DEVELOPMENT OF A UNIVERSAL WATER QUALITY INDEX AND WATER QUALITY VARIABILITY MODEL FOR SOUTH AFRICAN RIVER CATCHMENTS

By

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DECLARATION 1 - PLAGIARISM

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(1) The research reported in this thesis, except where otherwise indicated, is my original research;

(2) This thesis has not been submitted to the University of KwaZulu-Natal or other tertiary institution for the purpose of obtaining an academic qualification, whether by myself or any other party;

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As the candidate's Supervisor, I agree/do not agree to the submission of this thesis.

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Professor Muthukrishnavellaisamy Kumarasamy

DECLARATION 2 - PUBLICATIONS

The submission of the Doctor of Philosophy in Engineering Degree is by Monograph Thesis, but considering the number of publications emerging from this doctoral work, it has become necessary to include the list of publications. The research articles contained herein, are original work resulting from the development of a universal water quality index and water quality variability model for South African river catchments. All the articles are published in peer-reviewed journals, and the publication list is as follows:

(a) **Publication 1:**
Talent Diotrefe Banda and Muthukrishna Vellaisamy Kumarasamy, (2020). Development of Water Quality Indices (WQIs): A Review. *Polish Journal of Environmental Studies,* Volume 29, Issue 3, Pages 2011-2021. DOI: https://doi.org/10.15244/pjoes/110526. Submitted 10 February 2019, Accepted 08 July 2019, Published 23 January 2020.

(b) **Publication 2:**
Talent Diotrefe Banda and Muthukrishnavellaisamy Kumarasamy, (2020). Aggregation Techniques Applied in Water Quality Indices (WQIs). *Pollution Research,* Volume 39, Issue 2, Pages 400-412. Submitted 08 February 2020, Accepted 25 March 2020, Published 01 June 2020

(c) **Publication 3:**
Talent Diotrefe Banda and Muthukrishnavellaisamy Kumarasamy, (2020). A Review of the Existing Water Quality Indices (WQIs). *Pollution Research,* Volume 39, Issue 2, Pages 489-514. Submitted 18 February 2020, Accepted 30 March 2020, Published 01 June 2020.

(d) **Publication 4:**
Talent Diotrefe Banda and Muthukrishnavellaisamy Kumarasamy, (2020). Application of Multivariate Statistical Analysis in the Development of a Surrogate Water Quality Index (WQI) for South African Watersheds. *Water,* Volume 12, Issue 6, Page 1584. DOI: https://doi.org/10.3390/w12061584. Submitted 30 April 2020, Accepted 29 May 2020, Published 02 June 2020.

(e) **Publication 5:**
Talent Diotrefe Banda and Muthukrishnavellaisamy Kumarasamy, (2020). Development of a Universal Water Quality Index (UWQI) for South African River Catchments. *Water,*

Volume 12, Issue 6, Page 1534. DOI: https://doi.org/10.3390/w12061534. Submitted 30 April 2020, Accepted 26 May 2020, Published 28 May 2020.

(f) **Publication 6:**
Talent Diotrefe Banda and Muthukrishnavellaisamy Kumarasamy, (2020). Determination of Significant Water Quality Variables, Relative Weight Coefficients and Sub-Indices for Universal Water Quality Index (UWQI) Developed to Evaluate Surface Water Quality of South African River Basins. Publication in preparation.

(g) **Publication 7:**
Talent Diotrefe Banda and Muthukrishnavellaisamy Kumarasamy, (2020). Artificial Neural Network (ANN) Based Water Quality Index (WQI) for Assessing Spatio-Temporal Trends in Surface Water Quality – A Case Study of Umgeni, Umdloti, Nungwane and Umzinto River Catchments in KwaZulu-Natal, South Africa. Publication in preparation.

(h) **Publication 8:**
Talent Diotrefe Banda and Muthukrishnavellaisamy Kumarasamy, (2020). A Hybrid Water Quality Variability Model (WQVM) for Evaluating Surface Water Quality of South African River Catchments. Publication in preparation.

