

**MODELLING OF THE MARIANRIDGE WASTEWATER
TREATMENT PLANT**

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Engineering in the School of Chemical Engineering at the University of KwaZul-Natal*

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ABSTRACT

One of the consequences of the social and economic change due to industrialisation is the generation of industrial wastewater which requires treatment before being released into the natural aquatic environment. The municipality has wastewater treatment plants which were initially designed for the treatment of domestic wastewater. The presence of industrial wastewater in these treatment plants introduces various difficulties in the treatment process due to the complex and varying nature of the industrial wastewater.

A means needs to be developed, that will allow the municipality to evaluate if a wastewater treatment plant can adequately treat a particular composition or type of wastewater to a quality suitable for release to the environment. Developing a simulation model for a wastewater treatment plant and calibrating it against plant operating data will allow the response of the wastewater treatment plant to a particular wastewater to be evaluated. In this study a model for the Marianridge Wastewater Treatment Plant is developed in the WEST (Worldwide Engine for Simulation, Training and Automation) software package.

The sources of data for modelling were laboratory experiments, historical data from the municipal laboratory and modelling of experiments. Dynamic input files representing the properties of the influent wastewater were generated by characterising the influent wastewater through the use of batch respirometric tests and flocculation filtration on composite samples of wastewater. Kinetic and stoichiometric coefficients of the model were determined from batch respirometric tests on wastewater and activated sludge, and simulation of the batch respirometric experiment. To make the model plant-specific it is calibrated against plant operating data.

Influent characterisation and reliable ASM3 model parameters were determined from the respirometric batch test and modelling of experiments. The resulting plant model was able to closely predict the trends of the effluent COD concentration in the plant. Hence it was concluded that the use of laboratory experiments, historical data from the municipal laboratory and modelling of experiments in order to generate information for the modelling of wastewater treatment plants makes up a methodology which can be adopted and improved by additional experiments.

GLOSSARY

| | |
|-------------------------------|---|
| Activated sludge | Product that results when primary effluent is mixed with bacteria-laden sludge and then agitated and aerated to promote biological treatment, speeding the breakdown of organic matter in raw sewage undergoing treatment. |
| Aerobic | The condition of living or acting in the presence of molecular oxygen. |
| Autotrophs | Organisms which use inorganic carbon dioxide or bicarbonate as sole carbon source for growth and development. |
| Bacteria | Single-cell, prokaryotic micro-organisms. |
| Chemical oxygen demand | Chemical oxygen demand is a measure of the capacity of water to consume oxygen during the decomposition of organic matter. |
| Heterotrophs | Organisms that require organic substrates to get carbon for growth and development. |
| Inhibition | An impairment of bacterial function. |
| Kinetics | The branch of chemistry that is concerned with the rates of change in the concentration of reactants in a chemical reaction. |
| Pollution | The introduction of contaminants into an environment, of whatever predetermined or agreed upon proportions. |
| Respiration | A biochemical process by which living organisms take up oxygen from the environment and consume organic matter, releasing both carbon dioxide and heat energy. |
| Suspended solids | Un-dissolved non-settleable solids present in wastewater. |
| Trade effluent | Any liquid which is given off as a result of any industrial, trade, manufacturing, mining or chemical process or any laboratory research or agricultural activity and includes any liquid other than standard domestic effluent or storm-water. |
| Wastewater | Water that has been used in homes, industries, and businesses that is not for reuse unless treated by a wastewater facility. |

LIST OF ABBREVIATIONS

| Name | Description |
|-------------|--|
| ASM | Activated sludge model |
| ASM1 | Activated sludge model No. 1 |
| ASM2 | Activated sludge model No. 2 |
| ASM2d | Activated sludge model No. 2d |
| ASM3 | Activated sludge model No. 3 |
| ASU | Activated sludge unit |
| BOD | Biological oxygen demand |
| COD | Chemical oxygen demand |
| DO | Dissolved oxygen |
| IWA | International Water Association |
| IAWPRC | International Association on Water Pollution Research and Control |
| IAWQ | International Association of Water Quality |
| MSL | Model Specification Language |
| ODE | Ordinary differential equation |
| OP | Ortho Phosphorus |
| OUR | Oxygen Uptake Rate |
| TKN | Total Kjeldahl Nitrogen |
| TP | Total Phosphorus |
| UCT | University of Cape Town |
| WEST | World-wide Engine for Simulation and Training |
| WISA | Water Institute of South Africa |
| WRC | Water Research Commission of South Africa |
| WWTP | Wastewater treatment plant |

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1. INTRODUCTION

The major challenge for local authorities like the eThekweni Municipality in managing industrial wastewater is to have an optimal management strategy for achieving the ultimate goal of serving all clients while meeting the required quality of treated effluent.

The key elements available to the municipality for management of industrial wastewater are the wastewater treatment plants for remediation, trade effluent permits and discharge tariffs for financing the treatment and for providing incentives and penalties for the users of the system. The relationship between these elements is complex and at times poorly understood.

This challenge is the motivation for a broad project, initiated by the eThekweni Municipality in the context of an agreement between the municipality and the University of KwaZulu-Natal to provide scientific support for municipal policies. The project's immediate goal is to provide a means of determining the link between a particular industrial effluent and the capacity of the receiving wastewater treatment plant to treat the effluent, serve other clients and meet the set standard for treated effluent. The knowledge gathered would then be used to inform the municipality during the process of setting the conditions for the industrial discharge permits.

Achieving this goal will complement the efforts of eThekweni to codify its bylaws as per requirement of the local government (Municipal Structures Act, 1998 and the Local government: Municipal Systems Act, 2000) to ensure administrative justice which includes the issuing of discharge permits to industries.

The effort to provide a mechanism for assessing the impact of wastewater discharges from industries will contribute information to the Pollution and Environmental Branch of eThekweni Municipality in their new five year permitting system for sewer discharges introduced in December 2004.

1.1. Objective of study

The main objective of this study is to produce, a calibrated process model for the Marianridge Wastewater Treatment Plant (WWTP) of the Umhlatuzana Works. The simulation model will serve as a baseline model of the WWTP which describes the performance while treating the combined wastewater generated by its catchment. This will include domestic sewage together with a proportion of industrial effluent generated by the factories in the catchment. To avoid having to characterise effluents individually from all the other factories in order to evaluate the effect of the one of interest, the baseline model is based on experimental characterisation of the combined feed to the WWTP.

The model will be developed using the WEST (Worldwide Engine for Simulation, Training and Automation) software package which offers a modelling and simulation platform for wastewater modelling and simulation.

The model will simulate the processes which happen in the actual wastewater treatment plant and assess different scenarios that occur in the wastewater treatment plant, including examining how the treatment plant will respond to various types of influent wastewater, of mainly industrial origin. This model assisted assessment will inform the process of setting the conditions for the industrial wastewater discharge permit.

1.2. Project structure

This study includes four major sections:

- a) Introduction, Literature review and Site description,
- b) Determination of model parameters,
- c) Developing and calibrating the simulation model in WEST,
- d) Discussion, Conclusion and Recommendations.

The chapters dedicated to the four major sections of the study are outlined in the following section.

Introduction, Literature review and Site description

Chapter 1 Introduction

Chapter 2 Literature review

Chapter 3 Site description

Determination of model parameters

Chapter 4 Determination of model parameters

Chapter 5 Discussion of results

Developing the model in WEST and calibration

Chapter 6 Developing the plant model

Discussion, Conclusion and Recommendations

Chapter 7 Discussion

Chapter 8 Conclusion and Recommendations

2. LITERATURE REVIEW

The literature review of subjects relevant to this study is presented in this chapter under the following key headings:

- 2.1. Prevention and control of water pollution
- 2.2. Characterisation of influent wastewater
- 2.3. Wastewater treatment processes
- 2.4. Modelling of the activated sludge process
- 2.5. Simulators for wastewater treatment plants
- 2.6. Model calibration

2.1. PREVENTION AND CONTROL OF WATER POLLUTION

Pollution of water resources originates from different sources. These sources can be classified into two categories; point and non-point sources. Point-sources are identified with pollution traceable to specific sources, such as industrial outfalls, domestic drains, municipal sewers and wastewater treatment plants, whose entry point into specific water bodies, surface or underground, can be determined. The non-point sources have ill-defined origins which are difficult to determine, such as the runoff of agricultural land where fertilisers and pesticides are used, or the runoff of urban storm water, where the point of entry into water bodies is difficult or impossible to determine.

The decline in the quality of water resources has far-reaching implications to the economy, social life and public health, hence the prevention and control of water pollution, is now established as a function of government (Burchi et al., 2003).

2.1.1. Legislative approach to water pollution control

According to Burchi et al., (2003), government-directed pollution prevention and control is implemented through the adoption of legislation based on a variety of approaches. These approaches fall into the following categories;

- forbidding the discharging of untreated wastewater into bodies of freshwater, on the ground or underground,

- restricting discharges through permits, licenses, consents or authorisation granted by the government or local authority,
- charging for the discharging of wastewater in such a way that the external costs of pollution are factored into the discharger's decisions. These approaches are employed primarily in connection with the control of point-source pollution,
- prescribing precautionary measures with respect to selected land-based activities.

These water pollution control mechanisms work with other mechanisms designed to fight water pollution, such as the standards of quality for treated effluent. Other specific mechanisms include keeping inventories of the type, extent and sources of pollution, water quality management planning, and sampling and testing the quality of receiving water bodies. These mechanisms work closely with permit requirements (Burchi et al., 2003).

2.1.2. Management of water resources in South Africa

In terms of the Constitution of the Republic of South Africa (Act No. 108 of 1996) the management of water resources is a national responsibility. The National Water Act, 1998 (Act No. 36 of 1998) mandates the Minister of Water Affairs and Forestry to ensure that water is used, conserved, protected, and managed in a sustainable and equitable manner for the benefit of all people.

The Minister of Water Affairs and Forestry, supported by the Department of Water Affairs and Forestry (DWAF), acts as the public trustee of the nation's water resources. The directorate of Water Quality Management within DWAF, and various regional offices are jointly responsible for the governance of water quality in South Africa (www.dwaf.gov.za, 2008).

2.1.2.1. The Department of Water Affairs and Forestry

The Department of Water Affairs and Forestry (DWAF) is the custodian of the water resource and overall leader of the water sector. DWAF over sees the activity of all water sector institutions and regulates water resources and water services. It is primarily responsible for the formulation and implementation of policies governing water resources and water services (Water Affairs and Forestry, 2003). Water service authorities and municipalities play a role in the implementation of DWAF policies to ensure that water is used and managed in a sustainable and equitable manner.

2.1.2.2. Municipalities managing water resources

As part of managing water resources municipalities have to address water pollution through wastewater collection and treatment in sewage works. In order to exercise legislative authority in wastewater collection and treatment, municipalities operate in terms of the sewage disposal bylaws. One way of controlling water pollution in terms of the sewage disposal bylaws is the use of wastewater discharge permits.

Permit requirements may be directed at discharging wastewater into a water body or the carrying out of activities or processes resulting in the act of discharging wastewater (Burchi et al., 2003). In both approaches the aim is to prevent water pollution by reducing the polluting potential of wastewater released into a receiving water body.

The granting of waste discharge permits

The grant or refusal by the government or local authority of a waste discharge permit according to Burchi et al., (2003) is the result of a process which is structured in the legislation as a sequence of steps, outlined below:

- a) Fulfilling requirements precedent to the filing of applications
- b) Filing of applications
- c) Review of applications
- d) Deciding on applications
- e) Formatting of waste discharge permits
- f) Appealing from adverse decision
- g) Recording of decisions and permits

Charges for discharging waste under a permit

A charging mechanism can complement the use of wastewater-discharge permits. Charges can be paid at prescribed intervals while the permit is in use. The charges can be calculated based on the characteristics of the wastewater which is discharged in order to internalise the costs of dealing with that particular wastewater. Charging can also be used independently of a system of wastewater-discharge permits, as an alternative approach to achieve water pollution control goals essentially through a financial mechanism (Burchi et al., 2003).

2.1.3. eThekwini industrial effluent permitting system

eThekwini Municipality is the local authority responsible for the greater Durban Area. As part of its activities, it has authority to control the operations of industries within its area of jurisdiction. The Pollution Division of the municipality has duties to ensure that such industries operate in accordance with the guidelines and bylaws laid down by the municipality (Guidelines for permit application, 2006). In order to ensure this, eThekwini Pollution Division, formulated a five-year permitting system for sewer discharge in December 2004 in collaboration with the Norwegian Pollution Control Authority. The aim of the collaboration was to encourage the sharing of strategies in pollution control. The purpose of this permitting system is to provide a guideline for the operations of large and other high-risk industries.

High-risk industries must implement an environmental management system in their operations to meet part of the requirements of discharge permits. To implement such a system, industries must identify and prioritise their risks, and compile a five-year improvement program to address these risks. The municipality will then assess the program against recognised international benchmarks and incorporate it into the permit. The company's performance will then be measured through reporting mechanisms, compliance monitoring and annual audits.

2.1.3.1. Duty to apply for a trade effluent permit

The duty to apply for a discharge permit follows from sewage disposal bylaws which state that no person shall discharge, cause or permit to be discharged any trade effluent except with written permission of an authorised officer and in line with the sewage disposal bylaws (Guidelines for permit application, 2006).

2.1.3.2. Application for a permit

The information required in the application includes general information on the enterprise, production, plant and process information, a site water balance, details on releases to specific media such as air, sewer, storm-water and ground water. The applicant also needs to give information on waste preventive measures and contingency plans to deal with acute pollution, environmental management systems, occupational health and safety and major hazard installations present. With respect to potential releases to specific media the applicant should list all possible sources, and for

the significant sources, provide further information indicating how the impact will be minimised or managed (Guidelines for permit application, 2006).

2.1.3.3. Processing of application for a trade effluent permit

The Pollution and Environment Department of eThekweni Water and Sanitation is the responsible authority for processing and making decisions concerning applications for permits in terms of the sewage disposal bylaws. The permit applicant has the right of appeal and to make representation before a tribunal to ensure a fair administrative procedure. The eThekweni Water and Sanitation Authority charges a fee for processing applications for discharge permits in line with the sewage disposal bylaws.

2.2. CHARACTERISATION OF INFLUENT WASTEWATER

The objective of influent wastewater characterisation is to determine the volumes and concentration of the carbon, nitrogen, phosphorus and other constituents present in the wastewater, while characterisation of the effluent provides a way to assess the extent to which transformations of the wastewater constituents occur, in relation to achieving the required effluent standards.

The wastewater composition influences the actual wastewater treatment system performance, to a extent similar to that of system design (Henze et al., 1995). A detailed knowledge of the composition of influent going into the wastewater treatment system is essential for the development of a model which will be able to predict the performance of the wastewater treatment plant (WWTP).

The wastewater entering a wastewater treatment plant will have its detailed composition determined by the following factors:

- Input to the sewer
- Type of sewer system
- Transformation in the sewer
- Physical or chemical treatment prior to the activated sludge system

Input to the sewer

The input to the sewer depends on the community served. The relative contribution by industry and the types of industry discharging to the sewer have a major effect on the wastewater characteristics. For the domestic portion of the wastewater, limited water resources cause low water usage resulting in low volume and concentrated wastewater, of greater than 1 500 mgCOD/L (Wentzel and Ekama, 2006), while unlimited water resources result in higher volumes of wastewater with lower strength. Furthermore the socio-economic status of the community, its diet and the type of detergents used are some of the many factors that have a major influence on wastewater characteristics.

Type of sewer system

The use of separate or combined sewers has a major influence on wastewater characterisation, particularly on wastewater strength and flows. Combined sewers have greatly reduced strength due to dilution, and they also have larger flows which vary more due to storm flows, when compared to separate sewers. In South Africa separate sewers are mandatory by legislation (Wentzel and Ekama, 2006). The degree of infiltration into the sewer by rainwater will also influence the wastewater characterisation.

Transformation in the sewer

During transportation through the sewer, the wastewater may undergo transformations. The transformation process depends on the conditions prevailing in the sewer: temperature, residence time, oxygen supply to the wastewater, and scour velocity. In anaerobic sewers with long residence times, sulphate reduction and acid fermentation may occur, while in aerobic sewers, COD reduction and significant biological growth may occur. In South Africa, sewers are predominantly anaerobic and residence times are very short, so that usually little acid fermentation occurs (Wentzel and Ekama, 2006).

Physical or Chemical treatment prior to the Activated Sludge Unit

Preceding unit operations for physical treatment will influence the wastewater characteristics. The unit operations that have a dominant effect are primary sedimentation and flow balancing (Wentzel and Ekama, 2006). With primary sedimentation, the COD load on the activated sludge system is considerably reduced by approximately 40%, while a smaller reduction is observed for the Total Kjeldahl Nitrogen (TKN) and Total Phosphorus (TP) (approximately 15 to 20%) (Wentzel and

Ekama, 2006). This has the effect that settled wastewaters have higher TKN/COD and TP/COD ratios than raw wastewaters.

Primary sedimentation has a marked effect on the relative contribution of the COD, TKN and P fractions because some of the particulate components are removed while the soluble components are not, resulting in the soluble COD, TKN and TP fractions making up a large proportion of the remaining settled wastewater COD, TKN and TP concentrations than in the raw wastewater.

With flow balancing the daily COD, TKN and TP loads are not significantly affected, provided the equalising tank is operated in such a way that settleable solids do not accumulate in it (Wentzel and Ekama, 2006). However flow balancing reduces the amplitude in diurnal flow and organic (COD and TKN) load variations, which cause a marked reduction on peak oxygen demand.

2.2.1. Constituents in wastewater

Chemical characterisation of municipal wastewater is concerned with three major constituents, organic compounds, nitrogenous compounds and phosphorus (Wentzel and Ekama, 2006). The organic compounds include carbohydrates, proteins and fats, while nitrogen is principally present as ammonia and phosphorus is present in the form of phosphates from domestic waste. Municipal wastewater also has other constituents of particulate and dissolved nature, which include living biomass, grit, anions and cations. All these constituents have to be dealt with at the wastewater treatment plant, hence the need to characterise the wastewater.

The quantity and concentration of each constituent fraction is assessed bio-chemically. The chemical oxygen demand (COD) test forms the basis for specifying the various fractions of organic matter, the Total Kjeldahl Nitrogen (TKN) and the Free and Saline Ammonia (FSA) tests form the basis for specifying the various nitrogen (N) constituents and the total phosphorus (TP) and orthophosphate (OP) tests form the basis for specifying the phosphorus (P) constituents of the wastewater. Chemical characterisation also involves measurement of total alkalinity, and pH.

Physical characterisation involves separating wastewater into dissolved, suspended and settleable constituents through settling and filtration.

2.2.1.1. The organic fraction in municipal wastewater

The COD of municipal wastewater is divided into three main fractions, non-biodegradable, biodegradable and active biomass. The non-biodegradable COD has two fractions, the non-biodegradable particulate and non-biodegradable soluble. The biodegradable COD also has two fractions, the slowly biodegradable and readily biodegradable COD. The active biomass consists of heterotrophic and autotrophic organisms (Wentzel et al, 1995). Figure 2:1 shows the subdivision of the total COD of municipal wastewater.

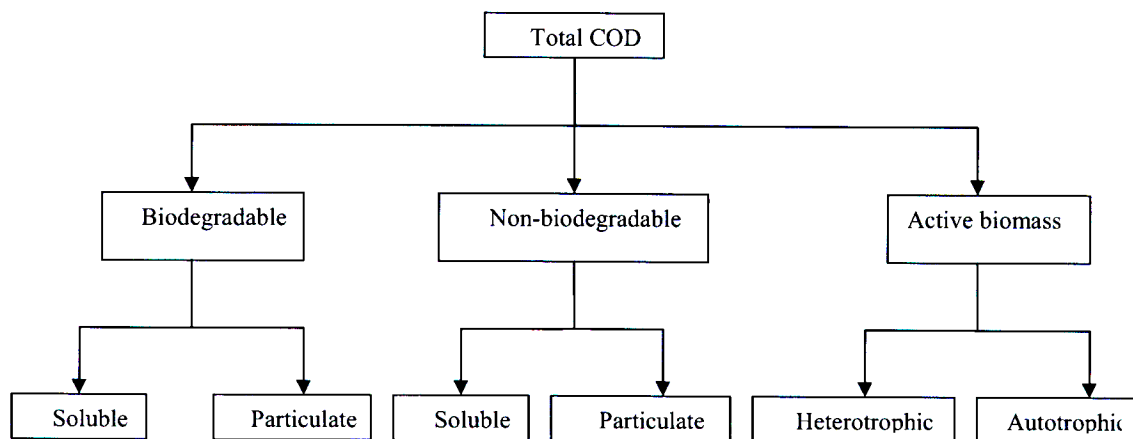


Figure 2:1 Fractions of the total COD of municipal wastewater adapted from (Petersen et al., 2000)

2.2.1.2. The nitrogen fraction in municipal wastewater

The total nitrogen concentration in municipal wastewater C_{TN} , is the sum of the Total Kjeldahl Nitrogen (TKN), and nitrite and nitrate (S_{NO}). The TKN includes organic nitrogen and Free and Saline Ammonia, but it excludes nitrate and nitrite which may be present in some wastewaters. The majority of South African municipal wastewaters will not contain nitrate or nitrite because in most sewage systems the wastewater will be in a deoxygenated state, and any nitrate entering the system is likely to be denitrified before it reaches the wastewater treatment plant (Wentzel and Ekama, 2006). The organic nitrogen is considered to be coupled to the organic COD components in the wastewater, so that it is sufficient to use fixed nitrogen fractions for the various COD components (Henze et al., 1995). The organic nitrogen is subdivided in the same way as the organic material as show in Figure 2:2.

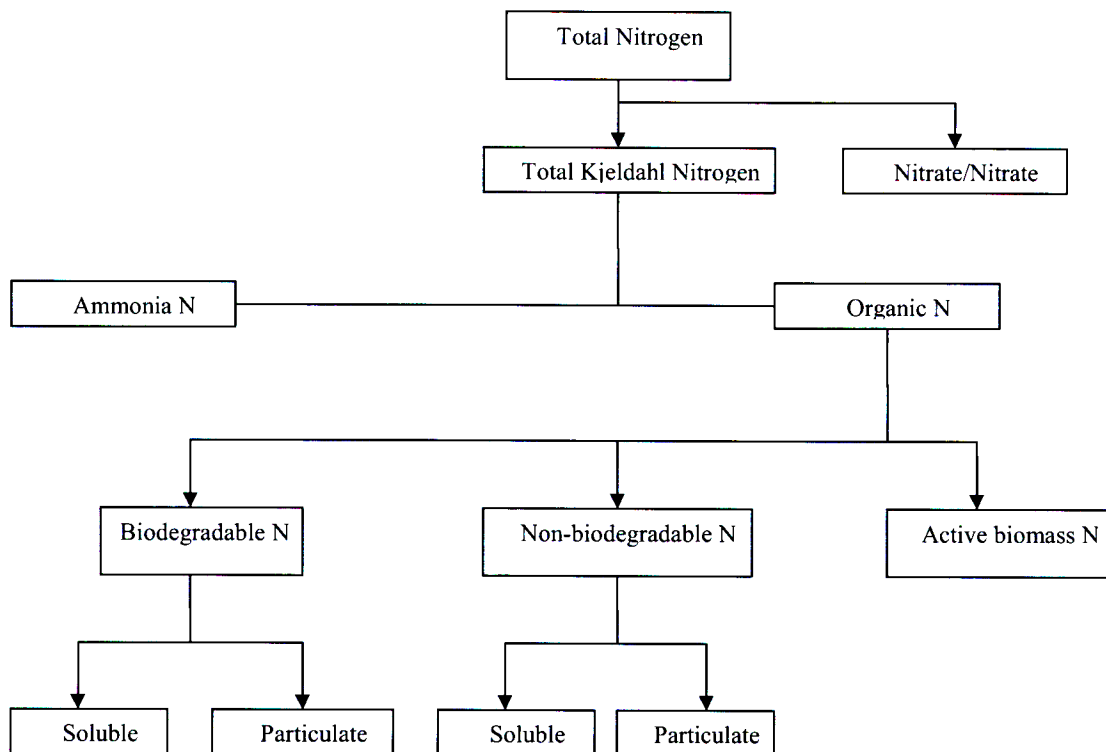


Figure 2:2 Subdivision of total nitrogen in municipal wastewater adapted from (Wentzel and Ekama, 2006)

2.2.1.3. The phosphorus fraction in municipal wastewater

The influent phosphorus is determined from the Total Phosphorus (TP) test, and Orthophosphate test. The total phosphorus test (TP) measures soluble orthophosphate, condensed orthophosphates and the phosphorus bound to organic compounds. The orthophosphate test measures the orthophosphates and a small fraction of some condensed phosphates may also be included. The difference in the P concentration between TP and orthophosphate test gives the organic P concentration (Wentzel and Ekama, 2006). The organic phosphorus is subdivided in the same way as the organic material as shown in Figure 2:3.

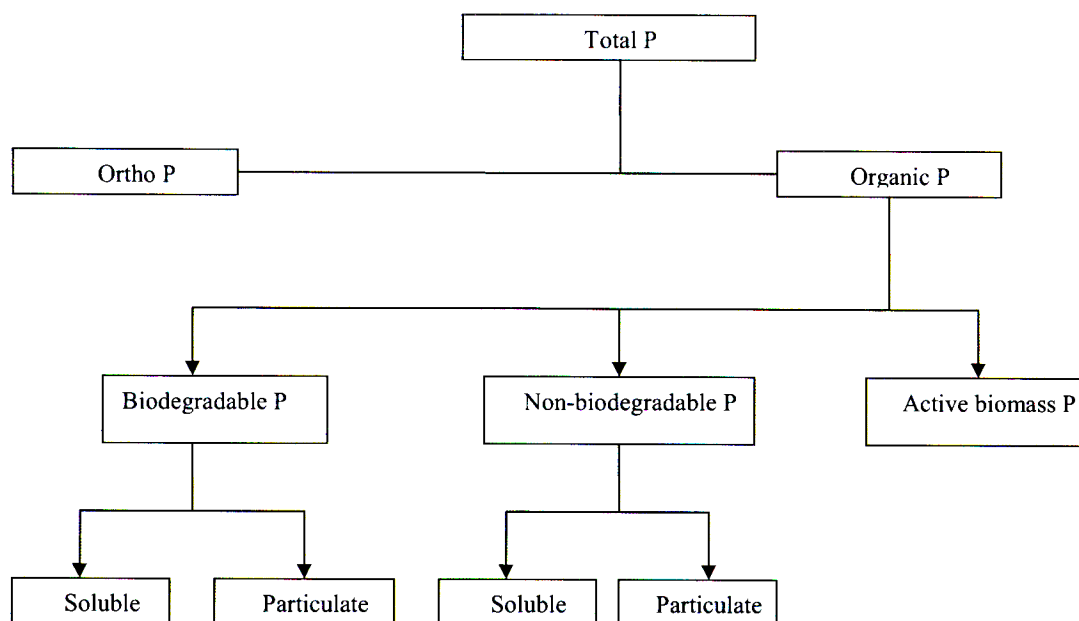


Figure 2:3 Subdivision of total phosphorus in municipal wastewater adapted from (Wentzel and Ekama, 2006)

2.2.1.4. Inorganic dissolved constituents and heavy metals

The wastewater contains other inorganic dissolved constituents which include magnesium, potassium, sodium, chloride and sulphates, which influences the performance of the wastewater treatment plants. These constituents are needed as trace elements for biological growth. A very low concentration, (5 to 20 mg/L) of elements such as Ca, Mg and K, is taken up biologically for growth (Wentzel and Ekama, 2006). These constituents are usually present well in excess of the bacteria requirements, and as a result a greater part of these constituents remain dissolved and leave the activated sludge system with the effluent stream.

Municipal wastewaters also contain potentially toxic metals and elements such as cadmium, lead, nickel, mercury, zinc, copper, chrome, cobalt, arsenic, fluorine, selenium, and boron. The greater part of these metals and elements are in particulate form and generally accumulate in the sludge formed at the treatment plant (Sneyders et al., 1998). If the final sludge produced contains potentially toxic metals and elements which exceed specified limits, then restrictions are placed on the final disposal of the sludge (WISA, 1993; WRC, 1997).

2.2.1.5. Temperature, alkalinity and pH

Temperature, alkalinity and pH of wastewater influence the behaviour of activated sludge system. The lower the temperature the slower the biological rates, in particular, the rates of nitrification and de-nitrification. Most biological reactions in activated sludge proceed optimally around a pH of between 7 and 8 (Wentzel and Ekama, 2006). Some of the biological reactions like nitrification and de-nitrification influence the pH by releasing or taking up hydrogen ions (H^+). This affects the buffering capacity of the wastewater, i.e. its ability to resist pH change. The alkalinity of the wastewater plays a central role in establishing the pH buffering capacity of the wastewater.

2.2.2. Test ratios of wastewater

Wastewater test ratios such as the TKN/COD ratio and the COD/BOD₅ ratio find application in the design of wastewater treatment plants as well as in assessing the biodegradability of wastewater.

2.2.2.1. TKN/COD ratio

The TKN/COD ratio is an important parameter to assess process nitrification/de-nitrification behaviour because it gives approximately the ratio of the nitrate generated to the de-nitrification potential. TKN/COD values less than 0.1 indicate good potential to denitrify the entire nitrate generated (WRC, 1984).

2.2.2.2. COD/BOD₅ ratio

The approximate COD/BOD₅ ratio of influent municipal wastewater, principally of domestic origin, based on data in several sources of literature is 2 (Wentzel and Ekama, 2006). The ratio indicates how biodegradable the wastewater is. The lower the ratio the more biodegradable the wastewater is. The ratio between COD and BOD varies with the type and quantity of industrial wastewater contribution, and other community practices.

2.2.3. Analytical formulation of wastewater components for modelling

The components of the influent wastewater are represented by specified components for modelling purposes. The break down of the major components in wastewater for modelling purposes using the IAW Activated Sludge Model No. 3, (ASM3) is presented in the following sections based on Gujer et al., (1999).

2.2.3.1. The organic fraction

The total organic content in wastewater is measured as the total chemical oxygen demand (COD), C_{TCOD} . For modelling based on ASM3, the influent wastewater total COD is split into seven components. The definition of each component and the typical concentrations for the organic fractions in municipal wastewater with a total COD concentration of 260 gCOD/m^3 are shown in Table 2.1.

Table 2.1 ASM3 components of total COD and their typical values in wastewater of total COD of 260 gCOD/m^3 , primary effluent (Gujer et al., 1999)

| Symbol | Component | COD [gCOD/m ³] |
|------------------|---------------------------------|-------------------------------|
| S_S | Readily biodegradable substrate | 60 |
| S_I | Soluble inert organics | 30 |
| X_I | Inert, particulate organics | 25 |
| X_S | Slowly biodegradable substrate | 115 |
| X_H | Heterotrophic biomass | 30 |
| X_A | Autotrophic, nitrifying biomass | >0 |
| X_{STO} | Organics stored by heterotrophs | 0 |

From this division the total COD is given by equation 2.3.

$$C_{\text{TCOD}} = S_S + S_I + X_I + X_S + X_H + X_A + X_{\text{STO}} \quad [2.3]$$

The concentration of autotrophic biomass, X_A , in the influent is in most cases very small, (Henze et al., 1995). The organics stored by heterotrophs, X_{STO} , is not considered to be present in the influent wastewater but it is only a functional compound required for modelling but not directly identifiable chemically (Gujer et al., 1999). Consequently the influent total COD is then represented by equation 2.4.

$$C_{\text{TCOD}} = S_S + S_I + X_I + X_S + X_H \quad [2.4]$$

Typical wastewater COD characteristics for South African municipal wastewater shows that about 7% of the total COD is non-biodegradable soluble, 13% non-biodegradable particulate, 60%

slowly biodegradable particulate and 20% readily biodegradable soluble (Wentzel and Ekama, 2006).

