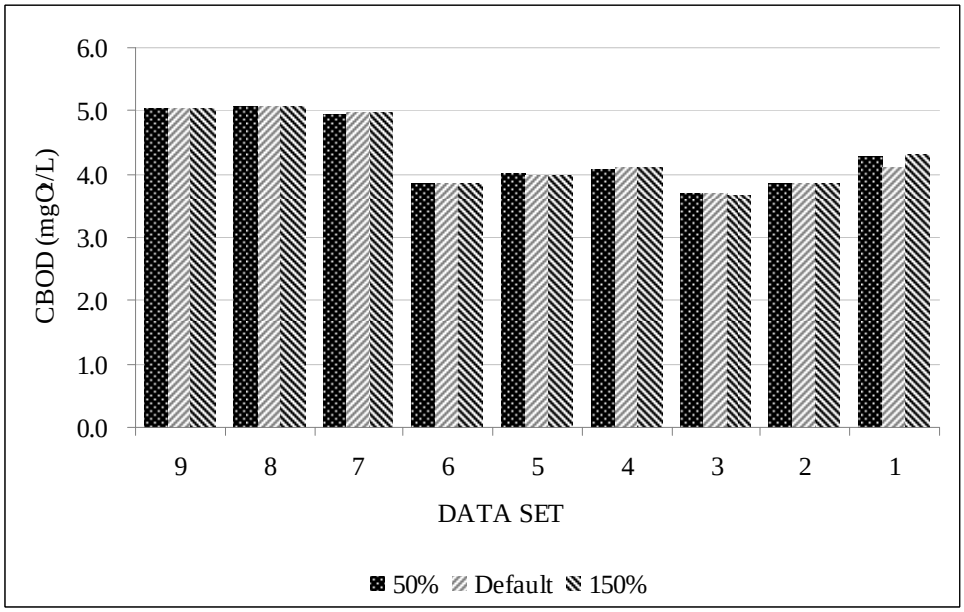

FIGURE 1.C.49: Effect of rate constant for storage of X_{PP} on the effluent CBOD concentration, where 100% =calibrated value, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value

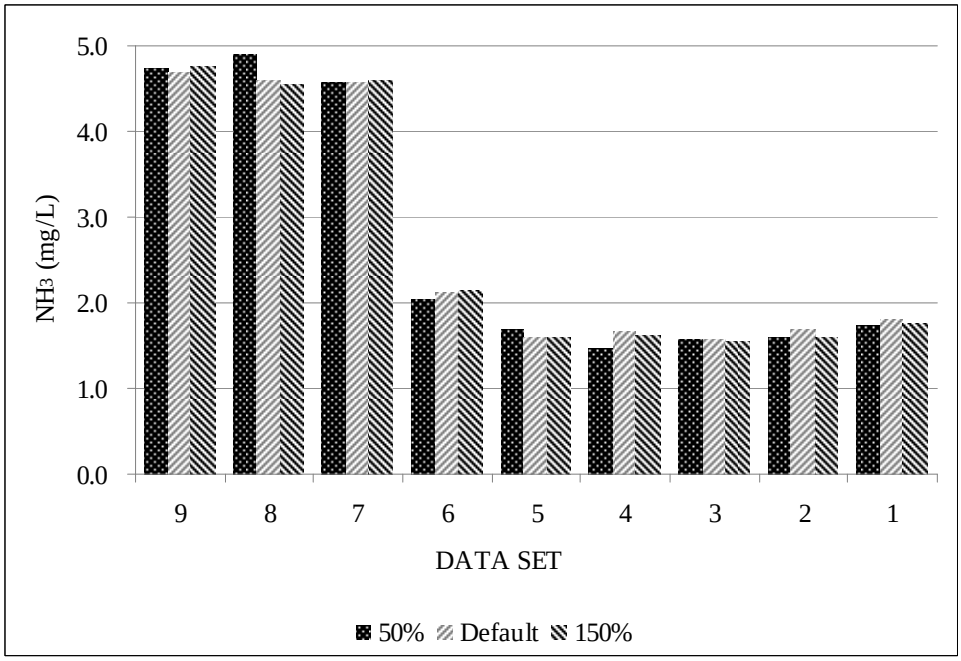

FIGURE 1.C.50: Effect of rate constant for storage of X_{pp} on the effluent NH_3 concentration, where 100% =calibrated value, 50% = 50% reduction in the calibrated value, 150% = 50% increase in the calibrated value