Signed: ______________________________

Talent Diotrefe Banda

DEDICATION

This study is dedicated to my late mother, Stella Kaseke. Your departure at such an early age caused indescribable grief, and it left a lasting imprint in my soul. But the consolation is that it eventually moulded my character to be the person I am today. I understand the meaning of life and believe that I had to experience what I did, just to become a better person. The principles you taught me always contribute towards every act, thought and decision I make. You are forever loved and always remembered with affection, rest peacefully.

REFLECTIONS

"There is something about losing a mother that is permanent and inexpressible – a wound that will never quite heal."

Susan Wiggs

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Lastly, I would like to thank my family and colleagues for instituting a hardworking and passionate attitude. Undoubtedly, your encouragement and sacrifices are priceless. Your continued patience and boundless support incited me to always struggle towards the pursuit of my academic goals, and your prayers have sustained me thus far. The sense of achievement is overwhelming, and I owe it to you; once again, thank you.

ABSTRACT

The assessment of water quality has turned to be an ultimate goal for most water resource and environmental stakeholders, with ever-increasing global consideration. Against this background, various tools and water quality guidelines have been adopted worldwide to govern water quality deterioration and institute the sustainable use of water resources. Water quality impairment is mainly associated with a sudden increase in population and related proceedings, which include urbanisation, industrialisation and agricultural production, among others. Such socio-economic activities accelerate water contamination and cause pollution stress to the aquatic environment. Scientifically based water quality index (WQI) models are then essentially important to measure the degree of contamination and advise whether specific water resources require restoration and to what extent. Such comprehensive evaluations reflect the integrated impact of adverse parameter concentrations and assist in the prioritisation of remedial actions.

WQI is a simple, yet intelligible and systematically structured, indexing scale beneficial for communicating water quality data to non-technical individuals, policymakers and, more importantly, water scientists. The index number is typically presented as a relative scale ranging from zero (worst quality) to one hundred (best quality). WQIs simplify and streamline what would otherwise be impractical assignments, thus justifying the efforts of developing water quality indices (WQIs). Generally, WQIs are not designed for broad applications; they are customarily developed for specific watersheds and or regions unless different basins share similar attributes and test a comparable range of water quality parameters. Their design and formation is governed by their intended use together with the degree of accuracy required, and such technicalities ultimately define the application boundaries of WQIs. Such an academic gap is perhaps the most demanding scientific need; that is, to establish universally acceptable water quality indices, which can function in most, if not all the catchments in South Africa. In cognisance of such, the study suggests four water quality models that are not limited to specific application boundaries, and such contribution is significant, not only to the authors but to the entire nation.

The first model, namely the universal water quality index (UWQI) developed based on conventional techniques using unequal weight coefficients and weighted arithmetic sum method. Model input parameters, relative weight coefficients and sub-index rating curves are established through an expert opinion by means of participatory based Rand Corporation's Delphi Technique and extracts from literature. The second developed artificial intelligence (AI) in the form of artificial neural network (ANN) has three neuron layers parallel-distributed to accommodate feedforward sequence and backpropagation. The multi-layer perceptron model architecture includes nineteen highly interconnected neuro-nodes and seventy weighted synapses operating in

a feedforward manner, from left to right. The study applied the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm to perform backpropagation training and optimising channel weights. The three-layered feedforward neural network indicated an increased performance registering an overall correlation coefficient of 0.985 and specific performance ratings of 0.987, 0.992 and 0.977 for training, testing and validation, respectively. The AI-based demonstrated an average target to an output error margin of ±0.242. Pointwise sensitivity analysis authenticated the robustness and computational aptitude of the suggested artificial neural network model. Both UWQI and ANN model functions with thirteen explanatory variables which are NH_3, Ca, Cl, Chl-a, EC, F, $CaCO_3$, Mg, Mn, NO_3, pH, SO_4 and turbidity (NTU).