2.2.3.2. The nitrogenous function

Total influent nitrogen, C_{TN} is divided into Total Kjeldahl Nitrogen, C_{TKN} and (Nitrate and nitrite), S_{NO3} .

$$C_{TN} = C_{TKN} + S_{NO3} \quad [2.5]$$

Total Kjeldahl Nitrogen C_{TKN} consists of particulate and soluble Kjeldahl nitrogen X_{TKN} and S_{TKN} , respectively.

$$C_{TKN} = X_{TKN} + S_{TKN} \quad [2.6]$$

Particulate Kjeldahl Nitrogen is the sum of nitrogen bound to all organic particulate fractions.

$$X_{TKN} = (X_I \cdot i_{N,XI}) + (X_S \cdot i_{N,XS}) + (X_H + X_A) \cdot i_{N,BM} \quad [2.7]$$

For this model where X_A is negligible in the influent, the expression for X_{TKN} simplifies to equation 2.8

$$X_{TKN} = (X_I \cdot i_{N,XI}) + (X_S \cdot i_{N,XS}) + (X_H) \cdot i_{N,BM} \quad [2.8]$$

Soluble Kjeldahl nitrogen is the sum of ammonium-nitrogen and the organic soluble fractions.

$$S_{TKN} = S_{NH4} + (S_S \cdot i_{N,SS}) + (S_I \cdot i_{N,SI}) \quad [2.9]$$

Analysis of South African raw unsettled wastewaters shows that about 75% of the TKN is Free and Saline Ammonia (FSA), and 25% Organic N, which as percentage of the TKN comprise 3% non-biodegradable soluble N, 10% non-biodegradable particulate N, and 12% biodegradable N (Wentzel and Ekama, 2006).

2.2.3.3. The phosphorus fraction

The main source of some of the orthophosphate is detergents which can contribute up to 50% of the total phosphate load (Wiechers and Heynicke, 1986). In both raw and settled South African municipal wastewaters, the soluble orthophosphate fraction predominates, ranging between 70 to 90% of the total phosphorus (Wentzel and Ekama, 2006).

2.2.4. Determination of COD fractions

The determination of the COD fractions making up the total COD of the influent wastewater is discussed in the following sections.

2.2.4.1. Readily biodegradable COD, S_s and heterotrophic active biomass, X_H

Several physical and bioassay methods to measure the readily biodegradable substrate, S_s , have been proposed in the past. The physical methods are based on the hypothesis that the difference in the bio-kinetic response of activated sludge to readily biodegradable substrate, (RBCOD) and slowly biodegradable substrate (SBCOD) is due to the difference in molecular size, while bioassay methods are based on the biological response of activated sludge to the COD fractions. Heterotrophic active biomass is determined from bioassay methods.

Physical method:

In the hypothesis of physical characterisation the RBCOD consists of relatively small molecules that are readily utilised by the microbial cells whereas SBCOD consists of larger and more complex molecules which need extra-cellular breakdown during the hydrolysis process, to smaller units before utilisation. Filtration methods outlined by Dold et al., (1986), Mamais et al., (1993) and Bortone et al., (1993) making use of different filter pore sizes, have been used on wastewater to determine the RBCOD. In filtration methods, both biodegradable and un-biodegradable COD may pass through the filter, and the un-biodegradable fraction has to be quantified independently and subtracted from the COD of the filtrate to give the RBCOD and this may require sequencing measurements of filtered COD over at least 10 d in batch tests (Wentzel et al, 1995), a more involving and time consuming task.

Bioassay Method:

The division between RBCOD and SBCOD is based on the biological response to the fractions rather than physical separation. Bioassay tests, which are based on the response of activated sludge to wastewater, can be used to determine the RBCOD. These tests have found wider application as either continuous flow through systems or batch experiments. The continuous flow-through systems can be run in the form of pilot plants which provide good estimations for RBCOD but they have been criticised for their cost and difficulty to operate (Wentzel et al., 1995), while for procedures using aerobic or anoxic batch experiments, sludge acclimatized to the wastewater has to be obtained, either generated in a special laboratory-scale continuous flow through reactor or from a full-scale plant.

To determine the quantity of heterotrophic active biomass in wastewater the procedure outlined by Wentzel et al., (1995) is useful. The procedure is a result of modification of the work by Kappelar and Gujer (1992) which described a batch test to quantify heterotrophic active biomass in activated sludge. In the test by Kappelar and Gujer (1992), a small quantity of activated sludge was mixed with centrifuged wastewater supernatant and the oxygen uptake rate (OUR) response monitored with time. Kappelar and Gujer (1992) noted that the test could be adapted to quantify the heterotrophic biomass in the wastewater by excluding the activated sludge. In this light Wentzel et al., (1995), refined and developed the bioassay test which can be used to determine the readily biodegradable substrate, S_S and heterotrophic active biomass, X_H . The bioassay test is discussed in detail in the section discussing the experiments that were carried out.

2.2.4.2. Soluble inert organics, S_I

Soluble inert organic compounds cannot be degraded further under normal operating conditions of the treatment plant. To determine the concentration of soluble inert organics, S_I , Ekama et al., (1986) suggested the use of a laboratory completely mixed reactor system operated at sludge ages between 10 to 20 d. It was assumed that the inert soluble organics will be equivalent to the COD of the filtered effluent.

Later Henze et al., (1995) suggested a different method for the determination of soluble inert fraction. It consisted of removing an aliquot from the mixed liquor from a continuously fed completely mixed reactor operating at a solids retention time (SRT) in excess of 10 d and aerating it in a batch reactor (Orhon et al., 1996). The final soluble residual COD concentration determined by

periodical sampling and analysis was assumed to be equal to the soluble inert COD concentration in the feed.

The major set back of both these methods is the inability to differentiate between the soluble inert COD of the effluent and the soluble residual fraction of microbial products which may not be biodegradable. The assumption and simplification may be tolerated for domestic wastewaters provided that the existence of residual products is accounted for in the determination of other organic fractions, but it is likely to cause serious problems during the characterisation of strong industrial wastes (Orhon et al., 1996).

2.2.4.3. Particulate inert organics, X_I

The procedures for determining the concentration of particulate inert organics involve the kinetic analysis of a laboratory scale completely mixed activated sludge unit operated at steady-state with a sludge age longer than 5 d (Orhon et al., 1996). Ekama et al (1986) proposed a calculation of the concentration of X_I which involves comparing the measured mixed liquor volatile suspended solids (MLVSS) concentration with the calculated value on the basis of calculated kinetics. The IAWPRC Task Group (Henze et al., 1987) recommends a similar approach based upon the comparison of observed and calculated sludge production (Orhon et al., 1996). For these procedures, the heterotrophic yield, Y_H the endogenous decay rate, b_H and the inert fraction of biomass must be correctly determined by independent experiments.

2.2.4.4. Slowly biodegradable substrate, X_S

When the slowly biodegradable substrate X_I is not further differentiated as rapid and slowly hydrolysable components, X_I is generally determined from mass balance. With the total COD known and the other COD fractions determined the mass balance principle can be applied to determine X_S . The slowly biodegradable substrate can be determined from equation 2.10.

$$C_{\text{TCOD}} = S_S + S_I + X_I + X_S + X_H \quad [2.10]$$

2.2.5. Physical characterisation of influent

Physical characterisation of the influent based on the relative size of the particles in the wastewater and the condition of the solid particles gives three broad divisions, dissolved, non-settleable

particulate and settleable particulate. Generally in wastewater, material of particle size less than 0.1 μm is considered dissolved, while material with particle size between 0.1 and 10 μm is considered as non-settleable particulates and material with particulate size larger than 10 μm is taken as settleable particulate.

This characterisation is mainly done in order to estimate the performance of settling tanks in the treatment plant. To obtain estimates of the settleable and non-settleable particulates and the dissolved material, Mbewe et al., (1994) states that pre-flocculation followed by filtration through 0.45 μm membrane filters or glass fibre filters appears to provide reasonable separation. A more practical procedure to estimate the mass of settleable solids in wastewater is the use of the Imhoff cone (Standards Methods, 1985). The Imhoff cone is similar to a 100 mm rain gauge with a volume of 1 L. During the test it is filled with a wastewater and allowed to settle for 1 h. The fraction of suspended solids (measured in mL/L) that can be removed by the gravity settling is called the settleable solids. The settleable solids can be decanted from the Imhoff cone and measured as total solids which include both the organic and the inorganic fractions. The difference between the total solids and the ash that remains when the total solids are incinerated in an oven at 600 °C for 30 min gives the volatile solids.

2.3. WASTEWATER TREATMENT PROCESSES

The objectives of wastewater treatment can be summarised as follows;

- reduce the organic matter in wastewater to a level which no longer sustains heterotrophic growth and thereby avoid de-oxygenation of the receiving fresh water body
- oxidize ammonia to nitrate to reduce its toxicity and de-oxygenation effects
- reduce eutrophic substances (ammonia, nitrate and phosphates)

Physical, chemical and biological methods are used in wastewater treatment processes. The methods are classified as physical unit operations, chemical unit processes and biological unit processes (Metcalf and Eddy, 2003). In physical unit operations, physical forces predominate, and the unit operations include screening, mixing, sedimentation, filtration and adsorption. In chemical unit processes, conversion of constituents or removal occurs as a result of addition of chemicals or other chemical reactions occurring. Chemical unit processes include disinfection, oxidation and precipitation. In biological unit processes, treatment of wastewater occurs as a result of biological

activity, which is mainly responsible for the removal of biodegradable organic matter and nutrients in the wastewater. Biological unit processes include activated sludge and trickling filter processes.

2.3.1. Physical unit operations

The physical unit operations in the wastewater treatment plant will be discussed in the following sections.

2.3.1.1. Equalising tank

An equalisation tank is located at the head of the wastewater treatment plant to dampen the variations of the influent flow-rate and achieve a constant or near constant flow rate. This helps to overcome operational problems caused by variations of influent flow rate, and improve the performance of down stream processes as well as reduce the size and cost of down stream treatment facilities in the works (Metcalf and Eddy, 2003).

2.3.1.2. Screening

Screening is used to remove coarse material from the influent wastewater in order to protect subsequent process equipment, and increase overall treatment process reliability and effectiveness. Two types of screens are used; coarse screens (with clear openings ranging from 6mm to 150mm) and fine screens (with clear openings less than 6mm) (Metcalf and Eddy, 2003). Screening elements may consist of, parallel bars, rods, wire mesh, grating, or perforated plate. Mechanically cleaned screens can also be installed in treatment plants to minimise manual labour required to clean the screens and reduce flooding due to clogging of screens.

2.3.1.3. Grit removal

Grit chambers are used to remove grit in order to protect moving mechanical equipment from abrasion and abnormal wear and to reduce formation of heavy deposits in pipelines, channels and conduits. Some treatment plants have units called digesters for the stabilization of solids and bio-solids such as sludge. In treatment plants where digesters are present, the presence of grit chambers reduce the frequency of digester cleaning when there is excessive accumulation of grit. Grit consists of sand, gravel, cinders and other heavy solid materials that have subsiding velocities or specific gravities substantially greater than those of the organic solids in the wastewater.

To protect the influent wastewater-pumps grit chambers should be located ahead of the wastewater-pumps, but this involves placing the grit chambers at increased depth with added expense. It is therefore more economical to pump the wastewater, including the grit, to grit chambers located at a convenient position ahead of the treatment plant units, recognizing that the pumps may require greater maintenance (Metcalf and Eddy, 2003).

2.3.1.4. Primary sedimentation

Primary sedimentation is used as a preliminary step before biological treatment of the wastewater. The objective of primary sedimentation is to reduce the suspended solids content by removing readily settleable solids and floating material.

2.3.2. Biological unit operations

Biological unit operations for wastewater treatment processes include the activated sludge process, oxidation ponds, trickling filters and wetlands. The activated sludge process is discussed in the following sections.

2.3.2.1. The activated sludge process

The basic configuration of an activated sludge process consists of an aeration tank and a settler. A schematic diagram of the activated sludge process is shown in Figure 2:4.

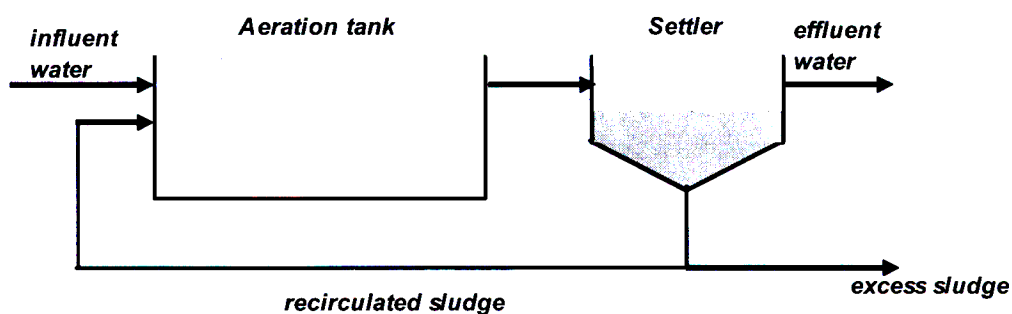


Figure 2:4 Basic configuration of an activated sludge process

The micro-organisms enter the system with influent wastewater and grow inside the aeration tank. The micro-organisms are kept suspended either by blowing air into the tank or by use of agitators. The micro-organisms use oxygen to oxidise organic matter which enters the activated sludge unit. The organic matter is converted to other forms by biological processes. Hydrolysis transforms

larger organic molecules of slowly biodegradable matter into smaller, more easily accessible molecules of readily biodegradable matter (Lindberg et al., 1997). The biomass growth rate depends on many variables such as the amount of biomass, the substrate, temperature, pH and the presence of toxins. During decay of micro-organisms, biologically inert matter is produced. This matter flows unaffected through the process and is collected and removed in the settler. The growth of the micro-organisms and influent particulate inert matter is removed from the process as excess sludge.

From the biological reactor the mixed liquor enters the secondary settling tanks so that the treated wastewater is separated from the biological sludge in order to produce a clear final effluent. The solid-liquid separation is achieved by gravity sedimentation in the secondary settling tanks. The secondary settler functions as a clarifier, to produce a clarified final effluent, and also as a thickener producing thickened sludge as under flow (Alkema et al., 1971). In order to maintain the required population of micro-organisms, and the right suspended solids concentration in the activated sludge process, the thickened sludge from the secondary settler is circulated back to the aeration tank (Lindberg et al., 1997). When the settling tanks fail to perform either of the two functions (clarification or thickening), sludge is carried over the settling tank weirs and escapes with the effluent, resulting in delivery of a poor quality effluent and uncontrolled reduction of sludge age to values below those required for efficient performance in the activated sludge unit (Alkema et al., 1971). Furthermore, secondary settlers also function as storage tanks to store sludge under high solids loading conditions and during times when there is high surface overflow rates.

Excess sludge is removed from the process to control sludge age and suspended solids concentration in the process. Sludge contains organic matter which has to be stabilised to avoid odour and reduce pathogenic content. Since the sludge contains about 95% water, it is dewatered before transportation to reduce transportation cost (Metcalf and Eddy, 2003). Stabilisation of sludge is usually done in anaerobic digesters where biogas, methane and carbon dioxide are produced during the digestion.

2.3.2.2. Extended aeration in the activated sludge process

Activated sludge process modifications exist. Each modification is done to address specific conditions or problems in the treatment process. Such modifications are characterised by differences in mixing and flow patterns in the aeration basin, and in the manner in which the

micro-organisms are mixed with the incoming wastewater. The major process modifications of the activated sludge process include extended aeration.

Extended aeration does not require primary treatment. It utilises a large aeration basin where a large population of micro-organisms is maintained. In an extended aeration basin the hydraulic retention time and the solids retention time are crucial. The hydraulic retention time (HRT) is a measure of the average length of time that a soluble compound remains in the bio-reactor, while the solids retention time (SRT) is the average time the activated-sludge solids are in the system. The extended aeration process has a long hydraulic retention time of 18 to 24h and a high solids retention time of 20 to 40d (Eckenfelder et al., 1998). This results in minimal sludge production but high oxygen requirements per amount of chemical oxygen demand (COD) removed. The process can be operated as a completely mixed reactor. Aeration is provided by rotating aerators. It is applicable during the treatment of poorly degradable organics that require high solids retention time to satisfy discharge limits (Eckenfelder et al., 1998) such as industrial wastewater with a high concentration of organics and low biodegradation rates (Woodside et al., 1999). Due to the high volume requirements of extended aeration basins the process is normally used for small flows and small communities.

2.4. MODELLING OF THE ACTIVATED SLUDGE PROCESS

Process modelling is fundamental in designing and managing wastewater treatment plants. The process model finds application in forecasting, design of the treatment plants, fault detection and monitoring plant operations (Lindberg et al., 1997). Modelling also finds application in research, where part of the natural and technical science includes developing and testing of models.

At a fundamental level a model may be a conceptual image of how a system functions, which alone cannot provide sufficient information about the behaviour of the actual system. To learn more about a system a pilot plant can be constructed. However the pilot plant may face limitations of time and resources which prevents exploration of all potentially feasible solutions of the system, hence the turn to mathematical models which allow relatively more exploration of the feasibility space (Henze et al., 1987).

The modelling of biological wastewater treatment systems has developed from fundamental concepts to mathematical models. The IAWPRC, later IAWQ and now IWA (International Water Association) task Group (Henze et al., 1987, 2000) has introduced an activated sludge model suit, which provides researchers and practitioners with a standard set of basic models for biological wastewater treatment processes.

The first model developed for municipal activated sludge WWTPs was the Activated Sludge Model No. 1 (ASM1) (Henze et al., 1987). It describes the removal of organic carbon compounds and ammonia-nitrogen, with facultative consumption of oxygen or nitrate as the electron acceptor, depending on the conditions in the activated sludge system. Other models, ASM2 and ASM2d, which include chemical precipitation processes and phosphorus removal, have also been developed. To correct a number of shortcomings of the ASM1 model, the ASM3 model was developed based on the ASM1 model. The ASM1 and ASM3 models are described in detail in the following sections.

2.4.1. Presentation of the activated sludge models-the Petersen Matrix

The IWA Activated Sludge Models are presented in a format called the Petersen Matrix. In the model, insoluble components are given the symbol X and the soluble components, S in conformity with IAWPRC nomenclature (Grau et al., 1982). Subscripts are used to specify individual components. An example of presenting and interpreting the Petersen Matrix is discussed below.

Considering the situation where heterotrophic bacteria, X_H , are growing in an aerobic environment (dissolved oxygen, S_O , will be consumed), by utilising a soluble substrate, S_S for carbon and energy the following interpretation can be done. The two fundamental processes occurring are biomass increase by cell growth and decrease by decay. The components of relevance are heterotrophic biomass, X_H , soluble substrate, S_S , and dissolved oxygen, S_O , and these are coupled to the processes through the system stoichiometry. The matrix representing the above situation is shown in Table 2.2.

Table 2.2 Petersen matrix showing the aerobic growth and decay of heterotrophic biomass (adapted from Henze et al, 1987)

| Components→ | i | 1 X _H [M(COD)L ⁻³] | 2 S _S [M(COD)L ⁻³] | 3 S _O [M(-COD)L ⁻³] | Process rate, ρ _j [ML ⁻³ T ⁻¹] |
|-------------|----|---|---|--|---|
| j Process↓ | | | | | |
| 1 Growth | 1 | | $-\frac{1}{Y}$ | $-\frac{1-Y}{Y}$ | $\mu \frac{S_S}{K_S + S_S} X_H$ |
| 2 Decay | -1 | | | -1 | $b_H \cdot X_H$ |

Where Y —yield of growth, μ —maximum specific growth rate, K_S —saturation coefficient, b_H —decay rate constant

i will take the values 1, 2 and 3 for the three components and j is equal to 1 or 2, for the two processes. The kinetic rate equations for the processes are also recorded in the matrix, and are denoted by ρ_j , where j corresponds to the process of concern. The elements within the matrix consist of the stoichiometric coefficients, v_{ij} , which give the mass relationships between the components in the individual processes. Stoichiometric coefficients are determined from experiment or predicted by applying the continuity equation provided other coefficients are known. The sign of the stoichiometric coefficient corresponds to either utilisation or formation. A negative sign representing utilisation while positive represents formation of compound.

The Petersen matrix can be used when working out the mass balances of the system. The basic equation for mass balance within a defined system boundary is:

Input - Output + Reaction (formation or consumption) = Accumulation

The input and output terms are transport terms which depend on the physical characterisation of the system being modelled. The system reaction term r_i of the component being considered in the mass balance is determined from the matrix as the sum of the product of the stoichiometric coefficients v_{ij} and the process rate expression ρ_j .

$$r_i = \sum v_{ij} \rho_j$$

For the biomass X_H ,

$$r_{XH} = \mu \frac{S_S}{K_S + S_S} X_H - b_H \cdot X_H$$

For the substrate S_s
$$r_{SS} = -\left(\frac{1}{Y}\right)\mu \frac{S_s}{K_s + S_s} X_H$$

For dissolved oxygen S_o
$$r_{SO} = -\left(\frac{1-Y}{Y}\right)\mu \frac{S_s}{K_s + S_s} X_H - b_H \cdot X_H$$

Using consistent units in the matrix allows continuity to be checked and to account for all components by moving across the matrix. The sum of stoichiometric coefficients for the particular process must be zero. Considering the decay process, and recalling that oxygen is being utilised hence its coefficient must be multiplied by (-1), the sum of the two coefficients for decay equal zero, indicating that all COD lost from the biomass due to decay must be balanced by oxygen utilization. Similarly, the continuity of the growth process can be checked.

2.4.2.ASM1

The IWA Activated Sludge Model No. 1 (ASM1) (Henze et al., 1987) is discussed in the following sections.

2.4.2.1.Organic components in ASM1

In ASM1 the total COD represent the organic matter in a wastewater, which is divided into three main fractions, non-biodegradable, biodegradable and active biomass. The non-biodegradable COD has two fractions, non-biodegradable particulate also known as particulate inert (X_I) and non-biodegradable soluble also known as soluble inert (S_I). The biodegradable COD also has two fractions, the slowly biodegradable (X_S) and readily biodegradable COD (S_S) while the active biomass consists of heterotrophic biomass, ($X_{B,H}$) and autotrophic biomass ($X_{B,A}$). Particulate products arising from biomass decay (X_P) also contribute to the total COD. Equation 2.1 gives the total COD.

$$C_{\text{TCOD}} = S_S + X_S + S_I + X_I + X_P + X_{B,H} + X_{B,A} \quad [2.11]$$

Figure 2:5 shows the COD fractions making up the total COD in ASM1.

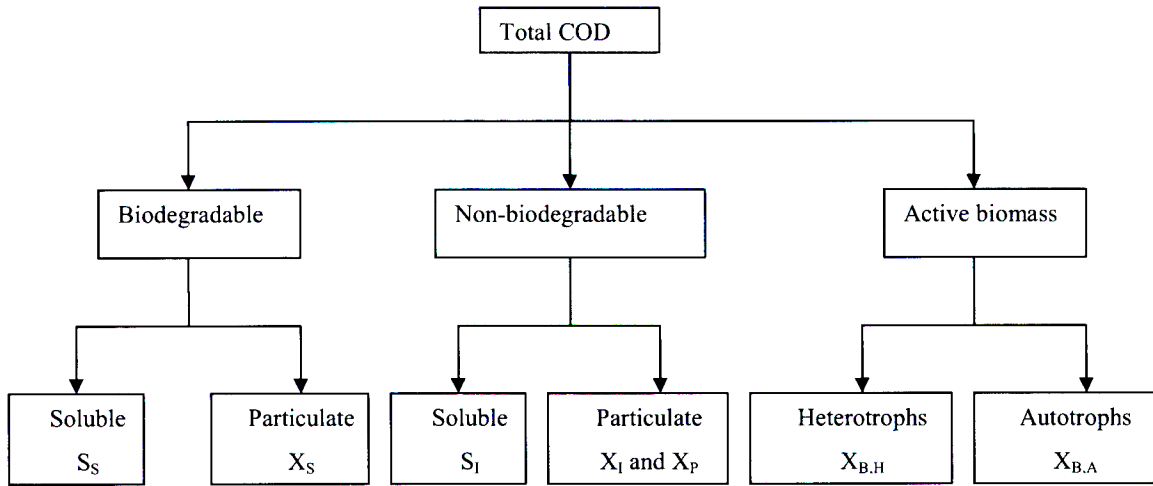


Figure 2:5 COD fractions making up the total COD in ASM1 (Petersen et al., 2000)

2.4.2.2. Nitrogen components in ASM1

For ASM1 the total nitrogen, C_{TN} in influent wastewater is divided into Total Kjeldahl Nitrogen (C_{TKN}) and nitrate and nitrite (S_{NO}). The Total Kjeldahl Nitrogen is then subdivided in a similar way as the COD, into three categories, the biodegradable, non-biodegradable and the active biomass. The biodegradable component consists of soluble ammonia nitrogen (S_{NH}) and two organic nitrogen fractions, soluble organic nitrogen (S_{ND}) and particulate organic nitrogen (X_{ND}). The non-biodegradable components are not included as separate components in the ASM1 model. The particulate non-biodegradable organic nitrogen (X_{NI}) is linked to non-biodegradable particulate components of COD and the soluble non-biodegradable organic nitrogen (S_{NI}) occurs in negligible amounts. The active biomass is also associated with a nitrogen fraction (X_{NB}) which is split between heterotrophic and autotrophic biomass ($i_{XB} \cdot X_{BH}$) and ($i_{XA} \cdot X_{BH}$) respectively. The particulate products (X_P) and inert particulate (X_I) are also associated with nitrogen fractions X_{NP} and X_{NI} respectively. Equation 2.2 gives the total nitrogen.

$$C_{TN} = S_{NH} + S_{ND} + X_{ND} + S_{NI} + X_{NI} + X_{NP} + i_{XB} \cdot X_{BH} + i_{XA} \cdot X_{BH} \quad [2.12]$$

Figure 2:6 shows the nitrogenous fractions making up the total nitrogen in influent wastewater, for ASM1.

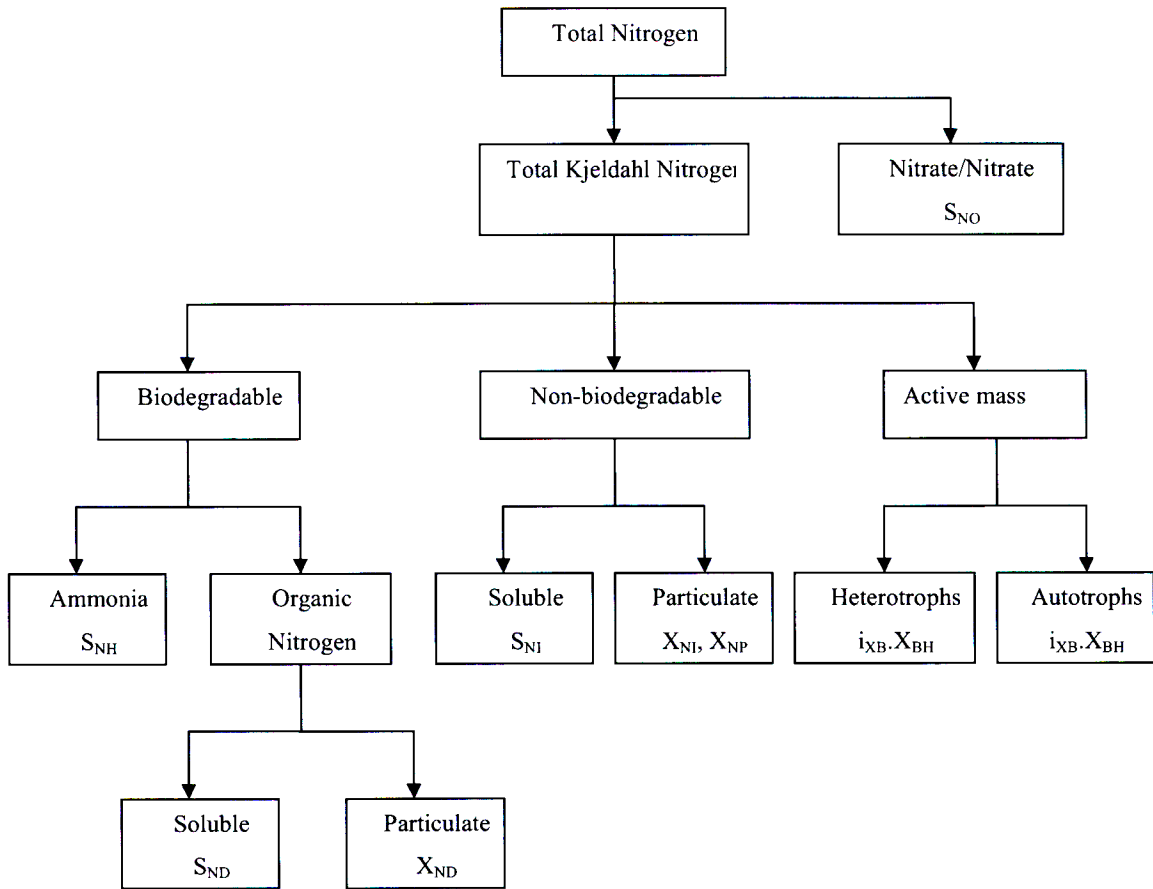


Figure 2:6 Nitrogenous fractions in influent wastewater for ASM1 (Petersen et al., 2000)

2.4.2.3. Processes in ASM1

Four processes are considered in ASM1, the growth of biomass, decay of biomass, ammonification of organic nitrogen and the hydrolysis of particulate organics which are entrapped in the bio-flocculation.

The growth of the biomass is represented by three processes; aerobic growth of heterotrophs, anoxic growth of heterotrophs and aerobic growth of autotrophs.

Aerobic growth of heterotrophs

Aerobic growth of heterotrophic biomass occurs at the expense of soluble substrate, S_s , and results in the production of heterotrophic biomass. It is associated with the utilization of oxygen, which is represented by the negative COD in the process model matrix. Ammonia nitrogen is removed from

solution and incorporated into cell mass. Monod kinetics is used to describe the process in the model matrix Table 2.3 Process 1.

Anoxic growth of heterotrophs

Anoxic growth of heterotrophs is the de-nitrification process which occurs at the expense of readily biodegradable substrate and results in heterotrophic biomass while nitrate nitrogen serves as the terminal electron acceptor. As in aerobic growth, ammonia nitrogen is converted to organic nitrogen in the biomass. The same Monod kinetics as the aerobic process is used to represent the process, but a correction factor, η_g is included to account for the anoxic process rates being slower than the aerobic process rates as shown in Table 2.3 Process 2.

Aerobic growth of autotrophs

Aerobic growth of autotrophs, results in autotrophic cell mass and nitrate nitrogen as end products. This is the nitrification process where ammonia nitrogen S_{NH} is oxidised to nitrate S_{NO} . Soluble ammonia nitrogen serves as the energy source for the growth of the nitrifiers. Oxygen is used in proportion to the amount of ammonia nitrogen oxidised as shown in Table 2.3 Process 3.

The decay of biomass is represented by two processes; decay of heterotrophs and decay of autotrophs.

Decay of heterotrophs

The decay of heterotrophic biomass is modelled using the death-regeneration concept of Dold et al., (1980). In the decay process, the biomass is converted to a combination of particulate products and slowly biodegradable substrate. The slowly biodegradable substrate is hydrolysed in the hydrolysis process. No loss of COD is involved in the split and no electron acceptor is utilised. The decay of heterotrophs is shown in Table 2.3 Process 4.

Decay of autotrophs

The decay of autotrophs is modelled in a similar manner to that of heterotrophs as seen in the model matrix shown in Table 2.3 Process 5.

Ammonification of organic nitrogen

In this process, organic ammonia (S_{ND}) is converted to ammonia nitrogen (S_{NH}) through a first order reaction accompanied by alkalinity changes. The ammonification of organic nitrogen is shown in Table 2.3 Process 6.

Hydrolysis of particulate organics is represented by two processes; the hydrolysis of entrapped organics and the hydrolysis of entrapped organic nitrogen.

Hydrolysis of entrapped organics

In this process slowly biodegradable substrate (X_S) is broken down into readily biodegradable substrate (S_S). A correction factor, η_h is included to account for the reduced hydrolysis rate under anoxic conditions. The rate of this reaction appears to saturate when the amount of entrapped substrate becomes larger in proportion to the biomass hence the importance of the ratio X_S / X_{BH} in the process rate. The hydrolysis of entrapped organics is shown in Table 2.3 Process 7.

Hydrolysis of entrapped organic nitrogen

The hydrolysis of entrapped organic nitrogen is modelled in a similar way to the hydrolysis of entrapped organics as shown in Table 2.3 Process 8.

2.4.2.4. The ASM1 matrix

The Petersen matrix for the Activated Sludge Model No.1 is shown in Table 2.3.