1. D. RESULTS OF MODEL RUN TO STUDY THE COMBINED EFFECT OF CALIBRATION OF KINETIC PARAMETERS:

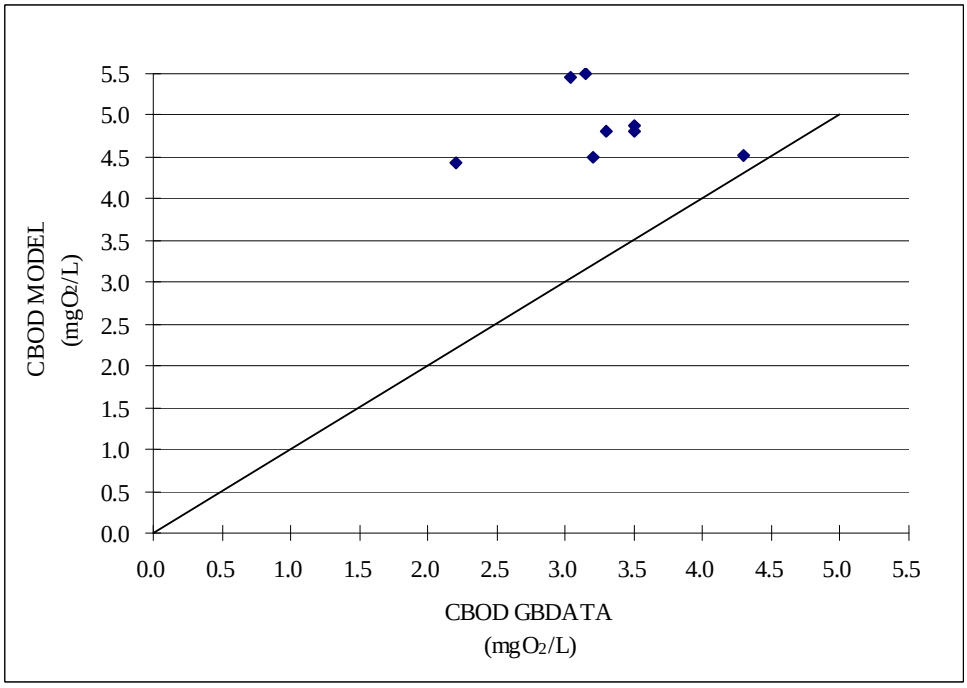

FIGURE 1.D.1: Comparison of measured and predicted CBOD concentration using default values of model kinetic parameter (hydrolysis rate constant, anoxic hydrolysis reduction factor, rate constant for storage of X_{PP}, lysis rate of X_{PP} and X_{PHA}, and inhibition coefficient for PP storage). Symbols lying on the 45^{o} line would indicate perfect agreement between modelled and observed values.