The third model entitled surrogate WQI works with four proxy water quality parameters comprising of chlorophyll-a, electrical conductivity, pondus Hydrogenium and turbidity. The proxy linear-based mathematical model is an abridged version of an outright WQI, purposefully established to substitute the UWQI and ANN model, thereby providing provisional index scores in the absence of extensive datasets. Water quality indices (WQIs) are customarily associated with massive data input demand, making them more rigorous and bulky. Such burdensome attributes are too taxing, time-consuming, and command a significant amount of resources to implement. Which discourages their application and directly influences water resource monitoring—making it increasingly indispensable to concentrate on developing compatible, more straightforward, and less-demanding WQI tools, but with equally matching computational ability. Surrogate models are the best fitting, conforming to the prescribed features and scope.

Consequently, the study proposes an alternative water quality monitoring tool requiring fewer inputs, minimal effort, and marginal resources to function. Multivariate statistical techniques which include principal component analysis (PCA), hierarchical clustering analysis (HCA) and multiple linear regression (MLR) are applied primarily to identify four proxy variables and define relevant regression coefficients. Resulting in Chl-a, EC, pH and turbidity being the final four proxy variables retained. The selected input parameters are conformable with remote monitoring systems; which is a vital feature allowing the surrogate index model to be considered for remote monitoring programs.

The fourth and final model suggested is a software-based water quality variability model (WQVM) established by integrating three distinctive water quality indices (WQIs) emerging from this study. The three WQIs are founded on different indexing methods, and they are documented as (a) universal water quality index, (b) artificial neural network, and (c) surrogate water quality index. Usually, most WQIs are presented as arithmetic formulas that are somewhat challenging to comprehend and apply in the real world. Therefore, the study attempts to address such research tendencies and set forth an excel-based hybrid water quality monitoring tool applicable at a national level. The WQVM enables the assessment of multiple water quality parameters, thereby solving practical water science problems. The proposed WQVM is earmarked for improving and promoting water quality monitoring programs, by providing a simple, convenient and user-friendly monitoring toolkit. Indeed, putting forward the WQVM has an increasing impact on water resource evaluation and optimising decision making amongst water scientists and professionals.

Suggested models yield one-digit index values rending from zero to one hundred, where zero denotes poor water quality, and one hundred represents excellent water quality. Furthermore, the index scores are classified using a categorisation schema having five classes. Whereby "class one" with a possible maximum score of hundred designate the highest degree of purity and vice versa, "class five" signifies water quality of the lowest degree with index scores nearing or equal to zero.

The WQIs and WQVM are developed and tested using water quality data from Umgeni Water Board (UWB) in KwaZulu-Natal Province, South Africa. From the original dataset, the current study retained 638 samples with 7,741 tests measured monthly over four years. The water quality records are from six sampling stations located within four different river basins identified as Umgeni, Umdloti, Nungwane and Umzinto/uMuziwezinto River catchments. The data samples are further curtailed to satisfy statistical requirements of each particular WQI model.

All four models are considered robust and scientifically stable, with minor divergence from the ideal values. Better off, the prediction pattern matches the exemplary graph having comparable index scores and identical classification ranks, which signifies their readiness to appraise water quality status across South African watersheds. The established models symbolise a significant milestone with the prospects of promoting water resource monitoring and assisting in capturing spatial and temporal changes within river systems. The study intends to substantiate the methods used and document results achieved.

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THESIS LAYOUT

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The preliminary section of the thesis documenting necessary study information that precedes the actual research work. These includes, (i) cover page, (ii) declaration, (iii) list of publications, (iv) dedication, (v) acknowledgements, and (vi) abstract, among others.

Chapter One: Introduction

This chapter describes the doctoral work and outlines the significance of the research. Specific study objectives, together with milestones achieved, are also contained in Chapter One. Research hypothesis forms part of chapter one, and this section delivers a brief explanation of methods used to achieve the study objectives.

Chapter Two: Literature review

Numerous existing water quality indices (WQIs) are discussed under literature review. The chapter focuses on the formation methods, selection of explanatory variables, application boundaries and even more importantly, the flaws in water quality science. Chapter Two assisted in identifying research objectives and provide direction in an attempt to envelop such research gaps.

Chapter Three: Methodology

Methods employed to develop the four water quality models are presented under Chapter Three, and the section intends to substantiate the techniques applied to achieve specific study objectives.