Table 2.3 The ASM1 model matrix

| component→ process ↓ | 1 S _I | 2 S _S | 3 X _I | 4 X _S | 5 X _{B,H} | 6 X _{B,A} | 7 X _P | 8 S _O | 9 S _{NO} | 10 S _{NH} | 11 S _{ND} | 12 X _{ND} | 13 S _{ALK} | Process rate, ρ _j |
|--|---------------------|---------------------|---------------------|---------------------|-----------------------|-----------------------|---------------------|--------------------------|----------------------|---------------------------|-----------------------|-----------------------------|---|---|
| 1 Aerobic growth of heterotrophs | | $-\frac{1}{Y_H}$ | | | 1 | | | $-\frac{1-Y_H}{Y_H}$ | | $-i_{XB}$ | | | $-\frac{i_{XB}}{14}$ | $\mu_H \left(\frac{S_S}{K_S + S_S} \right) \left(\frac{S_O}{K_{O,H} + S_O} \right) X_{B,H}$ |
| 2 Anoxic growth of heterotrophs | | $-\frac{1}{Y_H}$ | | | 1 | | | $-\frac{1-Y_H}{2.86Y_H}$ | | $-i_{XB}$ | | | $\frac{1-Y_H}{14 \cdot 2.86Y_H} - \frac{-i_{XB}}{14}$ | $\mu_H \left(\frac{S_S}{K_S + S_S} \right) \left(\frac{K_{OH}}{K_{OH} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \eta_k X_{B,H}$ |
| 3 Aerobic growth of autotrophs | | | | | | 1 | | $-\frac{4.57-Y_A}{Y_A}$ | $\frac{1}{Y_A}$ | $-i_{XB} - \frac{1}{Y_A}$ | | | $\frac{i_{XB}}{14} - \frac{1}{7Y_A}$ | $\mu_A \left(\frac{S_{NH}}{K_{NH} + S_{NH}} \right) \left(\frac{S_O}{K_{O,A} + S_O} \right) X_{B,A}$ |
| 4 Decay of heterotrophs | | | | $1-f_p$ | -1 | | f_p | | | | | $i_{XB} - f_p \cdot i_{XP}$ | | $b_H \cdot X_{B,H}$ |
| 5 Decay of autotrophs | | | | $1-f_p$ | | -1 | f_p | | | | | $i_{XB} - f_p \cdot i_{XP}$ | | $b_A \cdot X_{B,A}$ |
| 6 Ammonification of soluble organic nitrogen | | | | | | | | | | 1 | -1 | | $\frac{1}{14}$ | $k_a \cdot S_{ND} \cdot X_{B,H}$ |
| 7 Hydrolysis of entrapped organics | | 1 | | -1 | | | | | | | | | | $k_b \frac{X_S/X_{B,H}}{K_A + X_S/X_{B,H}} \left[\left(\frac{S_O}{K_{O,H} + S_O} \right) + \eta_n \left(\frac{K_{OH}}{K_{OH} + S_O} \right) \left(\frac{S_{NO}}{K_{NO} + S_{NO}} \right) \right] X_{B,H}$ |
| 8 Hydrolysis of entrapped organic nitrogen | | | | | | | | | | | 1 | -1 | | $\rho_7(X_{ND}/X_S)$ |

Table 2.3 shows the model components, processes and the process rate equations. The elements within the matrix consist of the stoichiometric coefficients. Stoichiometric coefficients are determined from experiment or predicted by applying the continuity equation.

2.4.3.ASM3

The IWA Activated Sludge Model No. 3 (Gujer et al., 1999) is discussed in the following sections.

2.4.3.1.Development of ASM3 from the ASM1

After developing ASM1, primarily for the removal of organic carbon compounds and ammonium nitrogen, a subsequent model ASM3 model (Gujer et al, 1999; Henze et al., 2000) was developed for organic carbon and biological N removal. This model was intended to correct shortcomings in the application of ASM1. The shortcomings of the ASM1 model as defined by Gujer et al., (1999) include the following:

- ASM1 does not include expressions to deal with nitrogen and alkalinity limitations.
- ASM1 considers biodegradable soluble and particulate organic nitrogen as model components. These can, however, not easily be measured and may in most cases unnecessarily complicate the use of ASM1.
- The ammonification kinetics cannot be easily quantified, and moreover this process is typically rather fast and does therefore not affect model predictions significantly.
- ASM1 differentiates between inert suspended organic matter present in the influent wastewater and produced within the activated sludge process. In reality, however, it is impossible to distinguish between these two components.
- Hydrolysis has a rather dominating effect upon the predictions of the oxygen consumption and de nitrification by heterotrophic organisms. In reality this process includes different coupled processes such as hydrolysis, lysis and storage of substrates. Therefore, the identification of the kinetic parameters of this combined process is difficult.
- The death regeneration concept is covering lysis combined with hydrolysis of released substrate and subsequently growth on this substrate. In reality it is difficult to determine the decay coefficient related to the death regeneration concept.
- Elevated concentrations of readily biodegradable organic substrates can lead to storage of polyhydroxy-alkanoates, lipids or glycogen. This process is not included in ASM1.
- ASM1 does not include the possibility to differentiate between decay rates of nitrifiers under aerobic and anoxic conditions. This may lead to problems with the predictions of the maximum nitrification rates in cases of high solids retention time and high fractions of anoxic reactor volumes.

ASM3 relates to the same dominant phenomena as does ASM1: oxygen consumption, sludge production, nitrification and de-nitrification in activated sludge systems treating wastewater of primary domestic origin (Gujer et al., 1999). The major difference between the two models is that ASM3 introduces the concept of storage-mediated growth of heterotrophic organisms assuming that all readily biodegradable substrate is first taken up and stored into an internal polymer component, X_{STO} , which is then used for growth and in ASM1 a single decay process (lysis) was introduced to describe the sum of all decay processes under all environmental conditions (aerobic, anoxic). A more realistic description of decay processes is introduced in ASM3 where the phenomena observed is close to endogenous respiration.

2.4.3.2. Components in the ASM3 model

The components of the ASM3 model are shown in Table 2.4 and the kinetic and stoichiometric coefficients of the model are also shown in Table 2.5.

Table 2.4 Short definitions for model components in ASM3 (Gujer et al., 1999)

| Soluble components | | Units |
|------------------------|--|--------------------------------------|
| S_O | Dissolved oxygen | mg O ₂ /L |
| S_S | Readily biodegradable substrate | mg COD/L |
| S_I | Inert, non-biodegradable organics | mg COD/L |
| S_{NH} | Ammonium | mg N/L |
| S_{NO} | Nitrate plus nitrite | mg N/L |
| S_{N_2} | Di-nitrogen N ₂ | mg N/L |
| S_{ALK} | Bicarbonate alkalinity | Mol HCO ₃ ⁻ /L |
| Particulate components | | |
| X_I | Inert, non-biodegradable substrate | mg COD/L |
| X_S | Slowly biodegradable substrate | mg COD/L |
| X_H | Heterotrophic biomass | mg COD/L |
| X_A | Autotrophic nitrifying biomass | mg COD/L |
| X_{STO} | Cell internal storage product of heterotrophic organisms | mg COD/L |
| X_{SS} | Suspended solids | mg TSS/L |

Table 2.5 Kinetic and stoichiometric coefficients in ASM3 (Gujer et al., 1999)

| Symbol | | Units |
|--------------|---|--|
| i_{NSI} | N content of inert soluble COD S_I | g N/g COD |
| i_{NSS} | N content of soluble substrate S_S | g N/g COD |
| i_{NXI} | N content of inert particulate COD X_I | g N/g COD |
| i_{NXS} | N content of particulate substrate X_S | g N/g COD |
| i_{NBM} | N content of biomass X_H, X_A | g N/g COD _{XBM} |
| $i_{SS,XI}$ | SS to COD ratio for X_I | g SS /g COD _{XI} |
| i_{SSXS} | SS to COD ratio for X_S | g SS /g COD _{XS} |
| i_{SSBM} | SS to COD ratio for X_S biomass X_H, X_A | g SS /g COD _{XBM} |
| f_{SI} | Production of S_I in hydrolysis | gCOD _{SI} /gCOD _{XS} |
| f_{XI} | Production of X_I in endogenous respiration | gCOD _{XI} /gCOD _{XBM} |
| $Y_{STO,O2}$ | Aerobic yield of stored product per S_S | gCOD _{XSTO} /gCOD _{SS} |
| $Y_{STO,NO}$ | Anoxic yield of stored product per S_S | gCOD _{XSTO} /gCOD _{SS} |
| $Y_{H,O2}$ | Aerobic yield of heterotrophic biomass | gCOD _{XH} /gCOD _{XSTO} |
| $Y_{H,NO}$ | Anoxic yield of heterotrophic biomass | gCOD _{XH} /gCOD _{XSTO} |
| Y_A | Yield of autotrophic biomass per NO_3^- -N | gCOD _{XA} /gN _{SNO} |

2.4.3.3. Processes in the ASM3 model

The processes in the Activated Sludge Model No.3 are discussed in the following sections.

Hydrolysis

This is the process which breaks down the slowly biodegradable substrate X_S into readily biodegradable substrate S_S . In ASM3, the hydrolysis process is assumed to be active independent of the electron donor present and it is of less dominating importance for the rates of oxygen consumption and de-nitrification.

Aerobic storage of readily biodegradable substrate

This process which requires energy from aerobic respiration, describes the storage of readily biodegradable substrate S_S in the form of cell internal storage products X_{STO} . It is assumed that all substrate first becomes stored material before it is later assimilated to biomass.

Anoxic storage of readily biodegradable substrate

This process is identical to aerobic storage, but de-nitrification rather than aerobic respiration provides the required energy, and a correction factor (η_{NO}) is included to account for the fact that only a fraction of the heterotrophic biomass maybe capable of denitrifying.

Aerobic growth of heterotrophs

Heterotrophic organisms grow off the substrate which is assumed to consist of entirely stored organics X_{STO} . Oxygen is utilized during the growth process and nitrogen is incorporated into biomass.

Anoxic growth of heterotrophs

This process is similar to aerobic growth but respiration is based on de-nitrification. A correction factor, η_{NO} is included to account for the reduced growth of biomass observed in anoxic respiration compared to aerobic respiration. The reaction rate also depends on the ratio of stored organics to heterotrophic biomass present X_{STO}/X_H .

Aerobic endogenous respiration

This process describes all forms of biomass loss and energy requirements not associated with growth by considering related respiration under aerobic conditions which include, endogenous respiration, lysis, predation, death and others.

Anoxic endogenous respiration

This process is similar to aerobic endogenous respiration but typically slower, because of lower activity under denitrifying conditions than under aerobic conditions.

Aerobic respiration of storage products

This process is analogous to endogenous respiration. It assures that storage products, X_{STO} decay together with biomass.

Anoxic respiration of storage products

This process is analogous to the aerobic process but occurs under denitrifying conditions.

2.4.3.4.ASM3 model matrix

The model matrix of the ASM3 is shown in Table 2.6.

Table 2.6 The ASM3 model matrix excluding the process rate equations

| Component i → ↓ Process j | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 |
|--|-----------|-------------|-----------|-------|-------|------------------------|-------|---|---------------------------|-------------------------------|---------------------------------------|------------------------------|---|
| | S_I | S_S | X_I | X_S | X_H | X_{STO} | X_A | X_{TSS} | S_O | S_{NO} | S_{NH} | S_{N2} | S_{ALK} |
| 1 Hydrolysis | f_{S_i} | $1-f_{S_i}$ | | -1 | | | | $-i_{TS,AS}$ | | | $i_{NAS} - i_{NSS} \cdot (1-f_{S_i})$ | | $\frac{i_{NAS} - i_{NSS} \cdot (1-f_{S_i})}{14}$ |
| 2 Aerobic storage of COD | | -1 | | | | Y_{STO,O_2} | | $0.6 \cdot Y_{STO,O_2}$ | $Y_{STO,O_2} - 1$ | | i_{NSS} | | $\frac{i_{NSS}}{14}$ |
| 3 Anoxic storage of COD | | -1 | | | | $Y_{STO,NO}$ | | $0.6 \cdot Y_{STO,NO}$ | | $-\frac{1-Y_{STO,NO}}{2.86}$ | i_{NSS} | $\frac{1-Y_{STO,NO}}{2.86}$ | $\frac{i_{NSS} + \frac{1-Y_{STO,NO}}{2.86}}{14}$ |
| 4 Aerobic growth | | | | | 1 | $-\frac{1}{Y_{H,O_2}}$ | | $i_{TS,BM} \cdot \frac{0.6}{Y_{H,O_2}}$ | $1 - \frac{1}{Y_{H,O_2}}$ | | $-i_{NBM}$ | | $-\frac{i_{NBM}}{14}$ |
| 5 Anoxic growth | | | | | 1 | $-\frac{1}{Y_{H,NO}}$ | | $i_{TS,BM} \cdot \frac{0.6}{Y_{H,NO}}$ | | $\frac{1-1/Y_{STO,NO}}{2.86}$ | $-i_{NBM}$ | $-\frac{1-1/Y_{H,NO}}{2.86}$ | $\frac{i_{NBM} + \frac{1-1/Y_{STO,NO}}{2.86}}{14}$ |
| 6 Aerobic endogenous respiration of heterotrophs | | | f_{X_i} | | -1 | | | $f_{X_i} \cdot i_{TS,X_i} - i_{TS,BM}$ | $-(1-f_{X_i})$ | | $i_{NBM} - f_{X_i} \cdot i_{NXI}$ | | $\frac{i_{NBM} - f_{X_i} \cdot i_{NXI}}{14}$ |
| 7 Anoxic endogenous respiration of heterotrophs | | | f_{X_i} | | -1 | | | $f_{X_i} \cdot i_{TS,X_i} - i_{TS,BM}$ | | $-\frac{1-f_{X_i}}{2.86}$ | $i_{NBM} - f_{X_i} \cdot i_{NXI}$ | $\frac{1-f_{X_i}}{2.86}$ | $\frac{i_{NBM} - f_{X_i} \cdot i_{NXI} - \frac{f_{X_i} - 1}{2.86}}{14}$ |
| 8 Aerobic respiration of X_{STO} | | | | | | -1 | | -0.6 | -1 | | | | |
| 9 Anoxic respiration of X_{STO} | | | | | | -1 | | -0.6 | | $-\frac{1}{2.86}$ | | $\frac{1}{2.86}$ | $\frac{1}{14 \cdot 2.86}$ |
| 10 Nitrification | | | | | | | 1 | $i_{TS,BM}$ | $1 - \frac{4.57}{Y_A}$ | $\frac{1}{Y_A}$ | $-i_{NBM} - \frac{1}{Y_A}$ | | $\frac{-i_{NBM} - 2/Y_A}{14}$ |
| 11 Aerobic endogenous respiration of autotrophs | | | 0.2 | | | | -1 | $f_{X_i} \cdot i_{TS,X_i} - i_{TS,BM}$ | $-(1-f_{X_i})$ | | $i_{NBM} - f_{X_i} \cdot i_{NXI}$ | | $\frac{i_{NBM} - f_{X_i} \cdot i_{NXI}}{14}$ |
| 12 Anoxic endogenous respiration of autotrophs | | | f_{X_i} | | | | -1 | $f_{X_i} \cdot i_{TS,X_i} - i_{TS,BM}$ | 1 | $-\frac{1-f_{X_i}}{2.86}$ | $i_{NBM} - f_{X_i} \cdot i_{NXI}$ | $\frac{1-f_{X_i}}{2.86}$ | $\frac{i_{NBM} - f_{X_i} \cdot i_{NXI} + \frac{1-f_{X_i}}{2.86}}{14}$ |

The ASM3 process rate equations are shown in Table 2.7.

Table 2.7 Process rate equations for ASM3

| j Process | Process rate ρ_j |
|--|--|
| 1 Hydrolysis | $k_h \cdot \frac{X_S / X_H}{K_X + X_S / X_H} \cdot X_H$ |
| 2 Aerobic storage of COD | $k_{STO} \cdot \frac{S_O}{K_O + S_O} \cdot \frac{S_S}{K_S + S_S} \cdot X_H$ |
| 3 Anoxic storage of COD | $k_{STO} \cdot \eta_{NO} \cdot \frac{K_O}{K_O + S_O} \cdot \frac{S_{NO}}{K_{NO} + S_{NO}} \cdot \frac{S_S}{K_S + S_S} \cdot X_H$ |
| 4 Aerobic growth of heterotrophs | $\mu_{mH} \cdot \frac{S_O}{K_O + S_O} \cdot \frac{S_{NH}}{K_{NH} + S_{NH}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{STO} / X_H}{K_{STO} + X_{STO} / X_H} \cdot X_H$ |
| 5 Anoxic growth of heterotrophs | $\mu_{mH} \cdot \eta_{NO} \cdot \frac{K_O}{K_O + S_O} \cdot \frac{S_{NO}}{K_{NO} + S_{NO}} \cdot \frac{S_{NH}}{K_{NH} + S_{NH}} \cdot \frac{S_{ALK}}{K_{ALK} + S_{ALK}} \cdot \frac{X_{STO} / X_H}{K_{STO} + X_{STO} / X_H} \cdot X_H$ |
| 6 Aerobic endogenous respiration of heterotrophs | $b_{H,O_2} \cdot \frac{S_O}{K_O + S_O} \cdot X_H$ |
| 7 Anoxic endogenous respiration of heterotrophs | $b_{H,NO} \cdot \frac{K_O}{K_O + S_O} \cdot \frac{S_{NO}}{K_{NO} + S_{NO}} \cdot X_H$ |
| 8 Aerobic respiration of X_{STO} | $b_{STO,O_2} \cdot \frac{S_O}{K_O + S_O} \cdot X_{STO}$ |
| 9 Anoxic respiration of X_{STO} | $b_{STO,NO} \cdot \frac{K_O}{K_O + S_O} \cdot \frac{S_{NO}}{K_{NO} + S_{NO}} \cdot X_{STO}$ |
| 10 Aerobic growth of Autotrophs, Nitrification | $\mu_{mA} \cdot \frac{S_O}{K_{A,O} + S_O} \cdot \frac{S_{NH}}{K_{A,NH} + S_{NH}} \cdot \frac{S_{ALK}}{K_{A,ALK} + S_{ALK}} \cdot X_A$ |
| 11 Aerobic endogenous respiration of autotrophs | $b_{A,O_2} \cdot \frac{S_O}{K_{A,O} + S_O} \cdot X_A$ |
| 12 Anoxic endogenous respiration of autotrophs | $b_{A,NO} \cdot \frac{K_{A,O}}{K_{A,O} + S_O} \cdot \frac{S_{NO}}{K_{A,NO} + S_{NO}} \cdot X_A$ |

The ASM3 was chosen as the mathematical model for the Marianridge WWTP, given that it is a more representative model developed to correct the shortcomings of ASM1 mentioned earlier in section 2.4.3.1. The ASM3 model matrix contains the relevant processes to model the activated sludge unit at Marianridge WWTP. In the event that the identified processes in the ASM3 model are not relevant or more processes are required to model the actual plant of concern, the model matrix can be modified by adding or removing processes together with the associated rate equations, components and stoichiometric coefficients. No modification was done to the original ASM3 model matrix.

2.5. SIMULATORS FOR WASTEWATER TREATMENT PLANTS

Different simulators for wastewater treatment plants have been developed and are commercially available. A few examples are shown in Table 2.8.

Table 2.8 A few examples of commercially available simulators for wastewater treatment plants

| Simulator | Company | Web address |
|------------------|--------------------|---|
| WEST | MOST for WATER NV | http://www.mostforwater.com/EN/index.php |
| Efor | DHI | www.efor.dk/efor/ |
| Simba | IFAK | www.ifak.fgh.de/regelung |
| JASS | Uppsala University | www.it.uu.se/research/project/jass/ |

2.5.1. WEST

This study was carried out under the Pollution Research Group (PRG). WEST (Worldwide Engine for Simulation, Training and automation) was the software package available for wastewater-treatment modelling purposes. In this study, the WEST program is used to simulate respirometric experiments that were carried out as well as to develop the process model for the plant and run simulations. Advantages of using WEST include the relative ease with which models can be modified or extended to accommodate new components like industrial wastewater components. WEST is a software package managed by MSL (Model Specification Language) which is used for developing simulations of environmental systems and processes taking place in wastewater treatment plants. WEST consists of four different subprograms where the user accesses the different utilities in order to set up a configuration for a system, launch an experiment and manage the project of concern. The subprograms are:

- WEST manager
- WEST configuration builder
- WEST experimental environment
- WEST model editor

2.5.1.1.WEST manager

The WEST manager gives the user an overview of the different projects created and allows for new projects to be created. For each created project, a list of the different configuration and or experiments assigned to that project can be viewed in the WEST manger (Amerlinck, 2004).

2.5.1.2.WEST configuration builder

The WEST configuration builder allows the user to select, drag and drop process nodes which represent the unit processes in the wastewater treatment plant being modelled. The selected process nodes are then connected to each other by connectors to form the plant layout (WEST tutorial, 2004).

2.5.1.3.WEST experimental environment

The WEST experiment environment is used to run simulations of the plant layout which has been generated in the configuration builder. Dynamic simulations of the plant model are run in the WEST experiment after specifying the values of model parameters for the initial conditions and choosing the required integrator settings (WEST tutorial, 2004).

2.5.1.4.WEST model editor

In the WEST model editor the user can design an alternative model by use of the matrix notation and implementing it in the WEST hierarchical structure. The WEST model editor is also used to program the different text files, which control the WEST hierarchical structure, in MSL (WEST MSL reference guide, 2004).

2.5.1.5.The WEST solution procedure

The sub-models in WEST model library use mass-fluxes as the reference unit. In processes dealing with liquids and suspension, concentrations are usually measured in the liquid phase and it is assumed that perfect mixing is achieved. Applying the mass conservation principle to the fluxes, the following is obtained:

$$\frac{d(M)}{d(t)} = 0 \text{ (WEST models guide, 2004)} \quad [2.13]$$

Where M = mass in the entire system for each component

The mass M can be broken down into the different components M_i ; water, biological and chemical components. The mass balance in a tank with a certain volume and different incoming and outgoing flows α can be expressed using ordinary differential equations as follows:

$$\begin{aligned} \frac{d(M_i)}{d(t)} &= \sum_{\alpha} (\phi_{i\alpha}) + r_i \cdot V \\ \frac{d(V)}{d(t)} &= \sum_i \left(\frac{1}{\rho_i} \cdot \sum_{\alpha} \phi_{i\alpha} \right) \end{aligned} \quad \text{(WEST models guide, 2004)} \quad [2.14]$$

Where:

- M_i = mass of component (g)
- V = volume of the tank (m^3)
- $\phi_{i\alpha}$ = net in/out flux of component i in the flow α (g/s)
- r_i = reaction speed of component i ($g/m^3 \cdot s$)
- ρ_i = density of component i (g/m^3)

Based on the sub-model selected for each unit WEST sets up differential equations for the entire plant using the methodology stated above; i.e. the set of equations that describe the system. When WEST performs a simulation, the system of ordinary differential equations is numerically integrated in time and the resulting algebraic equations are simultaneously solved. Three methods are available for WEST to perform the numerical integration (Amerlinck, 2004):

- Fixed step size integrator. This is an integrator that takes a constant step in order to solve the integration of the system of ordinary differential equations. The available fixed step integrators in WEST are; AB2, AB3, AB4, Euler, Heun, Midpoint, Milne, Modified Euler and Runge-Kutta of the 4th order)
- Adaptive step size integrator. This is an integrator that modifies its step size in order to obtain optimal calculation speed and optimal calculation accuracy. WEST only offers the Runge-Kutta 4th order adaptive step size controller (RK4ASC) as an adaptive step size integrator.
- Stiff solvers. This obtains a high performance gain for stiff systems. A stiff system is a system is where there is a large difference between the time constants of the processes (e.g.

biological and chemical processes). The two stiff solvers found in WEST are Rosenbrock and CVODE.

- The RK4ASC integrator was used in the WEST simulations carried out in this study for its speed and accuracy.

2.6. MODEL CALIBRATION

Model calibration is the adaptation of the model to fit a certain set of information obtained from the full-scale wastewater treatment plant under study (Petersen et al, 2002). The purpose of the model determines how to approach the calibration, as well as the quality and quantity of information required to achieve the calibration, hence the challenge in generalising the procedure of model calibration (Henze et al, 1995).

2.6.1. Calibration of activated sludge models

Successful calibration of activated sludge models involves collecting information for model calibration, parameter estimation and adopting a stepwise calibration procedure in which different parts of the model are calibrated in each stage (Petersen et al, 2002).

2.6.1.1. Information required for successful model calibration

The purpose of the model determines to a certain level the information required for calibration. For general purposes where a model does not have to describe a real existing plant, such as the use of a model for educational purposes, or comparison of design alternatives of non-existent plants, default (ASM) parameters for typical municipal sewage maybe sufficient (Henze et al., 1999). However when a plant-specific model has to be set up, a more accurate model calibration procedure is necessary to fine tune the default parameters. To achieve successful calibration in such a situation will require more plant specific information.

For successful model calibration, different classes of information are essential. Various sources which include, Henze et al., (1987), Lesouef et al., (1992), Stokes et al., (1993) and Kristensen et al., (1998) describe the information required for successful calibration as listed below:

- Design and operational data, which includes reactor volumes, aeration capacities, pump flows, recycle and waste flow rates.

- Characterization of the biological model includes wastewater compositions of influent, intermediate and effluent streams, as well as sludge compositions, as average or dynamic trajectories.
- Characterization of the settler model, which consists of zone settling velocities at different mixed liquor suspended solids concentration.
- Characterization of hydraulic model which can be achieved through the use of tracer tests.
- Reaction kinetics and stoichiometry information, which includes yield coefficients, growth and decay rates

The sources of information for model calibration include the following:

- Default values from literature
- Full scale plant data
- Average or dynamic data from grab or time-flow proportional samples
- Mass balances on the full scale plant
- On-line data
- Information from lab scale experiments with wastewater and activated sludge from the full scale plant under study

(Petersen et al., 2002)

2.6.1.2. Parameter estimation

The calibration of activated sludge models involves determining the optimal values of model parameters through the use of mathematical algorithms with the aid of measured data. Before starting the parameter estimation, the structure of the calibration procedure has to be defined. The model parameters have to be selected and the measured experimental data needs to be defined.

To initiate the estimation, an initial guess of concentrations and parameters need to be given. The routine of parameter estimation consists of minimising a defined objective function, such as the sum of squared error between the model output and the measured data. When the objective function reaches a minimum with a given accuracy the optimal parameter values are obtained (Petersen et al., 2002). Figure 2:7 illustrates the routine for parameter estimation.

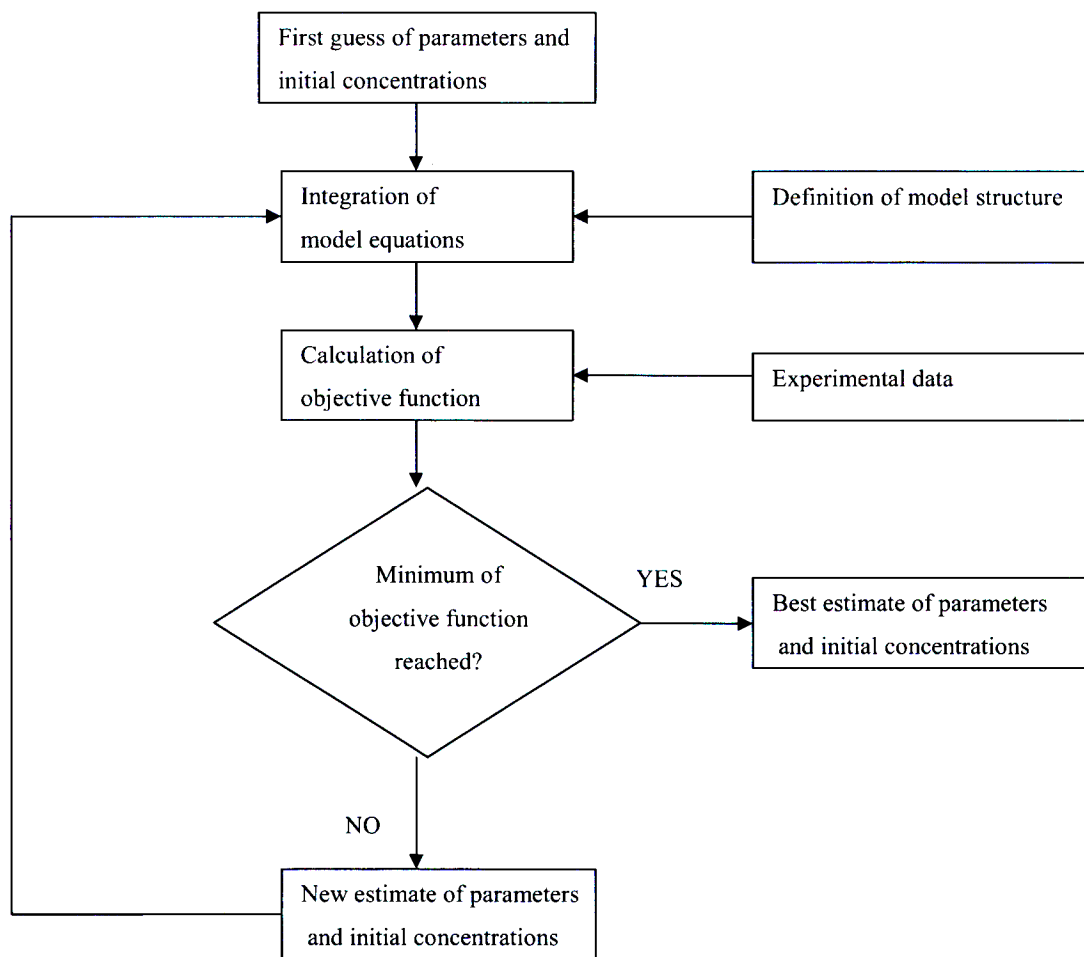


Figure 2:7 Illustration of the routine used for parameter estimation (Petersen et al., 2002)

2.6.1.3. Model calibration levels

A major challenge encountered in calibration of activated sludge models is the lack of identifiability of the model parameters, which is the ability to obtain a unique combination of parameters that fit the calibration data. Identifiability can be described as either theoretical or practical. Theoretical identifiability deals with the question whether it is possible to obtain unique parameter values from a selected set of ideal noise-free measurements, while practical identifiability includes the quality of the data. For instance, it has been shown that parameters may be unidentifiable in practice because of noise corrupted data, although these parameters are theoretically identifiable (Holmberg, 1982; Jeppsson, 1996).

Due to the identifiability problem a stepwise procedure is used to calibrate activated sludge models, where just a few parameters are changed at a time instead of applying an automatic mathematical optimisation routine for all the parameters. A steady state calibration is usually done and followed by a dynamic calibration (Petersen et al., 2000).

An overview of the general steps in an activated sludge model calibration is shown in Figure 2:8.

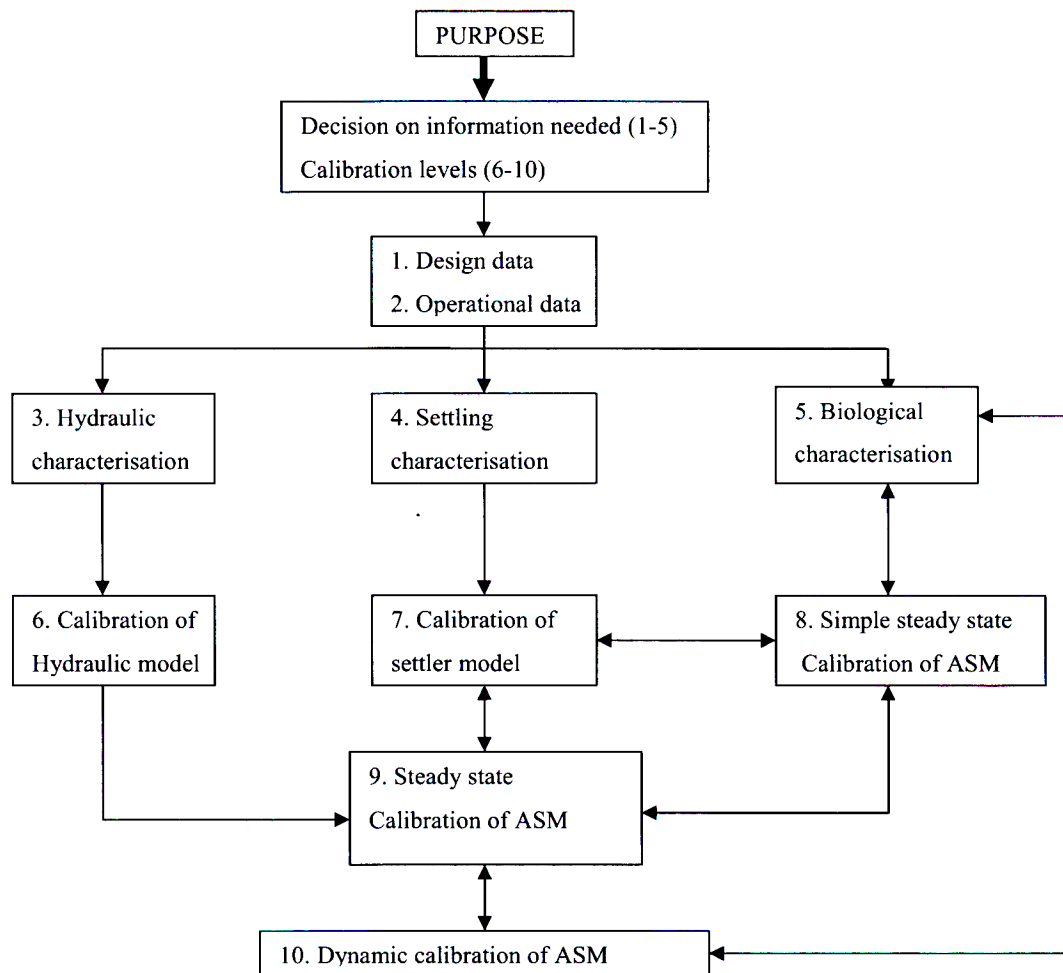


Figure 2:8 Overview of the different steps in an activated sludge model calibration procedure (Petersen et al., 2002)

Steps 1 to 5 shows the collection of information required for model calibration. Steps 6 to 10 illustrate the calibration levels. This involves the calibration of the hydraulic model settler model and the activated sludge model (ASM).