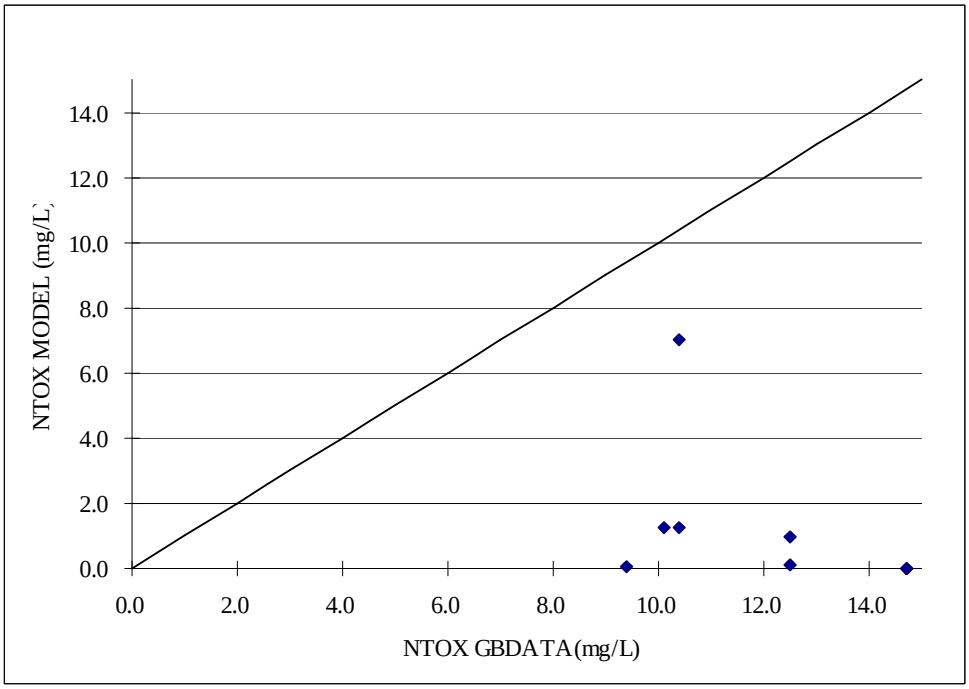

FIGURE 1.D.2: Comparison of measured and predicted NTOX concentration using default values of model kinetic parameter (hydrolysis rate constant, anoxic hydrolysis reduction factor, rate constant for storage of X_{PP}, lysis rate of X_{PP} and X_{PHA}, and inhibition coefficient for PP storage). Symbols lying on the 45^{o} line would indicate perfect agreement between modelled and observed values.

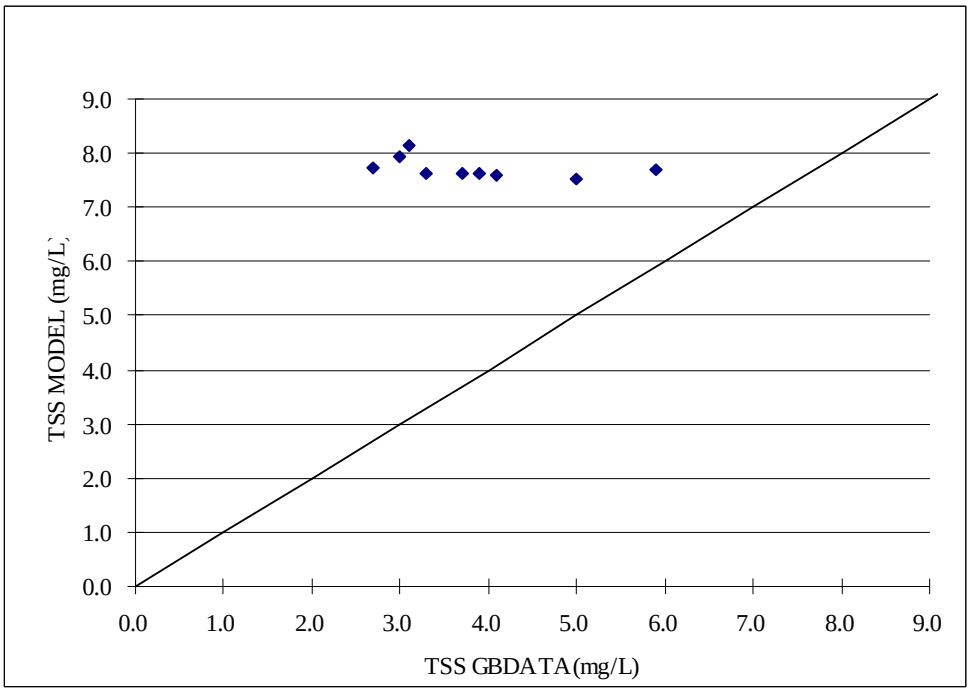

FIGURE 1.D.3: Comparison of measured and predicted TSS concentration using default values of model kinetic parameter (hydrolysis rate constant, anoxic hydrolysis reduction factor, rate constant for storage of X_{PP}, lysis rate of X_{PP} and X_{PHA}, and inhibition coefficient for PP storage). Symbols lying on the 45^{o} line would indicate perfect agreement between modelled and observed values.

