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In-Stream Water Quality Modelling and Optimisation by Mixed-Integer Programming: Simulation and Application in Actual system

by

Christopher Dumisani Mahlathi

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Department of Chemical Engineering
Faculty of Engineering, Built Environment and Information Technology
University of Pretoria

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I would like to dedicate this work to my mother Elisa Matumba for all the sacrifices she made to provide a stable home for us. To my mentor/friend/mother the late Mrs M.X. Mabunda for taking interest in my studies, motivating my interests in science and for inspiring me to be the person I am today.

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Declaration of Originality

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Abstract

Water scarcity has become a global problem due to diminishing water resource and pollution of the remaining resources. The problems arising fromwater scarcity are exacerbated rapid urbanisation and industrialisation. Water quality management systems are introduced. Numerous water management methods exist some of which, if applied effectively, can remedy these problems. In South Africa, water management systems are urgently needed to start addressing issues around the longterm sustainability of our limited water resource.

Water quality modelling is one of the tools employed to assist in validating decisions made during the planning phase of a water quality management system. It also provides a means of exploring viable options to be considered when these decisions are to be made. A range of management options exist and implementing all of them may prove costly, therefore optimisation techniques are utilised to narrow down options to the most effective and least costly among the available choices. Commonly, water quality models are used to predict concentrations in the river from which constraint equations are generated. The constraint equations are used in optimisation models to generate feasible solutions by either maximising or minimising the objective function. In this case the objective function is wastewater treatment cost. Constraints equations are based on the set in-stream water quality standard at selected theoretical measuring stations (checkpoints) in the stream and a feasible solution is one that suggests a treatment method that will ensure water quality standards are met at the lowest regional treatment cost.

This study focused on the Upper Olifants river catchment near Witbank in Mpumalanga province. This catchment is subjected to extensive wastewater effluents from various mining operations and wastewater treatment plants. The aim here was to develop a water quality model for predicting dissolved oxygen (DO) concentration in the river, and to use a modelling approach to generate constraint equations for the system.

A Streeter-Phelps stream simulation model was employed to predict DO concentration in the river. A mixed-integer programming technique was then used to evaluate the impact of nine wastewater treatment facilities discharging effluent into the river. Treatment levels were varied to test model reliability.

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The coupled stream simulation and optimisation model produced feasible solutions under 2 minutes, with each solution suggesting a range of treatment levels which ensured that the critical DO concentration was above 5 mg/L and the most stringent DO concentration the system could manage without violations anywhere else in the stream was obtained to be 7mg/L.

Keywords: dissolved oxygen, biochemical oxygen demand, Mixed Integer Optimisation, water quality modeling, wastewater treatment

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List of Nomenclatures

α	Momentum coefficient.
ε_x	Turbulent diffusion coefficient in the x direction.
ε_y	Turbulent diffusion coefficient in the y direction.
ε_z	Turbulent diffusion coefficient in the z direction.
η	Manning coefficient.
$\nabla \overrightarrow{c}$	Rate of change of determinants due to internal transformations.
$\triangle S$	Changes in the water body due to transport from external sources.
A	Wetted channel area (m^2).
A_c	Constant which varies for each treatment level monetary units/flow units.
B_p	A vector of pollution concentration limitations (stream standards) for c species, at each surveillance point p.
BOD	Biochemical oxygen demand in (mg/L).
c	Water quality species index.
C	Chezy coefficient.
C_{DO}	DO concentration in (mg/L).
C_l	A vector of treatment costs for treatment level n at load l.
D	Dissolved oxygen deficit (mg/L).
$D_{l,p}$	A matrix representing the change from the existing concentration of species c at surveillance point p when treatment level n is applied at load l.
C_D	Degassing of oxygen (mg/s).

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C_R	Aeration and re-aeration processes (mg/s).
C_s	Saturation concentration of DO in a liquid ($^{mg\,O_2}/_{L}$).
g	Gravitational acceleration (m^2/s).
H_e	Henry's constant ($^{mmHg}/_{mg\,O_2.L^{-1}}$).
K_a	surface re-aeration rate (day^{-1}).
K_d	oxidation rate in a stream (day^{-1}).
K_s	net rate of sedimentation and re-suspension of BOD (day^{-1}).
K_r	total removal rate of organic matter (day^{-1}).
l	load index.
L	oxidisable organic material as oxygen equivalents (BOD).
M_i	mass flux of DO entering a system ($kg/m^2.s$).
M_o	Mass flux of DO leaving the system ($kg/m^2.s$).
p	Surveillance point index.
p^*	Partial pressure of Oxygen gas (mmHg).
P	Wetted perimeter (m).
n	Treatment level index.
R	Hydraulic mean depth (m).
SOD	Sediment oxygen demand (mg/L).
T	Stream water temperature in degrees Celsius (^oC).
T_f	Final stream water temperature after addition of another stream (^oC).
T_L	Temperature of the load stream (^oC).
T_l	An integer vector ($t_n = 1$ or 0) indicating which treatment level, n, is provided.
T_r	Temperature of the river stream (^oC).
S_0	Bed slope.

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S_f	Fractional slope.
$\overline{U}$	Mean velocity (m/s).
U	Average stream velocity (m/s).
$\overrightarrow{c}$	Multi-dimensional mass concentration vector.
t	Travel time (s).
y	Stream depth (m).
q	Lateral flow per unit length (m^3/s.m).
Q	Flow discharge rate (m3/s).
Q_{B1H05}	Flow rate at the Olifants river stream with station B1H005 (m^3/s).
Q_{B1H021}	Flow rate at the stream joining the Olifants river with monitoring station B1H021 (m^3/s).
Q_{B1H029}	Stream flow rate of stream joining the Olifants river with monitoring station B1H029 (m^3/s).
Q_l	Load flow rate in the river (m^3/s).
Q_r	Water flow rate in the river (m^3/s).
Y_p^o	Vector of concentrations for c species, at each surveillance point p, resulting from existing stream loading.
$Y_{l,p}$	Matrix of species c concentrations occurring at surveillance point p, for treatment level n, being applied at load l and existing treatment at the remainder of the loads.
Y'_k	Vector of concentrations for each species c, at each surveillance point p, resulting from the optimal loading scheme determined by the mode.
Z	Vector with each element equals to 1.0.

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Part I.

Study Background

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1. Introduction

They say: "Three months at a laboratory saves one, two hours at a library". Similarly, time may be spent in a laboratory studying physical systems, but modelling allows one to evaluate systems virtually with less cost inputs thereby facilitating better planning before evaluating these physical systems. The content of this chapter provides the required background of the topic discussed, the problem statement, research objectives, study limitations as well as the summary of findings.

Background

Water quality management systems are designed to manage water utilisation and control pollution while maintaining good condition of the water body. Good condition of water environments usually refers to the ability of the water body to be used as a source of fresh water for humans and other organisms in the ecosystem which are affected (Saremi *et al*, 2010). Water quality management strategies include pollution prevention to maintain water quality standards and wastewater treatment before contaminated water is returned into a stream. Pollution prevention requires serious compliance by the water users as well as strong supervision by the guardians (water quality management department) of the water body. The limitation to this method is that most of the water used in industrial processes cannot be returned into a stream before treatment. That may be the reason why wastewater treatment forms a large part of the water quality management system. Some water users incorporate wastewater treatment systems into their operational processes in order to prevent discharge of waste which could result in violation of water quality standards.

Water quality standards are measured by monitoring the biological, chemical and physical properties of water of which Biochemical Oxygen Demand (BOD), ammonia and pH are examples of these properties respectively. Depending on the industrial or domestic processes taking place, different treatment schemes are employed to tackle specific parameters which may violate water quality of the receiving streams.

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It is common for more than one process effluent to be discharged into the same water body at a different location along the stream. Most of the times a stream may receive more that one effluent stream which creates complexity in managing the water body. Stream water quality depends on the dilution capacity and self-purification potential of the stream, the impact of the load and the location of a second discharge point. The amount of treatment required before an additional load is discharged is influenced by these stream properties. This observation influenced the earlier work of Streeter & Phelps (1925) and many other research work was developed around these stream properties. This is a common problem in some large rivers and streams receiving pollution from multiple sources and proper management of this is crucial the water quality management systems bares the full responsibility.

South Africa has numerous large rivers which receive multiple pollutant discharge from different municipal and industrial sources. Some of these pollutant discharges are not well regulated to meet the set quality standards. An example of such a river system is the Upper Olifants river catchment located in the Mpumalanga province. The stream receives pollutants from different mining properties and municipal wastewater treatment plants. A good water quality management system needs to be implemented to control and maintain compliance of water quality standards. A possible solution to this challenge could be to enforce high level treatment at all processes that discharge waste water into this stream. However, this could mean that a lot of investment will be spent on wastewater treatment and this may not be ideal for most industrial processes driven by profit. A more acceptable compromise would be to design an optimum treatment network that can be erected to ensure that all water users perform at least the minimum possible treatment and still maintain set water quality standards. In matching water quality and treatment, heuristics are often employed, which result mostly in temporal and sub-optimum solutions. A more systematic method is required to propose optimum water treatment levels at the lowest cost, while maintaining set stream standards. Optimisation techniques are therefore required to solve this problem, combined with water quality modelling.

Water quality modelling involves using mathematical equations to describe a water resource and solutions to these equations can be used to predict the behaviour of this water resource. This technique is popular since, when it is applied correctly, a lot of time and money can be saved. Having a sufficient model means that trial and error methods may be implemented at very little cost. Results from these sort of models may be used to determine the allowable amount of point or non-point source waste to be discharged into a river without violating water quality standards (Sasikumar & Mujumdar, 1998). Most optimisation methods aim to minimise or maximise certain quantities of the system studied. In the case of the Upper Olifants river system, it makes sense to minimise waste

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water treatment costs, which in most cases, present the largest barrier to stream and river water quality management.

Problem statement and study objectives

The Upper Olifants river catchment receives numerous waste discharges, most of these wastewater outfalls are of unknown water quality condition. A challenge arises for the water quality management system already in place to maintain set water quality standards. Better means of detecting these changes in water quality on time, and the ability to take corrective actions that will ensure compliance to stream water quality standards are required. It is imperative to device a plan which will ensure that these corrective actions will result in resolving the pollution problem completely while utilising minimum resources. It can be achieved through water quality modelling and optimisation.

The Objective for this study is to develop a simple stream simulation water quality model for a semi-hypothetical water stream (Upper Olifants river). This will depict the water quality along a river and its tributaries, based on wastewater loads. And to use this stream simulation model model to generate constraint for a wastewater treatment optimisation network problem. The constraints will be based on green drop standards and the objective function will be the cost of wastewater treatment (investment and running). A similar type of problem is the Waste Load Allocation based model, whereby the required contaminant treatment levels of waste sources discharge is determined in order to efficiently and economically maintain water quality standards on the receiving streams (Mujumdar & Vemula, 2004).

At the end of this study, a sufficient stream simulation model and a better load treatment optimisation network that will ensure water quality standards are met while minimising treatment costs are expected. In the system under study, the treatment plants existing will be designed to operate at a specific treatment level, which will serve to maintaining stream standards in rivers and also minimise treatment cost for the region under study.

Study limitation

The study only focuses on a selected section of the Upper Olifants river system where most of the discharges occur. The system studied was considered semi-hypothetical since some of the system properties were assumed and some relied on estimations. The data

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used for the simulation, as well as the river network and treatment plant locations, are all real representations of the Upper Olifants system. Empirical correlations have been employed for the dissolved oxygen and pH used in the stream simulation model, as well as other assumptions such as steady state flow, use of the BOD-DO model to represent treatment levels. The combination of real data and theoretical assumptions makes it semi-hypothetical. This has been necessitated by a paucity of data along the river system.

Research findings

The study produced a 1D steady state, mechanistic river stream simulation model for predicting DO concentration behaviour at the Upper Olifants catchment system. The model was calibrated to fit river stream data available at the Olifants river which resulted in a good fit at each water channel. Then the Streeter-Phelps equations were used with the re-aeration rate constant and de-oxygenation rate constants as the only model parameters. The final calibrated parameters for each different river stream section were found to be:

- The main Olifants river stream before addition of a branched stream produced a good fit when $k_d = 0.0410$ per day and k_a =0.0804 per day.
- Branched river stream produced a good fit when $k_d = 0.0280$ per day and $k_a = 0.0950$ per.
- Main Olifants river stream after adding the branched stream produced a good fit when $k_d = 0.1720$ per day and $k_a = 0.0902$ per day.

A mixed-integer programming technique for optimising waster water loads treatment by minimising treatment cost while maintaining in-stream DO concentration stream standards was applied to the semi-hypothetical treatment network at the Upper Olifants river catchment. The coupled stream simulation-optimisation model produced a feasible optimum solution which suggested the following application of treatment levels (Treatment level 1, 2 and 3 represents 25, 50 and 75% removal of untreated BOD at the treatment plants respectively) for BOD treatment facilities trying to maintain highest possible DO concentration standards:

- Treatment facilities 1, 2 and 3 should implement treatment levels 3, 2 and 3 respectively to maintain a DO concentration of 6.5 mg/L at all the checkpoints on the stream.

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- Treatment facilities 4-9 should implement treatment levels 3, 1, 1, 1, 3 and 3 respectively to maintain a DO concentration of 8 mg/L at all the checkpoints on the stream.

The minimum cost for the load treatments network was obtained for this system described under the given conditions.

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2. Literature Review

2.1. Introduction

Water quality modelling and optimisation are broad fields of study and both require basic understanding of the principles behind the theory to comprehend. This chapter focuses on providing the basis of the theory and also offers examples of applications of these principles to water management systems. Water quality modelling is used as a decision making tool in water resource management and planning. Optimisation assists in narrowing the possible options generated by water quality models down to feasible solutions which leads to better management decisions. Such decisions include selection of appropriate levels of treatment required from wastewater treatment works to maintain acceptable water quality standards at locations along the river where discharges from industrial process plants could be commissioned. Wastewater treatment is the preferred solution for water quality management since in-process pollution prevention may prove difficult to manage. This chapter also includes examples of treatment processes mostly considered by municipalities. A background on water quality modelling theory and application is provided as well as optimisation theory which will assist with understanding concepts developed in this study.

2.2. South African rivers condition

South Africa has limited water resources due to dramatic seasonal variations in rainfall and the uneven water distribution across the country. Factors such as South Africa's growing economy, population growth and rapid industrialisation due to mining opportunities also perform a significant role (Ashton *et al*, 2001) in water resource depletion. Fresh water demand is most likely to increase with these developments and more pollution could be expected. South Africa has many rivers across the provinces, of which most are used as portable sources for municipalities and industry. In this study the primary focus is on a section of the Upper Olifants river catchment.

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2.2.1. Water quantity and quality at the Olifants catchment

According to a report by Beumer *et al* (2011), the total national water resource in the Olifants catchment in 2010 was estimated to be at 948 million m^3/annum. Table 2.1 shows the contribution to the total by each management zone.

Table 2.1.: Summary of Total Current (2010) Water Resources within the Olifants River Catchment (Units: million m^3/annum)[Source: Beumer *et al* (2011)].

Management Zone	Yield from major dams (1 in 50 year)	Yield from Farm Dams and Diffuse Sources	Transfers in	Total
Upper Olifants	262	128	228	618
Middle Olifants	56	71	1	128
Lower Olifants	150	49	3	202
Total	468	248	232	948

The projected water requirements comprised the following users: domestic/industrial, irrigation, mining, Power Generation and Forestry. The summary of the requirements for each water management zone are listed on Table 2.2.

Table 2.2.: Summary of Total Current (2010) Water Resources requirements within the Olifants River Catchment (Units: million m^3/annum)[Source: Beumer *et al* (2011)].

Management zone	Domestic/Industrial	Mining	Irrigation (Adjusted to 98% assurance of supply	Power Generation	Total
Upper Olifants	109	21	254	288	612
Middle Olifants	39	24	93	-	156
Lower Olifants	21	36	161	-	218
Total	161	81	508	228	986

The flow data shows that at some instances, some rivers barely meet the demand while others like the Middle Olifants falls short of the requirement. This study focuses on

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the Upper Olifants where domestic and industrial use of water are most dominant. The aim of this study was to account for the water uses and how that is better managed through treatment network optimisation. Water quality concerns emerge mostly in areas immediately downstream of a point source or distributed source of pollution. The main causes of these low water quality standards include lack of treatment and poor management of water treatment works. Given enough time, the conditions will deteriorate more if appropriate intervention actions are not implemented. Table 2.3 shows the projected water balance for 2030.

Table 2.3.: Future(2030) Water balance based on the high Growth Scenario (Units: million m^3/annum)[Source: Beumer *et al* (2011)].

Management zone	Total water Resource	Water Requirement	Ecological Water Requirements	Water Balance
Upper Olifants	618	648	80	-110
Middle Olifants	227	214	51	-38
Lower Olifants	202	230	69	-97
Total	1047	1092	200	-245

Based on these projected values, it is clear that without proper management the water demand will exceed the supply by the available resources. A proposed approach by Beumer *et al* (2011) is to reduce the water requirements or increase the capacity of the source. This however could be difficult due to continuous growth in urbanisation and industrialisation (Ashton *et al*, 2001). Obtaining new sources is a huge challenge and could also be costly. Suggesting a better management of the current water resource seems a viable option at this stage and wastewater treatment optimisation could prove beneficial. This is in line with the school of thought that what we lack more is not water but rather water management.

2.2.2. The Upper Olifants catchment

Below is the description of the Olifants river catchment by the South African River Health Programme (SARHP,2008):

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"The Olifants Catchment covers about 54 570 km^2 and is subdivided into 9 secondary catchments. The total mean annual runoff is approximately 2400 million cubic metres per year. The Olifants River and some of its tributaries, notably the Klein Olifants River, Elands River, Wilge River and Bronkhorstspruit, rise in the Highveld grasslands. The upper reaches of the Olifants River Catchment are characterised mainly by mining, agricultural and conservation activities. Over-grazing and highly erodable soils result in such severe erosion, in parts of the middle section, that after heavy rains the Olifants River has a red-brown colour from all the suspended sediments.Thirty large dams in the Olifants River Catchment include the Witbank Dam, Renosterkop Dam, Rust de Winter Dam, Blyderivierspoort Dam, Loskop Dam, Middelburg Dam, Ohrigstad Dam, Arabie Dam and the Phalaborwa Barrage. In addition, many smaller dams in this catchment, have a considerable combined capacity. The Olifants River meanders past the foot of the Strydpoort Mountains and through the Drakensberg, descending over the escarpment. The Steelpoort and Blyde tributaries, and others, join the Olifants River before it enters the Kruger National Park and neighbouring private game reserves. Crossing the Mozambique border, the Olifants River flows into the Massingire Dam." Figure 2.1 shows the South African section of the Olifants catchment.

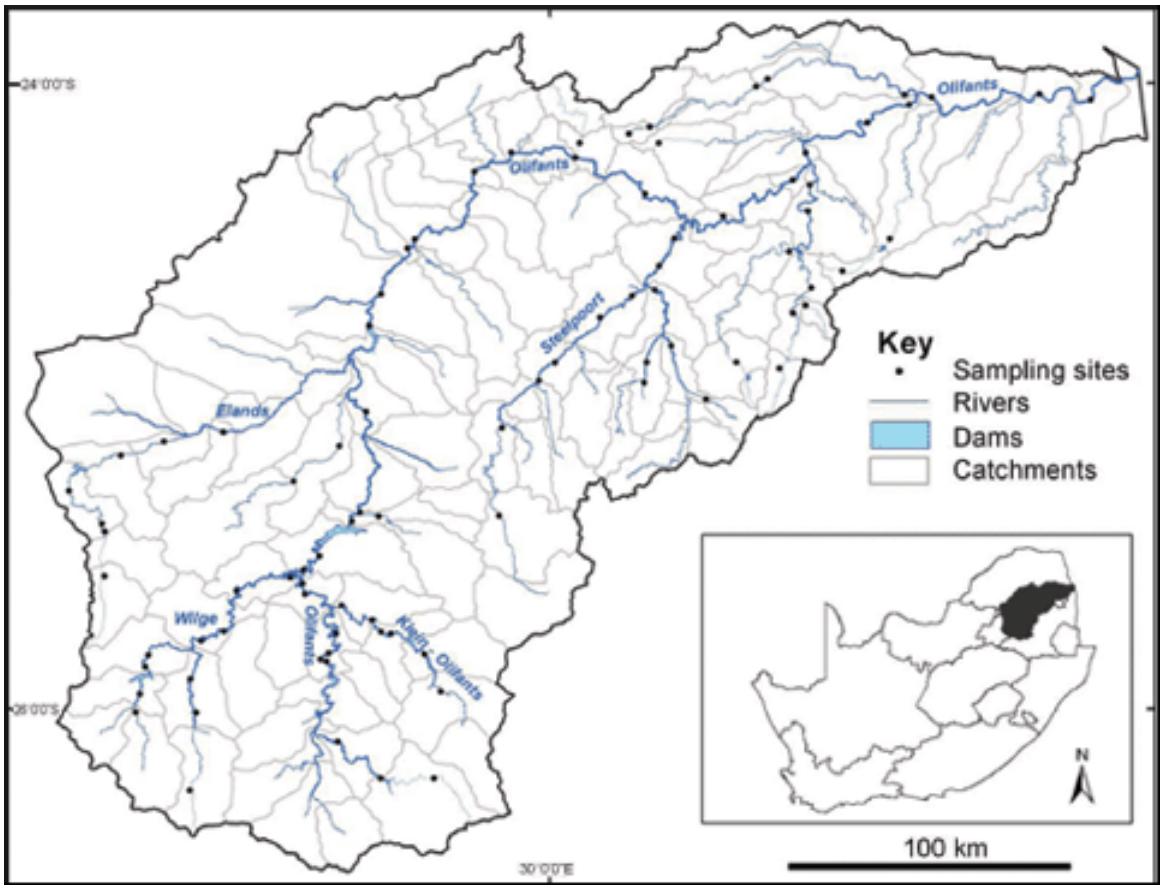

Figure 2.1.: The Olifants catchment map (Source: Rashleigh *et al* (2009)).

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The Upper Olifant catchment is one of the most exposed catchment to pollution in South Africa because relatively large treated domestic and industrial effluents from Witbank and Middleburg as well as other communities upstream of tributaries flow into these basins (Ashton *et al*, 2001). The high pollution activity at these particular tributaries draw more attention to environmental specialists since the potential of water quality standards violations is high. The Upper Olifants catchment is also subjected to high pollution due to mining of coal and other industrial activities (Beumer *et al* , 2011). The Department of Water Affairs has been monitoring this region for many years with the focus mostly on metals, nitrates, sulphates and phosphates. However, dissolved oxygen has not been included in these surveys.