To calibrate the activated sludge model the first level is usually a steady state calibration. During the steady state calibration, data from the full scale WWTP are averaged and it is assumed that this average is representative of a steady state. The model is then calibrated to average effluent and sludge data. During the steady state calibration parameters responsible for long term behaviour of the WWTP are determined. These include the yield of heterotrophic biomass Y_H , the decay constant for heterotrophic biomass b_H and the inert organics in the influent wastewater, X_I .

The model can not rely on steady state calibration only. During dynamic simulations the input variations are usually faster than the slow process dynamics on which the steady state calibration is based. There is need for dynamic calibration to achieve better dynamic simulations. A steady state calibration is useful in determining the initial values of model parameters for dynamic calibration. The values of model parameters obtained from a steady state calibration are used as initial guesses during dynamic calibration. During dynamic calibration the modeller uses information from laboratory experiments carried out on sludge and wastewater samples from the WWTP understudy to tune the model towards achieving acceptable predictions (Petersen et al., 2002). Validation of the model is done after calibration by evaluating how well the model out-put fits a set of measured data, which was not used to calibrate the model.

3. SITE DESCRIPTION

The site description of Umhlatuzana Works is presented in this chapter with focus on the Marianridge WWTP.

3.1. Layout of Umhlatuzana Works

Umhlatuzana Works consists of the two plants; Marianridge WWTP and Shallcross WWTP. The layout of Umhlatuzana Works is shown in Figure 3:1.

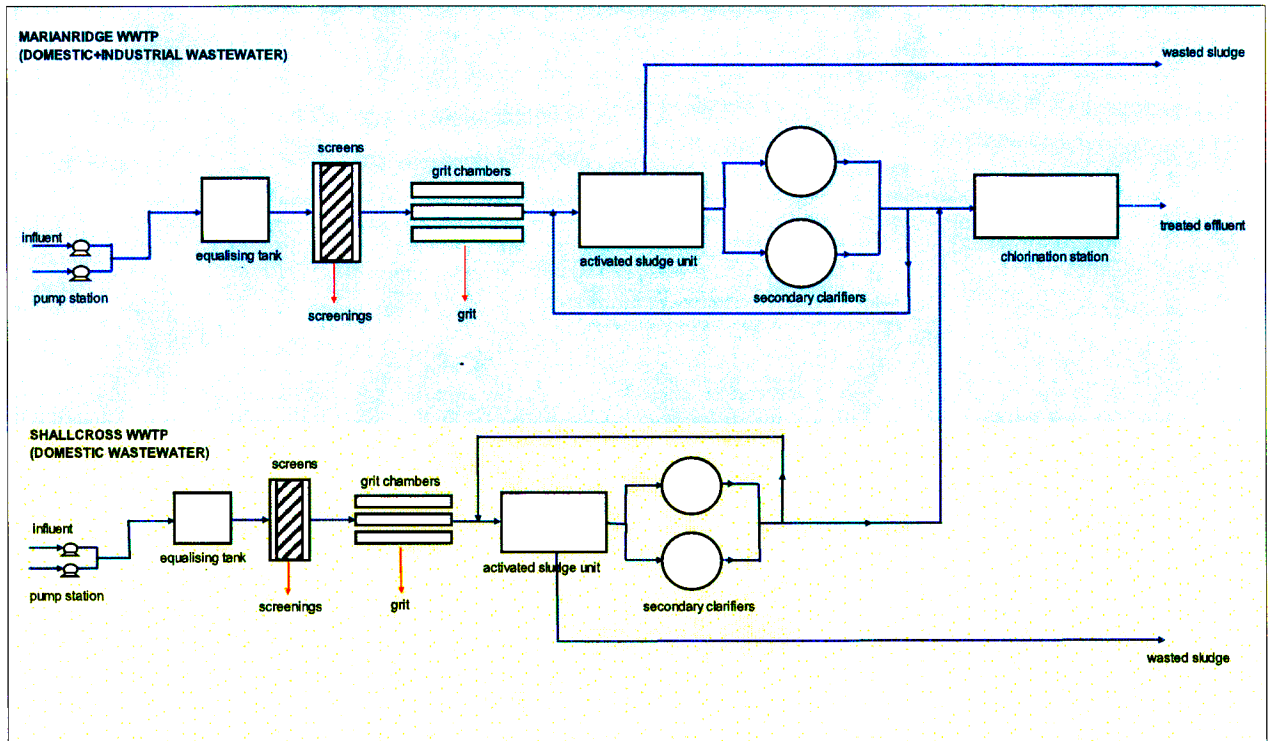


Figure 3:1 Lay-out of Umhlatuzana Works, showing Marianridge WWTP, Shallcross WWTP and the Chlorination Station

The layout in both wastewater treatment plants consists of identical unit operations but the units of the Shallcross WWTP are smaller than those of Marianridge WWTP. In both plants, the physical unit operations consist of screens, and grit chambers. The biological reactors used are operated as extended aeration basins, which are followed by secondary treatment in secondary settling tanks. The effluent from the two plants is combined and dosed with chlorine before it is released to the Umhlatuzana River.

3.1.1.The Marianridge wastewater treatment plant

The units making up the Marianridge WWTP are discussed in the following subsections.

3.1.1.1.Physical treatment

The influent wastewater is received at the raw sewage pump-station which has two pumps rated at 260 L/s and 33.8 m head. The wastewater is pumped to the equalising tank and then it flows through two hand raked screens with a bar spacing of 25 mm. The amount of screenings removed is 140 L/ML of wastewater. Screenings are removed daily and sent for disposal at a landfill.

After screening, the wastewater flows through a four-channel grit chamber where sand and other heavy particles settle in the channels. The grit is removed manually and sent to a landfill. A flow meter measures the flow rate of the wastewater after the grit chamber.

3.1.1.2.Biological treatment

The activated sludge unit at the Marianridge WWTP is an extended aeration basin with no phosphorus removal facilities. No chemical precipitation processes are employed in the unit. The basin capacity is 13 600 m³ with a depth of 4.5 m. There are eight aerators, each rated at 55 kW, producing an aeration capacity of 100 kgO₂/h. This provides the required oxygen for metabolic processes and the energy for mixing.

Four aerators are on line at any one time. The solids retention time of the Marianridge aeration basin is 21 to 25 d. This is in line with recommendations for extended aeration. The extended aeration basin operates at a hydraulic retention time between 18 to 24 h and a solids retention time of 20 to 40 d (Eckenfelder and Grau, 1998).

Ideally the aeration basin should be completely mixed and aerated so that no de-nitrification occurs. The operation of four aerators at a time instead of eight leads to anoxic zones in the basin which allow de-nitrification to take place. 500 m³/d of excess sludge is wasted from the aeration basin, and carried by pipeline to a larger works for further processing.

3.1.1.3. Secondary treatment

From the aeration basin the mixed liquor flows to two secondary settlers where particulate matter settles under gravity. The secondary settlers both have diameters of 29.4 m and depth of 3 m. The retention time in each secondary settler is approximately 6 h. The effluent which leaves as over-flow from the settlers is sent for chlorination before it leaves the treatment plant.

3.1.2. The Shallcross wastewater treatment plant

The Shallcross WWTP has similar units making up the treatment process but at a reduced scale since Shallcross WWTP handles about a quarter of the load received into Marianridge WWTP. The specifications of the Shallcross Plant were not investigated in this study.

3.2. Flow balance of Umhlatuzana Works

The nominal flow balance of Umhlatuzana Works is shown in Figure 3:2. Marianridge WWTP receives a nominal average of 8 000 m³/d of which about 30% is industrial wastewater and 70% domestic wastewater, while Shallcross WWTP receives a nominal average of 2 000 m³/d which is entirely domestic wastewater.

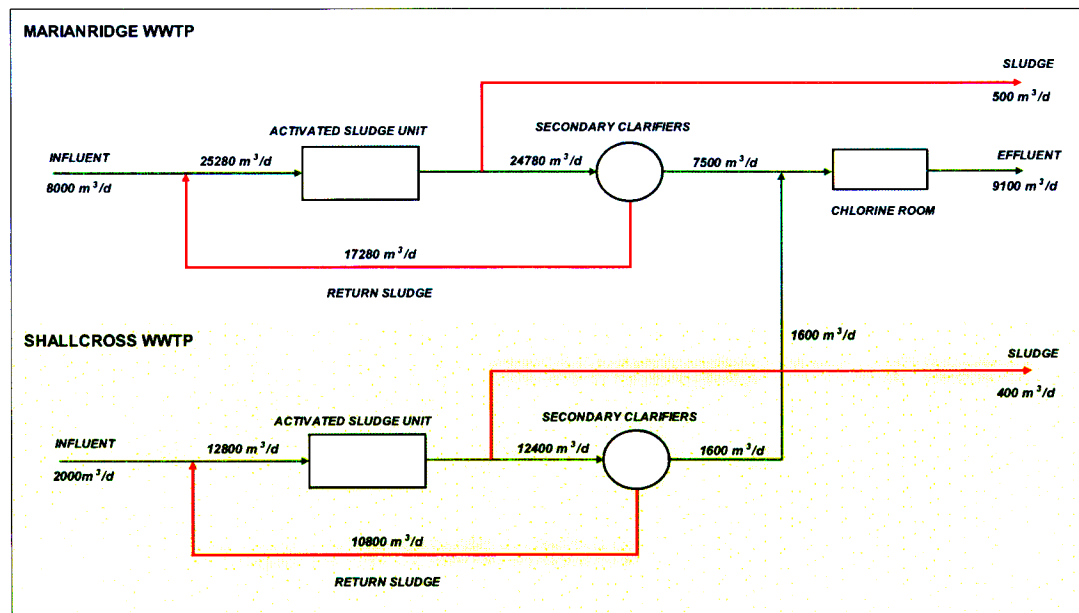


Figure 3:2 Nominal flow balance of the Umhlatuzana Works, showing the Marianridge and Shallcross WWTPs

The flow balance of Umhlatuzana Works was calculated using the nominal average values of the influent wastewater going to the two plants, the return sludge flow rate and the volume of excess sludge removed per day.

Combining the effluent streams from the two plants before chlorination means that to achieve acceptable final effluent composition from Umhlatuzana Works both plants should be operated properly, especially Marianridge WWTP which contains a significant portion of industrial wastewater.

3.3. Characterisation of Marianridge Waste Water Treatment Plant influent

The values for concentrations and flow-rate of the influent going to the Marianridge WWTP are discussed in the following sections.

3.3.1. Influent flow volumes

The typical daily flow rate of the influent wastewater going to the Marianridge WWTP is shown in Figure 3:3.

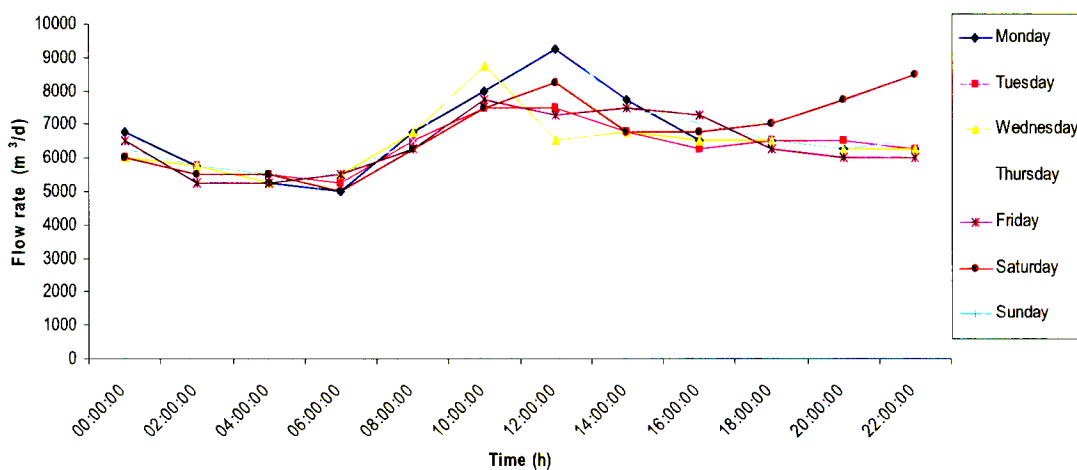


Figure 3:3 Typical daily flow rate of the influent to the Marianridge WWTP

The influent wastewater flow-rate going into the Marianridge Plant is measured using an online flow meter connected to an ultrasonic sensor which reads the depth of the wastewater passing through a constricted channel. The flow rate measure through out the day is recorded on charts. The

hourly flow-rates and average daily flow-rates can be determined from the recorded data. Figure 3:3 shows the daily flow pattern over a period of one week. The data indicates that the works receive the highest flow rate during the day, between 08:00 h and 14:00 h. The peak flow occurs at 12:00 h. The total monthly influent also varies through out the year. The monthly average flow-rate pattern for the year 2005 and 2006 is shown in Figure 3:4

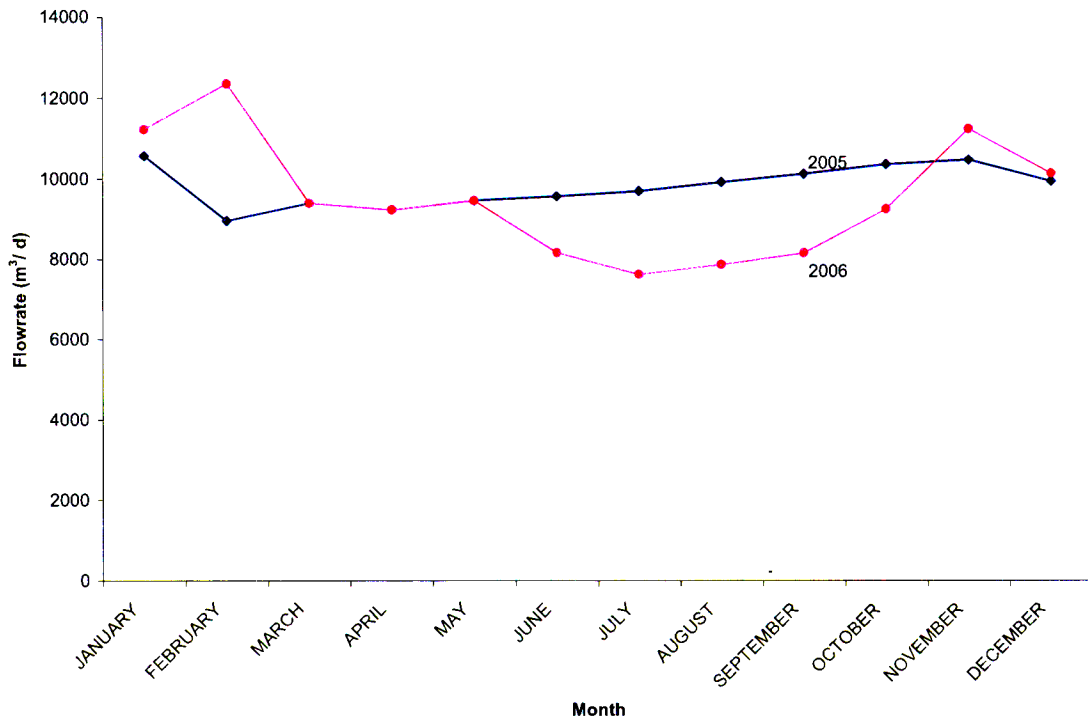


Figure 3:4 Monthly average flow- rates for the year 2005 and 2006

The highest load is experienced during the period of November to February, because of the contribution of the rainy season. The average monthly rainfall in the area around Durban in the summer period from December to February is approximately 3 times greater than during the winter season and the rest of the year (www.weathersa.co.za, 2007). When the influent flow rate goes above 10 000 m³/d during the rainy season at Marianridge WWTP, the excess influent is supposed to be diverted to Shallcross WWTP. The plotted graph indicates that in the year 2005 and 2006 influent flow rates above 10 000m³/d were allowed into Marianridge WWTP during the rainy season, and this might have resulted in overloading of the WWTP. The difference between the trends of the monthly average flow-rate between the year 2005 and 2006 might have been due to the different rainfall patterns experienced during the year 2005 and 2006.

3.3.1.1. Influent composition

Historical data obtained from the eThekweni municipal laboratory, of the composition of the influent wastewater for the Marianridge WWTP for the year 2006 is summarised in Table 3.1.

Table 3.1 Summary of historical data of the Influent composition going into Marianridge Treatment Plant for the year 2006 (Source: eThekweni Municipal Laboratory)

| Component | Units | Minimum | Average | Maximum | No. of samples |
|-------------------------------|------------------------|----------------|----------------|----------------|-----------------------|
| Chemical Oxygen Demand | | | | | |
| Total COD | mg O ₂ /L | 105 | 773 | 2709 | 291 |
| Nitrogenous Material | | | | | |
| Total Kjeldahl Nitrogen | mg N/L | 11 | 55 | 80 | 15 |
| Free ammonia | mg N/L | 1 | 25 | 82 | 325 |
| Nitrate | mg N/L | 0.4 | 0.8 | 1.6 | 15 |
| Phosphorus material | | | | | |
| Total phosphate | mg P/L | 1 | 8 | 15 | 113 |
| Orthophosphate | mg P/L | 6 | 9 | 12 | 15 |
| Solids | | | | | |
| Settleable solids | mg /L | 2 | 18 | 100 | 81 |
| Suspended solids | mg /L | 21 | 298 | 1592 | 62 |
| Total dissolved solids | mg /L | 212 | 570 | 934 | 9 |
| Total solids | mg/L | 319 | 1095 | 2426 | 48 |
| Other | | | | | |
| Colour | ADMI | 86 | 627 | 2720 | 105 |
| Alkalinity | mgCaCO ₃ /L | 83 | 268 | 798 | 338 |
| pH | | 6 | 7.2 | 10 | 336 |
| Conductivity | mS/m | 44 | 110 | 209 | 331 |
| Copper | µg Cu/L | 32 | 108 | 342 | 12 |
| Cadmium | µg Cd/L | <0.5 | <0.5 | <0.5 | 13 |
| Iron | µg Fe/L | 0.11 | 2 | 14 | 9 |
| Lead | µg Pb/L | 5 | 45 | 264 | 10 |
| Zinc | µg Zn/L | 26 | 162 | 316 | 13 |
| Sodium | µg Na/L | 53 | 140 | 233 | 104 |
| Chloride | mg Cl/L | 34 | 140 | 355 | 321 |

When the average influent characteristics shown in Table 3.1 are compared to the characteristics of domestic wastewater according to Henze et al., (2002) shown in **Appendix A**, the following conclusions can be made;

- Based on the average values of conductivity (110 mS/m) and the average concentration of settleable solids (18 mg/L) the influent wastewater going to the Marianridge WWTP is characterised as concentrated domestic wastewater.
- From the average values of alkalinity (268 mgCaCO₃/L), pH (7.2), total-phosphorus (8 mg P/L), ortho-phosphorus (9 mg P/L), the influent wastewater going to Marianridge WWTP is characterised as dilute domestic wastewater.
- From the average total COD value (773 mgO₂/L), the influent wastewater to Marianridge WWTP is characterised as concentrated domestic wastewater.
- From the average concentrations of heavy metals the influent wastewater to Marianridge WWTP is characterised as dilute domestic wastewater.

The comparison of the data in Table 3.1 with the characterisation by Henze et al., (2002) cannot provide a unique characterisation under the types specified by Henze et al., (2002), of the influent wastewater treated at Marianridge WWTP. This shows the varying nature of wastewaters containing domestic and industrial effluent.

3.3.1.2. Influent wastewater test ratios

The relationships between the Total Kjeldahl Nitrogen (TKN), total chemical oxygen demand (COD) and the biological oxygen demand (BOD₅) can also be used in characterisation of influent wastewater.

The COD/TKN ratio gives a measure of the de-nitrification potential. A ratio of between 10 and 14 mgO₂/mgN suggests the possibility of a fast de-nitrification process, while lower ratios between 6 and 10 mgO₂/mgN slower de-nitrification (Winther et al., 1998).

The COD/BOD₅ ratio indicates how readily biodegradable the wastewater is. A ratio of 1 means that all the organic material present in the wastewater will be broken down in an aerobic biological

treatment system in 5 days or less. A lower the ratio indicates that the wastewater is more biodegradable.

COD/BOD₅ and COD/TKN ratios of influent wastewater going to the Marianridge WWTP determined from tests carried out on the influent wastewater composite samples by the eThekweni municipal lab are shown in Table 3.2.

Table 3.2 Summary of test ratio data for Marianridge influent wastewater

| Value | COD/BOD₅ [-] | Classification | COD/TKN [mgO₂/mgN] | Classification | No. of samples |
|--------------|------------------------------------|-----------------------|--|-----------------------|---------------------------|
| Average | 6.8 | Less biodegradable | 11 | Good de-nitrification | 21 |
| Maximum | 11.0 | | 12 | | 21 |
| Minimum | 2.9 | | 10 | | 21 |

Table 3.2 shows an average COD/TKN ratio of 11 which suggests good de-nitrification potential. The COD/BOD₅ test ratio indicates an average of 6.8, as compared to a range of 2 to 2.5 for domestic influent wastewater according to Henze et al., (2002). The higher COD/BOD₅ ratio suggests that the influent at Marianridge WWTP is less biodegradable than normal domestic wastewater as describe by Henze et al., (2002), which is expected since the Marianridge WWTP influent contains industrial wastewater which includes textile effluent.

4. DETERMINATION OF MODEL PARAMETERS

It is important to determine model components and parameters that are specific to the Marianridge WWTP so that an accurate and specific model is developed.

The experimental work carried out was divided into two categories:

- determination of COD fractions in influent wastewater (influent characterisation)
- determination of kinetic and stoichiometric parameters

There are two approaches for the determination of model parameters and components; direct methods and indirect methods. When using direct methods, the model parameters and components are determined from the experiments carried out on wastewater and sludge samples from the WWTP. Indirect methods involve the use of numerical techniques on the model, to estimate model parameters and components.

Both direct and indirect methods were used in influent characterisation and to determine the kinetic and stoichiometric model parameters in this study. Influent characterisation was based on the batch respirometric experiments carried out on composite samples of wastewater, flocculation-filtration of composite samples of wastewater and simulation of the batch respirometric experiment carried out on the wastewater.

The model kinetic and stoichiometric parameters were determined from the batch respirometric experiments on composite samples of wastewater and sludge samples. The model representing the batch respirometric experiment was also used to determine some kinetic and stoichiometric parameters. An overview of the experiments done and the information determined from the experiments is shown in Figure 4:1.

The experimental work is described in detail in the subsequent sections.

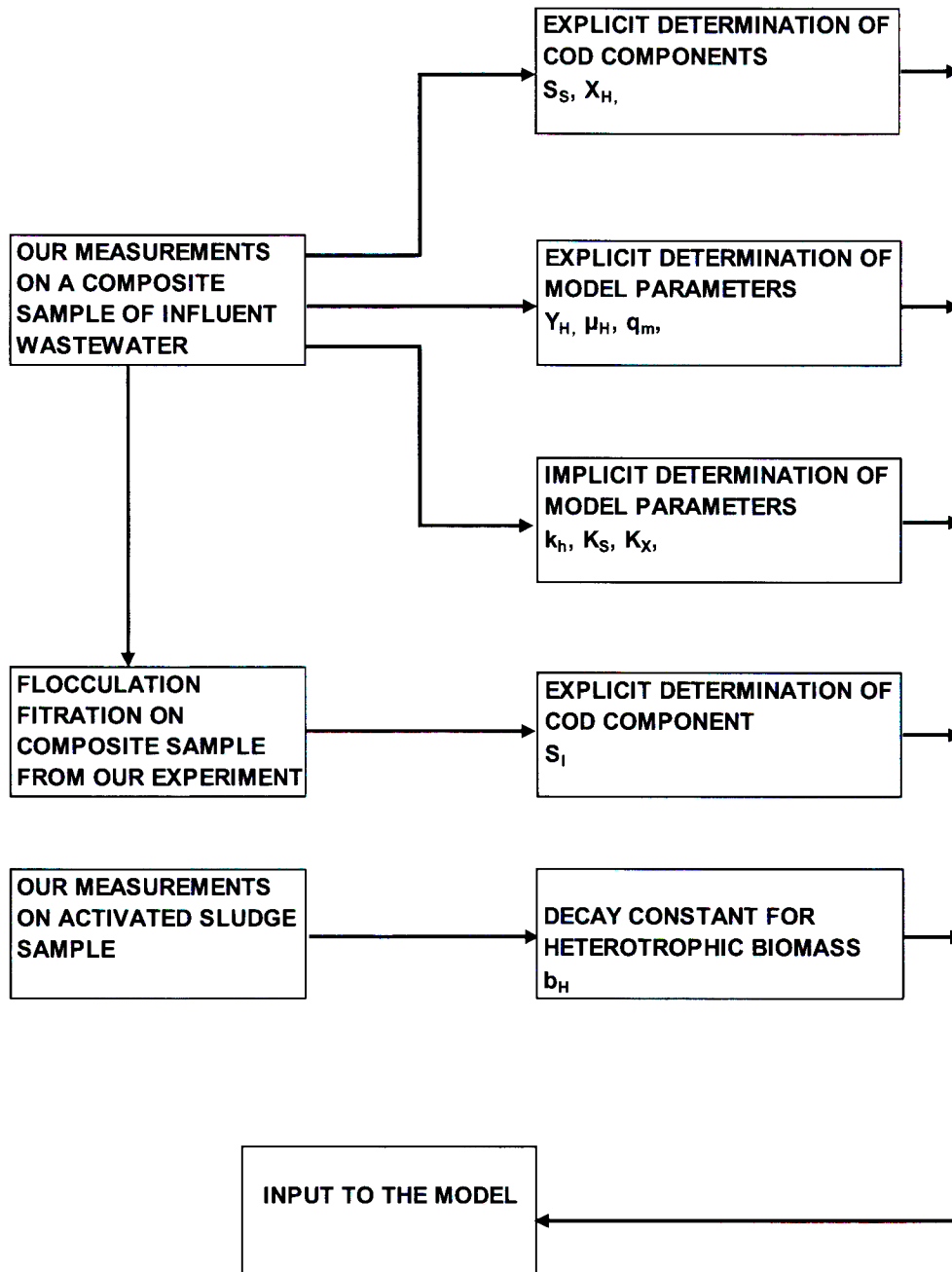


Figure 4:1 Overview of experimental work done and the information determined from each experiment.

4.1. Respirometry on activated sludge and wastewater

Respirometry is the measurement and interpretation of the biological oxygen consumption rate under well defined experimental conditions (Copp and Vanrolleghem, 2002). The respirometric experiments carried out were measurement of oxygen uptake rates (OUR) on activated sludge and raw wastewater. The OUR is an activity-related quantitative measure of the aerobic biomass influence on the relationship between the organic substrate and the dissolved oxygen, (Hvitved-Jacobsen, 2002). The OUR experiment reflects the different phases of activity that the heterotrophic biomass is exposed to, depending on the availability and quality of the substrate. The OUR-time relationship of wastewater samples and activated sludge samples is the basis for the analysis of the microbial system existing in the sample of concern. This relationship is crucial for the characterisation of the suspended wastewater phase in terms of COD components and the corresponding kinetic and stoichiometric parameters of the biological processes involved.

The bioassay test by Wentzel et al., (1995) outlined in section 2.2.4.1 is adopted in this study. It is based on the measurement of OUR in wastewater samples. The test is described as part of the outline of the experimental procedure in the following section.

4.1.1. Wastewater Sample Collection

Influent wastewater was collected from Marianridge WWTP. Hourly samples of raw unsettled wastewater were drawn from the inlet of the treatment plant after the screens and the degritting chambers. The hourly samples were kept anaerobic by sealing the sample bottles and placing them in a refrigerator to avoid significant biological transformation of the raw wastewater. After 24 h, the samples were carried to the laboratory in a cooler box with ice, and a 24 h composite sample was made from the hourly samples.

4.1.2. The batch respirometric experiment

The major components of the experimental set-up are the biological reactor, air supply, OUR-meter and the computer. The layout of the experiment is shown in Figure 4:2.

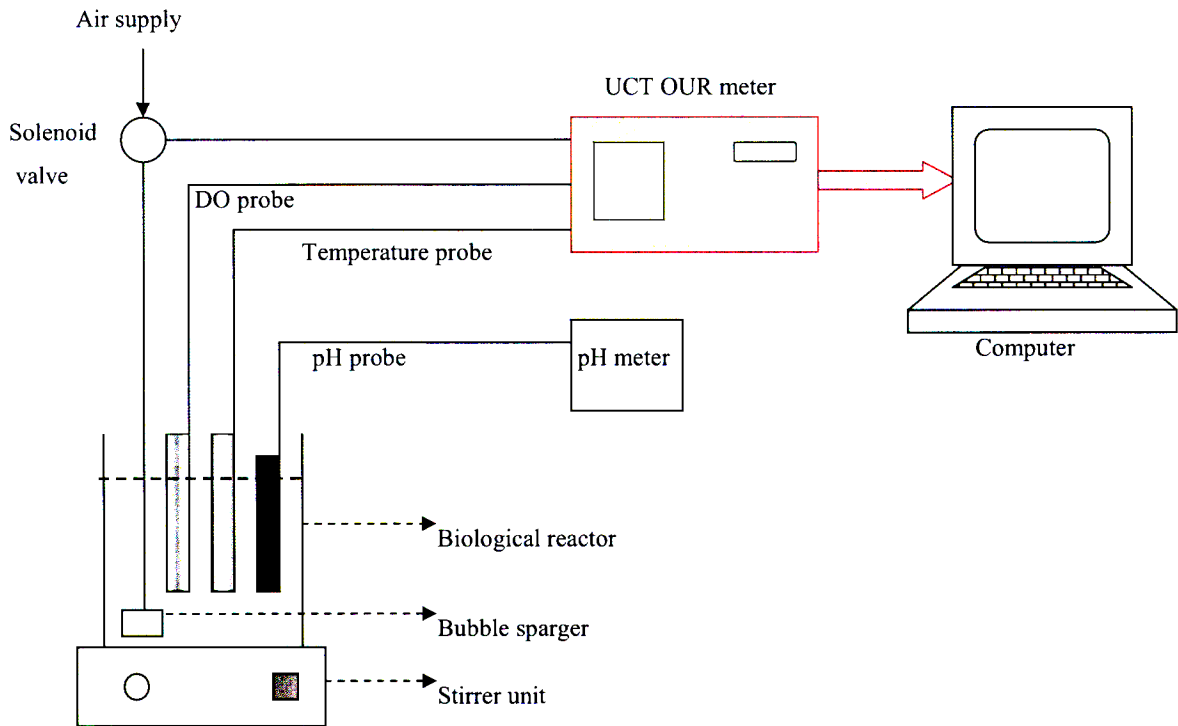


Figure 4:2 Schematic layout of the OUR meter and the completely mixed biological batch reactor

4.1.2.1. Biological reactor and air supply

The biological reactor (bio-reactor) consists of a 2 L continuously stirred vessel. The bio-reactor contains a dissolved oxygen probe and temperature probe connected to the UCT OUR meter and a pH probe connected to a pH meter to monitor pH. A bubble sparger is connected to the outlet of the air supply inside the reactor, so that the aeration occurs through small bubbles, hence preventing the formation of large bubbles on the surface of the liquid. The air supply to the bio-reactor is controlled by the OUR meter based on the measured dissolved oxygen concentration inside the bio-reactor. The air supply is switched on when the dissolved oxygen (DO) concentration reaches the lower set point and switched off when the DO concentration reaches the upper set point. The DO concentration value drops from the upper set point to the lower set point due biological activity which results on utilisation of oxygen in the sample of concern.