Chapter Four: Area of study

Chapter Four documents information relating to the study area and the various watersheds considered for doctoral work. The chapter outlines the importance of the research and socio-economic activities within the region.

Chapter Five: Results and discussion

This chapter presents the research results and discusses the processes followed during the development of three distinct water quality indices (WQIs), an index categorisation schema and an integrated water quality variability model (WQVM).

Chapter Six: Conclusion and recommendations

Chapter Six is the final chapter of the thesis, which provides closing remarks, conclusions drawn from the research and recommendations towards future studies.

Bibliography (References):

Listing of references cited throughout the thesis and the bibliography follows an alphabetical order in respect of the authors' surnames.

Annexures:

The last part of the booklet containing additional material and information relevant to the study and the thesis attachments are numbered for ease of reference.

CHAPTER 1

1. INTRODUCTION

1.1 Overview

The current study involves the establishment of various water quality monitoring tools functioning with predetermined explanatory physicochemical variables. Such vital scientific models are earmarked for assessing spatial and temporal water quality trends within the South African river catchments. Against this backdrop, Chapter One serves as an insight highlighting the background, purpose and significance of the doctoral work. Reasons justifying the inclusion of four different study regions are also discussed in this chapter. Lastly, Chapter One defines the study objectives, limitations and assumptions drawn to accomplish the primary purposes of the current study.

1.2 Background

Various physical, chemical and biological variables are considered detrimental to the aquatic environment, mainly if contained in excessive amounts. Such parameters originate from anthropogenic and natural sources. Though some might be essential in the aquatic ecosystem, however, they might pose a serious risk if present in excessive concentrations. Eventually, monitoring and assessment of water resources become mandatory to trace the levels and effects of such physio-chemical and biological parameters. And the standard practical method is through the application of water quality indices (WQIs). This prompt the need to further exploit the use of WQIs and continuously modify such essential tools, to become better, simpler and more appropriate towards water resource management needs; which needs are dynamic and forever changing (Banda and Kumarasamy, 2020e).

Water quality indices (WQIs) are necessary for simplifying the reporting of complex and technical water quality information. They are scientifically based communication models that are capable of converting multi-variable water quality data to produce a single unitless digit score that describes overall water quality. Deducing water quality into an index score is then crucial for providing a structured platform to evaluate and compare the quality of various water resources (Sarkar and Abbasi, 2006, Poonam et al., 2015, Banda and Kumarasamy, 2020e). Water quality indices are not aimed at replacing detailed water quality analysis. Instead, they are tools aimed at providing a quick guide to assist water quality experts, policymakers and the public, by communicating water quality data in a more consistent and on-going manner (Poonam et al., 2015, Luzati and Jaupaj, 2016, Banda and Kumarasamy, 2020e).

Water quality index (WQI) is a unique technique employed to describe water quality that has proven to be an effective method to evaluate spatial and temporal water changes in South African river catchments and the world at large. Water quality indices (WQIs) consolidate a large amount of complex water quality data and generates a single value in a simple and reproducible manner. Which then explains the successful application of WQIs over the past years, because they help to deduce a large amount of scientific data and describe water quality status to the public and policymakers, using a simple dimensionless score. Even non-technical stakeholders will understand the water quality rating scores, mostly when disseminated to classes presented as "poor," "fair," "medium," "good," and "excellent" (Banda and Kumarasamy, 2020d).

Water quality indices (WQIs) have been recognised as significant environmental performance indicators, and the concept of expressing water quality using a numerical value has been easily appreciated, leading to the suggestion of various indexing models. A considerable number of indices are developed for multiple applications, but mainly they are region-specific; thus limiting their implementation to drainage basins influencing their designs. Of lately, various countries have embarked on the process of developing composite universal indices to evaluate and describe the state of their domestic water. Which is, perhaps, the most demanding scientific need; that is, the development of a unified water quality index, that can work for most, if not all the watersheds of a given country (Banda and Kumarasamy, 2020d). An index that is not limited to certain application boundaries, and thus the aim of this current study.