2.3. Theory of water quality modelling

Mathematical modelling is generally a process of using mathematical concepts to describe a system and sometimes predict future behaviour of the system in response to disturbances. This method can be applied to different fields of study and water quality modelling is a specific example. Water quality modelling is defined as a process that applies mathematical techniques to describe systems in the water environment. A water quality model could be used to predict pollutant behaviour in polluted streams. The resulting model could be used as a decision making tool in water quality management and planning processes. A decision on which system to use requires broader knowledge of the system since, naturally, there are many water quality models available at one's disposal. An effort to study and accurately define the system is therefore crucial for modelling to avoid redundancy and to facilitate the most relevant model for a specific application. Figure 2.2 shows a typical example of a water environment system for which a water quality model can be developed.

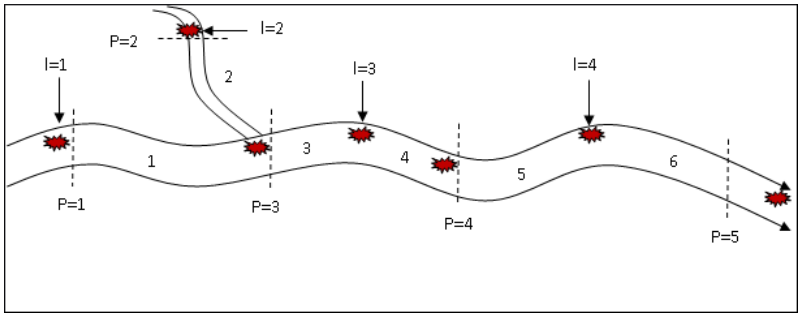

Figure 2.2.: A hypothetical river system with wastewater outfalls. (Image adapted from (Inney, 1977)).

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The Figure 2.2 shows a river system with four point sources being applied on different reaches. The river system is divided into six reaches with five theoretical measuring points where water quality is monitored. A water quality model for a river system such as the one represented in Figure 2.2 can be used to solve water pollution control problems and to evaluate load impacts along the river. By dividing the river into small river reaches the methods used to obtain solution could be simplified and the reach can realistically represent a solution in the river with uniform water quality parameters.

2.3.1. Basic concepts in water quality modelling

Water quality standards must be kept at recommended levels by monitoring each individual relevant water quality characteristics. Water quality can be characterised by:

- physical (colour, conductivity, temperature, and turbidity),
- chemical (COD, Ammonia, Carbon dioxide, and metals)
- and biological (Algae, BOD, and pathogens) properties.

Maintaining all these properties at compliant levels of standards for the intended water use is crucial for the safety of the users. Predictive modelling can be used in the implementation of pollution control by determining treatment levels for specific pollutants that will be required to achieve target ambient levels. This sections of the work focuses on some of the useful definitions and concepts of water quality modelling. According to Cox(2003a), classification of water quality models is based on a number of factors which include:

(1) The environment modelled;

(2) The purpose of the model;

(3) The number of dimensions considered;

(4) How the processes are described;

(5) Whether the data used are discrete, observed measurements or statistical distributions; and

(6) whether temporal variability is considered.

The options that could be selected and the sequence of selection criteria are illustrated in Figure 2.3.

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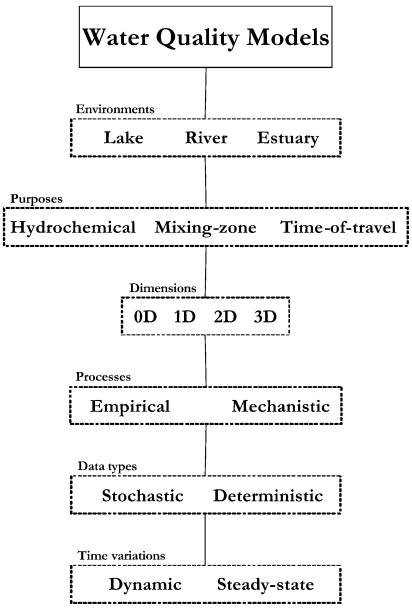

Figure 2.3.: Water quality model description of flow process (Cox, 2003a).

Water quality models can be developed and applied on different water environments including lakes, estuaries and rivers. These water environments play various roles in the ecosystem including supplying fresh water to organism. Rivers are the most used source of fresh water and some of the uses include:

- as a source of drinking water,
- irrigation of agricultural lands,
- industrial and municipal water supply and waste disposal,
- navigation and aesthetic value (Chapman, 1998: 243).

Lakes and estuaries also play significant roles in other aspects of life but rivers are mostly utilised for most domestic and industrial fresh water needs. According to Chapra (2008: 235), rivers can be categorised according to hydraulic (flow, velocity, dispersion) and geometric (depth, width, slope) properties. These parameters are used to describe unique water systems and can be obtained by using point estimate at a point or reach estimate at a reach. Temporal distribution of flow is another important aspect of stream physics. This is a time series which is quantified by a plot of flow rate versus time of the year called the annual hydro-graph (Chapra, 2008: 236). This relationship provides an estimate of flow variation over the course of a year at the river stream. The ability to estimate when extremely low and high flow conditions occurs can be used to decide what flows to use when developing a model. In a case of constructing a water quality model with the aim of

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evaluating point sources pollution control, the low flow conditions provide a sound design context (Chapra, 2008: 236).

Cox (2003a) mentioned in his study that models can be further classified according to the purpose they are meant to serve, and this provides useful information with regards to limitations of a particular model. This way a modeller will be able to design a model specifically for the intended purposes and the amount of time spent on model development may be reduced and also computational speeds may be improved. Three possible purposes were discussed in the study:

- Hydrological models whose purpose is to model the chemical and biological processes that affect the contaminants of interest, the aim of this type of model is to represent water chemistry.
- A mixed zone model which comprises only a portion of the stream that is immediately downstream of a discharge into the main water body. This type of model is ideal for impact analysis studies on the river after loading has been applied.
- And the time-of-travel model which provides the user with time of travel of pollutants downstream from where loading occurs.

The applicability of models can be limited by the level of complexity of the system modelled, deciding on the dimension in which the model is suppose to simulate is essential for the study. Most water quality models differ in stability and complexity whereby:

- 0D models representing volumes and concentrations assuming complete and instantaneous mixing in the water body,
- 1D models add advection and dispersion of solutes in one direction which is downstream the river to the 0D model,
- while a 2D model includes simulating dispersion across the width or depth of a stream but never both
- and lastly the most complex 3D models account for the flows and solute transport in all directions, because of their high sophistication they are usual reserved for deep and wide estuaries with complex mixing pattens.

Knowledge of the level of complexity of a model is essential for achieving the model objectives without using excessive resources. The use of complex models requires a broad understanding and numerous resources, therefore it is expected that simpler models are easy to understand (Tsakiris & Alexakis, 2012). There are two broad categories which

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describe the ways the determinants are influenced in the model. The model can be empirical or mechanistic and they are described as follows:

- Empirical models make no attempt to explicitly model hydro-chemical processes: instead the model inputs and outputs are by relationships obtained experimentally. These types of models are important for investigating causality relationships if they are used in formal statistics but they can only be used with any confidence within ranges of the data used to parametrise them.

- while mechanistic models simulate the changes in flow rate and water quality along a river by attempting to represent the processes that occur in a real system. These models are based on the underlying physics and chemistry that governs the behaviour of the process and does not require much data to model (Ming, 2000). Models can be further divided based on their inputs (i.e. Deterministic, stochastic). Deterministic models use fixed input variables and there is a predetermined relationship between inputs supplied by user and the outputs variables. The calculations made by the model assume that the input and output variables are fixed. Stochastic models rely on variable inputs of certain parameters, based on probabilities.

After careful consideration and examination of the problem, it may be easier to decide which modelling approach to consider and the level of complexity adequate to achieve the objectives of the modelling effort. More theory on the specific modelling approach selected for this study is discussed further and the possible alternatives were not described in detail.

2.3.2. Mechanistic modelling

In a situation where an attempt is made to represent processes with a primary focus on simulating flow and other water quality properties along a river, a mechanistic water quality modelling approach is considered. Mechanistic models are formulated from physical and chemical principles. All mechanistic models use the basic governing solute transport equation. The general form is represented by Equation (2.3.1) below :

$$\frac{\partial \overrightarrow{c}}{\partial t} = -\overrightarrow{u}\frac{\partial \overrightarrow{c}}{\partial x} - \overrightarrow{v}\frac{\partial \overrightarrow{c}}{\partial y} - \overrightarrow{w}\frac{\partial \overrightarrow{c}}{\partial z} + \frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial \overrightarrow{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_y \frac{\partial \overrightarrow{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_z \frac{\partial \overrightarrow{c}}{\partial z}\right) + \nabla \overrightarrow{c} \quad (2.3.1)$$

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where $\overrightarrow{c}$ is a multi-dimensional mass concentration vector for each of the contaminants ; t is the time; x, y and z are spatial coordinates; ε_x, ε_y and ε_z are turbulent diffusion coefficients for directions x, y and z respectively; and $\nabla\overrightarrow{c}$ represents the rate of change of determinants due to internal transformations in the reach (Cox, 2003a). The uniqueness of most mechanistic water quality models stems from the simplifying assumption made on Equation (2.2.1). Some of these assumption could be; to assume a one dimensional (1D) model where all the flow variations such as diffusion are considered to be dominant in one direction and variations in other directions negligible; or to avoid mixing by diffusion all together and only consider advection.

Hydrodynamics of the river system have to be modelled in order to determine and later predict the flow of water in the river. The mass conservation and momentum equations are used to describe flow in the river and are applied to conserve these properties within a river reach. Equation (2.3.2) and Equation (2.3.3) show the conservation of mass and momentum equations respectively, and are collectively called the Saint Venant equations (Cox, 2003a).

$$\frac{\partial A_x}{\partial t} + \frac{\partial Q}{\partial x} = q \tag{2.3.2}$$

Where A (m^2) is the wetted are (which is reach length per unit length), t (s) is the time, Q (m^3/s) is the discharge, x (m) is the distance downstream, q ($m^3/s.m$) is the lateral flow per unit length.

$$\frac{\partial Q}{\partial t} = gA\left(S_0 - S_f\right) - gA\frac{\partial y}{\partial x} - \frac{\partial\left(\alpha Q^2/A\right)}{\partial x} \tag{2.3.3}$$

where g is the gravitational acceleration, y is depth, α is a momentum coefficient, S_0 is the bed slope and S_f is the fractional slope. This method is known as the Navier-Stokes or Reynolds method, numerous methods are available to solve the equations with complex 3D solution attainable, but for fresh water the equations may be simplified since the terms describing diffusion of momentum due to turbulence are insignificant compared to the remaining term (MacDonald *et al*, quoted by Cox (2003a), 1995: 341), thus flow is often considered to be 1D assuming that the transverse or vertical accelerations are in significant relative to the longitudinal accelerations (Cox, 2003a). Further simplification

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may be performed on the hydrodynamic model with each simplification resulting in a less complex equation which is easier to solve. Careful consideration should be taken such that over-simplification does not affect the quality of the model. For steady state models, the stream hydrology equation can be reduced and further simplified by the use of the semi-empirical Equation (2.3.4) and Equation (2.3.5) of Manning and Chezy respectively:

$$Q = A\overline{U} = \frac{AR^{2/3}S_o^{1/2}}{n} \qquad (Manning) \tag{2.3.4}$$

$$Q = A\overline{U} = AC\sqrt{(RS_0)} \qquad (Chezy) \tag{2.3.5}$$

where $\overline{U}$ is the mean velocity, R is the hydraulic mean depth defined as ($R = {}^{A}/_{P}$ where P is the wetted perimeter), n and C are Manning and Chezy coefficients respectively which represents a roughness factor. The Table 2.4 taken from a table in (Chapra, Pelletier & Tao, 2008:16) showing some of Manning's coefficients values for different open channels.

Table 2.4.: Table showing Manning Coefficients for different open channels (Source Chapra , *et al* (2008)).

Material	**n**
Man-made channels	
concrete	0.012
Gravel bottom with sides:	
Concrete	0.020
mortared stone	0.023
Riprap	0.033
Natural Stream channels	
Clean, straight	0.025 - 0.04
Clean, winding and some weeds	0.03 - 0.05
Weeds and pools, winding	0.05
Mountain streams with boulders	0.04 - 0.10
Heavy brush, timber	0.05 - 0.20

All these simplifications are motivated by the need to arrive at simple and solvable equations which will require less resources to achieve the model objectives. Apart from simplicity, data availability plays a most important role on deciding the degree of simplification. All the possible simplifications in this study are mostly limited by the data available and this will become evident during the selection of a suitable dissolved oxygen model.

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2.4. Dissolved oxygen model

Dissolved Oxygen deficiency poses a serious threat to aquatic life which poises severe consequences to the water environment and users. Modelling and simulation of dissolved oxygen (DO) in rivers may assist in determining variation of parameter concentration along the water stream as well as indicate areas where critical concentration levels occur based on set water quality standards. Cox (2003b) reviewed dissolved oxygen modelling techniques, and from this study the theory of DO modelling was adapted. The review provides a modelling framework to describe processes affecting DO in lowlands in context of mass-balance techniques. The review states that sources of DO in rivers include:

1. Re-aeration from the atmosphere;
2. Enhanced aeration at weirs and other structures;
3. Photosynthetic oxygen production;
4. Other sources such as tributaries;

And main causes of DO depletion are:

1. Oxidation of organic material and other reduced matter in the water system;
2. Degassing of Oxygen in supersaturated water;
3. Respiration by aquatic micro-organisms;
4. The oxygen demand exerted by river bed sediments.

The total mass balance of Oxygen in water follows the general mass-balance equation:

$$Accummulation = Massenteringthesystem - Massleavingthesystem + SourcesofOxygen - Sinks\ of\ Oxygen$$

The sources and the sinks could be any of the four above listed or, a combination of some of them. Equation (2.4.1) best illustrates the mass balance mathematically.

$$\frac{\partial M}{\partial t} = M_i - M_o + \left(P - \bar{R}\right) + C_R - BOD - SOD - C_D \pm \triangle S \tag{2.4.1}$$

where t is the time, M_i is the mass flux of DO entering the system, M_o is the mass flux leaving the system,C_R represents the aeration and re-aeration processes,BOD is

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the biochemical oxygen demand representing oxidation of organic material, SOD is the sediment oxygen demand,C_D represents degassing of oxygen, P is the photosynthetic oxygen production rate, $\overline{R}$ is the respiratory oxygen uptake rate and $\triangle S$ represents changes in the water body due to transport from external sources. A model to represent all properties which contribute to DO balance may prove too complex and obtaining some of the required data may be very difficult. This is the reason most of the mechanistic models are semi-empirical even though they represent individual processes.

Most of the models which are developed employ modified or extended version of the classical Streeter-Phelps equations for BOD and DO profiles along natural water streams. The Streeter-Phelps model theory only considers (1) biochemical oxidation as the only oxygen sink in the water body and (2) atmospheric re-aeration as the only source ignoring all other possible sources. The simplest form of the model is for a reach in steady state characterised by plug flow with constant hydrology and geometry. The mass balance takes the form of Equations (2.4.2 and 2.4.3):

$$U\frac{dL}{dx} = -K_r L \tag{2.4.2}$$

$$U\frac{dD}{dx} = K_d L - K_a D \tag{2.4.3}$$

where U is the average stream velocity, L is the amount of oxidisable organic material as oxygen equivalents which is BOD, x is the distance along the reach moving downstream and D is the Oxygen deficit (the difference between saturation DO of the water body and the actual DO concentration), K_a is the surface re-aeration rate, K_r is the total removal rate of organic matter, K_d is the oxidation rate in the stream and $K_r = K_d + K_s$, where K_s is the net rate of sedimentation and re-suspension of BOD. The solution of the deferential Equations (2.4.2 and 2.4.3) can be obtained if $L = L_0$and $D = D_0$ at the time zero and the results are illustrated by Equations (2.4.4) and (2.4.5) respectively:

$$L = L_0 e^{\left(-K_r/U\right)x} \tag{2.4.4}$$

$$D = D_0 e^{\left(-K_a/U\right)x} + \frac{K_d L_0}{K_a - K_r}\left(e^{\left(-K_r/U\right)x} - e^{\left(-K_a/U\right)x}\right) \tag{2.4.5}$$

The model describes the DO sag curve that occurs downstream of where sewage is discharged in a stream and is illustrated by Figure 2.4:

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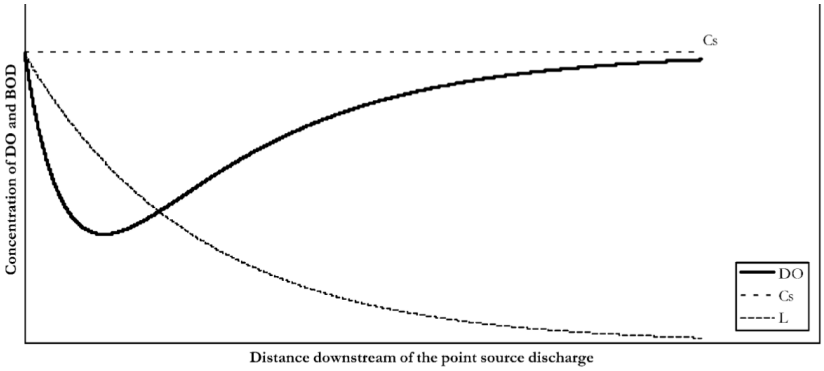

Figure 2.4.: Oxygen sag model diagram (Cox, 2003a).

From the Figure 2.4, L represents BOD concentration in the stream and C_s is the maximum equilibrium DO concentration the stream can achieve at a given temperature. The graphs shows the drop in dissolved oxygen after a sewage plant is introduced to the stream,and at some point oxygen depletion and re-aeration equate. When the critical point (lowest dissolved oxygen concentration) is reached, re-aeration rate dominates and the oxygen concentration rises until saturation is reached. The model has been found to be adequate to provide a representation DO concentration downstream of a point charge, however studies reviewed by Cox(2003b) indicated that other sources should be considered. Amongst the other suggested sources and sinks (Bennett and Rathburn, quoted by Cox (2003b), 1972: 306) suggested that the dominant sources and sinks are :

- the oxygen demand of the carbonaceous and nitrogenous wastes in the water;
- the oxygen demand of the bottom deposits;
- any immediate chemical oxygen demand (COD);
- the oxygen required for plant respiration;
- the oxygen produced by plant photosynthesis;
- the oxygen gained from atmospheric re-aeration.

Consideration of other models which include additional DO sources and sinks requires broad understanding of the processes that brings about these sources and sinks. More data will be required and also more parameters will have to be considered. An example of such a model would be the inclusion of BOD oxidation, sedimentation and re-suspension, with additional parameters such as: Algae biomass contributions and rate constant for BOD addition due to algal death. Another oxygen sink that could be considered is SOD (Sedimentation Oxygen Demand) which results from organic matter being deposited and

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incorporated in the channel bed. Modelling this property will require knowledge of the DO concentration in the overlying water, temperature, the characteristics of the bed as well as the interstitial (or pore) water. The more sinks and sources are included the more data is required about the system.

2.4.1. Parameter estimations

2.4.1.1. DO saturation concentration

The rate parameters on the equation vary for different reaches at different conditions. The re-aeration rate constant features in all open system based models for DO models as one of the sources of oxygen. The atmospheric re-aeration process involves absorption of atmospheric oxygen into the water and is regarded as one of the most important factors controlling the waste assimilation capacity of a river. If the water body is allowed to reach equilibrium with the atmosphere directly above, the DO concentration reaches a maximum and remains constant if additional disturbances do not occur. The DO concentration is known under these conditions as the saturation concentration, which can be described by Henry's law which states that the mass of any soluble gas at a given liquid volume, at constant temperature is directly proportional to the pressure that the gas exerts above the liquid. Equation (2.4.5) represents this relationship.

$$p^* = H_e C_s \tag{2.4.6}$$

where p^* is the partial pressure of Oxygen gas(mmHg), C_s is the saturation concentration of DO in a liquid ($^{\text{mg O}_2}/_{\text{L}}$) and H_e is Henry's constant ($^{\text{mmHg}}/_{\text{mg O}_2\text{.L}^{-1}}$). The saturation concentration of DO depends on the air pressure, salinity and temperature of the water. Temperature plays a more significant role in the saturation concentration and the most used Equation (2.4.6) in water quality modelling is the one developed by Elmore & Hayes (1960) for distilled water:

$$C_s = 14.652 - (0.41022T) + \left(0.007991T^2\right) - \left(7.7774 \times 10^{-5}T^3\right) \tag{2.4.7}$$

where T is the temperature in degrees Celsius.

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2.4.1.2. BOD oxidation, sedimentation and re-suspension rates

These rates are determined by experimental means in a lab where a BOD_5 test is performed. Another way of determining the rate constant is to use measurements of BOD at successive stations on a river and solving the BOD Equation (2.4.7) under constant flow and geometry conditions on the channel.

$$U\left(\frac{\partial L}{\partial x}\right) = -K_r L \tag{2.4.8}$$

where U is the mean reach velocity and K_r is the total removal rate (day^{-1}) of BOD, which is composed of oxidation and settling which can be represented by Equation (2.4.8):

$$K_r = K_d + K_s \tag{2.4.9}$$

The solution of Equation (2.4.8) is the resultant Equation (2.3.9):

$$L = L_0 e^{(-K_r/U)x} \tag{2.4.10}$$

Which can be linearised to Equation (2.4.10):

$$lnL = lnL_0 - (x/U)\, K_r \tag{2.4.11}$$

If lnL is plotted against $\frac{x}{U}$, K_r will be the gradient, which can be obtained from the graph

from the plotted log BOD data collected at successive stations. Although this technique does not require laboratory experiments, setting the conditions to match the ones used for this method would be difficult in a real system, and other means of estimating these constants have to be found. Additional estimation methods are available at the article by Cox (2003b) but were committed from the scope of this study. Appendix A shows a table with a list of available correlation for BOD re-aeration rate constant. Depending on the system being modelled, a more suitable correlation may be selected from the table.

The aim of each model is to obtain the most accurate representation of the system studied with whatever resources attainable. When modelling DO, a similar principle applies although the accuracy of this model is not guaranteed due to the difficulty in obtaining the required rate coefficients, modellers have to work with whatever data is available to still achieve a reasonable model that represent the system. The work in this

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study does value the accuracy of the model, but even a less accurate model can achieve the main objective of the overall study which is load stream treatment optimisation.