4.1.2.2.OUR meter and computer

The OUR meter comprises the DO and temperature probes, and a microprocessor unit. Specifications for the DO probe are given in **Appendix B**. The probes measure dissolved oxygen concentration and temperature. The microprocessor unit performs the timing functions, reads the DO concentration, temperature and time signals, and performs the data processing functions such as calculating the OUR. The OUR meter controls the DO concentration, between the specified upper and lower set points with an on-off solenoid valve in the air supply line and computes with the microprocessor the OUR from the change in DO concentration and time trace during the air-off period by means of a linear least squares regression analysis. The OUR meter has a local memory where up to 200 OUR readings can be stored. The OUR meter is connected to a computer for transfer of OUR data for storage and further processing.

4.1.2.3.Test procedure

A defined volume of 2 L of the unsettled 24 h composite of wastewater obtained from the treatment plant was poured into the continually stirred batch reactor. The initial total COD concentration is important to this test hence an aliquot was drawn from the composite sample and the initial total COD concentration was determined according the Standard methods procedure outlined in Eaton and Greenberg (1995). The OUR was measured continually using the automated UCT OUR meter. The DO concentration upper limit was set at 6 mgO₂/L and the lower set point at 4 mgO₂/L. The walls of the reactor were thoroughly brushed regularly during the experiment, to remove particulate matter adhered to the walls. During the operation of the batch test, the surface of the wastewater was covered with a plastic plate which was supporting the probes, to limit surface exchange of oxygen. The batch experiment was split into two stages. In the first stage the OUR was measured on the sample without addition of any substances and the second stage of the experiment involves addition of a readily biodegradable substrate, in order to investigate the growth of biomass. The two stages of the experiment are discussed in the following section 4.1.2.4. The complete OUR experiment took approximately 24 h. At the end of the test, the contents of the batch reactor were homogenised and, a sample was drawn and the total COD was measured according to Standard Methods set in Eaton and Greenberg (1995).

4.1.2.4. Addition of Substrate

The first stage of the test is based on the procedure by Wentzel et al., (1995). The first stage of the experiment involves measuring the OUR until the readily biodegradable substrate and the rapidly hydrolysable substrates are depleted. The amount of readily biodegradable substrate is considered depleted, when the OUR is approximately constant, i.e. when the maintenance energy requirements of the biomass corresponds to the readily biodegradable substrate resulting from the hydrolysis of slowly biodegradable substrate.

Hvitved-Jacobsen (2002) further extends the experiment by a second stage which involves addition of a readily biodegradable substrate to the wastewater sample. Sodium acetate was used as readily biodegradable substrate and the measurement continued, until this substrate is also depleted. Hvitved-Jacobsen (2002) concludes that there is no significant deviation between the values of the parameters based on adding a small amount of readily biodegradable substrate compared with the values when adding higher amounts. An amount of 100 mg acetate/L was chosen in the experiment, based on previous similar experiments (Poulsen and Lauridsen, 2005). The experiment ends, when the OUR curve declines to an almost constant value. The impact of the substrate addition was then evaluated from the OUR data.

4.1.3. Interpretation of experimental data

A typical OUR-curve plotted from the data obtained from OUR measurements on a composite sample of wastewater with addition of sodium acetate, a readily biodegradable substrate is shown in Figure 4:3.

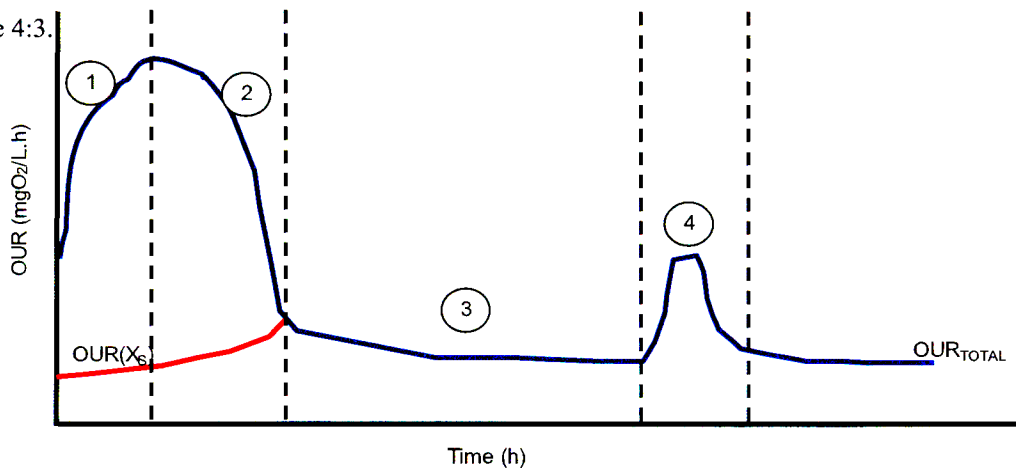


Figure 4:3 A typical OUR-curve on raw incoming sewage with addition of readily biodegradable substrate (Hvitved-Jacobsen et al., 2002)

The utilization of readily biodegradable and slowly biodegradable substrate results in the oxygen uptake rate shown by the curve OUR_{TOTAL} . The curve labelled $OUR (X_S)$ shows the oxygen uptake rate due to the utilisation of only slowly biodegradable.

The OUR curve is divided into four phases based on the substrate concentrations in the wastewater sample as shown in Figure 4:3.

- 1) Substrate non-limited condition.
- 2) Substrate non-limited condition is being terminated.
- 3) Substrate limited condition.
- 4) Addition of readily biodegradable substrate (sodium acetate)

The figure shows that during phase 1 the amount of readily biodegradable substrate present in the beginning is not limiting the growth of biomass. The amount of biomass increases in phase 1 and the OUR also increases. This is followed by a sharp decrease in OUR , when the readily biodegradable substrate is depleted in phase 2. After this period (phase 3) the readily biodegradable substrate is only available due to the hydrolysis of slowly biodegradable substrate. When the production of readily biodegradable substrate by hydrolysis corresponds to the required maintenance energy for biomass, i.e. the when the OUR is stable, an aliquot of readily biodegradable substrate is added. This addition results in immediate growth of the biomass under substrate non-limited conditions, where the OUR increases, followed by a rapid decrease to the maintenance value as seen in phase 4.

The purpose of addition of readily biodegradable substrate after phase 3 (the substrate limited conditions) in the experiment is to let the biomass growth rate change from zero to its maximum value. The experiment is then interpreted using a model which represents the processes which are occurring in the batch reactor.

4.1.3.1. Interpreting the experiment using the UCT and IWA models

The data from the first stage of the batch test before the addition of sodium acetate, (zone 1, 2, and 3) can be interpreted in terms of the UCT (Dold et al., 1980; 1991) and IWA model. Both the UCT model and the IWA model used by Hvitved-Jacobsen (2002) were used to interpret the results.

UCT model

For interpretation using the UCT model, the model was simplified by recognising the following specific conditions:

- the batch test is done under aerobic conditions so de-nitrification processes need not be included,
- there was no nitrification therefore, therefore the nitrification processes need not be included,
- excess ammonia is present in the wastewater so nitrite as an N-source for growth need not be considered and also transformations from organic to ammonium nitrogen does not need to be included.

The simplified UCT model based on the specific conditions is presented in **Appendix C**.

IWA model

For interpreting using the IWA model, the original model-matrix in Hvitved-Jacobsen (2002) is modified to suit, the COD fractions needed for this particular model. The modification means, that the originally two fractions of hydrolysable substrate are combined to one fraction of slowly biodegradable substrate. The modified IWA matrix model is shown in **Appendix C**.

The theory of the calculations to determine the COD fractions and model parameters is outlined in **Appendix C**.

4.1.3.2. Check of COD recovery

A mass balance of oxygen shows whether the data from the OUR measurements are acceptable. Before and after the experiment a sample was drawn to obtain the initial COD and end COD, also taking into account the readily biodegradable substrate added. A mass balance constructed, yields equation 4.1.

$$\% \text{ COD recovery} = \frac{COD_{t=T} + \int_{t=0}^{t=T} OUR \cdot dt}{COD_{t=0}} \cdot 100 \quad [4.1]$$

Where:

- t = Time (h)
- T = Time used at the end of the experiment (h)
- COD_{t=T} = Total COD concentration at the end of experiment (mg COD/L)
- COD_{t=0} = Total COD concentration at the beginning of experiment (mg COD/L)

A COD recovery in the range of 95 to 105 % indicates that the OUR measurements are reliable (Wentzel et al., 1995). COD recoveries of 95 to 97% were achieved in this study indicating that the experimental results were reliable. COD recovery data is presented in the compact disc accompanying the thesis.

4.1.4. Determination of inert soluble substrate, S_I

The inert soluble substrate, S_I in wastewater was determined by a flocculation-filtration procedure on the wastewater collected at the end of the batch respirometric test on composite wastewater described earlier in section 4.1.2.3. After running the batch test for 24 h, the only soluble COD remaining should be non-biodegradable soluble COD. Therefore, at the end of the batch test, 1 L of the batch reactor contents was drawn as sample to determine the inert soluble substrate. The sample was dosed with 10 mL of aluminium sulphate with a concentration of 50 g/L. The mixture was stirred rapidly for 2 min and then poured slowly into a Perspex cylinder (settling column) equipped with a magnetic stirrer. The content of the column were then stirred slowly for 30 min (flocculation phase). During the flocculation phase the flocs settled and leave a clear liquid zone. A 50 mL sample was drawn from the clear liquid zone and filtered through a glass fibre filter (Whatman GF/C) and the COD of the filtrate was determined. The COD of the filtrate gives the amount of the inert soluble substrate, S_I .

4.1.5. Inert particulate substrate X_I , and slowly biodegradable substrate X_S

From the batch OUR test, it is impossible to differentiate between inert particulate substrate and slowly biodegradable substrate. Furthermore, physical separation technique, such as flocculation-filtration can not separate the two COD fractions, since both are particulate. The inert particulate substrate, X_I is determined from the simulation model of the batch respirometric experiment. With four COD fractions known, the slowly biodegradable substrate X_S is determined from equation 4.2.

$$C_{\text{TCOD}} = S_I + S_S + X_I + X_S + X_H \quad [4.2]$$

4.2. Determination of kinetic and stoichiometric parameters from OUR test

The determination of kinetic and stoichiometric parameters for the model is discussed in the following sections.

4.2.1. Aerobic yield of heterotrophic biomass, Y_H

The aerobic yield of heterotrophic biomass, Y_H was determined from the OUR curve results obtained in the batch respirometric experiment outlined in section 4.1.2. The theory behind the data analysis is outlined in **Appendix C**.

4.2.2. Heterotrophic maximum growth rate μ_H

The heterotrophic maximum growth rate, μ_H is determined from the same OUR experiment where the aerobic yield of heterotrophic biomass, Y_H is determined. The theory behind the data analysis is outlined in **Appendix C**.

4.2.3. Decay rate constant, b_H

To determine the decay constant of the biomass in the activated sludge, an activated sludge sample is put in a batch reactor where the endogenous respiration rate is measured by measuring the oxygen uptake rate of the biomass over a period of 24 h or several days. Nitrification is inhibited during the test by addition of 20mg/L of thiourea. Since the endogenous respiration is proportional to the active biomass concentration, a plot of the natural logarithm of the endogenous respiration as a function of time describes the exponential biomass decrease as a straight line with slope b'_H which refers to the traditional decay coefficient described by Henze et al (1987).

In this study a sludge sample was taken from the outlet of the activated sludge unit and kept cool and anaerobic, to prevent significant transformation of the organic matter in the sample during the period of transportation and storing. OUR measurements were performed on the sample in the 2 L continuously stirred batch reactor, the upper set point of the dissolved oxygen was 6 mgO₂/L and the lower set point was 4 mgO₂/L. The OUR measured was done over a period of 24 h. Nitrification was inhibited during the test by addition of 20 mg/L of thiourea.

The plot of the natural logarithm of the recorded OUR values versus time showed the expected exponential decrease of the biomass as a straight line with the slope, b'_H . However when determining the model specific decay coefficient for activated sludge models which use the death regeneration model concept to describe the decay of biomass, like ASM1, the value of b'_H obtained from the experiment needs to be adjusted to get the model specific parameter b_H .

To obtain the model specific parameter, b_H , b'_H must be adjusted according to the values of the yield coefficient for heterotrophic biomass, Y_H , and the fraction of inert particulate biomass, f_p , as shown in equation 4.3 (Henze *et al.*, 1987).

$$b_H = \frac{b'_H}{1 - Y_H \cdot (1 - f_p)} \quad [4.3]$$

The change in ASM3 to the traditional endogenous respiration decay rate concept makes it more straight forward to determine the decay rate of the model from the experiment.

4.2.4. The hydrolysis constant, k_h

Attempts have been made to analyse hydrolysis in laboratory-scale experiments (Petersen *et al.*, 2002) in order to try and determine the hydrolysis constant, k_h . However the real enzymatic hydrolysis is not the same as the hydrolysis process in the model. The hydrolysis process in the model might also include consumption of storage polymer, hydrolysis of decayed biomass and other processes. Hence it remains difficult to design an experiment that is representative of both the model concept and the hydrolysis process as it takes place in the full-scale plant. Therefore in practice the value of the hydrolysis constant may have to be tuned during the model calibration (Petersen *et al.*, 2002). In this study k_h was estimated by fitting the OUR results predicted by the simulation model of the batch experiment, to the OUR results which were recorded in the batch experiment that was carried out on influent wastewater. The estimated value would further be adjusted during calibration if necessary.

4.2.5. Half saturation coefficients, K_S and K_X

In pure cultures the half saturation coefficients can be regarded as pure biological parameters that give measures of the affinity of the biomass for substrates (Petersen *et al.*, 2002). In activated sludge models where the biological meaning of the model half saturation coefficient is mixed with the hydraulics of the system, it becomes difficult to get values of half saturation coefficients from laboratory-scale experiments which are representative of the full-scale system. If a very detailed model is available to describe the hydraulics of system accurately it might be possible to separate the effects of biomass affinity for substrate and the hydraulic effects. The lumping of the biomass affinity for substrate and the hydraulics of the system means that processes such as mixing will

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affect the value of the coefficient. The different mixing characteristics of the laboratory-scale and full-scale system make it difficult to transfer the laboratory-scale observation to the full scale system. The coefficients may be estimated by laboratory-scale experiments but the values may not be very representative. Therefore in practice these values may have to be tuned during the model calibration (Petersen et al., 2002).

In this study the saturation coefficient for readily biodegradable substrate, K_S , and the saturation coefficient for particulate COD, K_X , are estimated by fitting the OUR results predicted by the simulation model of the batch experiment, to the OUR results which were obtained from the batch experiment that was carried out on wastewater. The curve fitting was done up to the point just before the addition of readily biodegradable substrate. The curve fitting is done by use of numerical techniques, during a trajectory optimisation run in the WEST software which is discussed in section 5.3.1. The results from the experimental and simulation work done are discussed in the following chapter. A summary of the determined model parameters and the method of determination is provided in Table 4.1 together with remarks on the need for adjustment of parameters.

Table 4.1 Summary of the determined model parameters and the methods used, with remarks

| Symbol | Description | Method used | Remark |
|---------------|--|--|---|
| Y_H | Yield coefficient | Batch OUR Test | May not require adjustment |
| μ_H | Maximum growth rate | Batch OUR Test | May not require adjustment |
| b_H | Decay rate constant | Batch OUR Test | May not require adjustment |
| k_h | Hydrolysis rate constant | Curve fitting of model predicted OUR data to measured OUR data | May require adjusted during model calibration |
| K_S | Saturation coefficient for S_S | Curve fitting of model predicted OUR data to measured OUR data | May require adjusted during model calibration |
| K_X | Saturation coefficient for particulate COD | Curve fitting of model predicted OUR data to measured OUR data | May require adjusted during model calibration |

5. DISCUSSION OF RESULTS

The results obtained from the experiments that were carried out are discussed in this chapter.

5.1. OUR measurements on activated sludge

The objective of the OUR measurements on activated sludge samples was to determine the decay rate constant for the heterotrophic biomass, b_H . Grab samples of activated sludge were used. From the theory outlined in **Appendix C**, the plot of the natural logarithm of the OUR against time should give a straight line with slope, b_H . The expected straight line profile was observed as shown in selected results in Figure 5:1 and Figure 5:2.

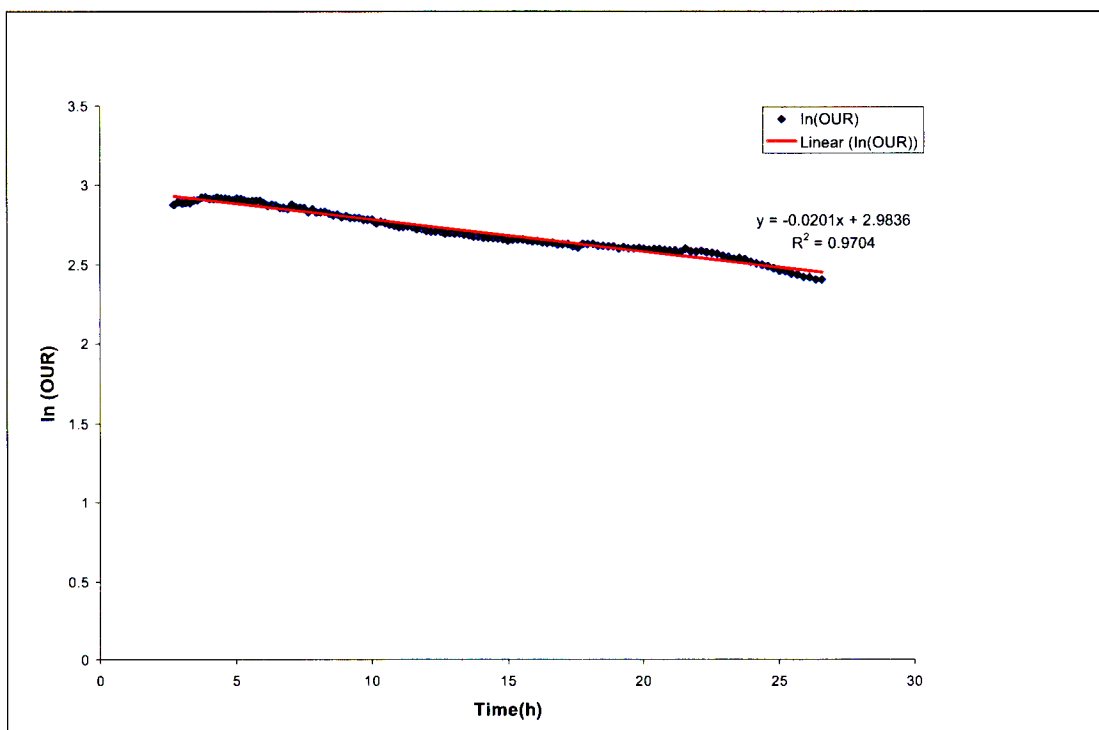


Figure 5:1 Endogenous respiration of heterotrophic biomass in a batch reactor

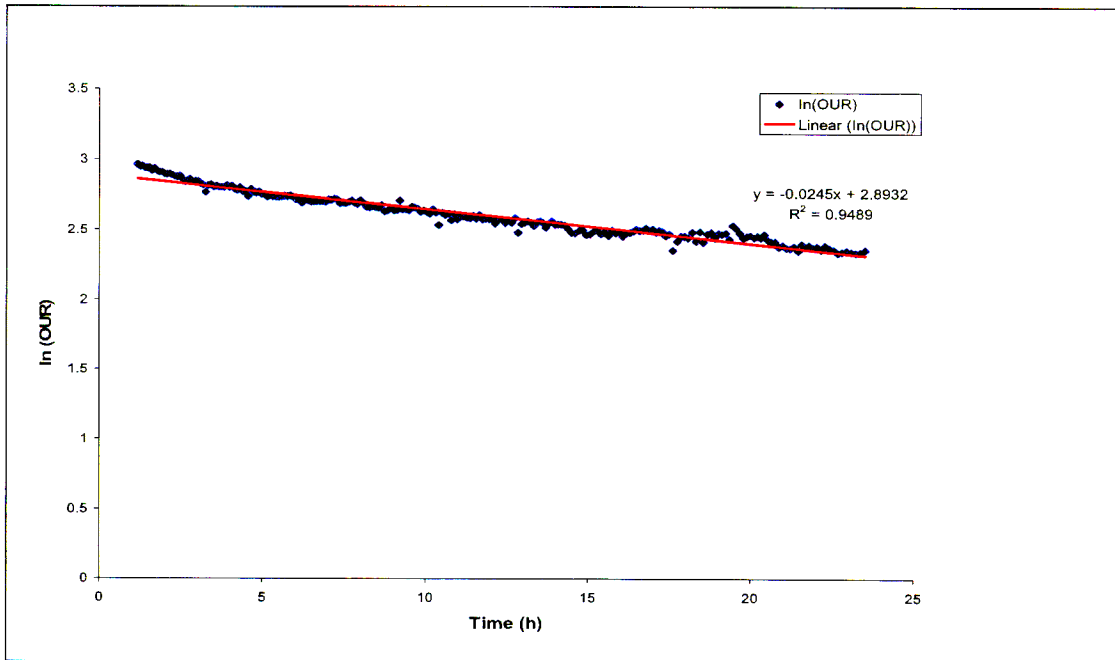


Figure 5:2 Endogenous respiration of heterotrophic biomass in a batch reactor

The results obtained for the decay rate constant, b_H are summarised in Figure 5:3 and Table 5.1.

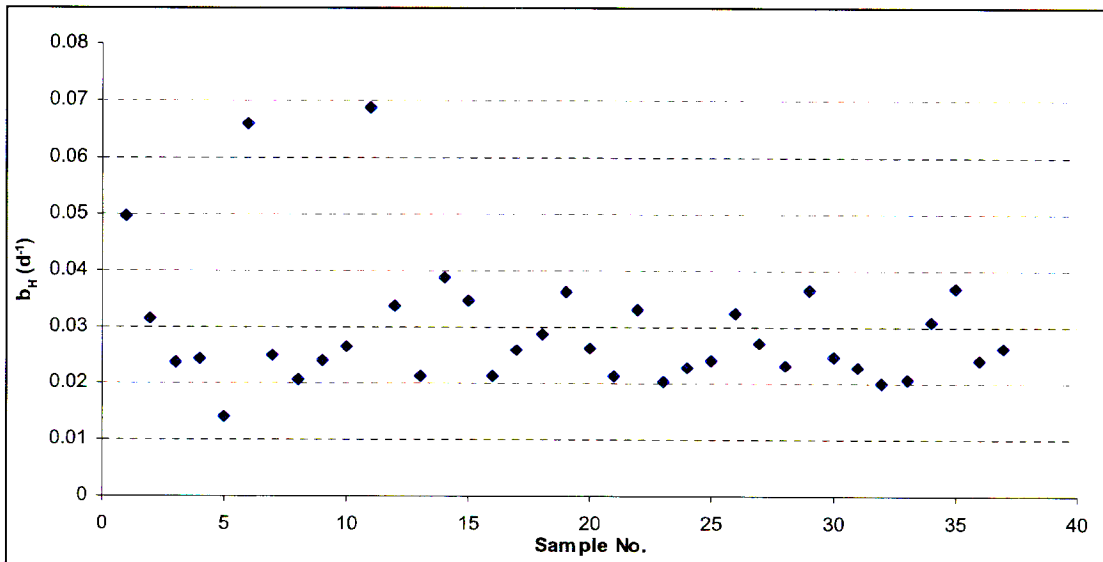


Figure 5:3 Values obtained for the decay rate constant in activate sludge from the Marianridge Plant

Table 5.1 Values obtained for the decay rate constant in activated sludge from the Marianridge Plant

| Symbol | Description | Unit | Mean value | Std. dev. | Samples | ASM3 default value |
|--------|---------------------|----------|------------|-----------|---------|--------------------|
| b_H | Decay rate constant | d^{-1} | 0.03 | 0.01 | 40 | 0.2 |

The results of the experiments indicate that the decay rate constant in the activated sludge unit at the Marianridge plant is lower than the ASM3 value, suggesting that for the same concentration of heterotrophic biomass, the rate of decay will be slower in the actual plant compared to a situation whose decay rate constant is defined by the ASM3 default value. However this does not imply abundant and unlimited biomass activity in the Marianridge WWTP because other factors such as the inhibitory effect of elements contained in the industrial portion of the wastewater going into the plant, still affect the performance of the biomass.

5.2. OUR measurement on wastewater with addition of substrate

OUR measurements on the daily composite samples of raw sewage with addition of readily biodegradable substrate were conducted over a period of nine months. The experiments carried out gave the expected OUR profile which was used to determine the COD fractions, S_S , X_H together with the stoichiometric and parameters, Y_H and μ_H . The kinetic parameters, k_b , K_X , and K_S , were determined by curve fitting based on the simulation of the OUR experiment

In order to estimate the concentration of readily biodegradable substrate in the influent wastewater, it is necessary to plot the OUR curve for the utilisation of slowly biodegradable substrate. Figure 5:4 and Figure 5:5 show the plots of OUR measured in the experiment as well the OUR curve due to utilization of slowly biodegradable substrate, $OUR(X_S)$. The OUR curve for utilisation of slowly biodegradable substrate is plotted from the theory outlined in **Appendix C**.

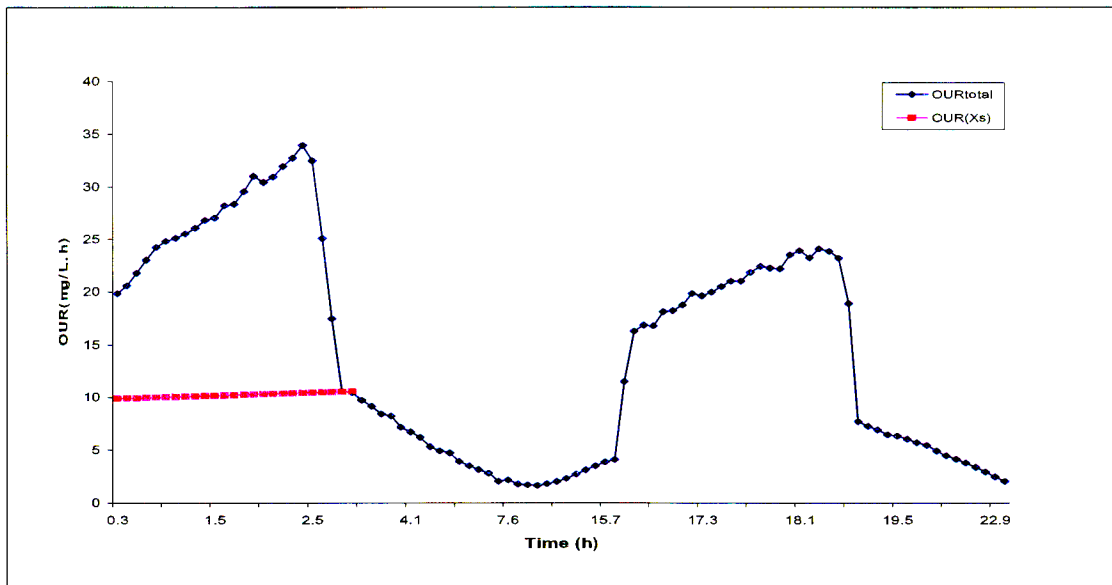


Figure 5:4: OUR-measurement results on influent wastewater with addition of readily biodegradable substrate showing the theoretical utilisation of slowly biodegradable substrate

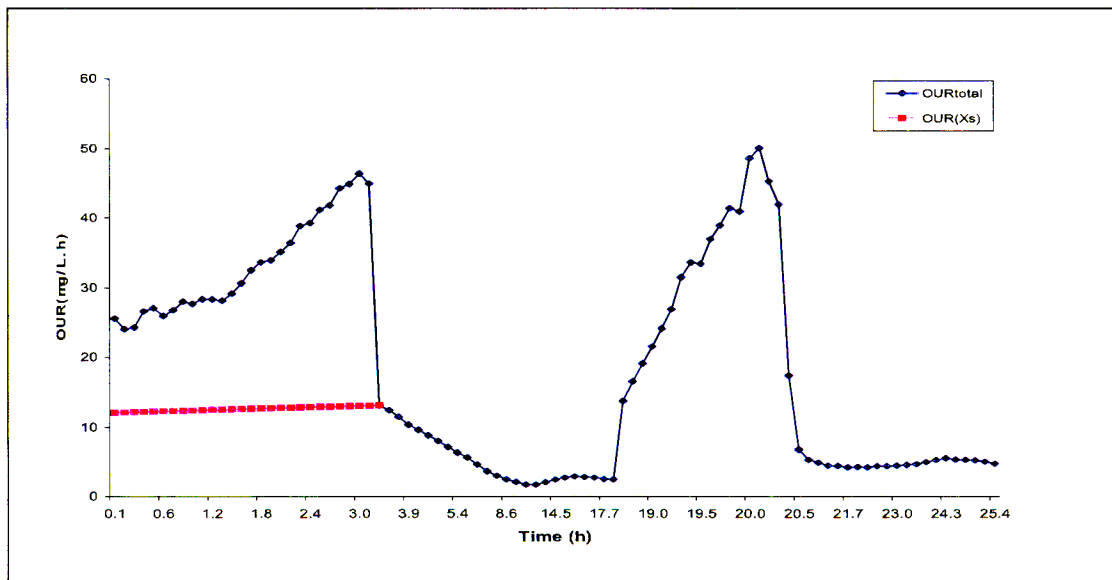


Figure 5:5 OUR-measurement results on influent wastewater with addition of readily biodegradable substrate showing the theoretical utilisation of slowly biodegradable substrate

During the first period of the batch test (less than 4 h), the OUR-time plots show that the OUR exhibits an exponential increase due to heterotrophic active biomass growth on readily biodegradable substrate. After 4 h the OUR drops precipitously due to depletion of readily

biodegradable substrate. For the next phase of the batch test (4 to 17 h) exhibits a pattern typical to saturation kinetics due to the utilisation of slowly biodegradable substrate. After the addition of acetate to the batch reactor the OUR exhibits an exponential increase similar to that observed at the start of the test, and then it drops towards the end of the test after the readily biodegradable substrate is used up.

5.3. Simulating the OUR experiment

The simulation model of the OUR experiment was developed and run in the WEST software package. The structure and operation of the WEST software package is outlined in detail in section 2.5.1.

A batch reactor containing wastewater under conditions similar to the experiment was set up in the ASM3 model base to model the biological processes occurring in the actual batch reactor used in the experiment. The batch experiment is only simulated up to the point just before the addition of readily biodegradable substrate. Only this section of the experiment is relevant to the determination of the required information. Figure 5:6 and Figure 5:7 show the measured and predicted OUR curves of two experiments, when the experiment was run with ASM3 default model parameters.