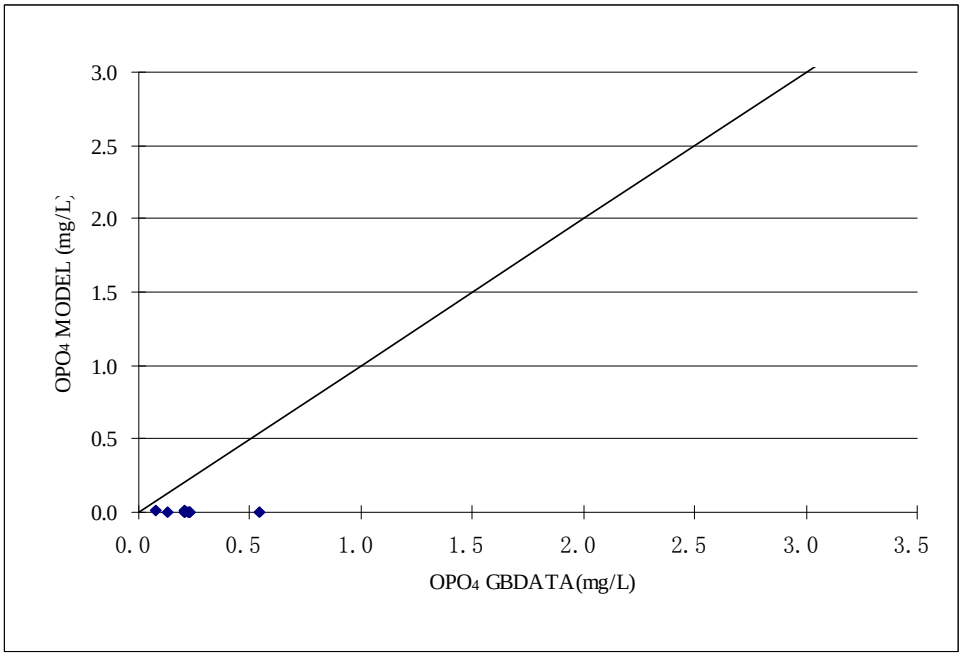

FIGURE 1.D.4: Comparison of measured and predicted OPO_4 concentration using default values of model kinetic parameter (hydrolysis rate constant, anoxic hydrolysis reduction factor, rate constant for storage of X_{PP}, lysis rate of X_{PP} and X_{PHA}, and inhibition coefficient for PP storage). Symbols lying on the 45^o line would indicate perfect agreement between modelled and observed values.

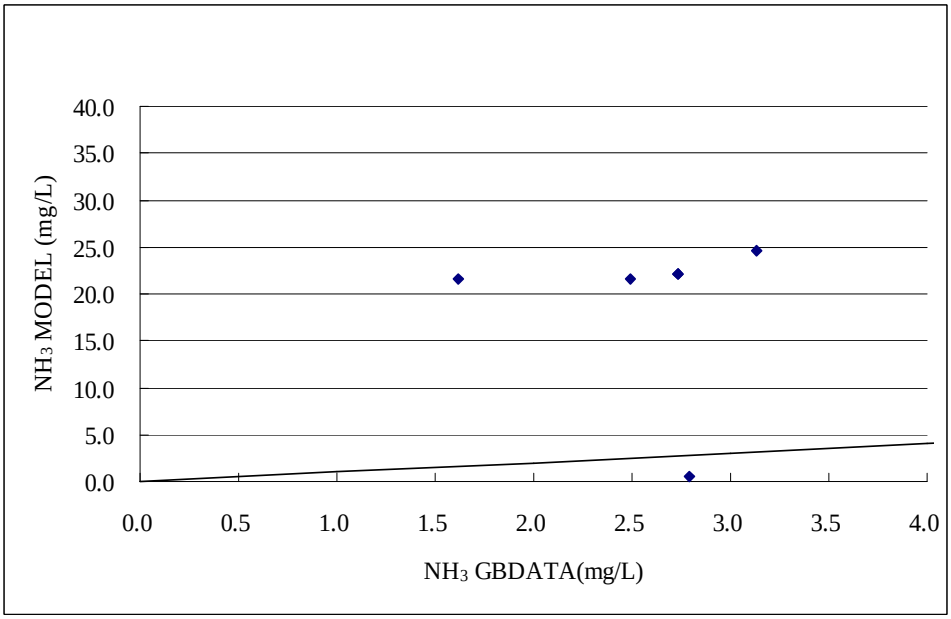

FIGURE 1.D.5: Comparison of measured and predicted NH_3 concentration using default values of model kinetic parameter (hydrolysis rate constant, anoxic hydrolysis reduction factor, rate constant for storage of X_{PP}, lysis rate of X_{pp} and X_{PHA}, and inhibition coefficient for PP storage). Symbols lying on the 45^o line would indicate perfect agreement between modelled and observed values.