2.4.2. Available water quality models for dissolved oxygen and applicability

Over the years many water quality models have been developed and improved. Some of the observed improvements relate to accuracy of the results generated by models and the ability to resolve multi-dimensional systems with a large number of parameters. Most of these models that solve complex systems require a lot of data which in most cases is not available. Scarcity of data poses a major challenge to development of water quality models (Marsili-Libelli *et al*, 2007). Hence when developing a model, it is very crucial to understand the challenges of data limitation on the system to be modelled. Cox (2003a) conducted a review on available in-stream water-quality models (SIMCAT, TOMCAT, QUAL2E, QUASAR, HERMES, QUESTOR, MIKE-11 and ISIS) and their applicability in modelling dissolved oxygen and also summarised the strengths and their weaknesses in dissolved oxygen simulations. The conclusion to this review indicated that Although numerous water quality models exist, the decision of which to apply lies on the type of problem to be modelled and the available resources, and data are one of those resources.

2.5. Model development and validation

During the modelling exercise numerous steps need to be followed to ensure that the model can be applied and produce reliable results. Based on the work of Chapra (2008: 317).The following steps need to be considered in a modelling environment :

- Problem specification and model selection
- Numerical specification and validation
- Preliminary application and calibration and
- sensitivity analysis

Following these steps guarantees an applicable and reliable model as a result. Each of these steps depends mostly on the problem the model is suppose to tackle.

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2.5.1. Problem specification and model selection

The first step in water quality modelling involves familiarity with the problem that needs to be addressed. This could be in the form of understanding what the outcome of the model should be and a clear scope of all possible technical elements to be considered. The modeller should be aware of the management objective, control options and constraints of the problem and these will be evaluated based on the the availability of data related to chemical, physical and biological parameters of the stream to be modelled. Having access to this information may provide an indication to the complexity of the intended model. This way it becomes easier to decide on the model approach to apply.

Since numerous water quality models exist for tackling different problems, it would be advisable to first consider evaluating all possible models which are readily available. The exercise of going through existing models can save both money and time and some of them have been evaluated and tested provided one of these models are capable of addressing the problem. However most of them are designed to target specific elements of different problems of which may not necessarily be similar to what is required. An alternative could be developing a theoretical model from fundamental principles.

2.5.2. Numerical specification and validation

After a model has been selected or developed, the model equations are computed. A process that according to Chapra (2008: 321) includes algorithm design, coding in computer language, debugging, testing and documentation. During this process it is the responsibility of the modeller to ensure that the results produced by the model are accurate and sufficiently stable. validation involves subjecting the model to a battery of test to ensure that they make sense physically. Some of the suggested tests include mass balance (to ensure the total mass of the system balances), simplified solutions (where model outputs are compared with simplified and verifiable cases of which closed-form solutions are possible and also graphical results to visualise where the model fails.

2.5.3. Preliminary application and calibration

Preliminary application is a necessary step for identifying data deficiencies, theoretical gaps as well as model parameters which are most important (Chapra, 2008: 322). The simple case for determining the parameters is conducting a sensitivity analysis whereby

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model outputs are varied with each parameter and the responses are compared based on which parameters impacts the most change.

Model calibration involves the process of tuning the model parameters to fit the system data. The calibration parameters may be obtained using various regression methods such as Gauss-Newton technique which attempt to find the best possible model parameters such that the square of the error between the model and data is minimised. The Gauss-Newton algorithm adapted from Siyakatshana (2006) is in Appendix D. After going through these processes, it is possible to guarantee with some level of confidence that the model may be able to perform satisfactorily to meet the required objective.

2.6. Industrial waste water treatment and cost

Over the past decades interaction between humans and the water environment in the form of industrial processes and basic individual use has been increasing. The result of such interaction destabilised the natural state of the environment and its ability to sustain life for other organisms which live or depend on the water body. Growth of industries and urbanisation may encourage high utilisation of clean water. Therefore, means to protect the sources of fresh water have to be implemented to maintain sustainability of the environment. Wastewater treatment could be considered a secondary means of pollution control to complete pollution prevention and waste minimisation. Since pollution prevention sometimes fails due to lack of suitable alternative process methods for certain industries to function without releasing pollutants, industrial water treatment is considered. Wastewater treatment unfortunately comes at high cost for most industries, since, sometimes it may be required that wastewater treatment plants should be built, managed and maintained in addition to current investments process plant equipment. Applying the minimum resources and using less capital should be the aim of most capital driven industries and municipalities. In this section some of background on the waste water treatment processes and cost estimates of such processes are discussed.

Wastewater treatment processes differ in unit process sequences depending on the contaminants to be treated. Contaminants may be removed by either physical, chemical and biological means, or a combination thereof. Some of the water quality variables considered either when designing wastewater treatment process sequences are pH, alkalinity, hardness, turbidity, natural organic matter, total dissolved solids and dissolved oxygen (Edzwald, 2011: 5.4). The processes required to treat these contaminants can be categorised under three main treatment stages which are Primary, Secondary and Tertiary treatment.

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Depending on the water quality requirement of a particular system, tertiary treatment, for example, is considered when stringent quality standards apply. Most common municipality treatment plants operate as primary, secondary, tertiary and physical-chemical treatment plants (Reynolds & Richards,1995:119). These treatment plants consist of numerous unit processes which ensure removal of certain contaminants at desirable removal efficiencies. Figure 2.5 shows an example of a municipal wastewater treatment plant process.

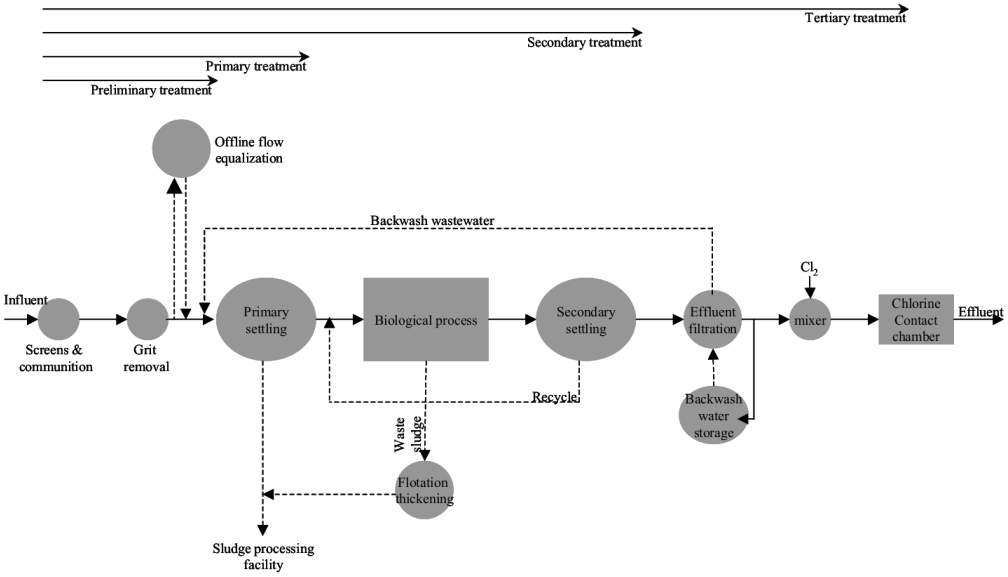

Figure 2.5.: Wastewater treatment process diagram (ESCWA,2003).

2.6.1. Primary treatment

Primary treatment process is responsible for the physical removal of most of the suspended solids in the wastewater. The treatment process takes place in three stages and unit processes namely:

- Bar screening whereby large objects such as stones, sticks and huge plastic bags which could block tank inlets or processes ahead or damage equipment.
- Grit removal process slows down flow such that all the grit in the water stream can fall out, and
- Sedimentation which occurs in a sedimentation tank or a clarifier whereby most suspended solids settle and are removed at the setting tank bottom outlet and the rest of the water proceeds to the secondary treatment.

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Depending on the state of the wastewater and the required water quality standards, there may be no need for additional treatment. in a case where further treatment is required, the outlet of the clarifier is fed into the secondary treatment process.

2.6.2. Secondary treatment

Secondary treatment consists of biological treatment processes, where remaining suspended solids from the primary treatment and dissolved organic wastes are bio-oxidised. At this stage biological treatment occurs, whereby micro-organisms convert suspended solids into settleable solids followed by sedimentation of the solids. The bio-oxidation may occur by a means of an activated sludge process, tricking filters, Oxidisation ponds (lagoons) or a combination of these processes.

Activated sludge process uses utilises micro-organisms to break down organics together with aeration and agitation. The reactors are usually fitted with a recycle stream that circulate the bacteria with activated sludge back to the aeration tank. The effluent stream goes through to the clarifier where the treated solids settle. Trickling filters similar to aeration basins, use mocro-organism to break down organics. They consist of a beds packed with stones or soft plastic whereby micro-organisms are attached. A wastewater stream goes through aeration and then get trickled past through the packed media. The effluent is collected and sent to the sedimentation tank. Lagoons consist of a large basin filled with micro-organism,algae as well as waterwater and relies on sunlight and the amount of oxygen available to treat the contaminated water. This a slow process but also relatively cheap.

Most municipal wastewater treatment plants disinfect the effluent stream from the secondary treatment with Chlorine before it reaches the final destination. The quality of water from the secondary treatment process may not be satisfactory depending on the required standards, therefore tertiary treatment may be required.

2.6.3. Tertiary treatment

Tertiary treatment involves further treatment of secondary treatment effluent usually by chemical means or expensive physical means such as filtration, nutrient removal processes and U/V radiation thereby providing increase in the water quality of the effluent. A common example of a tertiary treatment process is chemical water treatment. Chemical treatment consists of processes such as coagulation (chemical inducing suspended solids

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to coagulate), flocculation (forcing coagulated solids to form flocks which are easy to settle to the bottom of a settling tank) and sedimentation performed at different range of pH (to remove chemical compounds with properties that varies with pH).

The three treatment levels combined are considered for cost analysis of treatment plants. Based on the required water quantity, and quality standards, some of the advanced treatment levels may be omitted.

2.6.4. Treatment cost

The selection and design of wastewater treatment plants depend mostly on cost associated with the treatment process. Before these treatment plants are built and commissioned and appropriate water treatment technology is selected, a lot of work goes into technical feasibility studies that depend on the nature of the application (ESCWA, 2003). These studies include cost effectiveness, wastewater volumes and characteristics forecast, process alternatives for wastewater treatment, sludge and effluent management. All this is meant to determine a process that will minimise cost of resources required over the life span of the plant and minimise maintenance costs. Detailed knowledge of the process operations seems important in order to achieve reasonable conclusions. Wastewater treatment plants which already exit, possible changes which can be introduced to such a system could be the operational cost optimisation. Estimation of the operational cost of wastewater treatment plants is essential for optimisation studies for existing plants. Typical factors considered for estimating operational and maintenance cost are: labour, electricity, chemicals, residual management, taxes as well as insurance.

A link between the number of processes to required to achieve that water quality (treatment levels) and treatment efficiency may be deduced from the cost factors involved during plant operation. The relationship between treatment levels with cost associated with each level of treatment and efficiency can be used to perform a cost optimisation study.

2.7. Optimisation in water quality modelling

Mixed integer programming is a mathematical optimisation technique which only accepts integer values as optimisation variables in a feasible solution for a minimisation or maximisation optimisation problem. Figure 2.6 provides a holistic view of how the mathematical modelling process loop is conducted.

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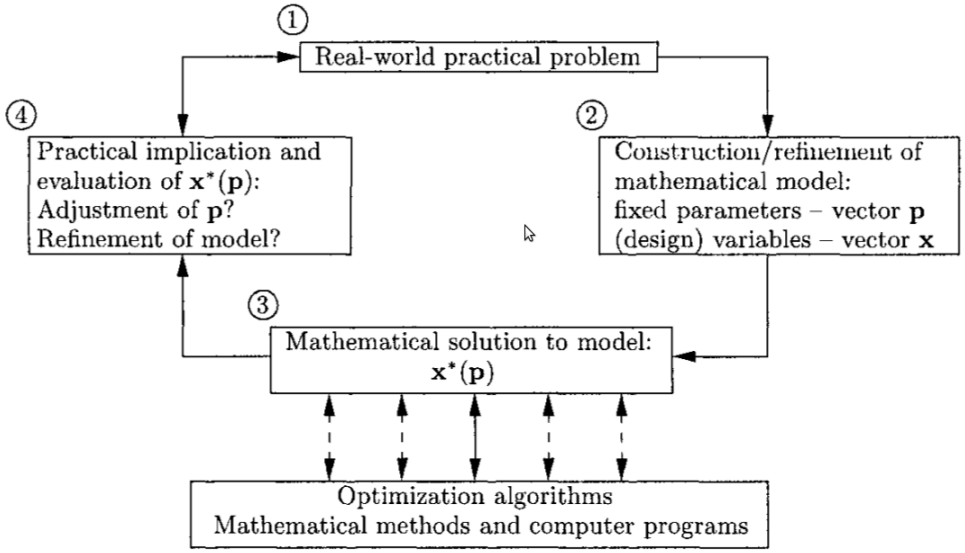

Figure 2.6.: The mathematical modeling process (Source:Snyman (2005: 5)).

The first step in the modelling process is to observe and study the real world problem, the second step is to represent the problem with mathematical equations (called problem formulation), the third step is to obtain the mathematical solution to the equations and optimisation, the last step is to determine if the optimised parameters are suitable representation for the system, otherwise the model has to be refined. This section provides a brief background on mathematical optimisation and available techniques that can be applied and also reviews some applications of mathematical optimisation in the water quality management field.

2.7.1. Mathematical optimisation: mixed integer

Mathematical optimisation also referred to as mathematical programming, non-linear programming or numerical optimisation according to (Snyman, 2005:1-3), can be described as the science of determining the best solutions for mathematically defined problems, which may be models of physical reality of a manufacturing or a management system. The process consists of a formulation and the solution of a constrained optimisation problem of a general mathematical form :

$$minimize_{w,r,t,x} f(X), X = [x_1, x_2, ..., x_n]^T \epsilon \mathbb{R}^n \tag{2.7.1}$$

subject to the constraints:

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$$g_j(X) \leq 0, \cdots j = 1, 2, ..., m \tag{2.7.2}$$

$$h_j(X) = 0, \cdots j1, 2, ..., r \tag{2.7.3}$$

where $f(X)$,$g_j(X)$ and $h_j(X)$ are the scalar function of the real column vector X. The

continuous components x of $X = [x_1, x_2, ..., x_n]^T$ are called the (design) variables, $f(X)$ is the objective function, $g_j(X)$ denotes the respective inequality constraint functions and $h_j(X)$ the equality constraint functions. The optimum vector X that solves problem shown by Equations (2.7.1 - 2.7.3) is denoted by X^* with corresponding optimum function value $f(X^*)$. If no constraints are specified, the problem is called an unconstrained minimization problem. This represents a typical formulation of an optimisation problem, depending on the optimisation algorithm used, a set of different mathematical problems can be optimised.The algorithm considered in depth in this study is the mixed integer programming scheme.

Luenburger *et al* (2008) describes three major types of optimisation problems which exist, namely: linear, unconstrained problems, and constrained problems. In the linear problem, the constraint and objective functions are linear. Most of the problems in the world fit the linear mathematical program. The problem may take the form of Equations (2.7.4 - 2.7.10).

$$minimise \quad wx_1 + w_2x_2 \tag{2.7.4}$$

$$subject \quad to \quad x_1 + x_2 \leq B \tag{2.7.5}$$

$$x_1 \geq 0, \qquad x_2 \geq 0, \tag{2.7.6}$$

Constrained problems take the form of the following Equations (2.7.7 - 2.7.10):

$$minimise \quad f(x) \tag{2.7.7}$$

$$subject \quad to \quad h_i(x) = 0, \qquad i = 1, 2, ..., m \tag{2.7.8}$$

$$g_j(x) \leq 0, \qquad j = 1, 2..., r \tag{2.7.9}$$

$$x \, \epsilon \, S. \tag{2.7.10}$$

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The last type of problem, the unconstrained problems are not common in practise because for many important problems, it can be argued that if the scope of a problem is broadened to the consideration of all relevant decision variables, there may be no constraints.

Mixed integer linear programming is only different from linear programming on the fact that some or all variable may only take integer values. This method is considered when dealing with complex systems where some of the decision variable represent real life quantities or parameters which strictly have to be integers. The process of modelling mixed integer programming problems as described by Smith & Taskin (2007) is done in three steps which are:

- defining a set of decision variables that represent choices to be optimised;
- statement of constraints in the model using mathematical equations;
- Defining the objective function.

Solving mixed integer problems can be done using available software like MIPLIB which is capable of solving both pure and mixed integer programs which arise from real world problems (Bixby *et al*, 1996) and Octave's built-in function *glpk* (Eaton, Bateman & Hauberg, 201: 487-491) which is an Open source software which can also applied to solve similar problems. Appendix B contains a document that explains how *glpk* works.

Chapter summary

The Upper Olifants catchment contains a network of unmonitored waste discharges form numerous different sources. The sources include wastewater treatment plants of which their state of operation was unknown. This provided a good case study of which the study aimed to research. The current wastewater management strategies applied at the catchment was not known to be applied such that set water quality standards are met and the cost of treatment is optimised.

DO was the parameter that was chosen since literature was available and methods of estimating the constituents playing a role were achievable. The Streeter-Phelps model has proven to be simple and reliable to model DO sag behaviour, and only contained two unknown parameters namely; reaeration rate coefficient and the de-oxygenation rate coefficient. This makes model calibration simpler and faster to produce parameters which will result in an acceptable fit to the data.

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Mixed integer programming was selected because the problem the study was attempting to solve fitted linear constrained mathematical problem, and the decision parameter chosen was conveniently chosen to take 0 when treatment was not applied and 1 at a location of the treatment levels (integer value between 0 and maximum number of treatment levels) vector. The location of the treatment and the 0 treatment criteria makes this a mixed integer problem hence this optimisation technique was selected.

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3. Methods

3.1. Introduction

The aim of this study is to develop a water quality simulation model for a section at the Upper Olifants catchment and also to design a optimal waste water treatment plants operational network by minimising operational cost. We have defined three sample modes of wastewater treatment plants (WWTP) operations, primary, secondary and tertiary. The key design question for an optimal regional system is to design a network such that each plant operates at either of the treatment levels and the cost of operating the whole system is minimised. All the while ensuring that water quality standards are not violated anywhere on the regional system under study. This is to be achieved by coupling a stream simulation model with a mixed integer optimisation model and dissolved oxygen is the chosen contaminant that will be monitored and modelled. DO is one of the most important parameters in water environment, it is used by fish and other large aquatic organisms for respiration. It is also utilised by micro-organisms for cellular activities.

The expected outcome of the study is a functional water simulation model that will estimate dissolved oxygen in-stream concentration profiles along the river catchment. Another outcome of this study is to track the point source loading of contaminants by municipal waste water treatment plants into the catchment and to use this data to determine the impact on the receiving water. The data collected from this exercise were used to determine the optimal contaminant treatment network for all contributing plants such that set water quality standards were not exceeded. This was achieved by a coupling the the simulation model and a mixed integer programming optimisation model, with the simulation model providing dissolved oxygen data in the streams and the optimisation model uses the DO data in the constraint equations for minimisation of the objective cost function. In this chapter a simple dissolved oxygen model is developed and a mixed integer programming scheme is designed for minimising treatment cost. Also, water quality data collected by the Department of Water Affairs from monitoring station at the catchment is analysed.

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3.2. Research design

This subsection illustrates the selection and design of methods which will be used to achieve the outcome of the study. These methods will be shows for the stream simulation model and the optimisation model.

3.2.1. Stream simulation model design

From the description given by Cox (2003a) of possible models Figure 3.1 shows the path followed in development of this model.

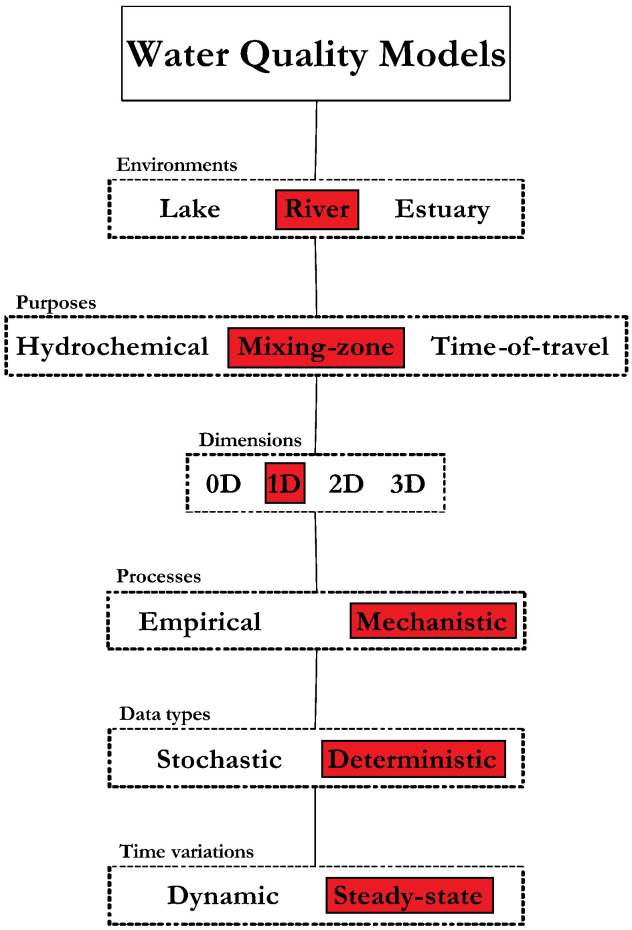

Figure 3.1.: Model selection diagram with highlighted model type.

This study was based on a river since it is an exposed source of fresh water and municipal waste water treatment plants around the Upper Olifants region provide a good example of a congested system with many treatment plants to apply this optimisation study. Other

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possible environments do not receive much contaminants and rivers are used as common source for fresh water supply.

- A mixing zone approach was considered since the aim of the study was driven mostly by the impact of different loading schemes by waste water treatment plants. Although a detailed hydrochemical study for the river could have been essential for understanding the system better,it does not focus on the impact areas where loading occurs.

- A one-dimensional (1D) model was selected for this study for the reason that since the flows were relatively high at the Upper Olifants river catchment the changes in water quality parameters on the direction of flow are much greater compared to the rest. The lack of resources and data encouraged development of a less complex model capable of estimating water quality well enough to represent the system.