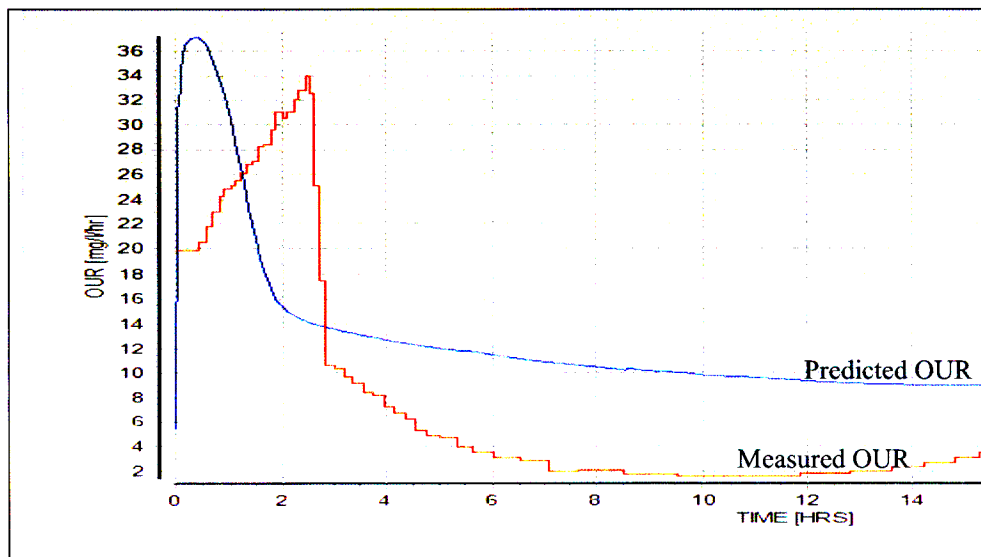


Figure 5:6 Predicted and measured OUR for a batch reactor containing raw wastewater

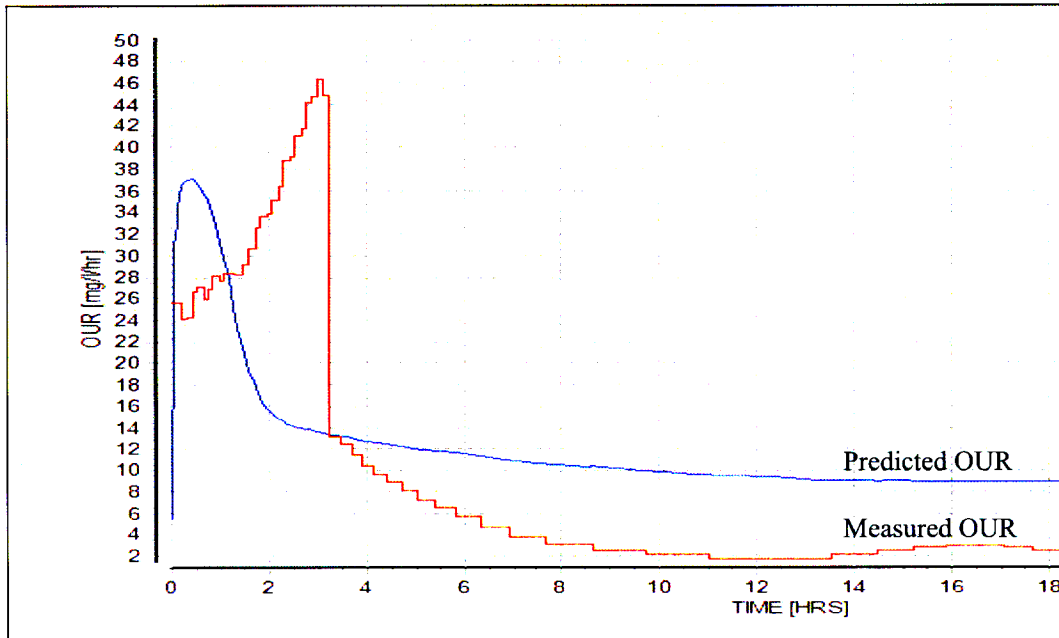


Figure 5:7 Predicted and measured OUR for a batch reactor containing raw wastewater

The simulated OUR curves shows a profile similar to that of the measured OUR. In the first part of the curve an exponential increase of OUR can be observed. The remainder of the curve exhibits the OUR corresponding to the utilisation of slowly biodegradable substrate.

The plots in Figure 5:6 and Figure 5:7, show that besides getting the characteristic profile of the OUR curve right, the model needs fine tuning at this particular stage, in order to get the simulated OUR curve to better fit the measured data closely. A trajectory optimisation was carried out on the simulation model in order to improve the prediction of the model.

5.3.1. Trajectory optimisation

In a trajectory optimisation a set of model parameters or components is tuned so that the model predictions match the measured data for a selected variable. A cost function is defined before estimating the values of model parameters or components. The cost function is a measure of the integrated difference between the simulated results and a measured data set of the selected variable. The best estimates of model parameters and components are those which correspond to the lowest value of the cost function.

During the trajectory optimisation in WEST a number of simulation runs with different parameter values, are executed. The optimisation algorithm, which chooses the different parameter values, attempts to minimise this cost function.

The squared error between the measured and predicted values was used as the cost function. The parameters that were tuned to minimise the OUR value cost function were selected based on their effect on the predicted OUR values and the relevance in the model matrix. The selected parameters are shown in Table 5.2. The parameters were tuned one by one and later combined for further adjustment.

Table 5.2 Parameters selected and used for trajectory optimisation

| Symbol | Parameter |
|----------|--|
| K_S | Saturation constant for substrate S_S |
| K_O | Saturation constant for oxygen S_O |
| K_X | Hydrolysis saturation constant |
| K_{NH} | Saturation coefficient for ammonia S_{NH} |
| K_{La} | Oxygen transfer coefficient |
| k_b | Hydrolysis rate constant |
| μ_H | Heterotrophic maximum growth rate of X_H |
| X_I | Inert particulate organics (initial concentration) |

5.3.1.1. Results of the trajectory optimisation

Two simulation curves, showing the results after tuning the model parameters during a trajectory optimisation exercise are shown against the measured OUR curve in Figure 5:8 and Figure 5:9.

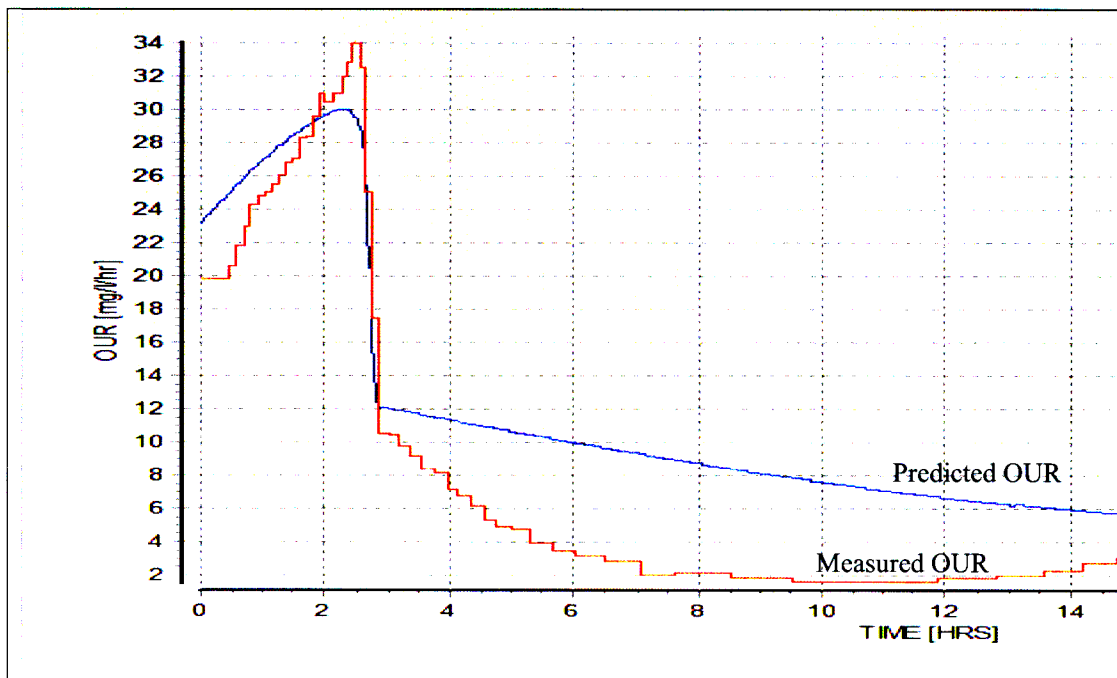


Figure 5:8 Model-predicted OUR and measured-OUR curves after tuning selected parameters using trajectory optimisation in WEST

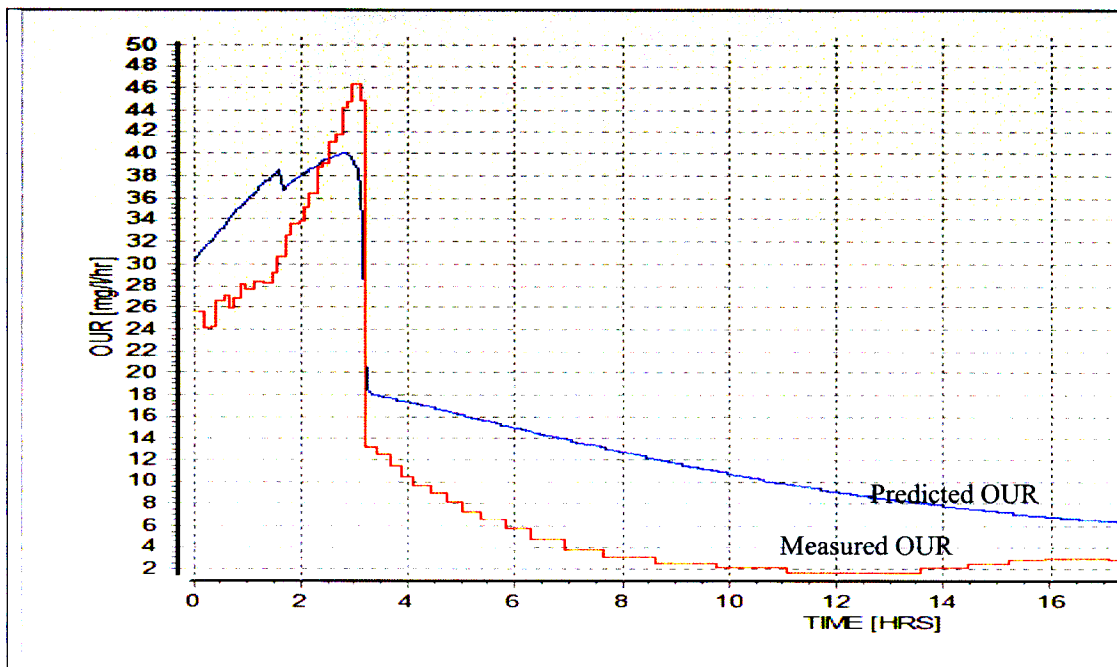


Figure 5:9 Model-predicted OUR and measured-OUR curves after tuning selected parameters using trajectory optimisation in WEST

The final accepted values of the selected parameters that were tuned in the trajectory optimisation are shown together with the initial ASM3 default values of the batch experiment, in Table 5.3.

Table 5.3 Parameter values derived from trajectory optimisation compared to the initial ASM3 values

| Parameter | Units | ASM3 value at 20°C | Derived value |
|------------------|---|----------------------------|----------------------------|
| K_S | $\text{gCOD}_{\text{SS}}/\text{m}^3$ | 2 | 2.31 |
| K_O | gO_2/m^3 | 0.2 | 0.0233 |
| K_X | $\text{gCOD}_{\text{XS}}/\text{gCOD}_{\text{XH}}$ | 1 | 1 |
| K_{NH} | gN/m^3 | 0.001 | 0.00107 |
| K_{La} | d^{-1} | 50 | 204 |
| k_b | $\text{gCOD}_{\text{XS}}/\text{gCOD}_{\text{XH}}$ | 3 | 3.03 |
| μ_{H} | d^{-1} | 2 | 2.40 |
| X_I | gCOD/m^3 | 0.15 of influent total COD | 0.15 of influent total COD |

The overall assessment of the simulated OUR curves as compared to the measured OUR curve indicates that the simulation model predicts the OUR curves satisfactorily in the beginning of the experiment during non-substrate limiting condition and in the beginning of the substrate limiting condition. The OUR model has problems simulating the rest of the substrate limiting condition zone, where the biomass primarily uses the slowly biodegradable substrate. The model tends to over estimate the OUR value under the substrate limiting conditions as shown in Figure 5:8 and Figure 5:9. A possible cause for this might be failure of the model to show adaptation of biomass behaviour to the conditions that exist in the water under the period of substrate limiting conditions. Another possibility is that the OUR model has one hydrolysable fraction and saturation coefficient for particulate matter as compared to suggestions which claim the existence of the two hydrolysable fractions, the fast hydrolysable and slowly hydrolysable fraction. The OUR model might be failing to simulate a point of discontinuity of the OUR curve, where the biomass change from utilising fast hydrolysable substrate to slowly hydrolysable substrate (Poulsen and Lauridsen, 2005).

The effect of mass transfer is also present in this system. Due to lack of predictive techniques to estimate the value of K_{La} in the process environment, K_{La} was deliberately adjusted from the default value of 50 d^{-1} to a higher value of 204 d^{-1} in order to obtain a more realistic simulation of the process

5.3.1.2. Summary of results: COD fractions

Table 5.4 shows results for the COD fractions determined in the characterisation of the influent from the Marianridge WWTP against the ASM3 values (Gujer et al., 1999) and the typical

municipal fractions of South African wastewater according to Wentzel and Ekama, (2006). The three COD fractions (S_S , X_H , S_I) determined experimentally and the two COD fractions (X_S , X_I) determined from the simulation model and mass balance, are expressed as a fraction of the total COD of the influent wastewater.

Table 5.4 COD fractions of the Marianridge influent wastewater compared to ASM3 values, and typical South African wastewater by (Wentzel and Ekama, 2006)

| Symbol | Description | % of Total COD in influent wastewater | | |
|--------|---------------------------------|---------------------------------------|---------------------------|------|
| | | Marianridge | (Wentzel and Ekama, 2006) | ASM3 |
| S_I | Soluble inert organics | 7.5 | 7 | 12 |
| S_S | Readily biodegradable substrate | 18.1 | 20 | 23 |
| X_S | Slowly biodegradable substrate | 44.2 | 60 | 44 |
| X_I | Inert particulate organics | 15.6 | 13 | 10 |
| X_H | Heterotrophic biomass | 14.6 | * | 12 |

**In the guide on the typical South African wastewater by (Wentzel and Ekama, 2006) the presence of heterotrophic biomass is considered negligible and is ignored because the greater portion of the micro organisms develop in the biological reactor.*

The major differences between the three influent wastewaters in Table 5.4 appears to be the fraction of soluble inert organics S_I and the fraction of slowly biodegradable substrate X_S . The Marianridge influent contains 7.5% soluble inert organics as compared to higher value of 12% for ASM3, while Wentzel and Ekama, (2006) provide a value of 7%.

The Marianridge influent contains 44.2% slowly biodegradable particulate X_S against the 60% of Wentzel and Ekama, (2006). ASM3 influent contains 44% X_S . For the readily biodegradable substrate S_S the Marianridge influent contains 18.1% against 20% as stated by Wentzel and Ekama, (2006) for South African wastewater. The COD fractions given by Wentzel and Ekama, (2006), are based on municipal wastewater of mainly domestic origin. The lower biodegradable component and higher non-biodegradable components in the influent to the Marianridge WWTP might be due to the industrial wastewater from factories discharging into the plant, with textile effluent making up a significant portion of the industrial influent wastewater to the plant. It is appreciated that, to make an accurate explanation with regards to the biodegradability of effluent components one would have to investigate the constituents in the industrial effluent since some industrial effluent can have high biodegradable content.

The COD fractions for ASM3 influent indicate more readily biodegradable substrate and less particulate inert organics because the fractionation is based on domestic municipal wastewater. The fraction of slowly biodegradable substrate is almost the same as the ASM3 value, indicating a 0.2% difference. Another source of the difference in COD fractionation between the obtained results and the ASM3 fractions might be that the ASM3 influent characterisation is related to European conditions, which are substantially different from South Africa, particularly in the issue of combined sewers with long residence times which exists in Europe. So it is expected that the sewage characteristics will be different.

The difference between the experimental results and the literature values from the ASM3 manual and Wentzel and Ekama, (2006) emphasises the need to carry out specific characterisation of influent in order to achieve more accurate modelling results for the chosen wastewater treatment plant.

5.3.1.3. Summary of results: Model parameters

Table 5.5 shows the results obtained for the selected model parameters, compared to ASM3 default values.

Table 5.5 Results obtained for model parameters compared with ASM3 default values at 20 °C

| Symbol | Description | Unit | Mean | Std. dev. | ASM3 | Samples |
|----------|--|---------------------------------------|---------|-----------|------|---------|
| Y_H | Yield coefficient | $\text{gCOD}_{XH}/\text{gCOD}_{XSTO}$ | 0.61 | 0.11 | 0.63 | 25 |
| μ_H | Maximum growth rate | d^{-1} | 2.4 | 0.24 | 2 | 30 |
| k_h | Hydrolysis rate constant | $\text{gCOD}_{XS}/\text{gCOD}_{XH}$ | 3.03 | 0.41 | 3 | 30 |
| K_S | Saturation coefficient for S_S | $\text{gCOD}_{SS}/\text{m}^3$ | 2.31 | 0.26 | 2 | 30 |
| K_X | Saturation coefficient for particulate COD | $\text{gCOD}_{XS}/\text{gCOD}_{XH}$ | 1 | ** | 1 | 30 |
| K_{NH} | Saturation constant for ammonium S_{NH} | gN/m^3 | 0.00107 | 0.0003 | 0.01 | 30 |
| K_O | Saturation coefficient for oxygen | gO_2/m^3 | 0.0233 | 0.0367 | 0.2 | 30 |

***The default value did not change during trajectory optimization, so the default value was taken.*

The average yield coefficient Y_H obtained was 0.61 against the ASM3 default value of 0.63. The experimental value is close to the ASM3 default value indicating the reliability of the experimental results. It is important to estimate the yield correctly because it influences the estimation of sludge

production, oxygen demand and other parameters whose determination depends on the value of Y_H , like the determination of S_S from respirometric experiments as well as the determination of the decay rate constant b_H .

The results for the maximum growth rate of heterotrophic, μ_H , and the hydrolysis rate constant, k_h , are comparable to the ASM3 default values. An average value of 2.4 d^{-1} as compared to the ASM3 value of 2 d^{-1} was obtained for μ_H , while the results of the hydrolysis rate constant indicate an average value of $3.03 \text{ gCOD}_{XS}/\text{gCOD}_{XH}$ compared to $3 \text{ gCOD}_{XS}/\text{gCOD}_{XH}$.

The value obtained for the saturation coefficient for the readily biodegradable substrate K_S , was $2.31 \text{ gCOD}_{SS}/\text{m}^3$ which is also a comparable value to the model default value of $2 \text{ gCOD}_{SS}/\text{m}^3$. The saturation coefficients of ammonium and oxygen, K_{NH} and K_O respectively, turned out to be lower in the actual experiment compared to the default values. A possible cause for the lower value is the presence of effective mixing in the batch experiment which improves the diffusion of substrate to the biomass cells, as compared to the values derived from the actual activated sludge unit where the presence of bigger flocs and different mixing characteristics will affect the diffusion of substrate, thus leading to different values of the saturation coefficients (Petersen et al., 2002).

Table 6.5 indicates that there was a slight change in the values of most of the parameters except the oxygen saturation coefficient K_O and oxygen mass transfer coefficient K_La which changed from 0.2 to $0.02 \text{ gO}_2/\text{m}^3$ and 50 to 204 d^{-1} , respectively, which suggests that these are critical model parameters deserving attention during the calibration of the plant model.

6. DEVELOPING THE PLANT MODEL

The plant model of Marianridge WWTP was configured in WEST. Sub-models were assigned to the different units in the configuration. There after simulations were run, evaluated and then the model was calibrated against plant operating data.

6.1. WEST configuration for Marianridge wastewater treatment plant

A model of Marianridge WWTP was configured using the WEST configuration builder by putting together the appropriate sub-models to represent the actual units of the treatment plant. The WEST configuration of the Marianridge Plant is shown in Figure 6:1.

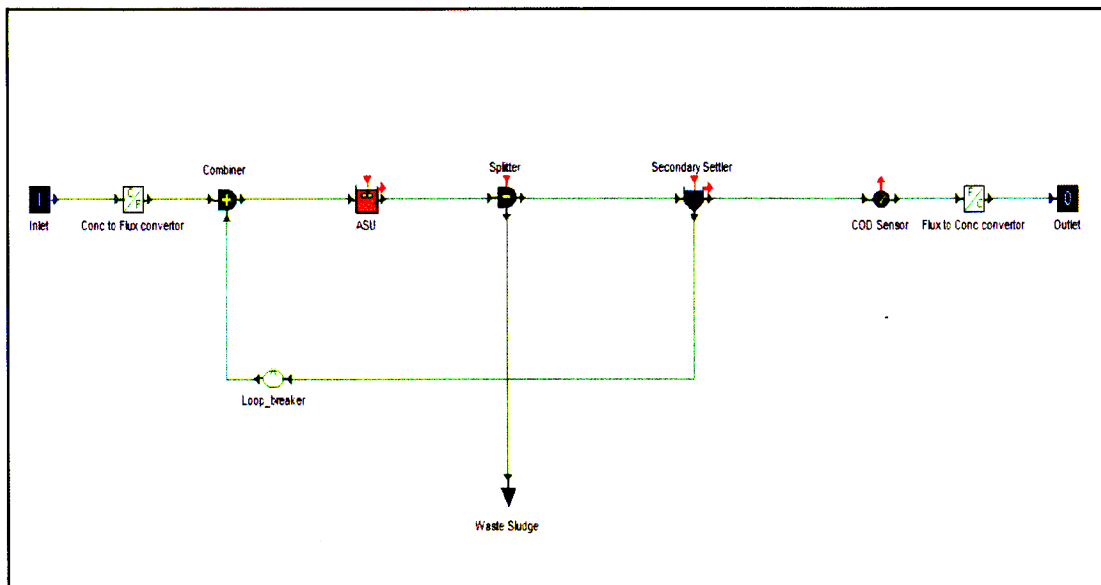


Figure 6:1 The WEST configuration for the Marianridge section of Umhlatuzana works

The configuration consists of the major units of the WWTP, the activated sludge unit (ASU) and the two secondary settlers. The secondary settlers are configured as one unit since it is assumed that they operate in the same way. Combiners and splitters have been added to combine and split flows, respectively. A COD sensor has been added to the outlet stream, to measure the COD concentration of the treated effluent. Converters in the configuration are used to convert concentrations of constituents in the wastewater to flux values, and flux to concentration values, as required by the following sub-models. The selection of sub models is outlined in the following sections.

6.2. Selection of sub-models

The selection of sub-models for the units making up the WEST configuration for Marianridge WWTP is discussed in the following sections.

6.2.1. Input

The *input* sub-model allows the influent to the wastewater treatment plant to be entered in terms of the volumes and composition of the raw sewage, either as constant values used in a steady-state simulation or as time dependant values which are used for a dynamic simulation.

6.2.2. Concentration to flux and flux to concentration converters

The *concentration to flux* sub-model is used to convert incoming data expressed as concentrations into flux values while the *flux to concentration* sub-model is used to convert flux values to concentrations. The input file representing the influent is given in concentrations hence the need to convert to fluxes which can be used in the differential equations in the model. To view the output from the simulation model in terms of concentrations the flux to concentration converter is used to convert the fluxes to concentrations.

6.2.3. Two-combiners

This sub-model combines the two incoming flows by summing up the inflow per component. For the calculation of the influent flow rate only water is considered.

6.2.4. WEST sub models for the activated sludge unit

Three types of sub-models are available for the activated sludge unit (ASU) in WEST. The *variable volume ASU* has one or more weirs and a variable volume and the effluent flow rate depends on the type, width, design and number of weirs. The *pumped volume ASU* has a volume which is controlled with a pump, between a maximum and minimum level. Between the two levels, the flow rate is constant (equal to the pump flow rate). The *fixed volume ASU* has a constant volume, and the influent flow rate to the ASU is the equal to the effluent flow rate.

At the head of the Marianridge Works there is an equalising tank which ensures constant flow into the activated sludge unit since there are flow variations coming into the works, therefore the fixed volume ASU is the most appropriate to model the near constant volume in the aeration basin.

6.2.5. Secondary settler

One-dimensional models based on the flux theory are used to model secondary settling tanks. These models assume a uniform horizontal velocity profile in the clarifiers, and that horizontal gradients in concentration are negligible. This results in modelling of only the processes in the vertical dimension, giving a settling cylinder which is viewed as a continuous flow reactor shown in Figure 6:2 where Q and X represent flow rate and suspended solids concentration respectively and the subscripts F,E and U represent feed, effluent and underflow respectively.

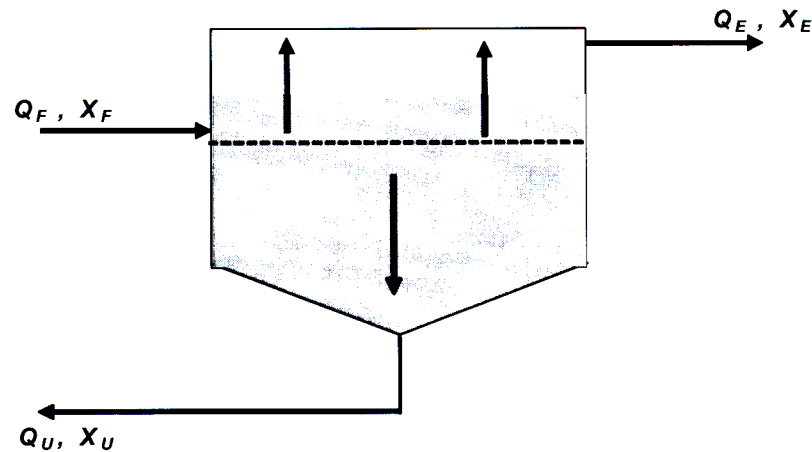


Figure 6:2 Schematic diagram showing the idealised secondary settler

The incoming mixed liquor is introduced through the inlet of the settling tank and the suspension is homogeneously spread over the horizontal cross section. The flow is divided into a downward flow towards the underflow exit at the bottom, and an upward flow towards the effluent exit at the top. It is further assumed that the concentration of suspended solids is completely uniform across any horizontal plane within the settler, and that the solid-liquid interface represents a physical boundary to separation and that the solids flux due to gravitational settling is zero at the bottom. It is also assumed that there are no significant biological reactions affecting the mass concentration inside the settler.

The sludge entering the settler is transferred to the bottom by two flux components the gravity flux G_S and the bulk flux G_B caused by the downward flow generated by the sludge being removed from the bottom of the settler tank. The total flux G_T is the sum of the two flux components.

$$G_T = G_S + G_B$$

$$G_T = v_s X + v_b X$$

Where: v_b is the vertical bulk velocity,
 v_s the settling velocity of the sludge,
 X the sludge concentration,

The flux theory is applied in simulation programs by splitting the tank into a number of horizontal layers and by applying the differential conservation equation on these layers.



6.2.5.1. WEST sub models for secondary settlers

There are six sub-models available in WEST for the representation of the secondary settlers

- Secondary point settler
- Marsili-Libelli
- Secondary Otterpohl Freund
- Takacs
- Secondary Takacs Solubles Propagator
- Secondary Takacs all fraction Propagator

The sub models are shortly introduced in **Appendix D**.

Choice of the secondary clarifier model

Grijnspeerdt et al., (1995) conducted a comparative study of several settler models available in literature. In this study, the settlers models were evaluated with respect to consistency and robustness and it was concluded that the double exponential settling velocity model proposed by Takacs et al., (1991) most realistically represents the sedimentation-clarification process. Based on the study by Grijnspeerdt et al., (1995) the Takacs model was initially adopted for modelling the secondary settling tanks and it was compared to the point settler model. The simulations of the plant model were similar for the two scenarios, hence it was opted to use the simpler point settler model.

The parameter which had to be determined in the point settler model was the non-settleable fraction of suspended solids f_{ns} . The non-settleable fraction of suspended solids was determined from mass balance of suspended solids across the secondary clarifier. The calculated value was 0.0052. The point settler model also offers more computing speed since it is mathematically simpler than the Takacs model, hence the use of the point settler model in the final plant model.

6.2.6. Two-splitter

The two-splitter sub-model divides the flow into two streams. Two sub-models are available for the splitters; an absolute splitter and a relative splitter. The absolute splitter has a constant value for one of the streams which result from the split, while in a relative splitter the ratio of the flow of the resulting streams is constant but the magnitude of the flows can vary. In Marianridge WWTP the splitter immediately after the activated sludge unit allows a constant flow of excess sludge to be wasted from the plant. Hence an absolute splitter is used to split the flow into two streams, one going to the settler and another representing the fixed flow of the wasted excess sludge.

6.2.7. Loop breaker

There are 2 sub-models available for the loop breaker unit; the loop breaker and differential loop breaker. Both sub-models are used to avoid circular algebraic dependencies during the modelling of recycle streams in the configuration of the wastewater treatment plant. The loop breaker introduces a time delay representing the retention time in the loop. The differential loop breaker was selected to represent the recycle stream in the WWTP configuration.

6.2.8. Online COD sensor

The effluent COD concentration is measured on line by an online *COD sensor* sub-model.

6.2.9. Output

The composition of the effluent from the WWTP model is accessed through the *output* sub-model. Results of pre-selected components of the effluent stream can be graphically depicted or written to an output text file. The user selects the components in the sub-model in order for the components to be plotted and sent to the output text file for further viewing.

6.2.10. Waste Flux

Waste Flux is a sub-model representing the excess waste-removal from a wastewater treatment plant. The inflow is expressed in fluxes. In the wastewater treatment plant simulation model it is used to represent the sludge wasted from the activated sludge unit.

6.3. Calibration of the model

The adequacy and reliability of the information available for the development of the model for the Marianridge WWTP was evaluated during the calibration of the model against plant operating data. The extent to which the model fits the plant data with the available modelling information will give a measure of how adequate the available information is for the purpose of modelling.

The purpose of the model in this study is to simulate the processes which happen in the WWTP. The calibration in this study aims to closely match the measured effluent COD concentration and the ammonia concentrations in the activated sludge unit, since the availability of consistent historical plant data is restricted to these two variables.

Matching the measured effluent COD and ammonia concentration gives a measure of how well the model can simulate the COD removal and nitrogen removal processes which occur in the activated sludge unit. Biodegradation of COD will also influence the concentration of nitrogen components such as ammonia and nitrates in the activated sludge unit; therefore it is important to look at the two variables, the effluent COD and ammonia concentration in the activated sludge unit.

A major challenge encountered in calibration of activated sludge models is the lack of identifiability of the model parameters, which is the ability to obtain a unique combination of parameters that fit the calibration data (Petersen et al., 2002). Due to the identifiability problems a stepwise procedure was used, where just a few parameters are changed at a time instead of applying an automatic mathematical optimisation routine. A steady-state calibration was done followed by a dynamic calibration.

6.3.1. Steady-state calibration

The information available for steady-state calibration and the steps taken during the steady-state calibration are discussed in the following sections.

6.3.1.1. Information for steady-state calibration

The available information for steady-state calibration is the design and operational data collected from Marianridge WWTP, average biological characterisation of influent wastewater and the average characterisation of the waste sludge stream from experiments and data collected from

eThekwini municipal laboratory. The information is summarised in Table 6.1, Table 6.2 and Table 6.3.

Table 6.1 Volume of the activated sludge unit and secondary clarifiers of Marianridge WWTP

| Design parameter | Unit | Value |
|---------------------------------|----------------|-----------|
| Volume of activated sludge unit | m ³ | 13 600 |
| Volume of secondary clarifiers | m ³ | 2 × 2 037 |

Table 6.2 The average influent wastewater characterisation of Marianridge WWTP for the year 2006

| Component | Unit | Mean | Standard deviation | No. of tests |
|---|--|-------|--------------------|--------------|
| Influent volume | m ³ /d | 9 800 | 4800 | 350 |
| Influent COD | gCOD/m ³ | 775 | 330 | 291 |
| Total suspended solids, X _{SS} | gSS/m ³ | 298 | 224 | 62 |
| Free ammonia, S _{NH} | gN/m ³ | 24.7 | 7.3 | 325 |
| Alkalinity, S _{ALK} | gHCO ₃ ⁻ /m ³ | 266.4 | 64.5 | 338 |

Table 6.3 Average total suspended solids concentration in the waste sludge from Marianridge WWTP (2006)

| Source of sludge | Suspended Solids | | | |
|-----------------------|--------------------|------|--------------------|--------------|
| | Units | Mean | Standard deviation | No. of tests |
| Activated sludge unit | gSS/m ³ | 455 | 245 | 81 |

6.3.1.2. Steady-state input file representing influent

To convert the collected data into an input file representing the influent wastewater going into the WWTP, for the steady-state calibration of the model, the average total COD was split based on the experimental results, into the ASM3 COD fractions (S_S + S_I + X_I + X_S + X_H + X_A). Components were added to the input file to represent concentrations for dissolved oxygen S_{O2}, di-nitrogen S_{N2}, organics stored by heterotrophs X_{STO}, and nitrate plus nitrite S_{NOX}. As earlier discussed in section 2.2 the concentrations of autotrophic biomass X_A, dissolved oxygen S_{O2}, nitrates + nitrites S_{NOX}, di-nitrogen S_{N2}, and organics stored by heterotrophs X_{STO} are assumed to be negligible in the influent wastewater hence they are equal to zero in the influent. The resulting steady-state input file is shown in Table 6.4. The source data for the values in Table 6.4 are Table 5.4 and Table 6.2.