1. E. Comparison of data from GBWWTP and model output using default and calibrated kinetic parameter value:

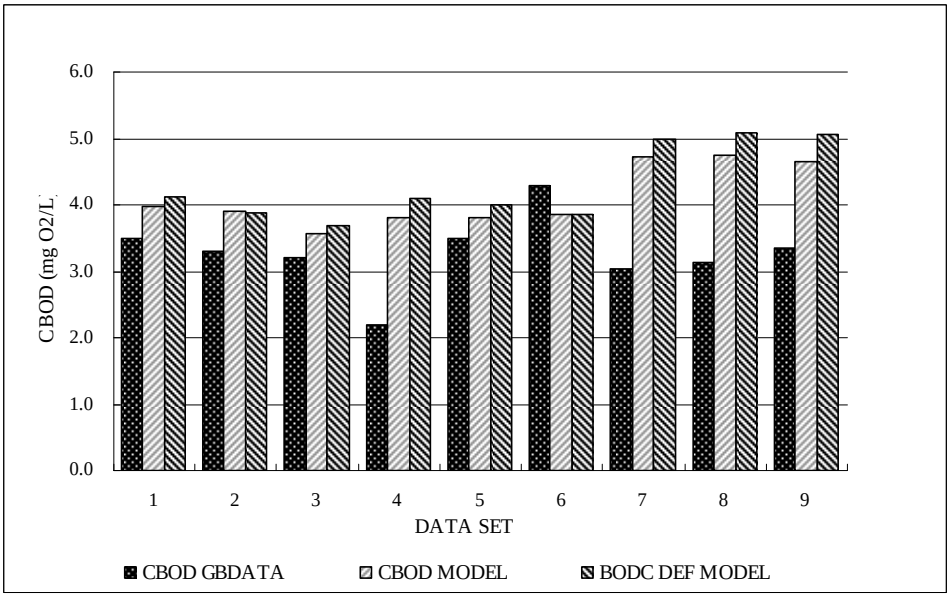

FIGURE 1.E.1: Comparison of measured and predicted CBOD concentration

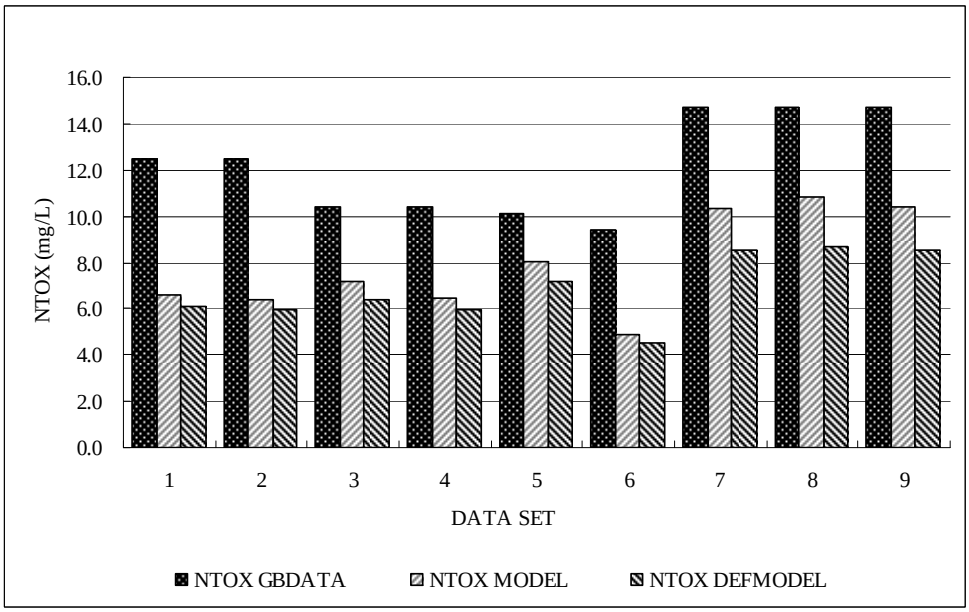