- Since there was no experiment conducted and limited data was available, a steady-state mechanistic approach was chosen since it did not require much data and was still able to represent the underlying physics and chemistry that govern the selected Olifants catchment system.

- A deterministic model was chosen since a few experimentally acquired data was not required for the model to yield valuable results.

The catchment were divided into reaches based on the following :

1. Monitoring station points, since water quality data was known for these regions and these sample data were used to calibrate the stream simulation model.

2. Waste water treatment plant discharge points, in order to track down the impact on the stream caused by point source loading.

3. Where stream additions or subtraction occurs, to track down possible changes in hydrology and contaminant concentration

Other models like the Qual2k divide reaches based on lengths which requires many computations to be performed. The dissolved oxygen model chosen for this study was the Streeter-Phelps model because it was easy to solve and had only two parameters (re-aeration rate constant k_a and de-oxygenation rate constant k_d) involved. This selection was inspired by the fact that the model covers both the major DO source and sink.

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3.2.2. Optimisation design: mixed integer programming

Mixed integer programming was selected for this study since the nature of the problem consists of a few variables which can take integer values and others which are not necessarily integers. The real motivation however, was the success of the model in designing optimisation networks in the past has been observed. The literature by Finney *et al* (1977) is a good example where development of mathematical models played an integral role. The literature starts off with the earliest model of Fan *et al*, (quoted by Finney *et al*, 1971:47) who discovered an optimal waste discharge policy along a stream by minimising the total cost of maintaining water quality standards on a regional basis. This work was followed by more similar work such as Arbabi & Elzina, (quoted by Finney et al, 1975: 48) who used a linear approach to meet system water quality standards for DO at minimum cost on the Willamette river. Finney *et al* (1977) succeeded is applying a similar model proposed by Bishop & Grenny, (quoted by Finney *et al*, 1976: 50) which used mixed integer programming to optimise water resources management. The model was able to determine a possible feasible wastewater treatment scheme that minimised cost. Recently the work of Saremi *et al* (2010) illustrated the use of a multi-optimal waste model with linear programming to model the environmental capacity of Haraz river with BOD being the parameter modelled. This work produced non-uniform removal rate for pollution based on the minimum cost method. The success of these models open doors for more work on using mathematical programming for waste water management.

The problem considered for this study was a system which receives point source loads from waste water treatment plants. The wastewater treatment works were considered to operate at three different treatment levels (Treatment level 1= Primary treatment, Treatment level 2 = Secondary treatment and Treatment level 3= Tertiary Treatment). The treatment levels were varied with Oxygen re-aeration efficiency levels assuming high re-aeration result in high treatment cost and the relationship is illustrated by Table 3.1.

Table 3.1.: Treatment levels with equivalent re-aeration efficiency and cost levels.

Treatment level	Re-Aeration efficiency(%)	Cost Level
1	25	Low
2	50	Medium
3	75	High

This study avoided using specific costs figures because of the varying nature of the cost parameter, instead treatment efficiency which will be linked to an arbitrary cost figure

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will be considered and thus any cost value can be assigned for efficiency at any given time.

3.3. Methodology

In this section a detailed stream simulation model was developed and a mixed integer optimisation problem was structured. Water quality data provided by the DWA were discussed and analysed for this problem.

3.3.1. Stream simulation model instruments

Dissolved Oxygen was the parameter considered in this study and the Steeter-Phelps model was chosen for this purpose since it was simple to compute and the required data could be estimated for the Klein Olifants catchment. The following Equations (3.3.1-3.3.2) of the model were considered for calculating the deficit oxygen concentration.

$$L = L_0 e^{\left(-\mathrm{K_r}/\mathrm{U}\right) x} \tag{3.3.1}$$

$$D = D_0 e^{\left(-\mathrm{K_a}/\mathrm{U}\right) x} + \frac{K_d L_0}{K_a - K_r} \left(e^{\left(-\mathrm{K_r}/\mathrm{U}\right) x} - e^{\left(-\mathrm{Ka}/\mathrm{U}x\right)}\right) \tag{3.3.2}$$

The Elmore & Hayes, (quoted by Cox, 1960: 310) model was considered for determining the saturation concentration at the river bed.The parameters given by Equation 3.3.3 were calibrated using in-stream water quality data by applying the Gauss-Newton method.

$$C_s = 14.652 - (0.41022T) + \left(0.007991T^2\right) - \left(7.7774 \times 10^{-5} T^3\right) \tag{3.3.3}$$

The temperature variation in the stream was only be considered for the areas where loadings were introduced and a mass balance type like equation will be used to estimate the temperature. The equations will take the form of Equation 3.3.4 :

$$T_f = \frac{Q_r T_r + Q_l T_l}{Q_r + Q_l} \tag{3.3.4}$$

where T_f is the final stream temperature, T_r is the temperature of the river stream before

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a load is introduced into there stream, T_l is the temperature of the load stream and Q_r and Q_l represent the flow rates of the river and the load stream respectively. The stream hydrology was determined using the Manning's equation since the steady state model approach was selected:

$$Q = A\overline{U} = \frac{AR^{2/3}S_o^{1/2}}{n} \qquad (Manning) \tag{3.3.5}$$

Most of these values were assumed values since the data was not available to validate them.

3.3.2. Octave stream simulation code

A code was written to perform all the necessary calculations. The code was designed to accept a file called input.csv as input. The input file contained data (reach length, cross-sectional area, mainstream and load flows and reach dependency) for each river reach. Reach length was estimated using google map scales, cross-sectional area was estimated using the channel average width and average water level depth. Average flows recorded on monitoring stations were used as river flow and load flows were assumed to be about 10% of the total stream flow for each load, while the stream dependency's main purpose was to inform the program , which one was the head reach and where calculation should begin.

After reading the input files the code solver computes the Streeter-Phelps equation along the reach length and gives the DO concentration as output. Instead of using time steps, the Streeter-Phelps equation was modified by making it to be a function of distance instead of time. This was achieved by replacing t by $\frac{x}{U}$ with x being distance in (m) and U is the stream velocity in (m/day). Before a calculation begins on a reach, mass balance is performed where loads are introduced. At the end, all DO concentrations are recorded at the end of each reach where checkpoints are assumed to be located. The full code with comments is available in Appendix (B and C).

3.3.3. Mixed Integer optimisation model development

The method used in this study was adopted from Finney *et al* (1977) and the following definitions are also from the study. Figure 3.2 shows a diagram representing some of the parameters used.

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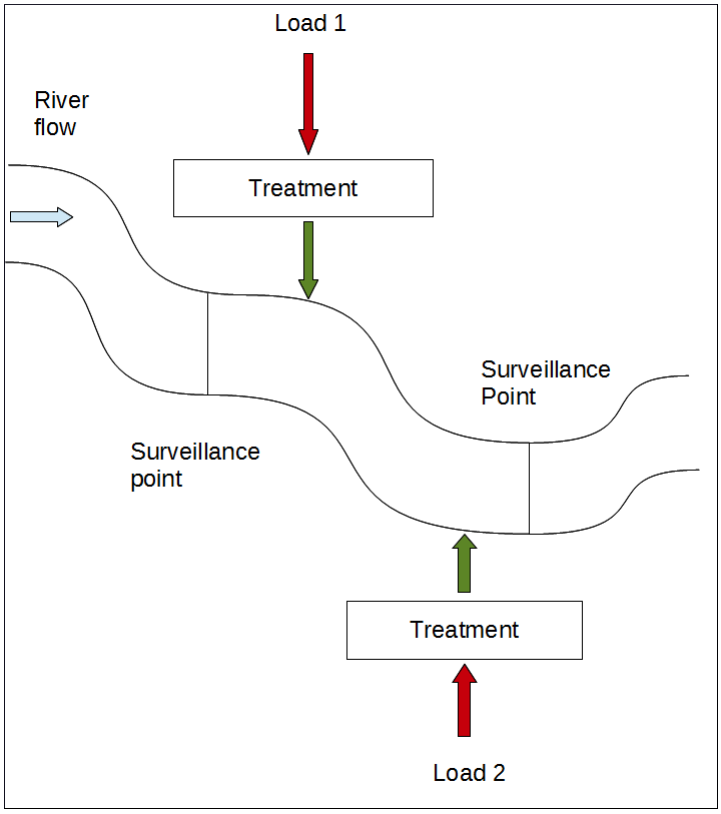

Figure 3.2.: Conceptual river system receiving two wastewater outfalls

The following is a list and definitions of parameters used.

- p =surveillance point index, 1,2,...P.
- n =Treatment level index = 1,2,...N
- l load index 1,2,...L
- $B_p = (b_c)_p$ = A vector of pollution concentration limitations (stream standards) for c species, at each surveillance point p.
- $Y_p^o = (Y_c^o)_p$= vector of concentrations for c species, at each surveillance point p, resulting from existing stream loading.

The following is a list and definitions of variables considered.

- c = water quality species index = 1,2,...C .
- $T_l = (t_n)_l$ = An integer vector ($t_n = 1$ or 0) indicating which treatment level, n,is provided: $t_n = 0$ if level not provided, $t_n = 1$ if level is provided.

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- $Y_{l,p} = (Y_{c,n})_{l,p}$ = Matrix of species c concentrations occurring at surveillance point p, for treatment level n, being applied at load l and existing treatment at the remainder of the loads. That is, it represents the concentrations resulting at p if only load l was given additional treatment.

- $Y'_k = (Y'_c)_p$ = Vector of concentrations for each species c, at each surveillance point p, resulting from the optimal loading scheme determined by the mode.

Assuming that the concentration of each species must be less than the stream standard at each surveillance point:

$$Y_p^{'} \leq B_p \qquad p = 1, 2 \ldots\ldots, P \tag{3.3.6}$$

For a linear system:

$$Y_p^{'} = Y_p^0 - \sum_{l=1}^{L} \left[Y_p^0 - Y_{l,p}T_l\right] \tag{3.3.7}$$

Therefore:

$$Y_p^0 - \sum_{l=1}^{L} \left[Y_p^0 - Y_{l,p}T_l\right] \leq B_p \qquad p = 1, 2 \ldots\ldots P \tag{3.3.8}$$

We define:$D_{l,p} = (d_{c,n})_{l,k}$ = a matrix representing the change from the existing concentration of species c at surveillance point p when treatment level n is applied at load l.

$$D_{l,p}T_l = Y_p^0 - Y_{l,p}T_l \tag{3.3.9}$$

Substituting into the previous Equation 3.3.9:

$$\sum_{l=1}^{L} D_{l,p}T_l \geq Y_p^0 - B_p \tag{3.3.10}$$

Finally we define: $C_l = (c_n)_l$ = a vector of treatment costs for treatment level n at load l. Non-linearities in cost functions are accounted for since a specific treatment cost

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is associated with each treatment scheme and load. The mixed integer programming problem to minimise treatment cost can then be structured as follows:

$$Minimise\ total\ cost = \sum_{l=1}^{L} C_l^T T_l \tag{3.3.11}$$

Subject to the set of constraints:

1. Water Quality stream standards

$$\sum_{l=1}^{L} D_{l,p} T_l \geq Y_p^0 - B_p \qquad p = 1.2, ...P \tag{3.3.12}$$

2. Integer solution for treatment levels and only one treatment level per load.

$$\sum_{n=1}^{N} (t_n)_l = 1 \qquad l = 1, 2 \ldots L \tag{3.3.13}$$

And $tn = 0$ or 1 for all values of n.

3.3.4. Combined simulation and optimisation model

Optimization model is linked to simulation model by a single parameter, the "D" matrices. The D matrix is conveniently generated by the stream simulation model using the following procedure:

1. Calculate Y_p^0 from existing loading
2. Apply the first treatment level at the first load and calculate $Y_{l,p}$
3. Calculate the "D" matrices, with

$$D_{l,p} = Y_p^0 Z^T - Y_{l,p} \tag{3.3.14}$$

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where vector Z is defined as follows $Z = z_l$ a vector with each element equals to 1.0, i.e. each element in $D_{l,p}$ is simply calculated as:

$$d_{c,n,l,p} = y^0_{c,p} - y_{c,n,l,p} \tag{3.3.15}$$

4. Repeat steps 2 and 3 for each treatment level. 5. Repeat steps 2, 3, and 4 for each load.

Constraint 1 is based on a linear system and is not necessary valid for non-linear quality relationships. For such relations, an iterative technique between simulation model and optimization model is required. The mixed integer problem was solved using Octave's built-in function *glpk* and more on the function is available in the Appendix A.

The relationship between treatment levels and efficiency was assumed and is represented in Table 3.1 and was also based on the fact that the higher the treatment level required, the more expensive the treatment.

Coupling of stream simulation models and mixed integer programming has proven to be a valuable tool in water management studies.The work of Finney *et al* (1977), which applied the method to optimise a waste water treatment network inspired work of Margeta (1984) where a similar model was applied on a different hypothetical problem. The approach to such problems is still appreciated with the work of Liu *et al* (2011) where mixed integer optimisation approach was used on an integrated resource management problem. The success of the method inspired the decision taken to apply it to the Olifants river catchment.

3.4. Data

The data used for this study was obtained from the Department of Water Affairs database where in-stream water quality data was provided using the Resource Quality Services (RQS). The site covers the national monitoring programs and is responsible for all the data processing (i.e Sampling, sample collection and analysis). The resource quality monitoring also involves management of the River Health Program in the country. The RSQ uses a data exploration tool where geographical water quality data can be obtained on Google Earth maps. The data were arranged based on Primary drainage regions, water

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management areas and hydrological sites (rivers, dams, estuaries, climate and "local"). The Primary drainage area data for the Olifants river were used on this study. More information on other data management programs can be obtained from the RSQ website (http://www.dwaf.gov.za/IWQS/).

The Olifants catchment was classified under water quality management area "B". Under this classification, river, dam_lake, wetland, water supply, waste, mine_industry and transfer water quality data were provided for the whole Olifants catchment. The main water quality data required for the study were: in-stream river water quality and water from waste water treatment works at the upper Olifants. The Figure 3.3 shows the river section on the Olifants river catchment where data is collected.

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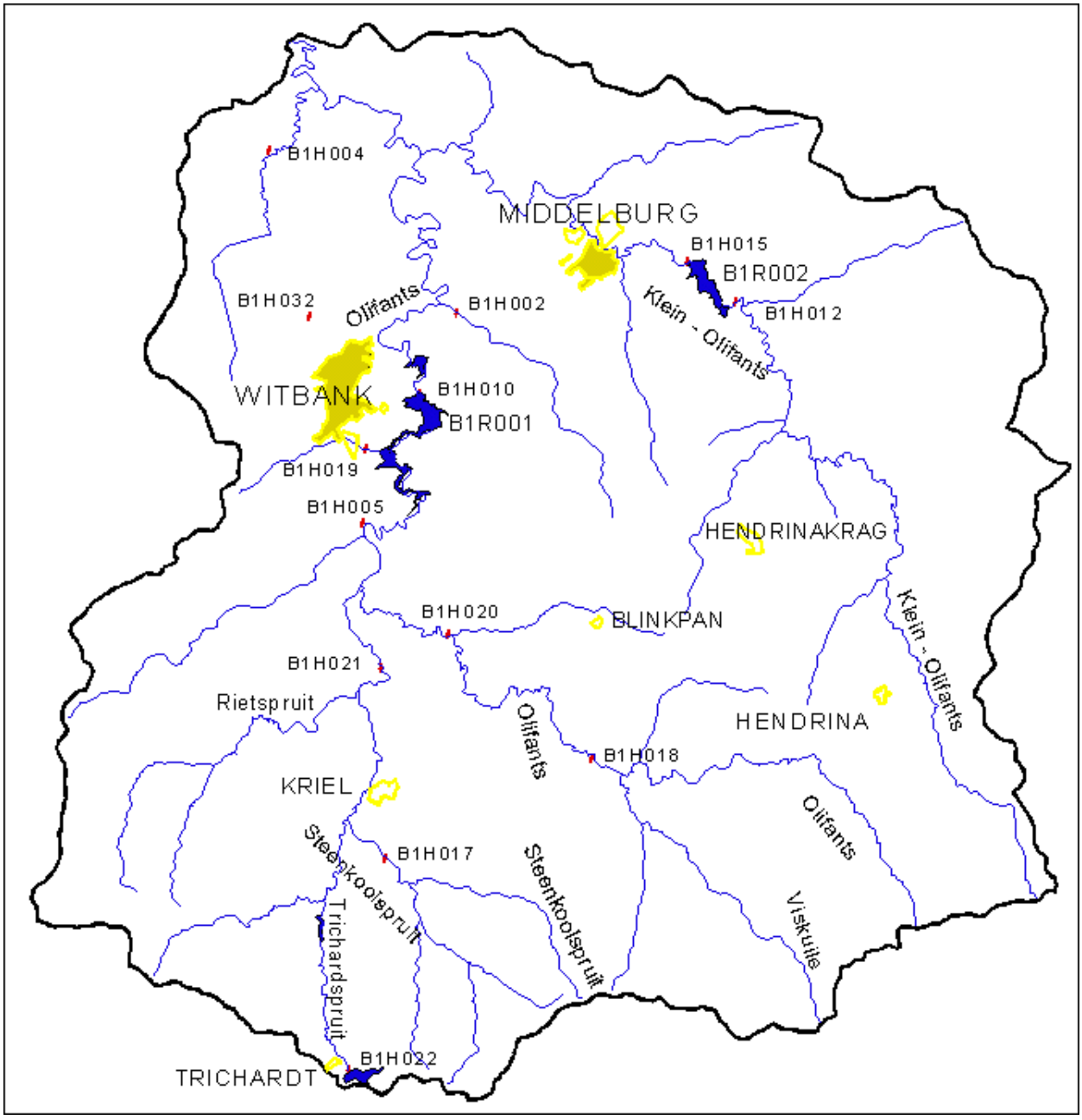

Figure 3.3.: The Upper Olifants river system (Source: DWA website).

The DWA has a selected number of monitoring stations which capture hydrological data. The station represented by the Table 3.2 are the ones closest to the selected catchment studies.

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Table 3.2.: Hydrological data at monitoring stations close to the studied catchment.

Monitoring station	Median flow rate (m^3/s)
B1H020Q01	0.013
B1H021Q01	0.281
B1H005Q01	0.243
B1H029Q01	not available

3.5. Data analysis

Data obtained required some re-work in order to obtain a realistic representation of the catchment studied. Since most of the data used on this study were acquired from the DWA monitoring program, an assumption was made that their sampling and sample analysis was of acceptable standards and thus in this section it will not be discussed. This section represents the manipulations performed on the data in order to suit the form required for this study.

3.5.1. Hydrological data

The hydrological data at the chosen area of study were estimated using a water balance of the river. The water balance however neglects the evaporation and transpiration effects by assuming that the contribution were negligible since this data were not available at the hydrological monitoring stations. The result of this was a material balance equation which only focuses on the water flowing at a given time. Figure 3.4 shows a map of the set up of the region studied and the location of the monitoring stations.

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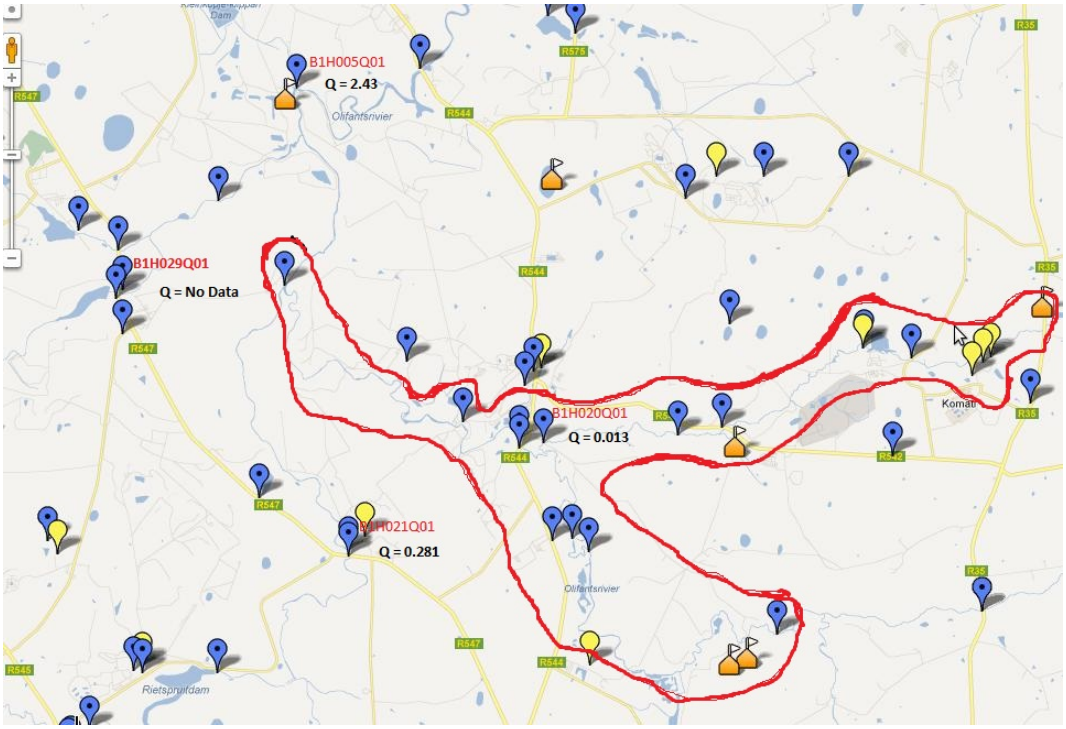

Figure 3.4.: Google map with marked Studied catchment with nearby monitoring stations.

The demarcated section of the map shows the selected river tributaries for this study. As the Figure 3.4 shows, the only monitoring station with hydrological data was B1HO20Q01 which was located at the end of the tributary that joined the Olifants river. The main stream had no monitoring stations with hydrological data, but further upstream it merged with other streams which had data. The water balance was performed upstream of the main Olifants river stream. The following material balance Equation 3.5.1 was used.

$$Q_{mainstream} = Q_{B1H005} - Q_{B1H029} - Q_{B1H021} \tag{3.5.1}$$

with Q_{B1H05} flow rate at the Olifants river stream with station B1H005, Q_{B1H021} flow rate at the stream joining the Olifants river with monitoring station B1H021 and Q_{B1H029} stream flow rate of stream joining the Olifants river with monitoring station B1H029. The flow was estimated assuming a linear relationship between catchment cross-sectional and flow rate, thus the sections with hydrological data were used to predict flows at streams with no data.