The current study focuses on developing nationally acceptable water resource monitoring tools that are applicable across all the watersheds in South Africa. Such a significant contribution facilitates water resource monitoring, thereby assisting in evaluating spatial and temporal trends in surface water. Accordingly, four water quality models are proposed, and these are:

(a) Universal water quality index (UWQI) developed using conventional methods involving parameter weights, sub-index functions and an aggregation formula;

(b) Artificial neural networks (ANN) model based on an artificial intelligence algorithm that simulates the functionality of human brains;

(c) Surrogate water quality index (proxy WQI) established through the application of multivariate statistical techniques. The proxy WQI functions as an abridged version of the outright UWQI and operates with limited input parameters; and

(d) Water quality variability model (WQVM) that combine the UWQI, ANN model and proxy WQI to become a software-based and practically-oriented monitoring tool.

Furthermore, the study suggested an index classification system aimed at interpreting WQI scores resulting from the newly developed water quality monitoring tools. The subsequent sections share an insight into the recommended water quality monitoring tools.

1.3 Establishment of water quality monitoring tools

1.3.1 Universal water quality index (UWQI) model

Water quality index (WQI) is the most popular method of exhibiting water quality of surface water bodies. WQI models are better known for delivering a comprehensive and explicit representation of water contamination for both surface water basins and groundwater reservoirs. The appraisal concept is concise and more straightforward, leading to wide acceptance across the water science community (Tripathi and Singal, 2019b). WQI provides a single numeric value that expresses the status of water quality through the integration of multiple microbiological and physicochemical parameters (Tripathi and Singal, 2019b, Paca et al., 2019). Water quality index scores are classified using a diverse array of rating scales; however, the frequently used grading system ranges from zero (bad quality) to hundred (excellent quality) (Boyacioğlu, 2007, Carvalho et al., 2011, Banda, 2015, Paca et al., 2019, Banda and Kumarasamy, 2020c).

WQI scores are dimensionless, and can further be categorised using descriptive ranks associated with terms like, “poor,” “marginal,” “fair,” “good” and “excellent” (Boyacioğlu, 2007, Carvalho et al., 2011, Banda, 2015, Unda-Calvo et al., 2019, Banda and Kumarasamy, 2020e). Water quality indices (WQIs) are typically used by water authorities, water scientists, policymakers and the general public for various activities. These include decision-making, delineating spatial and temporal trends, tracing contamination sources, appraising regulatory guidelines and environmental policies, and most importantly for suggesting future recommendations (Poonam et al., 2015, Unda-Calvo et al., 2019, Banda and Kumarasamy, 2020c).

The main objective of WQIs is to convert multiple parameter data into information that is understandable by both technical and non-technical personnel. The ability of WQIs to synthesis complex scientific data into simple and easily understood formats; which makes them the most fundamental and indispensable elements of water quality monitoring agenda. Hence, they are universally acknowledged as “lifeline” for water quality studies, and their development continues as an on-going affair (Banda and Kumarasamy, 2020e). Despite their range of application and variety of WQIs developed this far; there is still no definite and commonly acceptable methodology for setting water quality indices (Unda-Calvo et al., 2019, Sutadian et al., 2016).

Instead, numerous techniques and approaches exist in WQIs formation; nevertheless, the conventionally employed method involves, (a) determination of relevant water quality variables, (b) establishment of sub-indices, (c) generating significant weightage coefficients, (d) aggregation of sub-indices, and lastly (e) ascribing a water classification schema (Abbasi and Abbasi, 2012b, Tyagi et al., 2013, Poonam et al., 2015, Paun et al., 2016, Banda and Kumarasamy, 2020a, Banda and Kumarasamy, 2020e). Each step has alternative methods to consider, which becomes extremely important to decide the most suitable of each scenario. Notwithstanding having technical knowledge of WQIs, the developer should apply due diligence, avoid subjective judgements and biasness in the process of establishing WQIs. Otherwise, the WQI will inherit abnormalities and be considered dysfunctional (Banda and Kumarasamy, 2020e).