FIGURE 1.E.2: Comparison of measured and predicted NTOX concentration

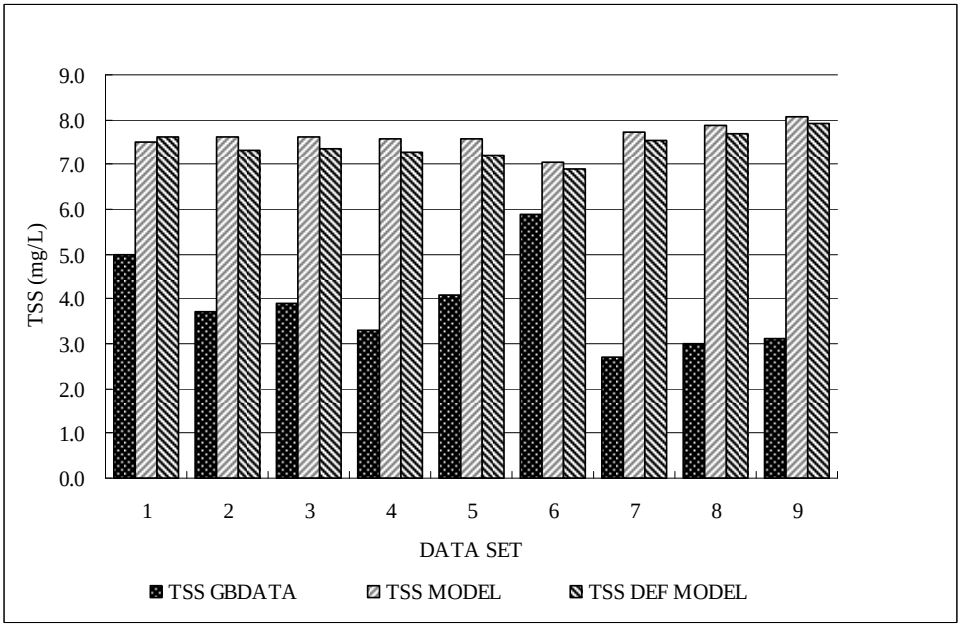

FIGURE 1.E.3: Comparison of measured and predicted TSS concentration

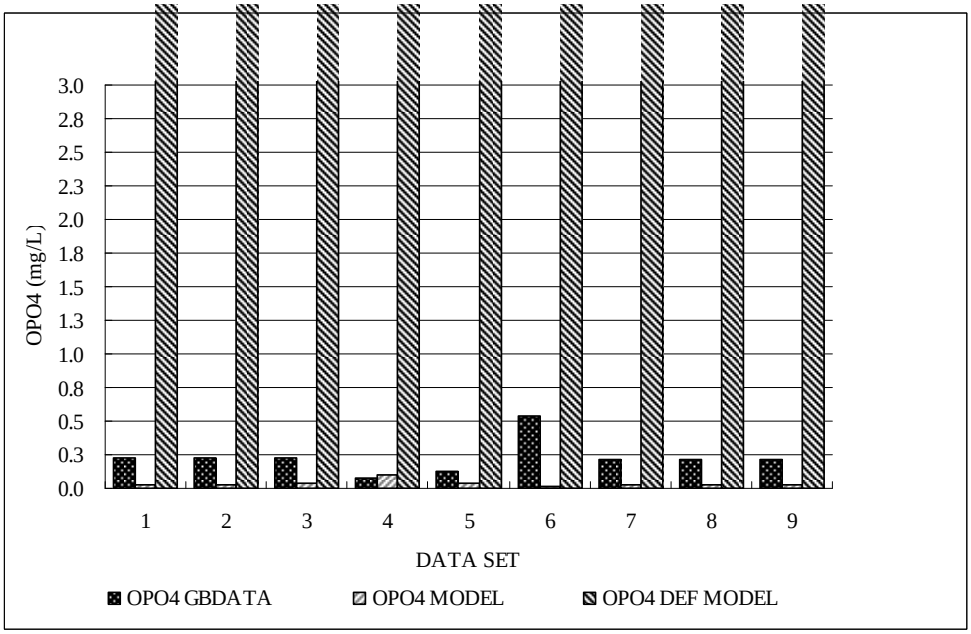