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3.5.2. Contaminant sampled data

The DWA monitoring system did not capture dissolved Oxygen and BOD and thus tracking dissolved oxygen became a challenge. The possible alternative was to find a correlation between some of the available sampled data and dissolved oxygen. Some of the available contaminants were nitrates and pH, However relationships on nitrates and dissolved oxygen correlation proved difficult to find compared to pH and dissolved oxygen. The study conducted by Zang *et al* (2010) contained different correlations for different water bodies relating pH to DO and the Equation (3.5.2) for river systems by Wang *et al* was selected for this study.

$$C_{DO} = 3.322e^{0.064}pH \tag{3.5.2}$$

where C_{DO} is DO concentration in (mg/L) and pH is the river water pH. Similar correlations were assumed to apply at the Upper Olifants catchment. However, lack of such studies have compelled us to use literature correlations for the benefit of this research. Figure 3.5 was produced using Equation (3.5.2) shows how the DO concentration correlates to pH.

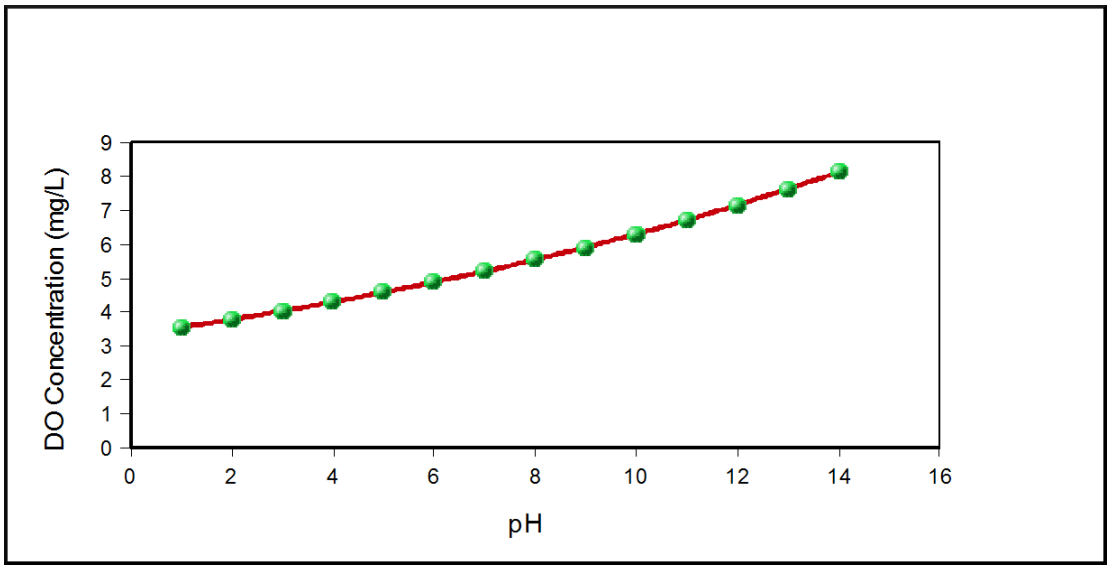

Figure 3.5.: DO and pH correlation (Zang *et al* (2010)).

The figure shows that along the full pH range, DO concentrations ranges between 3 - 8.5 mg/L which is an acceptable range since the river water temperature of the study was assumed to range between 15 - 22 °C. And the saturation DO concentration does not exceed 9.5 mg/L.

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3.6. Chapter summary

Based on the lack of data for this study and a number of assumptions made for some of the data, it is clear that the model model developed here might differ from the real system. Some of the major limitations of this study are:

- Due to lack of data, the results of the model are will be affected in a sense that it may be very dependant on the starting conditions during optimisation.
- The model does not take into consideration the complex mixing conditions where load streams are introduced, therefore an error is expected where mass balances are performed.
- The loads flow rate and BOD loading concentration assumed may not necessarily represent the real flows which has a great impact on the coefficients chosen during model calibration. Even though data exists for the actual DO concentration the effect might still be significant.
- The model only considers steady state conditions, which hardly exist at a large river stream like the Olifants.
- Waste water treatment level efficiencies are assumed, thus with a much better estimations of efficiencies a totally different feasible solution may be expected from the model.

With regards to all the assumptions made and some of these limitations outlined, the model was still considerably adequate to illustrate and the ideal optimised treatment network that could be applied to maintain water quality standards under given conditions. The resulting model and feasible treatment network solutions were strongly based on the assumptions made and took into consideration the limitations.

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Part II.

Results and discussion

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4. Water quality model

4.1. Introduction

The first Aim of this study was to develop a functional water quality model for predicting dissolved oxygen concentration in one of the sub-catchments of the Olifants river. The other objective was to use mixed integer optimisation strategy to determine the optimum operational mode of water treatment works on the catchment. So far the method of achieving these objectives has been discussed and applied to produce results which are outlined in this chapter. The findings recorded are at the selected theoretical measuring stations (checkpoints) of the river that illustrate the key components of the study.

4.2. Research findings

The water quality model presented in this study was developed in order to predict the concentration of dissolved oxygen and biochemical oxygen demand along the river. The key locations selected for this study were intersection of two streams and points immediately after outfalls from wastewater treatment plants. The findings comprise primarily the performance of the model in predicting dissolved oxygen concentration in the river. The first seed of results consisted of the model predictions of the concentration at the points of the river where data were available. This section only shows the model results in the stream with no treatment levels applied. The selected catchment for this study contained 16 in-stream data points with 9 samples from wastewater treatment plant outfalls. The stream simulation model (Streeter-Phelps) model contained four parameters (initial DO concentration, initial BOD concentration, k_a and k_d), only the two parameters (k_a and k_d) were optimised during model calibration. Table 4.1 shows the distributions of the sample data amongst the tree branches into which the catchment was divided and some of the statistical information which was gathered during applying regression technique for model calibration.

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Table 4.1.: Regression data and sample data distribution.

Catchment section	Sum of square errors	numbers of samples
Main stream (before confluence)	3.8842	5
Branched stream	8.4679	6
Main stream (after confluence)	1.5431	5

Figure 4.1 shows a conceptual diagram of the studied river channel with loads applied on the main and branched stream.

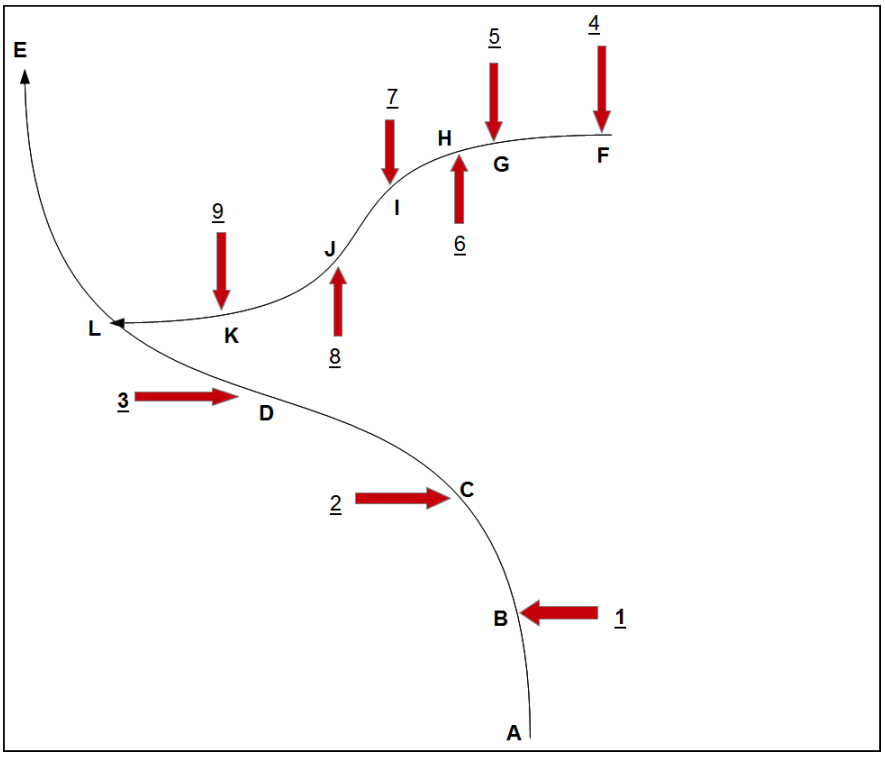

Figure 4.1.: Diagram showing conceptial catchment with wastewater outfalls indicated by arrows.

The catchment channel was divided into two sections with A-B-C-D-L-E along the channel representing the main stream (Olifants river) and F-G-H-I-J-K-L representing a tributary joining the Olifants river at point L. The main stream was divided into river reaches AB, BC, CD and DL, the branch was divided into reaches FG, GH, HI, IJ, JK and KL. Since most of the data of this streams were not accessible, random estimates were made. Table 4.2 shows reach data used for this model

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Table 4.2.: Data at Olifant reaches and branched stream reaches

Reach (Load number)	**Reach length (m)**	**Cross sectional Area (m^2)**	**Load flow rate (m^3/s)**	**Load DO concentration (mg/L)**	**Load BOD concentration (mg/L)**	**Flow (m^3/s)**
AB	6500	52.2	-	5.7045	14	0.245
BC(1)	1000	52.2	0.024	5.5180	50	-
CD(2)	3500	52.2	0.024	5.5281	50	-
DL(3)	9000	52.2	0.024	5.4087	50	-
LE	20000	52.2	-	-		-
FG(4)	2500	13.5	0.0013	5.2872	25	0.013
GH(5)	1000	13.5	0.0013	5.2578	50	-
HI(6)	1000	13.5	0.0013	5.8189	50	-
IJ(7)	1500	13.5	0.0013	5.4215	50	-
JK(8)	37500	13.5	0.0013	5.5266	30	-
KL(9)	2500	13.5	0.0013	5.74484	50	-

4.2.1. Main stream data and model results

The main stream was divided into four reaches and the fifth reach included the confluence with a tributary. Some of the reaches contained data points against which the model was calibrated. The following Figures (4.2 - 4.4) show data from river reaches A-D, with values of deoxygenation rate coefficient $k_d = 0.0410$ per day and re-aeration rate $k_a = 0.0804$ per day. The parameter values were obtained using the Gauss-Newton regression technique.

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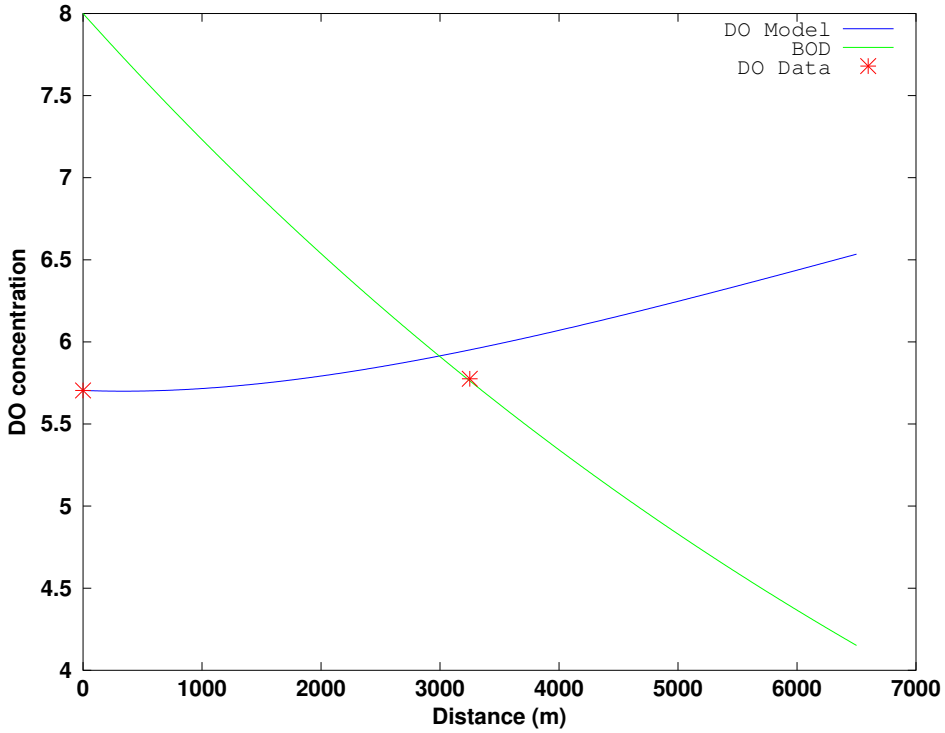

Figure 4.2.: Preliminary model fit of DO against distance at river reach AB.

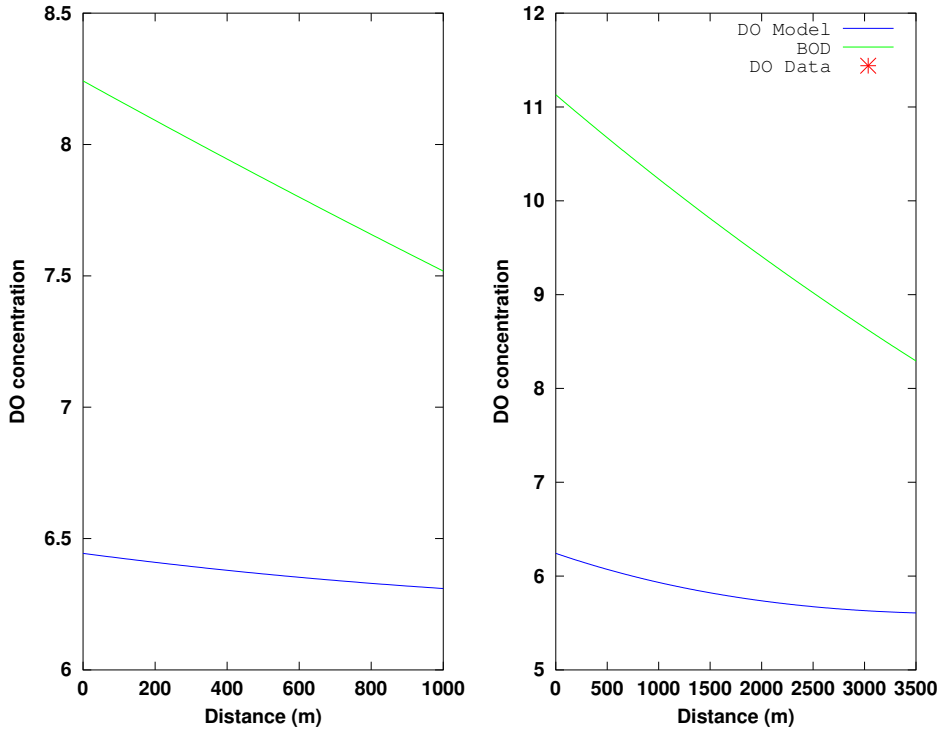

Figure 4.3.: Preliminary model fit of DO against distance at river reaches BC and CD.

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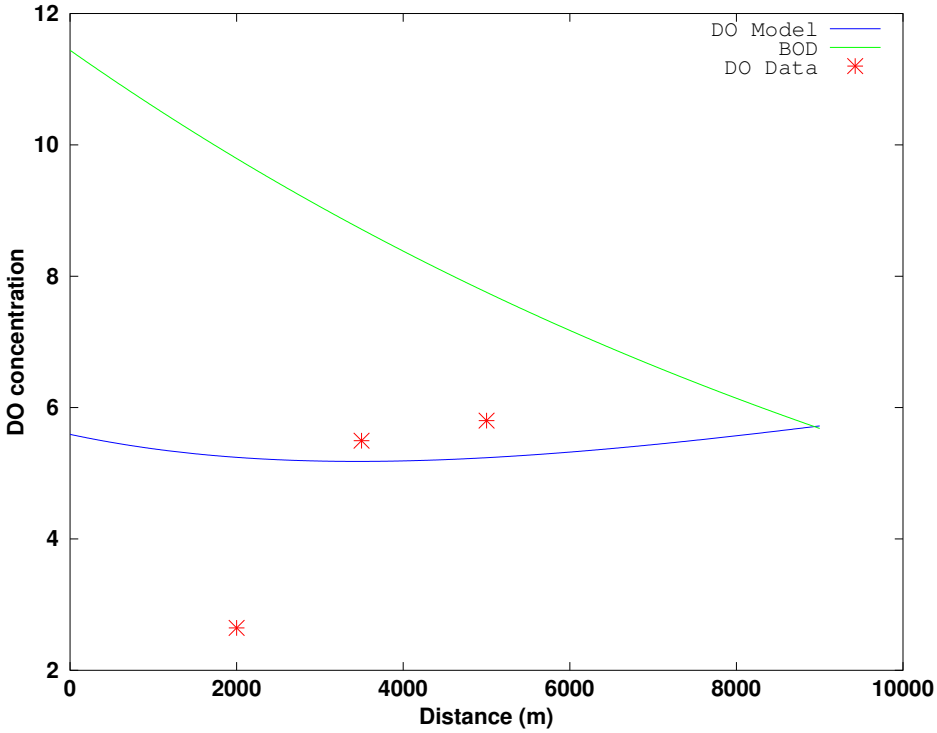

Figure 4.4.: Preliminary model fit of DO against distance at river reach DL.

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4.2.2. Branched stream data and model results

The branched stream was divided into six reaches. The following Figures (4.5 - 4.6) shows graphs of reaches A-D with rate coefficients values $k_d = 0.0280$ per day and $k_a = 1.0950$ per day.

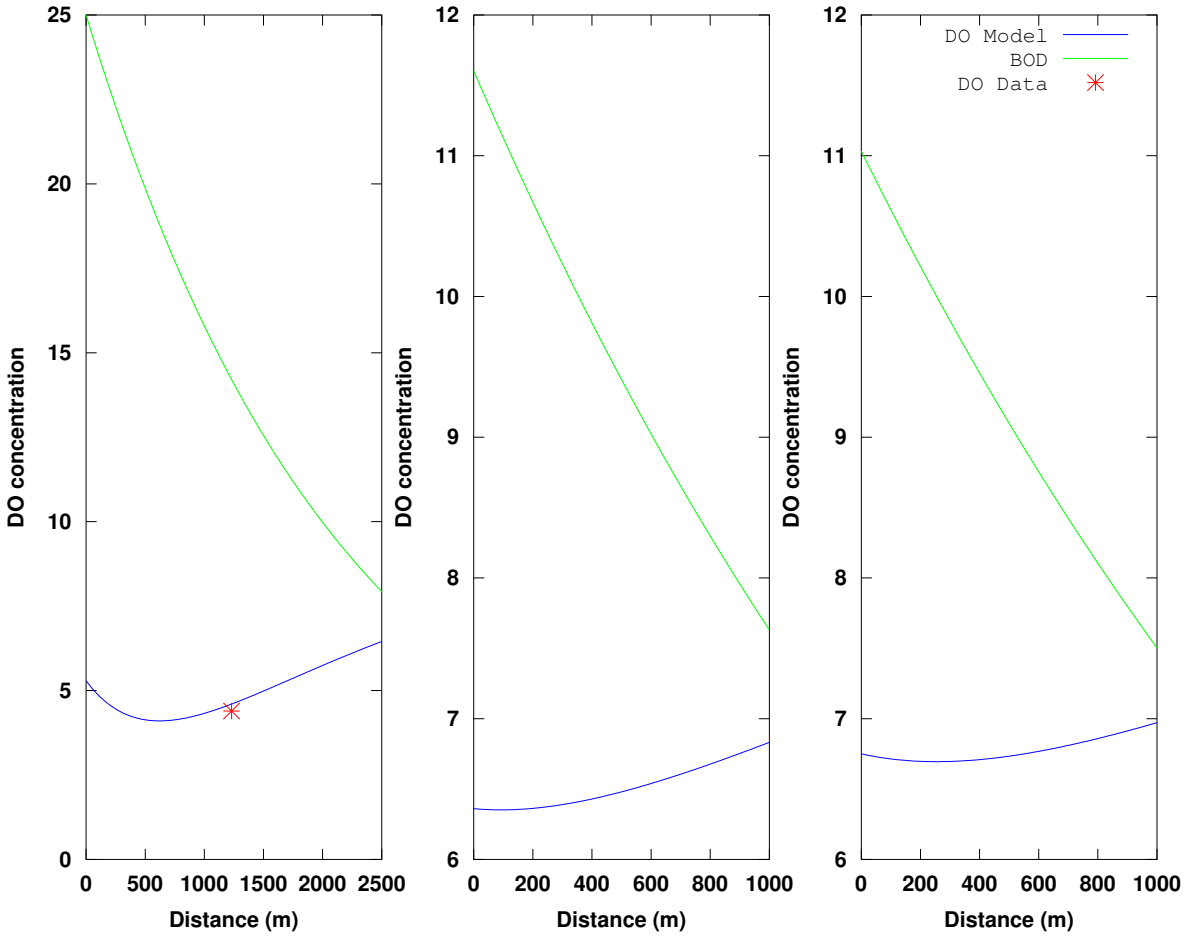

Figure 4.5.: Preliminary model fit of DO against distance at river reaches FG, GH and HI.