For the current study, an index model for water pollution control and river basin planning functions has been established using expert opinion in the form of participatory based Rand Corporation's Delphi Technique and extracts from existing literature. The process yielded thirteen input variables, namely NH_3, Ca, Cl, Chl-a, EC, F, $CaCO_3$, Mg, Mn, NO_3, pH, SO_4 and Turb (NTU). Additional to the parameter selection, the study also applied expert opinion to develop significant ratings and parameter weightage coefficients. The universal water quality index (UWQI) model is an increasing scale index founded on weighted arithmetic sum method with resultant values ranging from zero (very bad quality) to hundred (good quality). The overall classification is centred on five categories, with Class 1 rank denoting "good water quality" and Class 5 rank representing "very bad water quality" (Banda and Kumarasamy, 2020c).

Following the review by Banda and Kumarasamy (2020e), it has been noted that most WQIs are designed for a particular region and source-specific, thus creating a gap and ample scope to develop a universally acceptable WQI. However, it is a demanding task and extremely difficult to formulate a water quality model that is globally acceptable; hence the current studies only focus on national boundaries; that is, a model only applicable to South African river catchments. Though seemingly problematic to deal with in prospect; it is pertinent and recommended that water quality experts embark on developing a unified model that can be utilised across the globe. But the immediate mission is to develop nationally acceptable water quality indices and break the barrier of region-specific models (Banda and Kumarasamy, 2020e). And this study attempts to break such barriers, through the development of a universal index that applies to most river catchments in South Africa. Thereby promoting a standardised way of monitoring and comparing water quality of various watersheds at a national level, which eventually assists in the prioritisation of water resources across all the nine provinces in South Africa (Banda and Kumarasamy, 2020c).

Umgeni Water Board (UWB) provided water quality dataset used to test the UWQI. The data is from six sampling stations located in four different catchments under the jurisdiction of Pangola-Mtamvuma Water Management Area (WMA) in KwaZulu-Natal Province, South Africa. The four watershed regions are Umgeni, Umdloti, Nungwane and Umzinto/Umuziwezinto River catchments. The UWQI is earmarked for national application, but it is far-reaching and beyond the scope of the study to test the model against data from all the 148 catchments regions in South Africa. Nevertheless, the four catchments used are adequate to ascertain the functionality of the model and the process is a step towards the ultimate goal of testing the model against most, if not all the catchment areas in South Africa.

The model responded steadily to the variation in parameter values and managed to indicate spatial and temporal changes in water quality for the four Catchment areas considered for the study. Of great importance, the UWQI has been formed autonomously without being linked to neither a particular dataset nor specific region. The methods used are exclusively independent of such associations, and UWB dataset is entirely for testing purposes, which task can be performed using any other available data.

1.3.2 Artificial neural network (ANN) model

Artificial intelligence (AI), mostly artificial neural networks (ANNs) have become popular in evaluating surface water quality. AI-based are less demanding compared with traditionally orientated models and statistically established water quality indices which are associated with sub-index functions and aggregation formulae (Gazzaz et al., 2012). ANN are quick alternatives and more direct methods of appraising water quality, offering the possibilities of reducing computational errors, time and effort required to monitor water resources (Gazzaz et al., 2012, García-Alba et al., 2019).

Artificial neural networks (ANNs) uses predefined multidimensional parameter relationships in the form of mathematical coding. Its ability to understand and relate to variable dependency provides a unique analytical advantage and produces more accurate WQI values than the sub-indexing methods (Li and Liu, 2019). Similar to the human brains, Artificial Neuron Network (ANN) refers to a computing system designed based on the structure and functions of the natural biological neural networks. It obeys the same manner in which human brains analyse and process information; whereby layers of neurons are interconnected like a web (Singh et al., 2009, Khalil et al., 2011, Huo et al., 2013, Seo et al., 2016, Qaderi and Babanezhad, 2017, Bansal and Ganesan, 2019, Salari et al., 2018, Kadam et al., 2019, Isiyaka et al., 2019, Ramasubramanian and Singh, 2019, Soro et al., 2020). The first layer consists of input neurons, which functions to receive data, attempt to analyse the input information and filter to the relevant neurons in the second layer. The second set of neurons process the input data and convey the information to the third layer of neurons, which in turn combine the data into a single consolidated output report. These processing units are called the input and output units or neuro-nodes (García-Alba et al., 2019).