Table 6.4 Part of the steady-state input file representing the influent wastewater

| | | | | | | | |
|------------------|-----------------------|-----------------------|------------------------|------------------------|-----------------------|--|------------------------|
| Component | Influent | S_S | S_I | X_I | X_S | X_H | X_A |
| Units | m ³ /d | gCOD/m ³ | gCOD/m ³ | gCOD/m ³ | gCOD/m ³ | gCOD/m ³ | gCOD/m ³ |
| Value | 9 800 | 140.3 | 58.1 | 15.6 | 342.55 | 113.15 | 0 |
| Component | X_{SS} | S_{O2} | S_{NOX} | S_{NH4} | S_{N2} | S_{ALK} | X_{STO} |
| Units | gSS/m ³ | gCOD/m ³ | gN/m ³ | gN/m ³ | gN/m ³ | gHCO ₃ ⁻ /m ³ | gCOD/m ³ |
| Value | 298 | 0 | 0 | 25 | 0 | 266 | 0 |

The kinetic parameters determined from the respirometric experiments were used as input to the model. The kinetic parameters are summarised in Table 6.5.

Table 6.5 Model kinetic parameters obtained from experiments

| Symbol | Description | Unit | Mean | Std. dev. | ASM3 |
|-----------------|---|--|-------------|------------------|-------------|
| Y _H | Yield coefficient | gCOD _{XH} /gCOD _{XSTO} | 0.61 | 0.11 | 0.63 |
| b _H | Decay rate constant | d ⁻¹ | 0.03 | 0.01 | 0.2 |
| μ _H | Maximum growth rate | d ⁻¹ | 2.4 | 0.24 | 2 |
| k _h | Hydrolysis rate constant | gCOD _{Xs} /gCOD _{XH} | 3.03 | 0.41 | 3 |
| K _S | Saturation coefficient for S _S | gCOD _{SS} /m ³ | 2.31 | 0.26 | 2 |
| K _X | Saturation coefficient for particulate COD | gCOD _{Xs} /gCOD _{XH} | 1 | - | 1 |
| K _{NH} | Saturation coefficient, for S _{NH} | gN/m ³ | 0.00107 | 0.0003 | 0.01 |
| K _O | Saturation coefficient. for oxygen | gO ₂ /m ³ | 0.0233 | 0.0367 | 0.2 |

6.3.1.3. Steady-state simulation of the model before calibration

Using the information in the steady-state input file two steady-state simulations were run in the model. In the first simulation the model was fully defined by only default ASM3 model parameters. In the second simulation the experimentally determined parameters in Table 6.5 replaced the default parameters in the model. The results of the two simulations are compared to measured values from data collected from eThekwini municipal laboratory, in Table 6.6.

Table 6.6 Steady-state simulation results before calibration

| Component | Final effluent COD [gCOD/m ³] | Free ammonia in ASU [gN/m ³] | Waste sludge TSS [gSS/m ³] |
|----------------------------------|---|--|---|
| Measured values | 66 | 0.98 | 455 |
| Simulated values: | | | |
| With ASM3 default parameters | 81 | 0.79 | 608 |
| With parameters from experiments | 78 | 0.72 | 833 |

It was observed that for both simulations the model overestimated the final effluent COD concentration. The simulation with parameters determined from experiments predicts a closer value as compared to the simulation with ASM3 default parameters. The measured final effluent COD concentration was 66 gCOD/m³. The simulation with parameter-values from experiments predicted a final effluent COD concentration of 78 gCOD/m³ and the simulation with ASM3 default parameter-values predicted 81 gCOD/m³.

The free ammonia concentration in the activated sludge unit is underestimated in both simulations. The measure free ammonia concentration was 0.98 gN/m³. The simulation with ASM3 default parameter-values predicted a concentration of 0.79 gN/m³, while the simulation with parameter-values predicted a concentration of 0.72 gN/m³. The simulation with parameters-values determined from experiments underestimates the free ammonia concentration by a wider margin.

An overestimate of the concentration of total suspended solids (TSS) in waste activated sludge is also observed in both simulations. The measured concentration of total suspended solids was 455 gSS/m³. The simulation with ASM3 default parameter-values predicted a concentration of 608 gSS/m³ while the simulation with parameter-values from experiments predicted a concentration of 833 gSS/m³.

The results from the simulations show that there is need to adjust some model parameters in order to improve the models' predictions when compared to the measured data.

6.3.1.4. Adjusting model parameters

Three variables were evaluated during the steady-state simulations before calibration; effluent COD concentration, free ammonia concentration in the activated sludge unit and total suspended solids concentration in waste activated sludge.

To match the predicted effluent COD concentration and the free ammonia concentration in the activated sludge unit, with measured data requires dynamic calibration but the predicted concentration of total suspended solids in waste activated sludge can be made to fit measured data through steady-state calibration because the concentration of total suspended solids in waste activated sludge depends on the long term operation of the activated sludge unit which is being represented by the defined steady-state. Therefore a steady-state calibration was done to fit the predicted value of the concentration of total suspended solids concentration in waste activated sludge to the measured value.

This was done by adjusting parameters responsible for long-term biological behaviour in the activated sludge unit, running simulations and comparing for the improvement in the predicted value of the concentration of total suspended solids in waste activated sludge. These parameters are, the decay rate constant of heterotrophic biomass b_H , the anoxic endogenous respiration rate for heterotrophic biomass $b_{H,NOX}$, the aerobic respiration rate for cell internal storage products $b_{STO,O2}$ and the anoxic respiration rate for cell internal storage products $b_{STO,NOX}$. The ASM3 default values for the parameters are shown in Table 6.7 together with the values before and after calibration to fit the measured data.

Table 6.7 Steady-state calibration parameters: ASM3 default values, and values before and after calibration

| Parameter | Units | ASM3 default value | Value before calibration | Value after calibration | Change in value |
|---------------|----------|--------------------|--------------------------|-------------------------|-----------------|
| b_H | d^{-1} | 0.2 | 0.03 | 0.27 | + |
| $b_{H,NOX}$ | d^{-1} | 0.10 | 0.10 | 0.37 | + |
| $b_{STO,O2}$ | d^{-1} | 0.20 | 0.20 | 0.51 | + |
| $b_{STO,NOX}$ | d^{-1} | 0.10 | 0.10 | 0.10 | 0 |

Note: [0 indicates no change, + indicates increase]

After calibration the predicted value for the concentration of total suspended solids concentration in waste activated sludge was 456 gSS/m^3 as compared to the measured value of 455 gSS/m^3 which is acceptable for this model and this suggests a satisfactory calibration step.

The value of $b_{\text{STO,NOX}}$ remained at the default value while the rest of the parameters were adjusted to fit the measured data. The adjusted values indicate that the decay rate constant for heterotrophic biomass b_{H} , which was determined from experiments, turned out to be lower than the value after calibration. An explanation for this might be in line with suggestions that it is possible but difficult to determine a representative value of the decay rate constant of the full-scale WWTP (Petersen et al., 2002). In the experiment the decay constant is investigated under starving conditions, while in the actual plant there is substrate inflow, which enables decay and growth to take place simultaneously. The decay rate in the full-scale plant can be influenced by the presence of other micro-organisms such as protozoa, (Petersen et al., 2002) which may not be able to survive in the laboratory-scale experiment and this will result in different values of the decay rate constant.

The values of anoxic endogenous respiration rate for heterotrophic biomass $b_{\text{H,NOX}}$, the aerobic respiration rate for cell internal storage products $b_{\text{STO,O2}}$ and the anoxic respiration rate for cell internal storage products $b_{\text{STO,NOX}}$ were not determined from experiments but ASM3 default values were used before the calibration. After calibration the default values turned out to be lower than the values before calibration.

Underestimation of these rate constants resulted in slower rates of the decay reactions resulting in less inert particulate organics being produced. Inert particulate organics contribute to the sludge's total suspended solids concentration. Production of more inert particulate organics increases the suspended solids concentration in the waste sludge stream.

6.3.2. Dynamic calibration

The model needs dynamical calibration after steady-calibration. If the model is calibrated by steady-state calibration alone, problems may be encountered during dynamic simulations since the real input variations are usually faster than the slow process dynamics which are focused on, during the steady-state calibration (Petersen et al., 2002). The use of the model will include the prediction of short-term dynamics of the effluent total COD concentration and the free ammonia concentration in the activated sludge unit, hence the need for calibration to dynamic data.

The aim of model calibration based on dynamic data is to obtain a more reliable estimation of the maximum specific growth rates μ_H and μ_A (Henze et al, 1999), which are the most important parameters in predicting dynamic situations. Selected saturation coefficients and kinetic parameters were also tuned to improve the prediction of effluent total COD and free ammonia concentration in the activated sludge unit.

6.3.2.1.Saturation coefficients

In pure cultures, the saturation coefficients can be regarded as pure biological parameters that give measures of the affinity of the biomass for substrates (Petersen et al, 2000). However in activated sludge, bacteria grow in flocs, where the size and structure of the flocs affect the diffusion of substrate to the biomass cell, thereby affecting the apparent value of the saturation coefficients. Thus, the different mixing characteristics of laboratory-scale and full-scale systems make it difficult to transfer laboratory-scale observation to full-scale behaviour (Henze et al, 1999). This creates a challenge to obtain an accurate model value from laboratory experiments. With this knowledge in mind, the experimentally determined values are used as initial values in the model but are further tuned during model calibration.

6.3.2.2.Dynamic calibration strategy

The assessment before steady-state calibration, of how well the model can predict the effluent COD concentration and the free ammonia concentration in the activated sludge showed that the model overestimated the effluent COD concentration and underestimated the free ammonia concentration.

Dynamic simulations by the model before dynamic calibration also show that the model overestimates the final effluent total COD concentration during certain periods and underestimates the free ammonia concentration in the activated sludge unit. Figure 6:3, Figure 6:4 and Figure 6:5 show the dynamic simulations of the model before dynamic calibration. The model can follow the trend of measured values during some periods through the simulation period but it does not completely match the measure data.

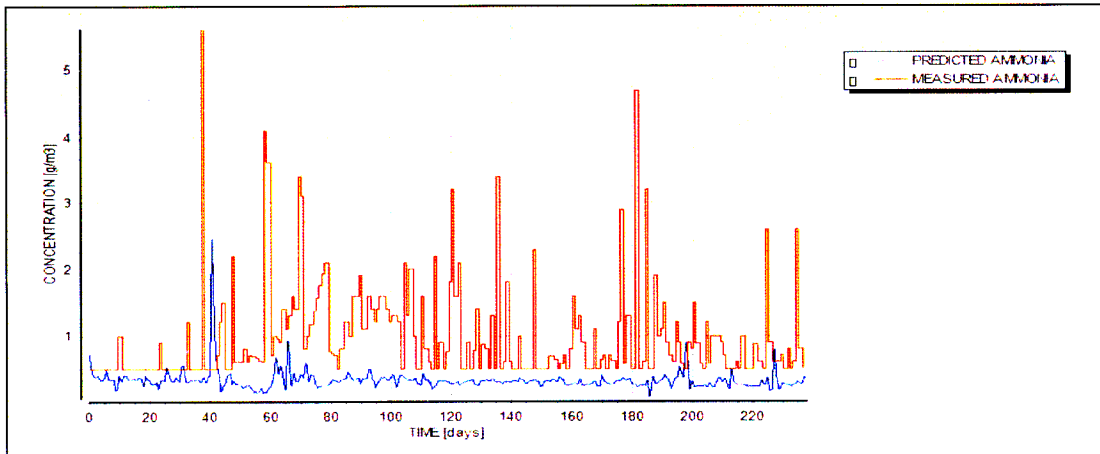


Figure 6:3 Predicted and measured free ammonia concentration before dynamic calibration year 2006

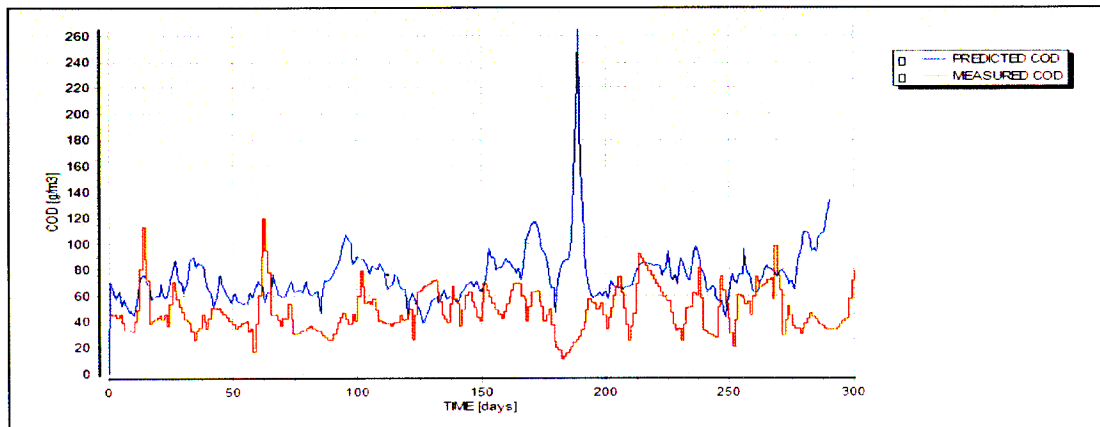


Figure 6:4 Predicted and measured effluent COD concentration before dynamic calibration for year 2005

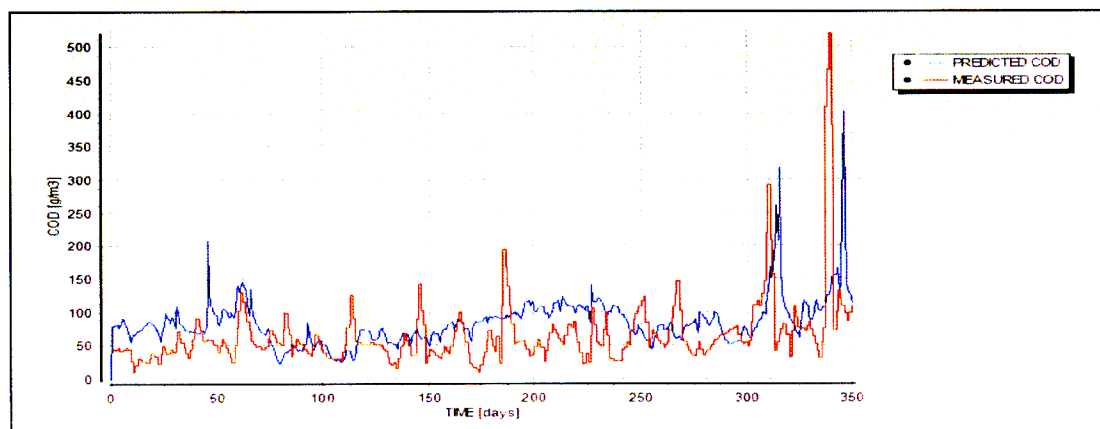


Figure 6:5 Predicted and measured effluent COD concentration before dynamic calibration for year 2006

From Figure 6:3, Figure 6:4 and Figure 6:5 it can be observed that the model's prediction does not match the sharp variations and the peaks shown by the measured data. A possible cause for this might be the fact that the measured data was missing for some of the days, so the gaps had to be filled in by interpolation. During the days when the values of effluent COD concentration or free ammonia concentration determined by interpolation differ from the actual values on the plant, the model's prediction will not match the measured data.

The predicted free ammonia concentration in the activated sludge unit is underestimated by the model as shown in Figure 6:3. This indicates that there is need to adjust kinetic parameters responsible for the reactions involving free ammonia in the activated sludge model. Since it is difficult to determine saturation coefficients from laboratory experiments which are transferable to full scale systems (Petersen et al, 2002), saturation coefficients are considered for adjustment during the dynamic calibration together with other parameters selected after running a sensitivity analysis.

6.3.2.3.Sensitivity analysis

The purpose of the sensitivity analysis is to establish how sensitive a chosen variable is to changes in the model parameters. In the sensitivity analysis, the selected variables were the predicted effluent COD concentration and free ammonia concentration in the activated sludge unit. A separate sensitivity analysis was run for each variable. The most sensitive parameters are then adjusted in a trajectory optimisation procedure in WEST to improve the curve fitting between the predicted and measured values.

In the sensitivity analysis the absolute and relative sensitivity of a selected variable due to a change in a particular parameter is calculated. This is done for a number of sensitivity functions. For each sensitivity function, the sensitivity is calculated as follows:

- First a reference simulation is run.
- Next the parameter, P, is altered by a certain factor (the perturbation factor) and a new simulation (the perturbation simulation) is run
- Then the absolute sensitivity is calculated for each time point as the difference between the variable value of the reference simulation and the variable value of the perturbation simulation divided by the difference between the parameter value of the reference simulation

and parameter value of the perturbation simulation. Equations 9.1 to Equation 9.3 show how absolute sensitivity, relative sensitivity and the average relative sensitivity of a variable, Y, respectively, are determined.

$$SF = \frac{Y_{pert} - Y_{ref}}{P_{pert} - P_{ref}} \quad [9.1]$$

$$RSF = \frac{Y_{pert} - Y_{ref}}{P_{pert} - P_{ref}} * \frac{P}{Y} \quad [9.2]$$

$$AS = \frac{\sum^N \left(\frac{Y_{pert} - Y_{ref}}{P_{pert} - P_{ref}} * \frac{P}{Y} \right)}{N} \quad [9.3]$$

Where:

- SF = absolute sensitivity
- RSF =relative sensitivity
- ASF = average relative sensitivity
- Y = variable value
- Y_{pert} = the variable value in the perturbation simulation
- Y_{ref} = the variable value in the reference simulation
- P = parameter value
- P_{pert} = the parameter value in the perturbation simulation
- P_{ref} = the parameter value in the reference simulation
- N = number of simulation steps

Since the model is non-linear a very small perturbation factor (1×10^{-6}) was used, in order to use the finite difference method, where the variable has to change linearly with respect to a change of the parameter. In order to quantify this problem a control simulation is performed. The parameter P is, again, altered by a certain factor (the perturbation factor multiplied with the control factor) for the control simulation.

The sensitivity analysis identifies the model parameters which influence the identified variables, but does not clearly indicate whether the influence results in an increase or decrease of the variable. Consequently, after identifying the parameters influencing the variables, a steady state run is

performed on the model and then each parameter is increased while other parameters are kept constant, to evaluate the effect of changing that parameter, against an initial steady state reference simulation run. The evaluation was based on increasing each parameter and observing the change in the variables (effluent COD and free ammonia concentration, S_{NH} in the activated sludge unit). The results of the evaluation on the model parameters are shown in Table 6.8.

Table 6.8 The effect of selected parameters on effluent COD and free ammonia in the ASU, when the parameters are increased

| Parameter | Description | Effluent COD | S_{NH} |
|-------------|--|--------------|----------|
| μ_H | Maximum specific growth (heterotrophs) | - | - |
| μ_A | Maximum specific growth (autotrophs) | - | - |
| K_X | Saturation coefficient for particulates | - | - |
| K_{La} | Mass transfer coefficient | - | - |
| K_O | Saturation coefficient for dissolve oxygen | * | - |
| K_S | Saturation coefficient for S_S | + | * |
| K_{A_NH} | Ammonium saturation coefficient for autotrophs | * | + |
| K_{A_O} | Oxygen saturation coefficient for autotrophs | - | + |

Note: [+indicates increase, - indicates decrease, *indicates no effect]

6.3.2.4. Adjusting of model parameters

Trajectory optimisation in WEST was used to complete the dynamic calibration by adjusting the selected model parameters to fit the measured effluent COD concentration and the concentration of free ammonia in the activated sludge unit, S_{NH} . The calibrated values are compared to default ASM3 values in Table 6.9.

Table 6.9 Model parameters after calibration, compared to default ASM3 values and value before calibration

| Parameter | Units | ASM3 value | Value before calibration | Value after calibrated value | Change in value |
|-------------|-----------------------|------------|--------------------------|------------------------------|-----------------|
| μ_H | d^{-1} | 2 | 2.4 | 2.4 | 0 |
| μ_A | d^{-1} | 1 | 1 | 1 | 0 |
| K_X | $gCOD_{XS}/gCOD_{XH}$ | 1 | 1 | 1 | 0 |
| K_{La} | d^{-1} | 50 | 50 | 50 | 0 |
| K_O | gO_2/m^3 | 0.2 | 0.02 | 0.02 | 0 |
| K_S | $gCOD_{SS}/m^3$ | 2 | 2.31 | 2.31 | 0 |
| K_{A_NH} | gN/m^3 | 1 | 1 | 2.0 | + |
| K_{A_O} | gO_2/m^3 | 0.5 | 0.5 | 0.8 | + |

Note: [0 indicates no change, + indicates increase]

The saturation coefficient for particulate COD K_X , the maximum specific growth rate of heterotrophic biomass μ_H , and the maximum specific growth rate of autotrophic biomass μ_A , had little effect on the variables and remained unchanged from their values before calibration. The maximum specific growth rate of heterotrophic biomass μ_H , determined from experiment remained unchanged after calibration at a value of is $2.4 d^{-1}$. The value is higher than the default ASM3 value.

The value for the saturation coefficient for oxygen K_O , remained as $0.02 gO_2/m^3$, after calibration indicating that the initial value is appropriate for the model as compared to the ASM3 default value of $0.2 gO_2/m^3$ which turned is higher. The value of the oxygen mass transfer coefficient K_{La} remained at the ASM3 default value of $50 d^{-1}$ after calibration. It is appreciated that K_{La} depends on plant operations and could not be determined experimentally, hence in the absence of measured values an attempt to tune K_{La} to fit the measured data of effluent COD was done.

The ammonium substrate saturation for autotrophic biomass, K_{A_NH} and the oxygen saturation for autotrophic biomass, K_{A_O} were adjusted to $2 gN/m^3$ and $0.8 gO_2/m^3$ respectively, to fit the predicted free ammonia in the activated sludge unit. The adjustment of these parameters related to autotrophic biomass was due to the fact that the laboratory experiments did not include determination of the kinetic parameters of autotrophic biomass.

The simulation results for the free ammonia concentration in the activated sludge unit before and after calibration are shown in **Error! Reference source not found.** and Figure 6:6 respectively.

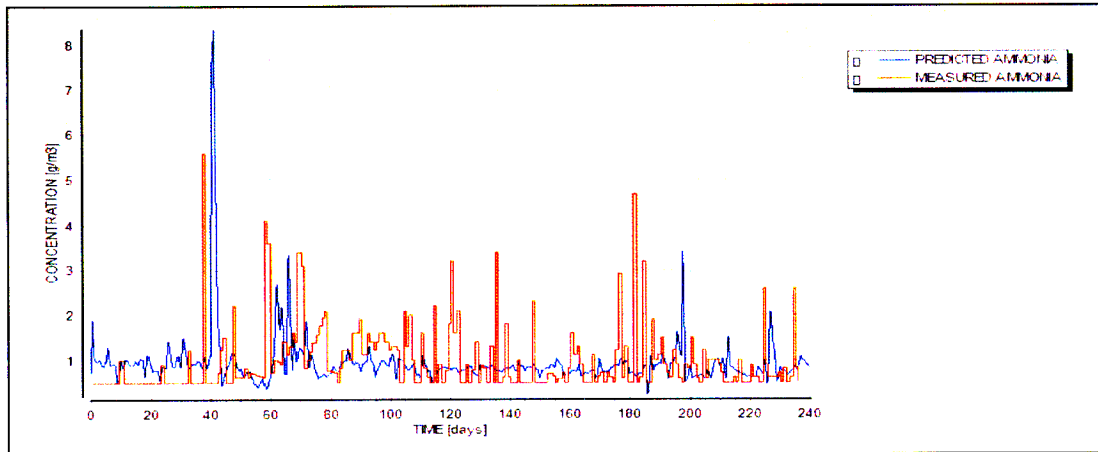


Figure 6:6 Predicted and measured free ammonia concentration after calibration for the year 2006

The calibrated model gives a better simulation of the free ammonia dynamics. The predicted curve matches the peaks of the measured data during certain intervals but fails during other periods, and it can be observed that the model manages to estimate the average trend of ammonia concentration after calibration.

During other intervals it can be seen that the measured ammonia concentration shows a constant value over a period of several days, while the model predicts fluctuations. The possible cause for this difference can be attributed to some inconsistency in the measured historical data collected from the municipal laboratory. A possible source of inconsistency might be the use of the previous day's measurements to fill in the gap of the next day caused by absence of measurements for that particular day.

The simulation results for the effluent COD concentration in the activated sludge unit before and after calibration are shown in Figure 6:7 and Figure 6:8 respectively

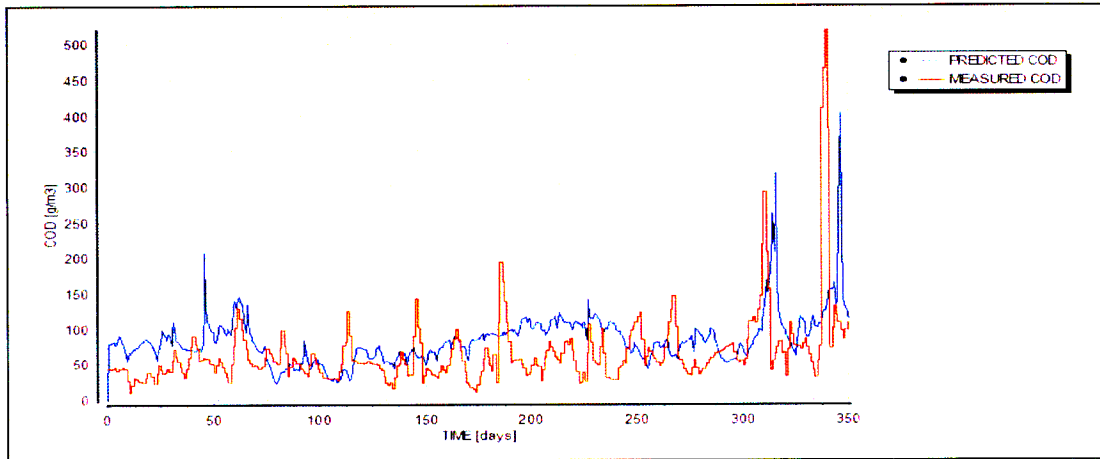


Figure 6:7 Predicted and measured effluent COD concentration before dynamic calibration for year 2006

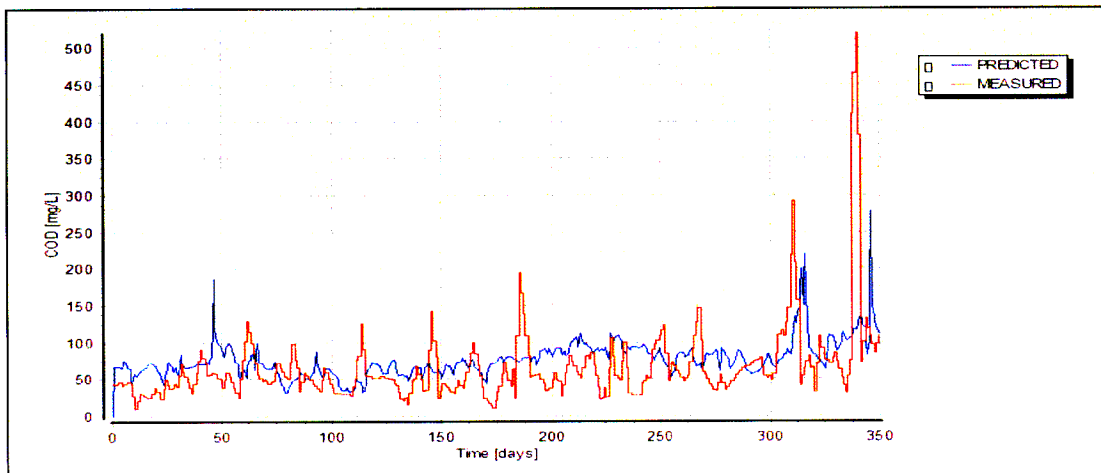


Figure 6:8 Predicted and measured effluent COD concentration after dynamic calibration for year 2006

The change in the predicted effluent COD concentration curve is more of a downward shift of the entire curve; the horizontal profile of the curve did not change. The model can still predict the trend of the measured effluent COD, but it predicts a higher effluent COD concentration during some of the time intervals. The description of the effluent COD concentration is good and the effect of high COD in the influent wastewater can be seen in the two sharp peaks shown after the 300 day mark. To further evaluate how well the model can predict effluent COD concentration validation of the model was done.

6.4. Validation of the model

After dynamic calibration, validation of the model was done using historical measured data for the year 2007 which was not used in calibration of the model. Validation gives an indication of how well the model can simulate the treatment plant after the calibration effort. The data for the free ammonia concentration in the activated sludge unit were not available for the year 2007, so the only data set of 2006 was used earlier to check for improvement in the prediction of the ammonia concentration. The effluent COD concentration data for 2007 were available for model validation.

6.4.1. Effluent COD concentration

Figure 6:9 shows that the calibrated model can simulate the trend and fluctuations of the effluent COD concentration.

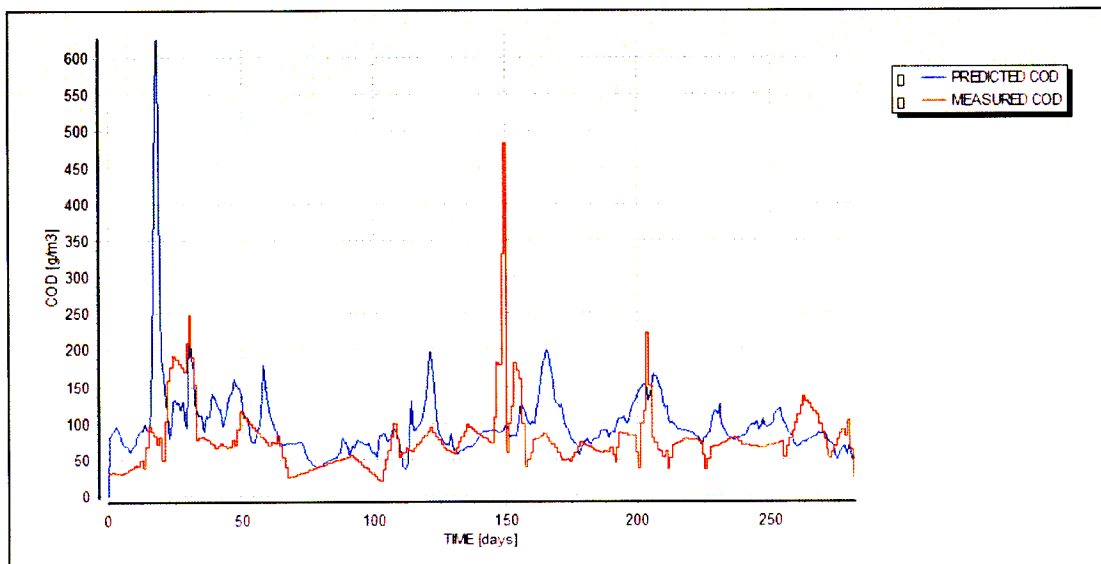


Figure 6:9 Effluent COD simulation after calibration for the year 2007

At the early stages of the simulation the model indicates a noticeable high peak far from the measured value. This peak is due to a high COD value in the input file based on the historical measured data of the influent COD concentrations of 2007 whose reliability could not be verified. The measured effluent COD does not indicate the peak, only the model shows how the high influent COD reflects in the effluent COD. For the rest of the simulation the model estimates the trends satisfactorily though the peaks during fluctuations turn out to be higher.

The effluent contains other component of interest like the nitrate + nitrite concentration and the free ammonia concentration. How well the model predicts the concentration of these components could not be assessed due to lack of measured data to compare with the model predictions. The data available for the effluent from the Marianridge WWTP consisted of only the COD concentrations.