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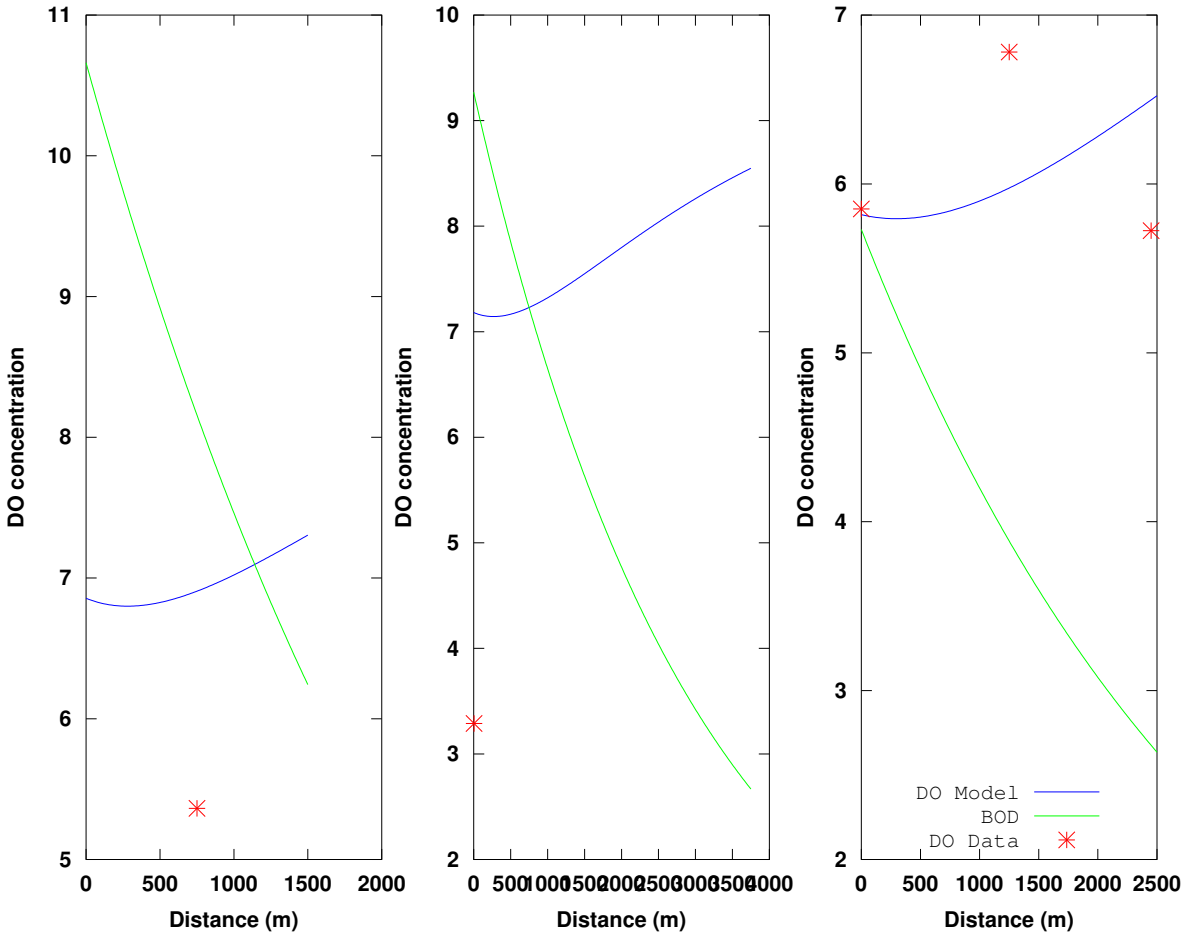

Figure 4.6.: Preliminary model fit of DO against distance at river reaches IJ, JK and KL.

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The last reach LE, represents the main stream after the tributary had been added. The coefficients were calibrated to $k_d = 0.1720$ per day and $k_a = 0.9020$ per day to fit the data at this reach. The Figure 4.7 shows DO and BOD concentration profiles and DO stream data.

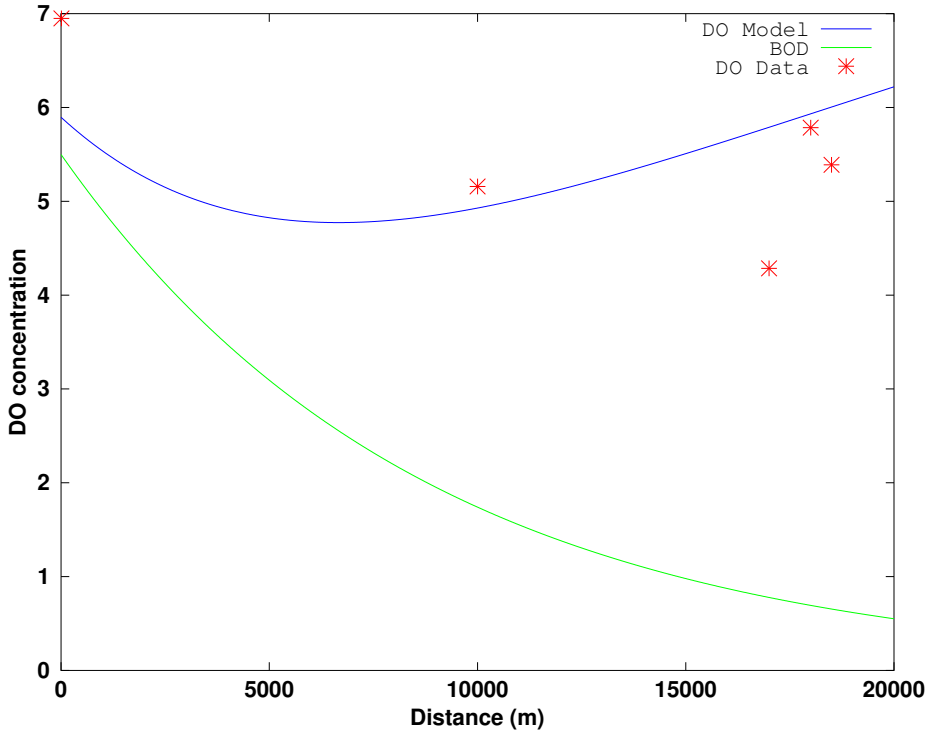

Figure 4.7.: Preliminary model fit of DO against distance at river reach LE.

4.3. Analysis and discussion

4.3.1. Main stream reaches analysis

The main stream contained only five in-stream data points which were spread out between reach AB and DL. The river reach AB contained two data values and the river reach DL contained three data points. Since there were no significant disturbances expected on the stream, it was assumed that the model should be governed by constant deoxygenation and re-aeration coefficients obtained during calibration of each stream. Thus the calibration performed included in one section was assumed to be applicable to the whole river (reaches AL). These assumptions were made for the sake of the study because it is understood that both coefficients may be affected by seasonal variations.

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At river reach AB, the initial sampled data point was located conveniently at the head stream of the main Olifants stream. At reaches BC and CD, no data were recorded but the model provided realistic DO concentration relationships, no non-positive concentrations were recorded. The last reach DL had three data points. The model managed match only only two data points. The first data point the model lie out of range of the model. The offset could be an error somewhere throughout the data analysis process, or it could be existence of a wastewater outfall which was not recorded by the DWA and therefore not considered in the model. There were no methods of verifying either one on the causes of the offset, for the benefit of this study we have attributed the error to the analytical processes performed on the data.

The model has shown capability to represent the channel based on these few available data and therefore was used to represent the Olifants system for the given conditions. This argument however could be strengthened by obtaining more data from the stream.

4.3.2. Branched stream reach analysis

The branched stream was divided into six reaches in accordance with existing outfalls. The stream contained six data points spread out between reaches FG, IJ, JK and KL. The branched stream was expected to have different coefficients from the mainstream since they had different flow rates and loading, but these coefficients were expected to be constant for the whole branched stream.

River reach FG contained only one data point which the model obtained a satisfactory fit and reaches GH and HI had no data points. The model failed to obtain a satisfactory fit with the parameters obtained after calibration for the sample point at reaches IJ and JK. The primary cause of this may be attributed to the fact that not enough data was available and some point the system had insufficient degrees of freedom. This type of offset could also be caused by the fact that the observed points were located immediately after wastewater outfalls occurred. At these points mixing conditions which the model did not include could have played a role, another reason could be the fact that the load flow rates were assumed and not based on the real values from the wastewater treatment plants. A higher offset could be that the actual load flow rate at JK was higher that the assumed value. A similar situation can be observed on the Figure 4.6 with reach KL. The model provided acceptable fit to some of the data but failed to predict the concentration immediately where loading occurred. The model was deemed acceptable for the sake of the study because even though it was not very accurate at these points, it was not complex and it did not require high computational power.

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4.3.3. Main stream after the confluence point

At this section of the catchment, different model parameters which best fitted the data were obtained. The re-aeration rate remained almost similar to the main stream before addition of the tributary stream, this was expected since the model catchment area did not change significantly. River reach LE contained five data points of which the model managed to predict the concentration profile closest to the data points even though a perfect fit was not obtained. This could have been a result of errors which came about during data analysis.

4.4. Chapter summary

The following was observed about the stream simulation model:

- The model calibration produced high sum of square errors values during calibration of the optimised parameters varied with different starting conditions.
- The model failed to predict accurate DO concentrations where load streams mix with the main stream.
- It did not produce a best fit to the available data but managed to predict the DO concentration profile at the reaches.
- However, the model was capable at predicting concentration profile along the length of a reach. This was illustrated by how there was a much better fit for data points located further from the initial points. This motivated the selection of checkpoints to be at locations towards the end of each river reach since the model had proven to predict better at those locations. The D-matrix produced by the model was used for generating constraints equations for the optimisation model.

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5. Coupling stream simulation and optimisation models

5.1. Introduction

In this chapter optimisation of wastewater treatment networks was performed using the D-matrix supplied by the stream simulation model. The purpose of the optimisation was to minimise wastewater treatment cost while maintain river stream DO concentration at environmentally acceptable levels. The target solution is that which ensures that the DO concentration at each selected checkpoint was equal or greater that the set water quality standards. The river system studied contained five wastewater treatment plants and four mining properties with each assumed to have had wastewater treatment facilities. This

treatment was assumed to be performed after the current normal operating conditions of the plants and water quality standards checkpoints were assumed to be located towards the end of each river reach. Table 5.1 shows the initial conditions at each wastewater treatment facility.

Table 5.1.: Waste water facilities with initial operation conditions.

Load no	**DO concentration (mg/L)**	**BOD concentration (mg/L)**	**Load flow (m^3/s)**
1	5.518	50	0.024
2	5.5408	50	0.024
3	5.4087	50	0.024
4	5.7045	50	0.0013
5	5.2450	50	0.0013
6	5.8189	50	0.0013
7	5.4215	50	0.0013
8	5.5266	50	0.0013
9	5.7448	50	0.0013

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The effluent BOD concentrations without additional treatment applied were assumed, as well as the treatment facility effluent discharge flow rate. These initial conditions were applied to the stream simulation model to generate the D-matrix for the system in order to solve the optimisation problem. Equation (5.1.1) provided the objective function cost coefficients for each treatment level, the assumption was not based on any theoretical equation but only used as tool for optimisation. The adaptation of this equation was derived from Finney *et al*, (1977) which was a used as a basis for cost calculations.

$$Treatment\ Cost = A_c * Q^{0.6} \tag{5.1.1}$$

with Q as effluent discharge flow rate in m^3/day and A_c is a constant which varies for each treatment level monetary units/flow units and $Treatment\ Cost$ is assumed to be the total operation cost for each treatment level. This simplified equation was selected based on the fact that it illustrates the fundamental elements (flowrate and a constant that signifies the effect of higher treatment levels on cost) in cost studies of wastewater facilities. Table 5.2 shows values of A_c for each treatment Cost. The values of A were assumed considering the fact that at higher treatment levels more cost is expected than at lower treatment levels hence the numerical values increase with treatment levels.

Table 5.2.: Treatment cost constant for each treatment level.

Treatment Level (n)	**Treatment cost constant** (A_c)
0	0
1	40000
2	60000
3	80000

Under these conditions, the optimisation model was constructed suitably to be solved using Octave's built-in function glpk for solving mixed integer problem.

5.2. Research findings

The following Tables (5.3 - 5.8) represent the initial conditions of at each checkpoint before optimisation was performed as well as the final DO concentration when the feasible solutions were applied.

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Table 5.3.: Initial DO concentrations at check points and water quality standards.

Checkpoint (Load no)	**DO concentration (mg/L)**	**DO concentration standards (mg/L)**
1(1)	6.3037	6.5
2(2)	5.6001	6.5
3(3)	5.7112	6.5
4(-)	6.2175	6.5
5(4)	6.4520	6.5
6(5)	6.8318	6.5
7(6)	6.9171	6.5
8(7)	7.3052	6.5
9(8)	8.5483	6.5
10(9)	8.6213	6.5

The number of checkpoint represented on the table are only 10 instead of eleven because at the first checkpoint which was located at the end of reach AB, no wastewater outfall existed therefore there was no load to treat and optimise. A similar argument was presented for river reach LE, but since the reach depended on loadings from the branched (reach KL) and main (reach DL) stream, the DO concentration was changed by manipulating treatment levels at those streams. Checkpoints 1 - 4 violated the set stream standards, therefore treatment was required. The Figure 5.1 and Figure 5.2 shows the graphs of DO concentration, green drop standards as well as the location of checkpoints. The sub-plots are arranged as follows:

- the top left sub-plot represents the first river reach where the stream begins.
- the top right sub-plot shows the river reach that follows the fist reach.
- The red solid lines represents checkpoints where water quality standards are measured for optimisation.
- GD (Standards) is the green drop standards at the river reach and
- critical, is the minimum allowable critical deficit concentration set for this study.

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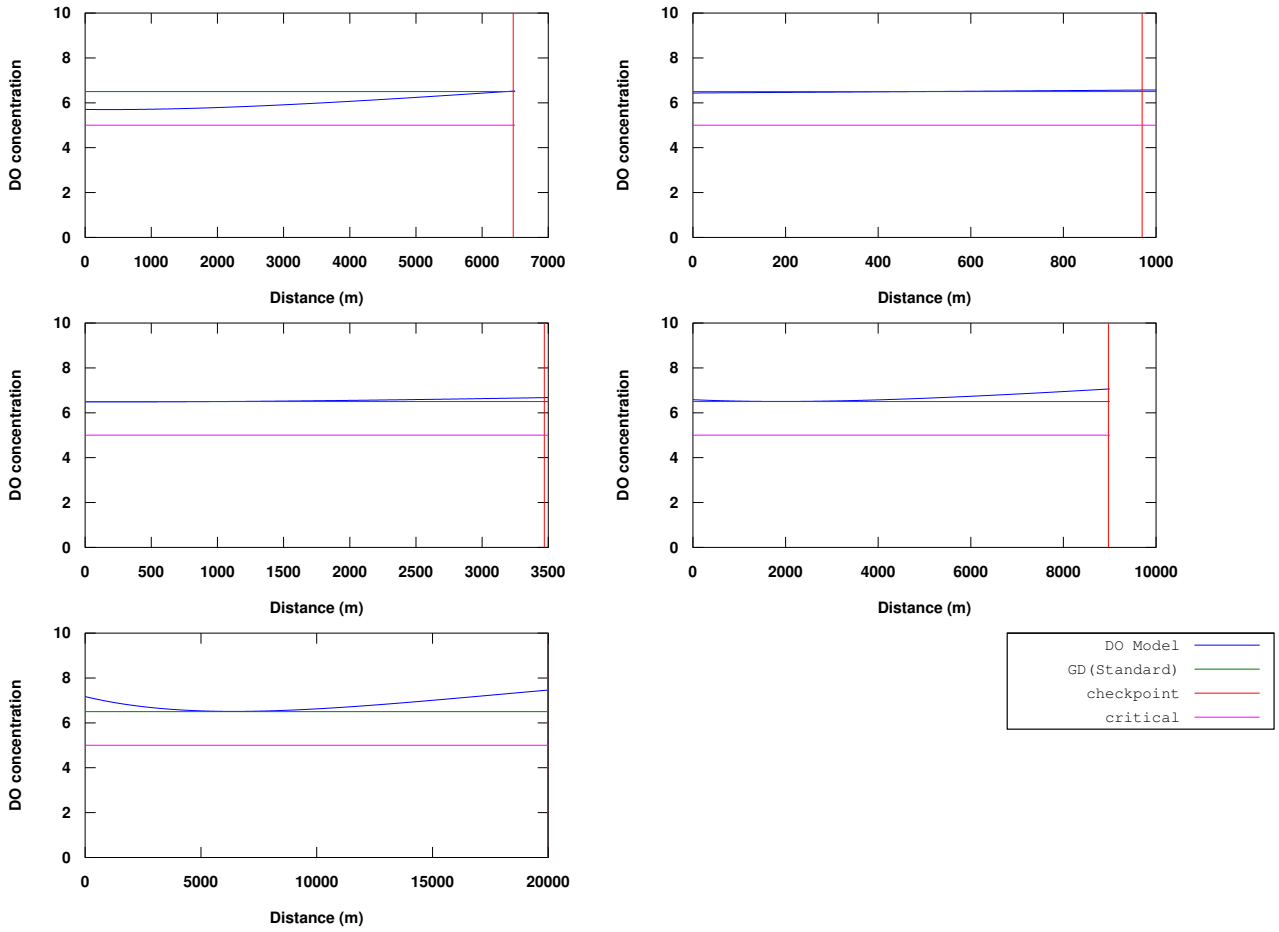

Figure 5.1.: Main Olifants stream optimised to maintain 6.5 mg/L green drop standard.

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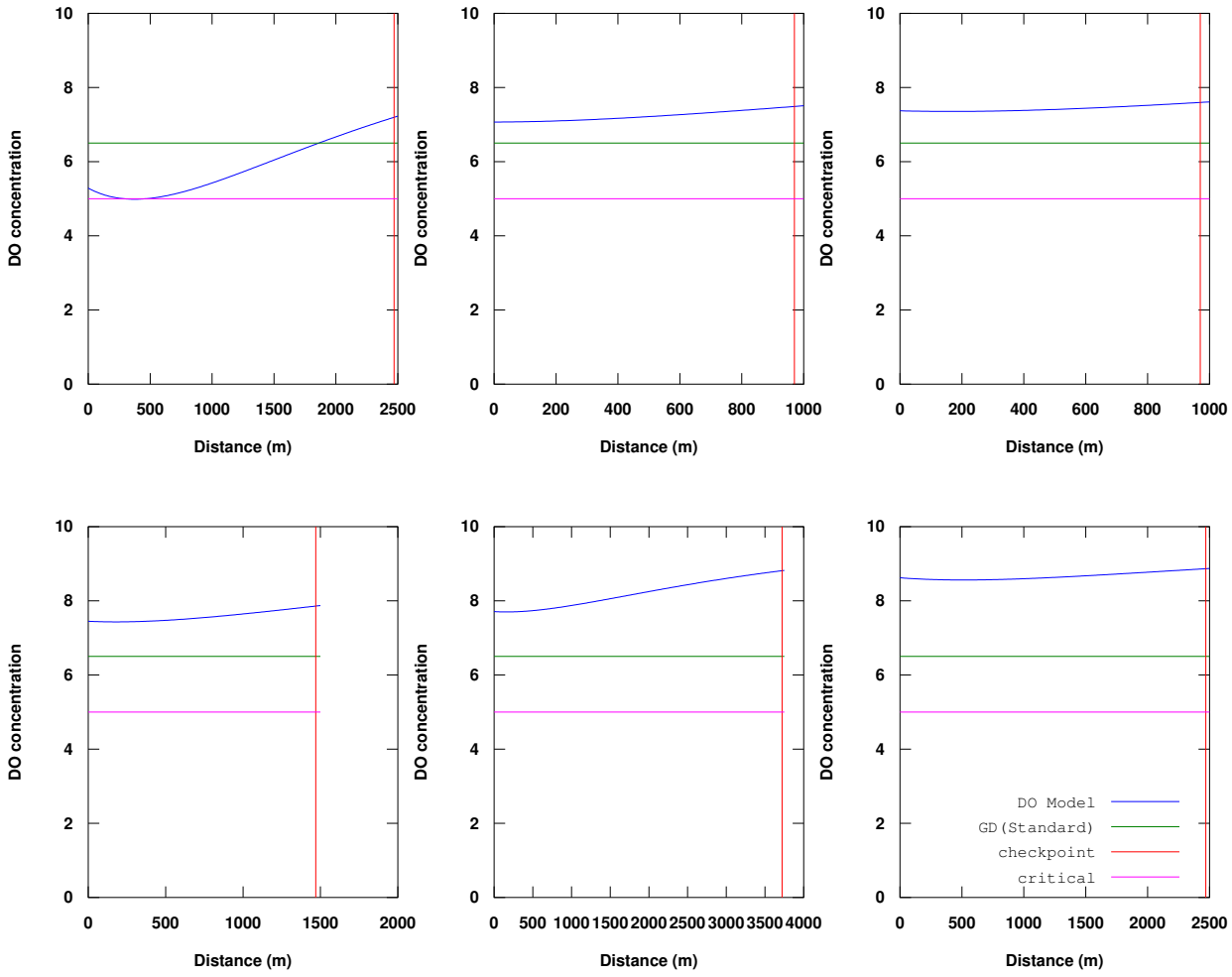

Figure 5.2.: Branched stream optimised to maintain 6.5 mg/L green drop standard.

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The set initial conditions and results from the optimisation model of each system are represented on the tables. The Tables (5.4 - 5.8) show different the feasible solutions obtained after implementing different stringent DO water quality standards at the main and branched stream.

Table 5.4.: Solution obtained with total $Treament\ cost = 244860\ monetary\ units$.

Checkpoint (Load no)	**Treatment level (n)**	**DO concentration (mg/L)**
1(1)	3	6.5722
2(2)	2	6.6783
3(3)	1	7.0624
4(-)	0	7.4646
5(4)	1	7.2275
6(5)	1	7.5073
7(6)	1	7.6117
8(7)	1	7.8726
9(8)	1	8.8206
10(9)	1	8.8720

Table 5.5.: Initial conditions with more stringent DO concentration standards at the branched stream.

Checkpoint (Load no)	**DO concentration (mg/L)**	**DO concentration standards (mg/L)**
1(1)	6.3037	6.5
2(2)	5.6001	6.5
3(3)	5.7112	6.5
4(-)	6.2175	6.5
5(4)	6.4520	7.5
6(5)	6.8318	7.5
7(6)	6.9171	7.5
8(7)	7.3052	7.5
9(8)	8.5483	7.5
10(9)	8.6213	7.5

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Table 5.6.: Solution obtained with total *Treament cost* = 25928 *monetary units*.

Checkpoint (Load no)	**Treatment level (n)**	**DO concentration (mg/L)**
1(1)	3	6.5722
2(2)	3	6.8815
3(3)	1	7.2957
4(-)	0	7.6747
5(4)	2	8.0030
6(5)	1	7.9929
7(6)	1	7.9198
8(7)	1	8.0408
9(8)	1	8.8657
10(9)	1	8.8914

Table 5.7.: Initial conditions with more stringent DO concentration standards at the branched stream.

Checkpoint (Load no)	**DO concentration (mg/L)**	**DO concentration standards (mg/L)**
1(1)	6.3037	6.5
2(2)	5.6001	6.5
3(3)	5.7112	6.5
4(-)	6.2175	6.5
5(4)	6.4520	8.0
6(5)	6.8318	8.0
7(6)	6.9171	8.0
8(7)	7.3052	8.0
9(8)	8.5483	8.0
10(9)	8.6213	8.0

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Table 5.8.: Solution obtained with total *Treament cost* = 284280 *monetary units*.

Checkpoint (Load no)	**Treatment level (n)**	**DO concentration (mg/L)**
1(1)	3	6.5722
2(2)	2	6.6783
3(3)	3	7.5405
4(-)	0	8.0011
5(4)	3	8.7784
6(5)	1	8.4785
7(6)	1	8.2280
8(7)	1	8.2089
9(8)	3	9.1083
10(9)	3	9.2621

These results only considered situations where DO concentrations were above 6.5 mg/L in order to represent the ability of the method to produce feasible solution.