FIGURE 1.E.4: Comparison of measured and predicted OPO_4 concentration

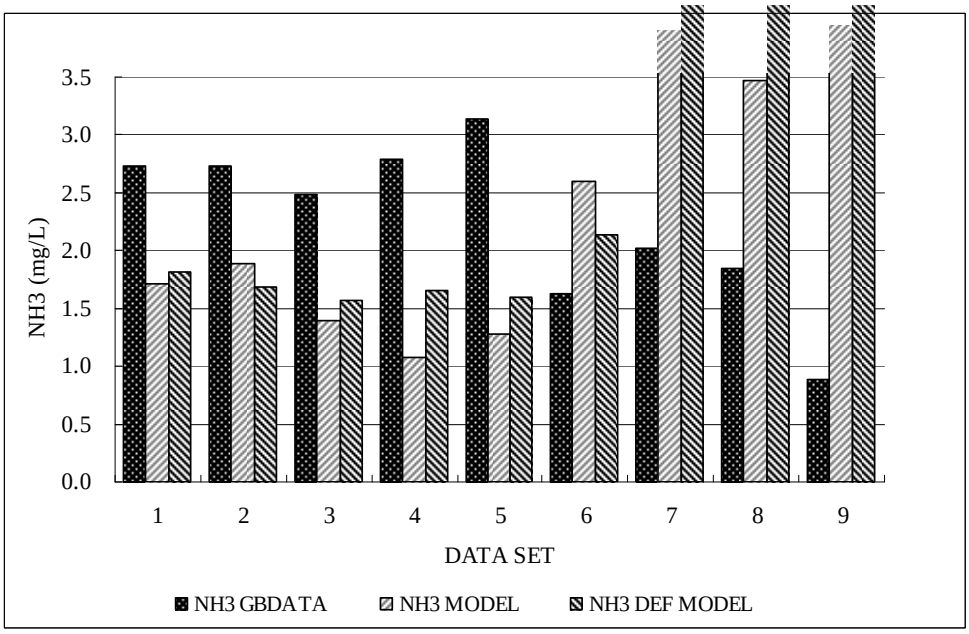

FIGURE 1.E.5: Comparison of measured and predicted NH_3 concentration

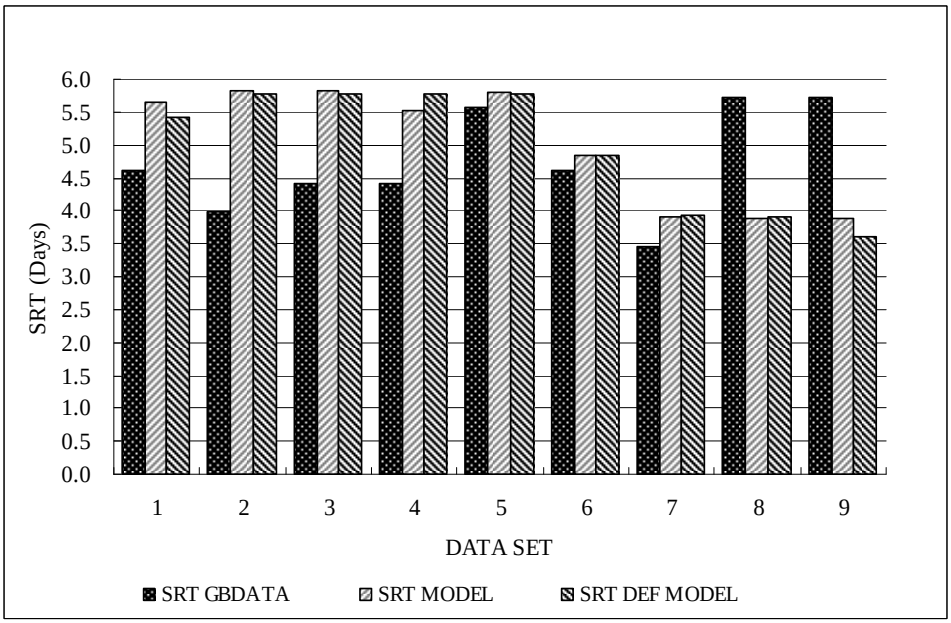

FIGURE 1.E.6: Comparison of measured and predicted SRT