7. DISCUSSION

The main objective of this study was to produce, a calibrated process model for the Marianridge WWTP treating influent wastewater with a significant portion of industrial wastewater. A methodology was adopted where laboratory experiments, historical data from the municipal laboratory and modelling of experiments are employed to generate information for the development and calibration of the plant model.

Respirometric batch test

Respirometric experiments carried out on influent wastewater and activated sludge were used to determine the yield coefficient Y_H , the maximum growth rate μ_H and the decay rate constant b_H . The mean value obtained for Y_H was 0.61 which is close to the ASM3 default value of 0.63, while μ_H was found to be 2.4 d^{-1} as compared to the ASM3 value of 2 d^{-1} and b_H was found to 0.03 d^{-1} as compared to the ASM3 value of 0.2 d^{-1} . The value obtained for b_H suggested that there might be need to adjust the value during the calibration of the model.

The influent COD fractions S_S and X_H were also found to be 18.1 % and 14.6 % of total COD respectively, from the respirometric batch test on 24 h composite samples of the influent wastewater. The influent COD fraction S_I was determined to be 7.5 % of total COD by flocculation-filtration of the composite sample at the batch of the respirometric batch test.

Modelling of respirometric batch test

The hydrolysis rate constant k_h , saturation constant for readily biodegradable substrate K_S and the saturation coefficient for particulate COD K_X were determined from the modelling of the batch respirometric experiment. The mean value of k_h was found to be $3.03 \text{ gCOD}_{XS}/\text{gCOD}_{XH}$ as compared to the ASM3 value of $3 \text{ gCOD}_{XS}/\text{gCOD}_{XH}$. The value obtained for K_S , was $2.31 \text{ gCOD}_{SS}/\text{m}^3$ which is also a comparable value to the ASM3 value of $2 \text{ gCOD}_{SS}/\text{m}^3$. The saturation coefficient for particulate COD retained the ASM3 default value of $1 \text{ gCOD}_{XS}/\text{gCOD}_{XH}$.

The influent COD fraction X_I was determined by curve fitting in the modelling of the respirometric batch test, as 15.6 % of total influent COD. With four COD fractions known at this point, the

slowly biodegradable substrate X_S was then determined as 44.2 % of total influent COD by a COD balance based on the average influent COD and the other known fractions.

Model Calibration

During model calibration against measured effluent COD and ammonia concentration in the ASU, these experimentally determined model parameters did not change significantly except b_H which was adjusted from 0.03 d^{-1} to 0.27 d^{-1} . The sensitivity analysis on kinetic parameters related to autotrophic biomass, during model calibration indicated significant effect on the effluent COD and ammonia concentration. This indicates the need to carry out experiments to determine model parameters related to the activity of autotrophic biomass which would definitely improve the performance of the model.

The simulation results indicate that the model can predict the trends of the effluent COD concentration, though the model cannot accurately predict some of the sharp fluctuations that are shown by the collected data for effluent COD concentrations and free ammonia concentration. This may be due to some suspect points in the historical measured data from the municipal laboratory as well as the need for a measuring campaign in which the frequency of sampling during the collection of plant operation data is increased as compared to the current routine by the municipal laboratory.

It was noted that characterisation of the effluent from each of the two wastewater treatment plants at Umhlatuzana Works is limited to COD concentration only. Other tests for nitrate, total suspended solids, ammonia are not performed on a regular basis, except on the final combined effluent. The presence of historical measured data containing total suspended solids concentrations of effluent from Marianridge WWTP, will improve the calibration of secondary settler models selected to represent the secondary settler. In the event of modelling both plants separately, more tests need to be done on the individual effluent streams from the plants so that more information is available for modelling the different sections of the plant.

Validation of model

After dynamic calibration, validation of the model was done using historical measured data for the year 2007 which was not used in calibration of the model. The data available for validation of the model was limited to effluent COD concentration for the year 2007. The data for the free ammonia concentration in the activated sludge unit were not available for the year 2007, so the only data set

of 2006 was used earlier to check for improvement in the prediction of the ammonia concentration. During validation the model predicted the trends of effluent COD concentration satisfactorily though the peaks during periods of intense fluctuations turned out to be higher.

8. CONCLUSION AND RECOMMENDATIONS

The procedure for the development of a baseline model for a WWTP receiving a significant proportion of industrial effluent, based on a combination of laboratory tests and plant operating data was presented. The conclusion of this study was focused on three key points:

- The adequacy of the available data for the modelling of Marianridge WWTP
- The transferability of experimentally determined model parameters to the model
- The implication results on the bigger permitting project

The adequacy of the available data to for the modelling of Marianridge WWTP

- There is need for more reliable and complete data with fewer gaps in order to preserve the integrity of the data when used for modelling. A lot of gaps in the data lead to loss of vital information especially for dynamic simulations, as experienced in this study. More accurate data collected frequently will improve the calibration process of the model. The sampling frequency should be chosen in relation to the time constants of the process and the influent variations. One of the important time constants of the process is the hydraulic retention time. Ideally, one should choose to sample about five times faster than the hydraulic retention time (Ljung et al 1987). Using an auto-sampler at the WWTP set to draw samples every hour for laboratory tests, over a period of 1 year will generate sufficient information for modelling.
- During steady-state calibration the most relevant model parameters include the decay constant b_H and the non-settleable fraction of suspended solids which leave with the secondary settler over flow f_{ns} . The decay constant b_H was determined from experiment but there was not sufficient measured data f_{ns} , so that mass balance calculations had to be used. Daily measurements of the average total suspended solids concentration in leaving with the settler over-flow for a period of 1 year would allow f_{ns} to be determined more accurately. Data collected over a period of 1 year would include diurnal, monthly and seasonal variations of the total suspended solids concentration which will allow sufficient dynamic calibration to be done on the secondary settler.
- During dynamic calibration the model parameters relevant for short term predictions, include the specific growth rates of heterotrophic and autotrophic biomass, μ_H and μ_A respectively as well as the saturation coefficients for readily biodegradable substrate, ammonia and oxygen

for both heterotrophic and autotrophic organisms. The results of this study indicate that determining the model parameters only for heterotrophic biomass is not sufficient. There is need to carry out experiments to determine model parameters related to the activity of autotrophic biomass.

The transferability of experimentally determined model parameters:

- In order to develop input files representing the influent wastewater characteristics for the modelling of a wastewater treatment plant using ASM3, COD fractionation of the influent wastewater to WWTP can be done through carrying out a batch respirometric test on the influent wastewater to determine the readily biodegradable fraction and the heterotrophic biomass. Flocculation-filtration can be used to determine the soluble inert fraction. The particulate inert and slowly biodegradable fractions can be determined by using a simulation model of the batch respirometric experiment and carrying out a COD balance in the influent wastewater.
- The COD fractionation of the influent wastewater based on the OUR measurements, flocculation-filtration, and simulation of the batch experiment, on the wastewater, is assessed to be satisfactory for modelling, because of the modelling response achieved even before calibration.
- Reliable values of the maximum yield of heterotrophic biomass Y_H , and the maximum specific growth rate for heterotrophic biomass μ_H , for ASM3 modelling, can be determined from the respirometric batch test on composite samples of the influent wastewater.
- In this study the value of the decay constant of the biomass b_H in the activated sludge, determined by monitoring the endogenous respiration of the biomass turned out to be lower than the calibrated value of the developed model. Literature suggests that it is difficult to obtain reliable values of b_H from laboratory-scale experiments, therefore the values determined from experiment may need to be adjusted during the model calibration procedure.
- Since it is difficult to determine values of half saturation coefficients from laboratory experiments which are transferable to the model representing the full scale system, the approach of tuning the values of these coefficients during model calibration can be used. If an

attempt is made to determine the values of half saturation coefficients using laboratory experiments, the values obtained from the experiments can be used as initial estimates during the calibration procedure.

The implication of the modelling results on the bigger permitting project:

- The use of laboratory experiments, historical data from the municipal laboratory and modelling of experiments in order to generate information for the modelling of wastewater treatment plants makes up a methodology which can be adopted and improved by implementing the suggested recommendations so that simulation models can be a significant source of information for municipal policies in wastewater management. The idea of the methodology is summarised in Table 8.1.

CONCLUSION AND RECOMMENDATIONS

Table 8.1 Summary of how laboratory experiments modelling of experiments and, historical data can be used for modelling of WWTP's

| | Type | Variable determined |
|--|--|--|
| Influent characterisation | | |
| Laboratory experiment | Respirometric batch test | COD fractions S_S X_H |
| | Flocculation-filtration | COD fraction S_I |
| Modelling of experiment | Simulation of respirometric batch test | COD fraction X_I |
| Historical data | Influent wastewater volumes and concentrations | TSS, COD, N, P, TKN, NH_4-N , NO_3-N , PO_4-P , VSS etc |
| Determination of model parameters | | |
| Laboratory experiment | Respirometric batch test | Y_H , μ_H , b_H , |
| Modelling of experiment | Simulation of respirometric batch test | K_b , K_S , K_X , |
| Historical Plant data | Design data and Operational data | Reactor volumes, pump flows, aeration capacities, effluent, recycle flow rate, |
| Calibration and Validation of model | | |
| Historical Plant data | Wastewater concentrations of the influent and effluent as well as some intermediate streams between the WWTP unit processes, as averages or as dynamic trajectories Sludge compositions | Calibrated model parameters and validated model. |

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10. APPENDICES

10.1. APPENDIX A

Characteristics of different types of domestic wastewater according to Henze et al., (2002) are shown in Table A: 1.

Table A:1 Characteristic of different types of domestic wastewater according to Henze et al., (2002)

| Characteristic | Unit | Wastewater type | | | |
|--|-------------------------|-----------------|----------|--------|-------------|
| | | Concentrated | Moderate | Dilute | Very dilute |
| Physical | | | | | |
| Conductivity | mS/m | 120 | 100 | 80 | 70 |
| Settleable solids | mg/L | 10 | 7 | 4 | 3 |
| Inorganic chemical | | | | | |
| Alkalinity | mg CaCO ₃ /L | 150 – 350 | | | |
| Free ammonia | mg N/L | 50 | 30 | 18 | 12 |
| pH | - | 7 – 8 | | | |
| Ortho phosphorus | mg P/L | 14 | 10 | 6 | 4 |
| Total phosphorus | mg P/L | 23 | 16 | 10 | 6 |
| Total Kjeldahl Nitrogen | mg N/L | 80 | 50 | 30 | 20 |
| Organic Chemical and Biological | | | | | |
| Biological oxygen demand (BOD ₅) | mg O ₂ /L | 350 | 250 | 150 | 100 |
| Chemical oxygen demand (COD) | mg O ₂ /L | 740 | 530 | 320 | 210 |
| Heavy metals and halogens | | | | | |
| Cadmium | µg Ca/L | 4 | 2 | 2 | 1 |
| Chloride | mg Cl/L | 500 | 360 | 280 | 200 |
| Chrome – total | µg Cr/L | 40 | 25 | 15 | 10 |
| Copper | µg Cu/L | 100 | 70 | 40 | 30 |
| Lead | µg Pb/L | 80 | 65 | 30 | 25 |
| Manganese | µg Mn/L | 150 | 100 | 60 | 40 |
| Nickel | µg Ni/L | 40 | 25 | 15 | 10 |
| Zinc | µg Zn/L | 300 | 200 | 130 | 80 |

10.2. APPENDIX B**Dissolved oxygen (DO) probe specifications**

| | |
|---------------------|----------------------|
| Type: | YSI 5739 Field Probe |
| Membrane: | FEP Teflon |
| Cathode: | Gold |
| Anode: | Silver |
| Electrolyte: | Half-saturated KCL |
| Temperature Range: | -5 to 45 °C |
| Polarizing Voltage: | 0.8 V |
| Probe Current: | 19mA |

10.3. APPENDIX C

The theory of determining COD fractions from a batch respirometric experiment carried out on wastewater, with addition of a known amount of sodium acetate is presented, in the following section. A typical OUR plot on which the calculations are based is shown in Figure C:1.

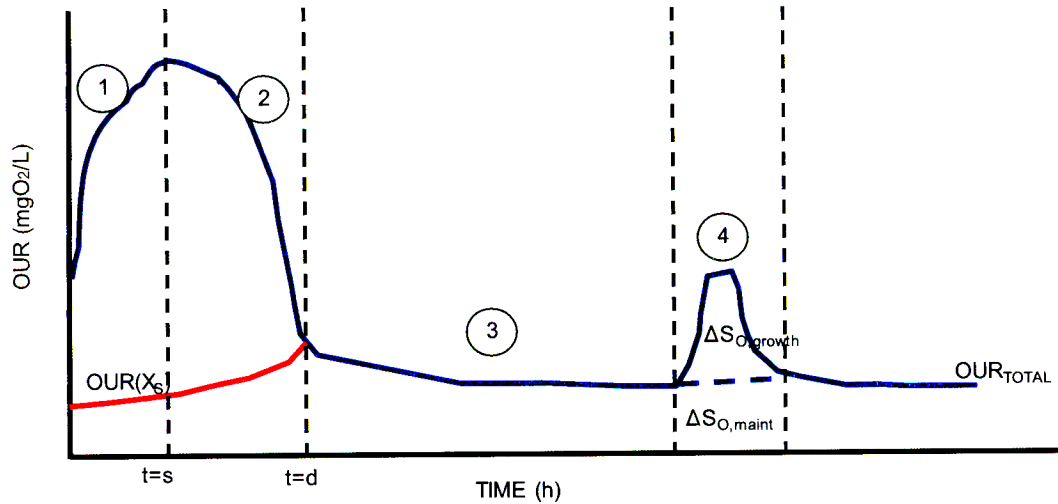


Figure C:1 A typical OUR-curve on raw incoming sewage with addition of readily biodegradable substrate.

The curve is divided into different substrate concentration conditions:

1. Substrate non-limited condition,
2. Substrate non-limiting condition is being terminated,
3. Substrate limited condition,
4. Addition of readily biodegradable substrate.

Interpretation using the IWA model matrix

Table C:1 The model matrix describing the aerobic utilisation of substrate in wastewater in a batch reactor.

| Process | COD fractions | | | | Rate |
|--|------------------|-------|-----------------|-----------------------|---|
| | S_S | X_S | X_H | $-S_O$ | |
| Biomass growth | $\frac{-1}{Y_H}$ | | 1 | $\frac{(1-Y_H)}{Y_H}$ | $\mu_H \cdot \frac{S_S}{K_S+S_S} \cdot X_H$ |
| Maintenance energy requirements | -1 | | -1 ¹ | 1 | $q_m \cdot X_H$ |
| Hydrolysis of slowly biodegradable substrate | 1 | -1 | | | $k_h \cdot \frac{x_s/x_H}{K_x+x_s/x_H} \cdot X_H$ |

¹: If S_S is not present in sufficient concentration, X_H is used for endogenous respiration.

q_m : Maintenance requirements rate constant [h^{-1}]

Theory for determination of the parameters, Y_H , μ_H , and q_m

The yield constant, Y_H , relates the mass of COD biomass produced to the mass of COD totally consumed. The yield constant can be found from zone 4 using equation C.1.

$$Y_H = \frac{\Delta S_{S,add} - \Delta S_{S,growth}}{\Delta S_{S,add}} \quad [C.1]$$

Where:

$\Delta S_{S,add}$ = Amount of added readily biodegradable substrate (mg O₂/L)

$\Delta S_{S,growth}$ = Oxygen uptake for growth (mg O₂/L)

$\Delta S_{S,growth}$ is calculated from zone 4 as the area under the OUR curve in zone 4 minus the area corresponding to the oxygen uptake for maintenance energy $\Delta S_{O,maint}$.

During the first part of the experiment, zone 1, the biomass undergoes an exponentially increased growth and the OUR can at this stage be described as an exponential function, equation C.2.

$$OUR(t) = OUR(t_0) \cdot \exp(\mu_H \cdot \Delta t) \quad [C.2]$$

The maximum specific growth rate, μ_H , is isolated from equation C.2 and determined by equation C.3.

$$\mu_H = \frac{\ln\left(\frac{OUR(t)}{OUR(t_0)}\right)}{t - t_0} \quad [C.3]$$

q_m is the maintenance requirements rate constant that is determined using equation C.4.

$$q_m = \frac{\mu_H \cdot \frac{1-Y_H}{Y_H} \cdot \Delta S_{O,maint}}{\Delta S_{O,growth}} \quad [C.4]$$

Theory for determination of the COD fractions, S_S , X_H and X_S

According to the division of the OUR-curve in Figure C:1, S_S is calculated from equation C.5. The concentration of S_S is given by $1/(1-Y_H)$ times the area between the observed OUR_{total} and the

calculated theoretical OUR (X_S) from when the measurement starts and to the precipitous drop time ($t = d$), i.e. where no readily biodegradable substrate is left. OUR (X_S) is the OUR used to utilise slowly biodegradable substrate and is a theoretical calculated value. The method for determining the curve of OUR (X_S) is on the UCT model (Wentzel et al., 1995).

$$S_S = \frac{1}{1 - Y_H} \cdot \int_{t=0}^{t=d} (\text{OUR}_{\text{total}} - \text{OUR}(X_S)) \cdot dt \quad [C.5]$$

$$S_S = \frac{1}{1 - Y_H} \cdot \int_{t=0}^{t=d} \text{OUR}(S_S) \cdot dt$$

S_S is determined by integrating graphically thus calculating the difference between the area under the $\text{OUR}_{\text{total}}$ curve and OUR (X_S), between the starting time, $t=0$ and $t=d$.

Referring to the IWA model matrix model in Table C:1 the OUR is divided into two parts, an uptake for growth and a corresponding uptake for maintenance requirement energy of the biomass. The interpretation of this division is shown under stage (4) in Table C:1. Consequently the OUR at a time t , can be described by equation C.6.

$$\text{OUR}(t) = \frac{dS_{O,\text{growth}}}{dt} + \frac{dS_{O,\text{maint}}}{dt} = \left(\frac{1 - Y_H}{Y_H} \cdot \mu_H \cdot \frac{S_S}{K_S + S_S} + q_m \right) \cdot X_H \quad [C.6]$$

When readily biodegradable substrate is added, the growth process corresponds to substrate non-limited condition, hence S_S becomes much greater than K_S and the monod-expression, $S_S/(K_S + S_S)$, is simplified to a unity. The initial heterotrophic biomass at $t = 0$ is then isolated and found by equation C.7.

$$X_H = \frac{\text{OUR}_{t=0}}{\frac{1 - Y_H}{Y_H} \cdot \mu_H + q_m} \quad [C.7]$$

Because the OUR is carried out over only approximately 24 h, the duration is not sufficient to measure the degradation of slowly biodegradable substrate, X_S . Furthermore the degradation of produced biomass will create interference. Hence an alternative method is use to estimate X_S .

Interpretation using the UCT model matrix

The UCT model (Dold et al., 1991), used to interpret the experiment is shown in Table C:3.

Table C:3 .The UCT model (Dold et al., 1991) matrix describing the aerobic utilisation of substrate in wastewater during OUR measurements in the batch reactor

| i COMPOUND → | Z _{BH} | Z _E | Z _I | S _{ads} | S _{enm} | S _{bs} | S _{us} | O | PROCESS RATE, ρ _j |
|---|------------------------------|---------------------------|---------------------------|---|---|---|------------------------------------|------------------------------|--|
| ↓ j PROCESS | | | | | | | | | |
| Aerobic growth of Z _{BH} on S _{bs} | 1 | | | | | $\frac{-1}{Y_{ZH}}$ | | $-\frac{(1-Y_{ZH})}{Y_{ZH}}$ | $\mu_H \cdot \frac{S_{bs}}{K_{SH} + S_{bs}} \cdot Z_{BH}$ |
| Aerobic growth of Z _{BH} on S _{ads} | 1 | | | $\frac{-1}{Y_{ZH}}$ | | | | $-\frac{(1-Y_{ZH})}{Y_{ZH}}$ | $K_{MP} \cdot \frac{S_{ads} / Z_{BH}}{K_{SP} + S_{ads} / Z_{BH}} \cdot Z_{BH}$ |
| Death of Z _{BH} | -1 | f _E | | | 1- f _E | | | | $b_H \cdot Z_{BH}$ |
| Adsorption of S _{enm} | | | | | | | | | $K_A S_{enm} Z_{BH} (f_{MA} - S_{ads} / Z_{BH})$ |
| Stoichiometric constants | | | | | | | | | Kinetic constants |
| Y _{ZH} – Heterotrophic yield | (M COD. L ⁻³) | (M COD. L ⁻³) | (M COD. L ⁻³) | (M COD. L ⁻³) | (M COD. L ⁻³) | (M COD. L ⁻³) | (M COD. L ⁻³) | (M COD. L ⁻³) | μ _H -heterotrophic max. |
| f _E –Endogenous residue | | | | | | | | | specific growth rate on S _{bs} |
| f _{MA} - Max. ratio S _{ads} / Z _{BH} | | | | | | | | | K _{SH} –heterotrophic half saturation on S _{bs} |
| | Active heterotrophic biomass | Endogenous mass | Inert mass | Adsorbed slowly biodegradable substrate | Emmeshed slowly biodegradable substrate | Readily biodegradable soluble substrate | Un-biodegradable soluble substrate | Oxygen | K _{SP} -heterotrophic half saturation on S _{ads} |
| | | | | | | | | | b _H -heterotrophic specific death rate |
| | | | | | | | | | K _A -S _{enm} specific adsorption rate |

Theory for determining heterotrophic active biomass Z_{BH}

From the simplified UCT model shown Table C:2 the rate of growth of heterotroph biomass is given by equation C.8.

$$\frac{dZ_{BH}}{dt} = \text{growth on RBCOD} + \text{growth on SBCOD} - \text{death}$$

$$\frac{dZ_{BH}}{dt} = \mu_H \cdot \frac{S_{bs}}{K_{SH} + S_{bs}} \cdot Z_{BH} + K_{MP} \cdot \frac{S_{ads} / Z_{BH}}{K_{SP} + S_{ads} / Z_{BH}} \cdot Z_{BH} - b_H \cdot Z_{BH} \quad [C.8]$$

It can be accepted that during the initial stages of the batch test, (before the readily biodegradable COD is depleted and the OUR drops precipitously) $S_{bs} \gg K_{SP}$ and $S_{ads}/Z_{BH} \gg K_{SP}$ (Wentzel et al., 1995), therefore:

$$\frac{dZ_{BH}}{dt} = (\mu_H + K_{MP} - b_H) \cdot Z_{BH} \quad [C.9]$$

Separating variables and integrating and solving equation C.9 yields the active organism concentration at a time t, ($Z_{BH(t)}$; mgCOD/L) in terms of the initial active organism concentration ($Z_{BH(0)}$; mgCOD/L), time (t, in h) and the net specific growth rate ($(\mu_H + K_{MP} - b_H)$, d). The factor 24 converts time t in hours to days.

$$Z_{BH(t)} = Z_{BH(0)} e^{(\mu_H + K_{MP} - b_H) t / 24} \quad [C.10]$$

The OUR at a time t is a function of $Z_{BH(t)}$ and the net specific growth rate:

$$OUR_{(t)} = \frac{1 - Y_{ZH}}{Y_{ZH}} (\mu_H + K_{MP}) \cdot Z_{BH(t)} / 24 \quad [C.11]$$

Substituting equation C.10 for $Z_{BH(t)}$ in equation C.11 and taking natural logarithms yields:

$$\ln OUR_{(t)} = \ln \left[\frac{1 - Y_{ZH}}{Y_{ZH}} (\mu_H + K_{MP}) \cdot Z_{BH(0)} / 24 \right] + (\mu_H + K_{MP} - b_H) \cdot t / 24 \quad [C.12]$$

This equation represents a straight line with:

$$\text{Slope} = (\mu_H + K_{MP} - b_H) \cdot t / 24$$

$$\text{Y-intercept} = \ln OUR_{(t=0)}$$

$$= \ln \left[\frac{1 - Y_{ZH}}{Y_{ZH}} (\mu_H + K_{MP}) \cdot Z_{BH(0)} / 24 \right]$$

From the plot of $\ln OUR_{(t)}$ versus time in hrs, the influent active heterotrophic biomass $Z_{BH(0)}$ can be obtained as shown in equation C.13.

$$Z_{BH(0)} = \frac{e^{(y-int \text{ intercept}) \cdot 24}}{1 - \frac{Y_{ZH}}{Y_{ZH}} \cdot (slope \cdot 24 + b_H)} \text{ mgCOD/L} \quad [C.13]$$

The biomass yield Y_{ZH} and the death constant b_H are determined from experiment.

Theory for determining the influent readily biodegradable COD

The theory for determining the influent readily biodegradable COD is presented in the following section.

Heterotroph maximum specific growth rate on SBCOD, K_{MP}

The RBCOD concentration is calculated from the concentration of oxygen utilised in its degradation. This requires the OUR before the precipitous drop to be separated into its RBCOD and SBCOD contributions, which is equivalent to separating the overall growth rate ($\mu_H + K_{MP}$) into its μ_H and K_{MP} components.

In terms of the UCT-model, growth of heterotrophic micro-organisms on readily biodegradable substrate, and slowly biodegradable substrate, is independent. The only thing that separates them is the respective maximum growth rates on the two substrates. The oxygen uptake rate, OUR ($\text{mgO}_2/\text{L/h}$), of the two growth processes are given by equation C.14 and C.15.

$$OUR_{RBCOD(t)} \cdot 24 = \frac{1 - Y_{ZH}}{Y_{ZH}} \cdot \mu_H \cdot Z_{BH(0)} \cdot e^{(\mu_H + K_{MP} - b_H)t/24} \quad [C.14]$$

$$OUR_{SBCOD(t)} \cdot 24 = \frac{1 - Y_{ZH}}{Y_{ZH}} \cdot K_{MP} \cdot Z_{BH(0)} \cdot e^{(\mu_H + K_{MP} - b_H)t/24} \quad [C.15]$$

Where:

- Y_{ZH} = Yield coefficient for heterotroph (mg COD/mg COD)
- μ_H = Maximum specific growth rate of heterotroph on readily biodegradable substrate (d^{-1}).
- K_{MP} = Maximum specific growth rate of heterotrophs on slowly biodegradable substrate (d^{-1}).
- $Z_{BH(0)}$ = Initial concentration of heterotroph (mg COD/L).
- b_H = Lysis and decay rate for heterotroph (d^{-1}).

Before the precipitous decrease the total OUR, $OUR_{(t)}$, is the sum of the two growth processes, equation 10.14 and 10.15. When RBCOD is depleted the OUR shows the precipitous decrease and if this occurs at $t = d$ K_{MP} can be calculated from equation C.16.

$$K_{MP} = \frac{OUR_{SBCOD(t=d)} \cdot 24}{\frac{1 - Y_{ZH}}{Y_{ZH}} \cdot Z_{BH(0)} \cdot e^{(\mu_H + K_{MP} - b_H) \cdot (t=d) / 24}} \quad [C.16]$$

Where:

$OUR_{SBCOD(t=d)}$ = OUR value due to utilization of SBCOD only, immediately following the precipitous drop i.e. at $t=d$

($t=d$) = The time immediately following the precipitous drop in OUR in h

$(\mu_H + K_{MP} - b_H) \cdot t / 24$ = the slope of the $\ln OUR_{(t)}$ vs. time (h) plot.

Heterotroph maximum specific growth rate on RBCOD, μ_H

The maximum growth rate is calculated from the value for K_{MP} derived earlier and the slope of the $\ln OUR$ versus time plot as shown in equation C.17.

$$\mu_H = \text{slope} \cdot 24 - K_{MP} + b_H \quad [C.17]$$

Determination of the influent RBCOD concentration

Knowing K_{MP} and μ_H , the OUR_{SBCOD} can now be calculated and subtracted from OUR_{total} to give the OUR_{RBCOD} . The RBCOD then is given by $1/(1 - Y_{ZH})$ times the area between the observed OUR and the theoretical OUR_{SBCOD} from the start of the batch test $t=0$ to the precipitous drop $t=d$:

$$RBCOD = \frac{1}{1 - Y_{ZH}} \int_0^d (OUR_{total} - OUR_{SBCOD}) \cdot dt \quad \text{mgCOD/L} \quad [C.18]$$

The RBCOD concentration can be found by doing the integration in equation C.18 graphically, i.e. determining the area between the two curves in the OUR plot.

COD analysis

The principle of the experiment is that organic matter is oxidized by a mixture of boiling chromic and sulphuric acids. A sample taken before and after the OUR experiment is refluxed in strong acid solution with a known excess of potassium dichromate ($K_2Cr_2O_7$). After digestion, the remaining unreduced $K_2Cr_2O_7$ is titrated with ferrous ammonium sulphate to determine the amount of $K_2Cr_2O_7$ consumed. The oxidisable matter is then calculated in terms of the oxygen equivalent.

10.4. APPENDIX D

The models for the secondary settler available in the WEST are outlined below. The source of the outline is the WEST models guide (Amerlinck 2004).

Secondary point settler

The modelling of a settler by means of a point settler is a large simplification of the actual process. The settler is only a phase separator, and has no real volume. Hence, the model does not take into account the retention time in the settler. It is not a dynamical model but only based on mass balances.

The effluent particulate concentration is calculated as a fraction of the influent concentration to the settler. To calculate the underflow concentration a mass balance over the settler is solved. The soluble fraction is divided according to the flow rates. It is assumed that there are no biological reactions (WEST models guide).

Marsili Libelli

In this model, the settling process exists of two sub-processes, thickening and clarification, of which the first is the most important one. A clarification failure is always the result of a thickening failure. The model is a dynamic presentation for the transfer and accumulation of sludge mass in the secondary clarifier based on the theory of hindered settling without the use of layers. The total downward mass transfer is calculated from a gravitational component F_g and a bulk flux component F_b . The total flux F_t is the sum of F_g and F_b . (WEST models guide).

Secondary Otterpohl Freund

The Secondary Otterpohl Freund model for a secondary clarifier aims to give good results for the following points.

- The sludge settling must be near reality both for concentrations and stored masses.

- The effluent solids concentration should have reasonable values for dry and wet weather flows.

To satisfy the first condition the Secondary Otterpohl Freund model includes the model of Hartel which satisfies the condition. Hartel uses a correcting function that limits the amount of sludge in each layer. The function allows the model to describe the settling in the transition and the compressing zone. Then the model of Otterpohl and Freund provides a solution for the second goal by using two components, micro- and macro-flocs, in modelling the sedimentation behaviour. The macro-flocs settle with a velocity according to the Hartel function and the settling velocity of the small solids is constant.

The model divides the settler into 10 layers. The volume of the layers must be at least one order of magnitude larger than the flow rate in one time interval. For each layer a mass balance is formed. The change of mass depends on the bulk flux and the settling flux (gravitational flux). Every layer has a maximum capacity for sludge storage. So the amount of settling sludge cannot exceed the amount of sludge that the layer below can handle.

Secondary Takacs Solubles Propagator

The Secondary Takacs Solubles Propagator model is an extension of the Takacs model. In this model, the propagation of the soluble components is taken into account. The propagation of the soluble components is caused by the flow rate. Under the feed layer, the propagation is due to the underflow rate, above the feed layer the propagation is due to the overflow rate.

Secondary Takacs all fraction Propagator

The Secondary Takacs All Fraction Propagator model is an extension of the Takacs model. In this model the propagation of the all the components, solubles as well as particulates, is taken into account. The propagation of the soluble components is caused by the flow rate. Under the feed layer, the propagation is due to the underflow rate, above the feed layer the propagation is due to the overflow rate. The propagation of the particulate components is caused partially by the flow rate and partially by the gravitational settling.

Takacs

The model of Takacs is based on the model of Vitasovic. The settler is modelled with a number of layers around which a solids balance is made, while assuming that the incoming solids are distributed immediately homogenous over the feed layer and that only vertical flow is considered.

The settling velocity of the sludge blanket is taken as a non-linear function of the solids concentration. In Vitasovic's model, the settling flux is due to the gravity settling and also due to the bulk flux. The bulk flux is upward above the feed layer and resulting from the overflow rate. Beneath the feed layer, the bulk flux is downward and resulting from the underflow rate. The calculation of the settling velocity depends on the concentration of particulates. Beneath a minimum concentration, there is no gravitational settling. Above the minimum concentration, the settling velocity follows the equation of Vesilind for the large particles with a correction for the smaller particles. For the layers above the feed layer a threshold suspended solids is added. The threshold concentration is the maximum concentration that the layer below can handle. This is a limitation for the downward solids flux. It is assumed that the particulate matter is always present in the influent.