5.3. Analysis and discussions

The method managed to produce feasible solutions for the semi-hypothetical treatment network system described for the Olifants catchment. The aim of the optimisation was to maintain DO concentration at each checkpoint above set standards while minimising treatment cost. The DO model has similar characteristics to the DO sag model in literature, which means that at some point after a wastewater outfall occurs, there exist a point where minimum DO concentration occurs (critical deficit). The aim of the study was to maintain the set standard only at the selected checkpoints, however, we do acknowledge the existence of the critical deficit, hence the minimum water quality standards at the checkpoints were constrained such that at the critical deficit, the concentration should be above 5 mg/L.

When all the DO water quality standards to be maintained were set at 6.5 mg/L at all checkpoints, the code took 1.3492 minutes to produce a feasible solution on Table no 5.4 . The solution suggested that at checkpoints 1,2 and 3, treatment levels 3, 2 and 1 should be applied respectively. And at checkpoints 5-9 only treatment level 1 was suggested for all these checkpoints.At checkpoint 1 the most expensive treatment solution was selected which was expected since the initial concentration was very low compared to the stream standards and at checkpoint 2 a least expensive solution was suggested. Since no violations occurred at treatment levels 5-10, the lowest treatment levels were suggested. The final concentration after the suggested treatment levels were applied was

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above 6.5 mg/L with no notable variables around this value. At lower that 6.5 mg/l DO concentration standard, the method did not produce any feasible solution.

When the DO water quality standards to be maintained above 7.5 mg/L for checkpoints 5-10, the code took 1.3445 minutes to produce a feasible solution on Table no 5.6. The solution suggested that at checkpoints 1,2 and 3, treatment levels 3,2 and 1 should be applied respectively which was expected since the standards remained the same. And at checkpoints 5-10 only treatment level 2, 1, 2, 1, 1 and were suggested. The changes in water quality standard resulted in a change of treatment methods. At higher required standards a more expensive treatment methods was suggested by the model.

A further increase in DO water quality standard to 8 mg/L for checkpoints 5-10 while maintained at 6.5 mg/L at other checkpoint, the code took 1.3367 minutes to produce a feasible solution on Table no 5.8. The solution remained the same for the other checkpoints. And at checkpoints 5-10 only treatment levels 3, 3, 3, 1, 1 and 1 were suggested. The final concentration at after the suggested treatment levels were applied were above the standards minimum concentration.

The behaviour of the feasible solutions produced by the model has shown the independence between checkpoints 1-3, and 5-10 since these streams are only connected to each other at checkpoint 4 where the tributary joins the main Olifants river. If checkpoint 4 did not exist , two independent feasible solution would be expected form the model. Making DO concentration standards more stringent at the confluence point and keeping the rest at 6.5 resulted in a high treatment levels requirements for both streams. Tables 5.9 and 5.10 illustrate this effect when only stringent conditions are applied at checkpoint 4.

Table 5.9.: Initial conditions with more stringent DO concentration standards at checkpoint 5.

Checkpoint (Load no)	**DO concentration (mg/L)**	**DO concentration standards (mg/L)**
1(1)	6.3037	6.5
2(2)	5.6001	6.5
3(3)	5.7112	6.5
4(-)	6.2175	6.5
5(4)	6.4520	8
6(5)	6.8318	6.5
7(6)	6.9171	6.5
8(7)	7.3052	6.5
9(8)	8.5483	6.5
10(9)	8.6213	6.5

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Table 5.10.: Solution obtained with total *Treament cost* = 282160 *monetary units*.

Checkpoint (Load no)	**Treatment level** (n)	**DO concentration (mg/L)**
1(1)	3	6.5722
2(2)	2	6.6783
3(3)	3	7.5405
4(-)	0	8.0001
5(4)	1	7.2275
6(5)	1	7.5073
7(6)	1	7.6117
8(7)	2	8.0368
9(8)	3	9.0781
10(9)	3	9.2493

DO concentration standards could only go as high as 8 mg/L and at 8.5 mg/L no feasible solution existed.

5.4. Chapter summary

The optimisation solutions provided results which could lead to the following sub-conclusions :

- Mixed integer programming has proven useful in obtaining a feasible solution for a semi-hypothetical system at the Olifants river catchment with 9 loads which could implement 3 different treatment levels.
- The methods did not take too long (averaging at 1.35 minutes) to yield a feasible solution for the system.
- If the treatment cost magnitude per treatment level increases with treatment levels, The Olifants river system could be optimised provided the DO concentration standards are not more stringent than 8 mg/L.
- The main stream treatment network has more impact on the maintaining stream standards at a checkpoint where the main Olifants stream was combined with the branched stream.
- All streams meet water quality standards when the feasible treatment network method optimum solution was applied.

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- The method managed to converge to a feasible solution for the stream simulation model selected to represent DO concentration.

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6. The Conclusion

6.1. Summary of findings

The work was structured to solve two main issues. The first of which was developing a stream simulation model for a section at the Olifants river catchment and the second of which was finding an optimum solution for wastewater treatment while maintaining set stream water quality standards. The following findings summarise the study:

- The Olifants river receives many waste loading with most loads not treated to acceptable levels by the available wastewater treatment facilities.
- Many DO oxygen models exits with different complexity and the Streeter-Phelps method was the most basic as well as a well understood model and it was capable of producing a reasonable oxygen sag model for the studied streams.
- Water quality data was difficult to acquire for the Olifants river system and hydrological data proved even more difficult to obtain.
- The stream simulation model was capable of predicting satisfactory Olifants river system behaviour under the given circumstances but failed to properly represent mixing where loading were applied.
- A combined stream simulation and mixed-integer programming model was capable of producing a feasible solution for a treatment system with 9 treatment facilities operating at 3 treatment levels by minimising treatment cost.

6.2. Conclusions

The study produced a 1D steady state, mechanistic river stream simulation model for predicting DO concentration behaviour at the Upper Olifants catchment system. The model was calibrated to fit river stream data available at the Olifants river which resulted

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in a good fit at each water channel. Then the Streeter-Phelps solve equations were used with the re-aeration rate constant and de-oxygenation rate constants as the only model parameters. The final calibrated parameters for each different river stream section were found to be:

- The main Olifants river stream before addition of a branched stream produced a good fit when $k_d = 0.0410$ per day and k_a =0.0804 per day.
- Branched river stream produced a good fit when $k_d = 0.0280$ per day and $k_a = 0.0950$ per.
- Main Olifants river stream after adding the branched stream produced a good fit when $k_d = 0.1720$ per day and $k_a = 0.0902$ per day.

A mixed-integer programming technique for optimising waster water loads treatment by minimising treatment cost while maintaining DO concentration stream standards was applied to the semi-hypothetical treatment network at the Upper Olifants river catchment. The coupled stream simulation-optimisation model produced a feasible optimum solution which suggested the following application of treatment levels for BOD treatment facilities trying to maintain highest possible DO concentration standards:

- Treatment facilities 1, 2 and 3 should implement treatment levels 3, 2 and 3 respectively to maintain a DO concentration of 6.5 mg/L at all the checkpoints on the stream.
- Treatment facilities 4-9 should implement treatment levels 3, 1, 1, 1, 3 and 3 respectively to maintain a DO concentration of 8 mg/L at all the checkpoints on the stream.

The minimum cost for the load treatments network was obtained.

6.3. Recommendations and further research

The Olifants river catchment can be better represented by a more complex model that will consider the un-steady state nature of the system and also take into consideration the other possible sources and sinks of Oxygen. Future work on the model for the Olifants river network should include more that just one contaminant and also need to take into consideration the effect of distributed sources. The coupled stream simulation-optimisation model should consider load streams with varying flows and optimisation

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should be done also based on other contaminants such as ammonia, nitrates, phosphorus as well as Chemical Oxygen Demand.

One of the constraints found in this research was data collection. If this can be improved, it will markedly improve model accuracy and proper techno-economics can be performed. Data required are especially flow, contaminant concentration, river morphology and wastewater loads. To fully optimise the whole system, even at a sub-catchment level, more contaminants will have to be included. The ultimate goal of such a bigger project would then be to consider a larger catchment, which would make the problem several orders of magnitude more complex but with adequate data, can prescribe a solution for optimal WWTP operations at regional level for multiple contaminats.

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Appendix

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Appendix A : Octave 3.2 built-in function *glpk*

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Next: Quadratic Programming, Up: Optimization

25.1 Linear Programming

Octave can solve Linear Programming problems using the `glpk` function. That is, Octave can solve

```
min C'*x
```

subject to the linear constraints A*x = b where x ≥ 0.

The `glpk` function also supports variations of this problem.

— Function File: [*xopt*, *fmin*, *status*, *extra*] = **glpk** (*c, A, b, lb, ub, ctype, vartype, sense, param*)

Solve a linear program using the GNU GLPK library. Given three arguments, `glpk` solves the following standard LP:

```
min C'*x
```

subject to

```
A*x  = b
  x >= 0
```

but may also solve problems of the form

```
[ min | max ] C'*x
```

subject to

```
A*x [ "=" | "<=" | ">=" ] b
  x >= LB
  x <= UB
```

Input arguments:

c
A column array containing the objective function coefficients.

A
A matrix containing the constraints coefficients.

b
A column array containing the right-hand side value for each constraint in the constraint matrix.

lb
An array containing the lower bound on each of the variables. If *lb* is not supplied, the default lower bound for the variables is zero.

ub
An array containing the upper bound on each of the variables. If *ub* is not supplied, the default upper bound is assumed to be infinite.

ctype
An array of characters containing the sense of each constraint in the constraint matrix. Each element of the array may be one of the following values

"F"
A free (unbounded) constraint (the constraint is ignored).

"U"
An inequality constraint with an upper bound (`A(i,:)*x <= b(i)`).

"S"
An equality constraint (`A(i,:)*x = b(i)`).

"L"

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An inequality with a lower bound (`A(i,:)*x >= b(i)`).

"D"
An inequality constraint with both upper and lower bounds (`A(i,:)*x >= -b(i)` *and* (`A(i,:)*x <= b(i)`).

vartype
A column array containing the types of the variables.

"C"
A continuous variable.

"I"
An integer variable.

sense
If *sense* is 1, the problem is a minimization. If *sense* is -1, the problem is a maximization. The default value is 1.

param
A structure containing the following parameters used to define the behavior of solver. Missing elements in the structure take on default values, so you only need to set the elements that you wish to change from the default.

Integer parameters:

`msglev (LPX_K_MSGLEV, default: 1)`
Level of messages output by solver routines:

0
No output.

1
Error messages only.

2
Normal output.

3
Full output (includes informational messages).

`scale (LPX_K_SCALE, default: 1)`
Scaling option:

0
No scaling.

1
Equilibration scaling.

2
Geometric mean scaling, then equilibration scaling.

`dual (LPX_K_DUAL, default: 0)`
Dual simplex option:

0
Do not use the dual simplex.

1
If initial basic solution is dual feasible, use the dual simplex.

`price (LPX_K_PRICE, default: 1)`
Pricing option (for both primal and dual simplex):

0
Textbook pricing.

1

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Steepest edge pricing.

round (LPX_K_ROUND, default: 0)
Solution rounding option:

0
Report all primal and dual values "as is".

1
Replace tiny primal and dual values by exact zero.

itlim (LPX_K_ITLIM, default: -1)
Simplex iterations limit. If this value is positive, it is decreased by one each time when one simplex iteration has been performed, and reaching zero value signals the solver to stop the search. Negative value means no iterations limit.

itcnt (LPX_K_OUTFRQ, default: 200)
Output frequency, in iterations. This parameter specifies how frequently the solver sends information about the solution to the standard output.

branch (LPX_K_BRANCH, default: 2)
Branching heuristic option (for MIP only):

0
Branch on the first variable.

1
Branch on the last variable.

2
Branch using a heuristic by Driebeck and Tomlin.

btrack (LPX_K_BTRACK, default: 2)
Backtracking heuristic option (for MIP only):

0
Depth first search.

1
Breadth first search.

2
Backtrack using the best projection heuristic.

presol (LPX_K_PRESOL, default: 1)
If this flag is set, the routine lpx_simplex solves the problem using the built-in LP presolver. Otherwise the LP presolver is not used.

lpsolver (default: 1)
Select which solver to use. If the problem is a MIP problem this flag will be ignored.

1
Revised simplex method.

2
Interior point method.

save (default: 0)
If this parameter is nonzero, save a copy of the problem in CPLEX LP format to the file `"outpb.lp"`. There is currently no way to change the name of the output file.

Real parameters:

relax (LPX_K_RELAX, default: 0.07)
Relaxation parameter used in the ratio test. If it is zero, the textbook ratio test is used. If it is non-zero (should be positive), Harris' two-pass ratio test is used. In the latter case on the first pass of the ratio test basic variables (in the case of primal simplex) or reduced costs of non-basic variables (in the case of dual simplex) are

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allowed to slightly violate their bounds, but not more than `relax*tolbnd` or `relax*toldj` (thus, relax is a percentage of tolbnd or toldj.

tolbnd (LPX_K_TOLBND, default: 10e-7)
Relative tolerance used to check if the current basic solution is primal feasible. It is not recommended that you change this parameter unless you have a detailed understanding of its purpose.

toldj (LPX_K_TOLDJ, default: 10e-7)
Absolute tolerance used to check if the current basic solution is dual feasible. It is not recommended that you change this parameter unless you have a detailed understanding of its purpose.

tolpiv (LPX_K_TOLPIV, default: 10e-9)
Relative tolerance used to choose eligible pivotal elements of the simplex table. It is not recommended that you change this parameter unless you have a detailed understanding of its purpose.

objll (LPX_K_OBJLL, default: -DBL_MAX)
Lower limit of the objective function. If on the phase II the objective function reaches this limit and continues decreasing, the solver stops the search. This parameter is used in the dual simplex method only.

objul (LPX_K_OBJUL, default: +DBL_MAX)
Upper limit of the objective function. If on the phase II the objective function reaches this limit and continues increasing, the solver stops the search. This parameter is used in the dual simplex only.

tmlim (LPX_K_TMLIM, default: -1.0)
Searching time limit, in seconds. If this value is positive, it is decreased each time when one simplex iteration has been performed by the amount of time spent for the iteration, and reaching zero value signals the solver to stop the search. Negative value means no time limit.

outdly (LPX_K_OUTDLY, default: 0.0)
Output delay, in seconds. This parameter specifies how long the solver should delay sending information about the solution to the standard output. Non-positive value means no delay.

tolint (LPX_K_TOLINT, default: 10e-5)
Relative tolerance used to check if the current basic solution is integer feasible. It is not recommended that you change this parameter unless you have a detailed understanding of its purpose.

tolobj (LPX_K_TOLOBJ, default: 10e-7)
Relative tolerance used to check if the value of the objective function is not better than in the best known integer feasible solution. It is not recommended that you change this parameter unless you have a detailed understanding of its purpose.

Output values:

xopt
The optimizer (the value of the decision variables at the optimum).

fopt
The optimum value of the objective function.

status
Status of the optimization.

Simplex Method:

180 (LPX_OPT)
Solution is optimal.

181 (LPX_FEAS)
Solution is feasible.

182 (LPX_INFEAS)
Solution is infeasible.

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183 (`LPX_NOFEAS`)
Problem has no feasible solution.

184 (`LPX_UNBND`)
Problem has no unbounded solution.

185 (`LPX_UNDEF`)
Solution status is undefined.

Interior Point Method:

150 (`LPX_T_UNDEF`)
The interior point method is undefined.

151 (`LPX_T_OPT`)
The interior point method is optimal.

Mixed Integer Method:

170 (`LPX_I_UNDEF`)
The status is undefined.

171 (`LPX_I_OPT`)
The solution is integer optimal.

172 (`LPX_I_FEAS`)
Solution integer feasible but its optimality has not been proven

173 (`LPX_I_NOFEAS`)
No integer feasible solution.

If an error occurs, *status* will contain one of the following codes:

204 (`LPX_E_FAULT`)
Unable to start the search.

205 (`LPX_E_OBJLL`)
Objective function lower limit reached.

206 (`LPX_E_OBJUL`)
Objective function upper limit reached.

207 (`LPX_E_ITLIM`)
Iterations limit exhausted.

208 (`LPX_E_TMLIM`)
Time limit exhausted.

209 (`LPX_E_NOFEAS`)
No feasible solution.

210 (`LPX_E_INSTAB`)
Numerical instability.

211 (`LPX_E_SING`)
Problems with basis matrix.

212 (`LPX_E_NOCONV`)
No convergence (interior).

213 (`LPX_E_NOPFS`)
No primal feasible solution (LP presolver).

214 (`LPX_E_NODFS`)
No dual feasible solution (LP presolver).

extra
A data structure containing the following fields:

`lambda`
Dual variables.

`redcosts`
Reduced Costs.

`time`
Time (in seconds) used for solving LP/MIP problem.

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mem

Memory (in bytes) used for solving LP/MIP problem (this is not available if the version of GLPK is 4.15 or later).

Example:

```
c = [10, 6, 4]';
A = [ 1, 1, 1;
     10, 4, 5;
      2, 2, 6];
b = [100, 600, 300]';
lb = [0, 0, 0]';
ub = [];
ctype = "UUU";
vartype = "CCC";
s = -1;

param.msglev = 1;
param.itlim = 100;

[xmin, fmin, status, extra] = ...
   glpk (c, A, b, lb, ub, ctype, vartype, s, param);
```


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Appendix B : Stream simulation model Code file and Sub-routine

Input file

input.csv - LibreOffice Calc

File Edit View Insert Format Tools Data Window Help

Liberation Sans 10

	A	B	C	D	E	F	G
1	Reach						
2	Label	Length	Dependency 1	Dependency 2	Dependency 3	Initial concentration DO2	Initial concentration BOD
3	A	6500				5.704528	14
4	B	1000	A				
5	C	3500	B				
6	D	9000	C				
7	E	20000	D	K			
8	F	2500				5.7233314566	13
9	G	1000	F				
10	H	1000	G				
11	I	1500	H				
12	J	3750	I				
13	K	2500	J				
14							
15	Load						
16	Label	Q(m3/s)	Location	Area	D0	BOD	
17	startA	0.245	A	12.2	5.704528	8	
18	startT	0.0138	F	10.8	5.28728329	25	
19	1	0.024	B	11.6	5.51807719	50	
20	2	0.025	C	17.5	5.518	50	
21	3	0.024	D	20	5.408702317	50	
22							
23	5	0.00132	G	13.9	5.408702317	50	
24	6	0.00132	H	1.25	5.818969174	50	
25	7	0.00132	I	11.4	5.421512012	50	
26	8	0.00132	J	9.2	5.526613837	50	
27	9	0.00132	K	13.7	5.74484289	50	
28							
29							
30							
31							
32							
33							
34							
35							
36							
37							
38							

Sheet1

Sheet 1 / 1 Default STD

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Input read code

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```
function [ loadMat, reachTable, root ] = inputRead( fname, delim = "," )

    noY        = 2     # Number of contaminants
    indexDO    = 4
    indexBOD   = 5

#   % Initialize the variable output argument
#     varargout = cell(nargout, 1);
#
#     % Initialize elements of the cell array to nested cell arrays
#     % This syntax is due to {:} producing a comma-separated
#     [ varargout{:}] = deal( cell() );

    fid = fopen(fname, 'r');

    sect = "none";

    lnames = {};
    rnames = {};

    reachTable = [];    % Reaches with indices substituted for names
    loadTable = [];     % Loads with indices substituted for names

    while true
        % Get the current line
        ln = fgetl(fid);

        % Stop if EOF
        if ln == -1
            break;
        endif

        % Split the line string into components and parse numbers
        elems = strsplit( ln, delim );

        % Determine which section of the file are reading
        if strcmpi( elems{1,1}, "reach" )
            disp( "Reading reach section" )
            sect = "reach";  %Skip headings
            ln = fgetl(fid);
            ln = fgetl(fid);
            elems = strsplit( ln, delim );
            cols = columns( elems );
        elseif strcmpi( elems{1,1}, "load" )
            disp( "Reading load section" )
            sect = "load";
            ln = fgetl(fid);    %Skip headings
            ln = fgetl(fid);
            elems = strsplit( ln, delim );
        endif

        % Capture reaches
        if strcmpi( sect, "reach" ) && ( length( elems{1} ) > 0 )
          rnames( end+1 ) = elems{1};
          reachTable{ end+1 } =  elems( 1:cols );
         endif

        % Capture loads
        if strcmpi( sect, "load" ) && ( length( elems{1} ) > 0 )
          lnames( end+1 ) = elems{1};               # Name of load
          loadTable{ end+1 } =  elems( 1:cols );
         endif

    endwhile

    row = length( reachTable );
    col = 1 + length( reachTable{1}( 3:end ) );
    reachMat = zeros( row, col );

    loadMat = zeros( length( loadTable ), 2 + noY );
```

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```
  % Convert reach table to matrix
  for r = 1:length( reachTable )

    dep = zeros( 1, length( reachTable{r}( 3:end ) ) );

    for d = 3:length( reachTable{r} )    % Each dependency

      if length( reachTable{r}(d) ) > 0  % Has value

        % Find the index of the reach with that name and update dep
        for n = 1:length( rnames )

          if strcmpi( rnames{n}, reachTable{r}(d) )
            dep( d-2 ) = n;
            break
          endif

        endfor
      endif
    endfor

    reachMat( r, 1:end ) = [ str2num( reachTable{r}{2} ) dep ];

  endfor

  % Convert load table to matrix
  for l = 1:length( loadTable )

    Q = str2num( loadTable{l}{2} );

    % Find the concentrations of the Y
    Y = [];
    for n = [1:noY] + 4
      Y = [ Y str2num( [ "0" loadTable{l}{n} ] ) ];
    endfor

    L = [];
    % Find the code for its location
    for n = 1:length( rnames )

      if strcmpi( rnames{n}, loadTable{l}(3) )
        L = n;
        break
      endif

    endfor

    loadMat( l, 1:end ) = [ Q L Y ];

  endfor

  % Find the end reach (no reach depends on it) by elimination
  rootI = complement( reachMat(:,2:end)(:), 1:rows( reachMat ) );

  % Populate the fields of the root branch
  root.no = rootI;
  root.Length = reachMat( rootI, 1 );

  root.Load = findLoads( loadMat, rootI );                  % Get root loads
  root.branches = findBranches( reachMat, loadMat, rootI ); % Child branches


% Find all loads at beginning of reach with index r
% ========================================================================%
function [ loads ] = findLoads( loadMat, r )

  loads = [];
  for l = 1:rows( loadMat )
    if loadMat(l,2) == r
```

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```
    loads = [loads; [ loadMat(l,1) loadMat(l,3:end) ]];
  endif
endfor

endfunction


% Find all branches that branch r depends on and return them as a cell array
% ============================================================================%
function [branches] = findBranches( reachMat, loadMat, r )

  branches = {};

  % Read off the appropriate row from reachMat
  for d = reachMat( r, 2:end )

    if d == 0
      continue      % Leave out empty dependency fields
    endif

    branch.no = d;
    branch.Length = reachMat( d, 1 );
    branch.Load = findLoads( loadMat, d );
    branch.branches = findBranches( reachMat, loadMat, d );

    branches = { branches{:}, branch };        % Add branch to list

  endfor

endfunction
```

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Reach concentrations calculations

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```
function [Y_End, Q_End,Y_mat]= ReachCalc(branch,L,levelNo,LoadNo,Y_mat)

 elapsed_time = tic ();

   disp( [ "Branch length: " num2str( branch.Length ) ] )
   disp( [ "Branch no: " num2str( branch.no ) ] )
   disp( repmat( ["*"], 1, 80 ) )


  Q_Start = 0;
  Y_Start.BOD = 0;
  Y_Start.DO2 = 0;

        tL = L(levelNo);

  # Look for a load
  if LoadNo == branch.no

     if ~isempty(branch.Load)
        Y_Load.DO2 = branch.Load(2);
        Y_Load.BOD = branch.Load(3) * (1 - tL);
        Q_Load = branch.Load(1);

        # Mass balance with Q_Start and Y_Start
        Y_Start = MassBalance(Y_Start, Q_Start,Q_Load, Y_Load);
        Q_Start = Q_Start + Q_Load;


    endif
  else
     if ~isempty(branch.Load)
     Y_Load.DO2 = branch.Load(2);
     Y_Load.BOD = branch.Load(3);
     Q_Load = branch.Load(1);

     # Mass balance with Q_Start and Y_Start
      Y_Start = MassBalance(Y_Start, Q_Start,Q_Load, Y_Load);
      Q_Start = Q_Start + Q_Load;

  endif
  endif

#   Determining initial conditions for each branch (Reach)

  for b = 1:length( branch.branches)

#      disp( [ "Going to child branch: " num2str( branch.branches{b}.no ) ] )
#      disp("Branch calaculated")
#
#      branch.branches{b}.Reach_start = [Q Y.DO2 Y.BOD];

     [Y_branch, Q_branch,Y_mat] = ReachCalc( branch.branches{b},L,levelNo,LoadNo,Y_mat);

      # Mass balance with Q_Start and Y_Start and put answer in Q_start, Y_start

      Y_Start = MassBalance(Y_Start,Q_Start, Q_branch, Y_branch);
      Q_Start = Q_Start + Q_branch;

  endfor

  # Now we have Y_start, Q_start

  # Run model, generate Y_End, Q_end

  Reach_start = 0;
  Reach_end = branch.Length;

  if branch.no >= 5

      CA = 133000; %
```

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```
        Length = 10000;
        H_reach = 1.470412;

        Catchment_width = CA/Length;
        A_reach = Catchment_width*H_reach;
    else

        CA = 3256000;%Olifants river catchment area (Wilge river catcment area)
        Length = 40000;
        H_reach = 2.084167;

        Catchment_width = 25;% CA/Length;
        A_reach = Catchment_width*H_reach;
    endif

    T_reach = 20;
    U = Q_Start/A_reach;

    X = [];
    y.DO2=[];
    y.BOD=[];
    for x = Reach_start:10:Reach_end %%Model

        Y_ReachSolver = ReachSolver(x, Y_Start,T_reach,H_reach, U,branch.no);

        X=[X x];
        y.DO2=[y.DO2 Y_ReachSolver.DO2];
        y.BOD=[y.BOD Y_ReachSolver.BOD];


    endfor

#    Preparation of data for plotting

    Real_data = [5.704528 5.7754313045 2.6448 5.49604 5.8019140743 5.7233314566 6.78124 5.85185 3.2888646153
                 5.3629866664 4.3911911112 6.9492000001 5.15808 4.2848363634 5.7848699999 5.388464]';

    X_data = [0 3250 2000 3500 5000 2450 1250 0 5 750 1230  10 10000 17000 18000 18500]';

    Y_End = Y_ReachSolver;
    Q_End = Q_Start;
    Y_mat.BOD(branch.no) = Y_ReachSolver.BOD;
    Y_mat.DO2(branch.no) = Y_ReachSolver.DO2;

    if branch.no == 1

        x_data = X_data(1:2,1);
        y_data = Real_data(1:2,1);

      elseif  branch.no == 4

        x_data = X_data(3:5,1);
        y_data = Real_data(3:5,1);

        elseif  branch.no == 9

        x_data = X_data(10,1);
        y_data = Real_data(10,1);

        elseif  branch.no == 10

        x_data = X_data(9,1);
        y_data = Real_data(9,1);

        elseif  branch.no == 11

        x_data = X_data(6:8,1);
        y_data = Real_data(6:8,1);

        elseif  branch.no == 6
```

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```
        x_data = X_data(11,1);
        y_data = Real_data(11,1);


        elseif  branch.no == 5

        x_data = X_data(12:16,1);
        y_data = Real_data(12:16,1);

        else

        x_data = nan;
        y_data = nan;

   endif

#    hold on
#
# if LoadNo == branch.no
#
#        if branch.no <= 5
#
#              figure(1)
#              subplot(3,2,branch.no)
#              plot   (X,y.DO2,'--4')
#              xlabel ("Distance (m)")
#              ylabel ("DO/BOD concentration (mg/L)"), title ("branch.no")
#              title  ("Reach DO Profile")
#              legend ("DO Model","DO Data","location","outside")
#              legend ("boxon")
#
#        elseif branch.no > 5
#
#            figure (2)
#            subplot(2,3,branch.no - 5)
#            plot   (X,y.DO2,'--4')
#            xlabel ("Distance (m)")
#            ylabel ("DO/BOD concentration (mg/L)")
#            title  ("Reach DO Profile")
#            legend ("DO Model","DO Data","location","outside")
#            legend ("boxon")
#     #
#       endif
#
# else
#
#
 # plots

   if branch.no <= 5

          figure(1)
          subplot(3,2,branch.no)
          plot   (X,y.DO2,X,y.BOD,'--2',x_data,y_data,'*1')
          xlabel ("Distance (m)")
          ylabel ("DO/BOD concentration (mg/L)"), title ("branch.no")
          title  ("Reach DO and BOD Profile")
          legend ("DO Model","BOD","DO Data","location","outside")
          legend ("boxon")

       elseif branch.no > 5

          figure (2)
          subplot(2,3,branch.no - 5)
          plot   (X,y.DO2,X,y.BOD,'--2',x_data,y_data,'*1')
          xlabel ("Distance (m)")
          ylabel ("DO/BOD concentration (mg/L)")
          title  ("Reach DO and BOD Profile")
          legend ("DO Model","BOD","DO Data","location","outside")
```

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```
            legend ("boxon")

        endif
endif
    disp ("reach final values")
    disp( repmat( ["-"], 1, 80 ) )

  print -depsc2 Main_stream.jpg


endfunction
```

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```
function [ init_Y ] = mass_balance( Y, Q_stream, Q_Reach_mat, Y_Reach_mat, Load )

    Y_vector =( Y2vec( Y ) *Q_stream + Y2vec( Y_Reach_mat(Load) ).*Q_Reach_mat(Load))/(Q_stream +
    Q_Reach_mat(Load));

    init_Y = vec2Y( Y_vector );

endfunction

function [ vector ] = Y2vec( Y )
    vector = [ Y.BOD, Y.DO2 ];
endfunction

function [ Y ] = vec2Y( vector )
    Y.BOD = vector(1);
    Y.DO2 = vector(2);
endfunction
```

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```
function Y_value = ReachSolver(x,Y_init,T_reach , H_reach, v,loc)


% K_a=11.507*( ( (S^0.25)/(H^1.25) )*1.016^(T-20));


if loc < 5

    k_d_20 = 0.03785; % deoxygenation rate
    k_a_20 = 1.54042;%5.5773*((U^(0.607))/(H_reach^(1.1689))); %Reaeration rate Bennett and Rathburn

elseif loc == 5

    k_d_20=0.08; % deoxygenation rate
    k_a_20 = 1.54042;%5.5773*((U^(0.607))/(H_reach^(1.1689))); %Reaeration rate Bennett and Rathburn

else
    k_d_20=0.08; % deoxygenation rate
    k_a_20 = 1.4508;%5.5773*((U^(0.607))/(H_reach^(1.1689))); %Reaeration rate Bennett and Rathburn

endif

k_r_20=0.56;

Theta=1.024;

#  Reach Dissolved oxygen rate constants

 U=v*(24*3600);% Convert velocity from (m/s) (to m/day}

k_a_20 = 0.093081;%5.5773*((U^(0.607))/(H_reach^(1.1689))); %Reaeration rate Bennett and Rathburn

k.r=k_r_20*Theta^(T_reach - 20);

k.a=k_a_20*Theta^(T_reach - 20);

k.d=k_d_20*Theta^(T_reach - 20);

#
||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||

DO_saturation = 14.652 - ( 0.41022*T_reach ) + ( 0.007991*(T_reach^2) ) - ( (7.7774*( 10^(-5) ))*(T_reach)
);


# Streeter-Phelps Model Calculation

                    Deficit_0=DO_saturation - Y_init.DO2;

                    L = Y_init.BOD*e^(-(k.d*x)/U);

                    Deficit=Deficit_0*e^(-(k.a*x)/U) + ( (k.d*Y_init.BOD)/(k.a - k.d) )*( (
                    e^(-(k.d*x)/U) ) - ( e^(-(k.a*x)/U) ) );

#||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||

                    DO_2=DO_saturation - Deficit;

                    Y.BOD = L;
                    Y.DO2 = DO_2;


        Y_value = Y;


endfunction
```

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Appendix C : Coupled stream simulation model Code files

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```
clear all
close all

 tic ();

[l,r,R]=inputRead("input.csv",";");

noLevels = 4;
TotalLoads = 11;
L = [0 0.25 0.50 0.75];

Y_checkpoint.BOD = {};
Y_checkpoint.DO2 = {};
Y_mat = {};


for LoadNo = 1:TotalLoads


    for levelNo = 1:noLevels

      [o,p,q] = ReachCalc(R,L,levelNo,LoadNo,Y_mat);

      Y_checkpoint.BOD{levelNo,LoadNo} = [q.BOD]';
      Y_checkpoint.DO2{levelNo,LoadNo} = [q.DO2]';

    endfor

endfor


#       D-matrix
      f=Y_checkpoint.DO2;

    for LoadNo = 1:TotalLoads

#   Y_matrix = [];
        for levelNo = 1:noLevels

            Y_matrix(:,( ((LoadNo-1)*(noLevels)) + levelNo ) ) = f{levelNo,LoadNo}(:);

#               Y_matrix = [Y_matrix y_matrix];

      endfor

endfor

 Dmatrix = Y_matrix(:, [repmat([1:noLevels:(TotalLoads * noLevels)]',1, (noLevels-1))]'(:)) -
          Y_matrix(:, [repmat([2:noLevels], TotalLoads, 1) + repmat([0:(TotalLoads - 1)]' * noLevels, 1,
          (noLevels - 1))]'(:));

 Y0 = f{1,1}(:);
 B0 = [7 7 7 7 7 8.5 8.5 8.5 8.5 8.5 8.5]';
 B = (Y0 - B0);
g = blkdiag([1 1 1],[1 1 1],[1 1 1],[1 1 1],[1 1 1 ],[1 1 1],[1 1 1],[1 1 1],[1 1 1],[1 1 1],[1 1 1]);


#  OPTIMISATION
#            min C'*x
#
#      subject to
#
#           A*x  = b
#             x >= 0
#
#      but may also solve problems of the form
#
#           [ min | max ] C'*x
#
#      subject to
```

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```
#
#           A*x [ "=" | "<=" | ">=" ] b
#             x >= LB
#             x <= UB
# Treatment cost
flows =(3600*24)*[0 0.024 0.024 0.024 0 0.0013 0.0013 0.0013 0.0013 0.0013 0.0013];

Cost= [];

for p =1:length(flows);

    T1 = (40000*flows(p)).^(0.594);
    T2 = (60000*flows(p)).^(0.594);
    T3 = (80000*flows(p)).^(0.594);

    tcost =[T1 T2 T3];

    Cost = [Cost tcost];

endfor

C = Cost';

A =[(Dmatrix);g];
b1 = [0 1 1 1 0 1 1 1 1 1 1]';
b =[B;b1];
lb = []';
ub = [];
ctype = "FUUUUUUUUUUSSSSSSSSSSS";
vartype = "IIIIIIIIIIIIIIIIIIIIIIIIIIIIIII";
s = 1;
param.msglev = 1;
param.itlim = -100;
[xmin, fmin, status, extra] = glpk (C, A, b, lb, ub, ctype, vartype, s, param);

Checkpoint1 = disp('no treatment plant load')
Loadno1 = find(xmin(4:6));
Loadno2 = find(xmin(7:9));
Loadno3 = find(xmin(10:12));
Checkpoint5 = disp('no treatment plant load')
Loadno4 = find(xmin(16:18));
Loadno5 = find(xmin(19:21));
Loadno6 = find(xmin(22:24));
Loadno7 = find(xmin(25:27));
Loadno8 = find(xmin(28:30));
Loadno9 = find(xmin(31:33));

Ymat={};

Optimum_sol=[0 Loadno1 Loadno2 Loadno3 0 Loadno4 Loadno5 Loadno6 Loadno7 Loadno8 Loadno9]

# Checking if stream standards are met

[Y_End, Q_End,Ymat]= ReachCalc_optimum(R,L,Optimum_sol,Ymat)

left = Ymat.DO2'
right = B;
elapsed_time_seconds = toc();
```

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Appendix D: Gauss-Newton Algorithm

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D.1 Model evaluation

The assessment of a model involves the estimation of the parameters in that model which conform to the measured response curves of the system under study. Several formulations exist in literature for this task, among them the maximum likelihood estimation, robust estimation, the Bayesian estimation or least absolute differences estimator, which are applicable depending on the situation. However most methods are based on the least squares criterion, and chief among them is the Gauss-Newton algorithm, which will be discussed in further detail.

D1.1 The Gauss-Newton algorithm

This method belongs to the class of the so-called gradient methods. It is based on a minimization criterion, where the squares of the residuals, i.e. the differences between the observed (experimental) values and the model values are minimized to obtain the best fit of the model to experimental data. The non-linear regression algorithm is based on the following minimization criterion:

$$Q(a,b) = \sum_{i=1}^{n} H(t_i)\left[E(t_i) - E_m(t_i,a,b)\right]^2 = \min \qquad \text{(d1)}$$

where $E(t_i)$ are the experimentally observed or recorded response values, $E_m(t_i,a,b)$ are values determined from the model for the specific values of coefficients a and b and $H(t_i)$ are the statistical weights and n is the number of experimental data. Consequently, the nonlinear equation E_m is expanded around an estimated solution into a Taylor series, which is truncated after the first term. For Equation (d1) this leads to the expansion of E_m about $E(t, a_0, b_0)$ at a_0 and b_0, hence

$$E_m(t_i,a_0,b_0) \approx E_m(t_i,a_0,b_0) + D_1(t_i,a_0,b_0)(a_1 - a_0) + D_2(t_i,a_0,b_0)(b_1 - b_0) \qquad \text{(d2)}$$

where the partial derivatives with respect to the sought after parameters are designated

$$D_1(t_i,a,b) = \frac{\partial E_m(t,a,b)}{\partial a} \quad \text{and} \quad D_2(t_i,a,b) = \frac{\partial E_m(t,a,b)}{\partial b} \qquad \text{(d3)}$$

After substituting m_1 for (a_1 - a_0) and m_2 for (b_1 - b_0) in Eq. (d2), we obtain a minimizing function dependent on two variables m_1 and m_2

$$Q(a,b) = \sum_{i=1}^{n} H(t_i)\left[E(t_i) - E_m(t_i,a_0,b_0) - D_1(t_i,a_0,b_0)m_1 - D_2(t_i,a_0,b_0)m_2\right]^2 \qquad \text{(d4)}$$

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The minimizing principle hinges on the reality that the partial derivative of $Q(a,b)$ with respect to each of these two new variables must be zero at the minimum i.e. for the initial approximations:

$$\frac{\partial Q(a,b)}{\partial m_1} = 0 = \sum_i H(t_i) D_1(t_i, a_0, b_0) E(t_i) - \sum_i H(t_i) D_1(t_i, a_0, b_0) E_m(t_i, a_0, b_0) - m_1 \sum_i H(t_i) [D_1(t_i, a_0, b_0)]^2 - m_2 \sum_i H(t_i) D_1(t_i, a_0, b_0) D_2(t_i, a_0, b_0) \quad \text{(d5)}$$

$$\frac{\partial Q(a,b)}{\partial m_2} = 0 = \sum_i H(t_i) D_2(t_i, a_0, b_0) E(t_i) - \sum_i H(t_i) D_2(t_i, a_0, b_0) E_m(t_i, a_0, b_0) - m_2 \sum_i H(t_i) [D_2(t_i, a_0, b_0)]^2 - m_1 \sum_i H(t_i) D_1(t_i, a_0, b_0) D_2(t_i, a_0, b_0) \quad \text{(d6)}$$

This is in essence a system of two simultaneous equations, whence after solving for the two variables m_1 and m_2, we obtain new approximations for the sought after parameters a and b from the relation

$$a_{k+1} = a_k + m_{1k} \quad \text{(d7)}$$

$$b_{k+1} = b_k + m_{2k} \quad \text{(d8)}$$

written here for the k^{th} iteration. The new approximations of m_1 and m_2 are then again fed into the system of Eqs (d5) and (d6) and the process is repeated until a preconditioned convergence criterion or criteria are fulfilled, i.e. until $m_1 \leq \alpha$ or $m_2 \leq \beta$ – where α and β are relatively small increments – whereupon the iteration stops and the final, optimized values of the parameters are retained.

Iterative solution of equations (d5) and (d6) can give rise to problems, one of them being the initial guesses a_0 and b_0. Under certain conditions, the selection of a_0 and b_0 leads to a neighboring minimum, or is so unfavorable that iteration does not lead to convergence. The first of these problems requires a more precise investigation of the sum of the squares of the deviations or repetition of the calculation with various initial values of a_0 and b_0. In order to avoid divergence of the iterative method, choice of the parameter λ_k <1 can be made such that the value $\lambda_k m_{jk}$ is acceptable.

The sum of the squares of the deviations can contain terms of differing orders of magnitude, which lead to very different gradients in the direction of the individual parameters. In such cases scaling of the parameters is necessary, whereby the individual components in equation (d7) and (d8) are brought to the same order of magnitude by linear transformation.

The minimizing algorithm employed is outlined below

1. Approximation of the initial value of a, b

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2. Determination of m_{1k} and m_{2k} for the k^{th} iteration
3. Choice of the parameter λ_k such that the value $\lambda_k m_{1k}$ and $\lambda_k m_{2k}$ are acceptable i.e. such that for

   $a_{k+1} = a_k + \lambda_k m_{1k}$ and $b_{k+1} = b_k + \lambda_k m_{2k}$

   the condition:

   $Q(a_{k+1}, b_{k+1}) < Q(a_k, b_k)$

   must be fulfilled
4. Criteria test and end of algorithm. If the criteria are fulfilled, the sought after values are $a = a_{k+1}$ and $b = b_{k+1}$, if not then the algorithm repeats from step 2.

The derivations with respect to the parameters are usually carried out numerically for convenience, if the main function is too complex. These are of course subject to error, even though they can be neglected in most cases; however, analytical derivations are always more precise and herein lies the advantage of the sequence leading to the analytical derivations presented in section 2.4, which can be applied conveniently to Eq. (d3) and further substituted into Eqs. (d5) and (d6).

D.1.2 Assessment of estimated parameter values

Although we are chiefly interested in estimated parameters of the model, it is essential to evaluate the quality of the model too. A primary indication is provided by the final residual function $Q(a,b)$ after the regression process or the mean square of the residuals s_r^2, which is given by dividing the sum of the squares of the residuals by the number of degrees of freedom, these are equal to the number of measured observations minus the number of conditions constraining the minimization, in our case it is the number of parameters, which is equal to two, i.e.

$$s_r^2 = \frac{Q(a,b)}{n-2} \tag{d9}$$

This quantity can be used as an estimate of the variance, i.e. mean square deviations from the regression curve. In addition to the variances, which are a measure of the scatter of the estimated values, the asymptotic errors and confidence limits of the estimated values are used and can be calculated from the variances for further assessment.

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D1.2.1 Parameter errors

This is based on the computation of the covariance matrix of the parameters, which is obtained from the Jacobian of the model function after termination of the regression. The covariances of the parameters are then estimated from the product of the covariance matrix and the variances, i.e. mean square of the residuals. The asymptotic errors of the estimated values of parameters are then estimated from the square roots of the diagonals of the covariances i.e.

$$\boldsymbol{Cov} = \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \sigma^2_{\boldsymbol{E_m}} \tag{d10}$$

where $\boldsymbol{X}$ is the Jacobian

$$\boldsymbol{X} = \left(\frac{\partial \boldsymbol{E_m}}{\partial a} \quad \frac{\partial \boldsymbol{E_m}}{\partial b} \right) \tag{d11}$$

$\boldsymbol{E_m}$ is a column vector and $\sigma^2_{\boldsymbol{E_m}}$ is the variance for the model, which can be estimated by Eq. (2.3.9). In our case ***Cov*** results in a 2×2 matrix and the square roots of its diagonals represent an estimate of the asymptotic errors for the two parameters.

D.1.2.2 Confidence intervals

The *t*-distribution is used to calculate confidence intervals, i.e. the interval, within which we believe, with a stated confidence, that the unknown parameter lies. This can be expressed as

$$a \pm t^{n-2}_{\alpha/2} s_a \quad \text{and} \quad b \pm t^{n-2}_{\alpha/2} s_b \tag{d12}$$

where s_a and s_b are the standard errors and $t^{n-2}_{\alpha/2}$ is the value of the *t* distribution with *n*-2 degrees of freedom exceeded by an area of $\alpha/2$, which implies that 100(1-α)% of the sample averages from a normal distribution would fall into this interval. In our case, because *n* is very large, for a 95% confidence interval, we get from the *t* distribution $t^{\infty}_{0.025} = 1.96$.

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