ANNs are considered relatively simple non-linear statistical models to enhance Artificial Intelligence (AI) and solve analytical problems that would prove challenging and close to impossible by human or statistical standards (Khalil et al., 2011, Huo et al., 2013, Kim and Seo, 2015, Salari et al., 2018, Ramasubramanian and Singh, 2019, Sousa et al., 2019, Tiyasha et al., 2020). ANNs are evolving the traditional way of computing water quality indices, creating convenient analytical platforms and making water quality information accessible using minimal effort. Henceforth, the study focuses on developing an artificial neural network (ANN) based water quality index (WQI) for examining spatial and temporal trends in surface water.

The ANN model utilises thirteen variables similar to universal water quality index (UWQI) input parameters, and these include NH_3, Ca, Cl, Chl-a, EC, F, $CaCO_3$, Mg, Mn, pH, SO_4 and turbidity. The neural network delivers a scientifically justifiable non-dimensional single-digit score ranging from zero to hundred, with lower scores relating to poor water quality and higher values symbolising water resources of good quality. Index ratings are graded using a five-class ranking whereby class 1 corresponds to the highest degree of purity, and class 5 status designates severely contaminated water body. The index scores and ranking scales are identical and affiliated with gradings suggested for the UWQI and surrogate water quality index (proxy WQI) both designed for investigating South African watersheds.

The scope of establishing an ANN model intended to (1) confirm the capabilities of artificial intelligence (AI) in water science through the application of an ANN-based WQI free from sub-indexing and lengthy calculations, (2) define a holistic framework for creating neural networks, (3) compare the performance of ANN model against conventional WQI, and (4) propose an optimum artificial neural network WQI model for analysing and monitoring water quality status within South African river systems. Therefore, the study involves the design, training, validation, testing and application of ANNs towards computing index scores.

1.3.3 Surrogate water quality index model (Proxy WQI)

Regular water quality sampling and analysis is a costly and demanding task, hence acquiring large volumes of water quality data is often a challenge and requires a significant amount of financial resources (Pegram and Görgens, 2001, Ochieng, 2007). The challenge has initiated a common duty to examine alternative water monitoring techniques that are concise and possibly relieve sampling assignments (Banda and Kumarasamy, 2020b). The ultimate goal is to put forward cost-effective and flexible water assessment models, with significant attention being given to the optimisation of parameter input and mathematical simplicity.

Often, water quality index (WQI) models are heavily parameterised, requiring an extensive amount of data, thereby limiting their application due to input parameter demand. To govern such tendencies, a surrogate WQI is proposed. A surrogate model is an abridged version of an outright WQI, thereto function with limited input data. It represents a quick and easy method of translating complex water quality data into simple, but yet testable measure. Though less-detailed, proxy models are equally competent and fundamentally identical to the original unbridged models, but with reduced computational precision (Razavi et al., 2012, Banda and Kumarasamy, 2020b). Although having less accurate arithmetic aptitude, the advantages of surrogate models outbalance such unfavourable attributes and compensate for the numerical divergence. Based upon the review by Razavi et al. (2012), Asher et al. (2015), and Bhosekar and Ierapetritou (2018), a variety of surrogate models exist and documented in existing literature, with Schultz Martin et al. (2004), Shamir and Salomons (2008), Castelletti et al. (2010), Preis et al. (2011), and Sreekanth and Datta (2011) being practical examples of proxy models developed for water resource management functions.

The proposed proxy WQI has been established to be rationally implemented in lieu of the high-fidelity model for surface water pollution control and river basin planning functions, referred here as the universal water quality index (UWQI). The primary objective of developing and applying the suggested surrogate WQI is to make better use of typically restricted water resource monitoring budgets (Razavi et al., 2012, Banda and Kumarasamy, 2020b). Therefore, the proposed surrogate WQI aims to provide a more straightforward and cost-effective model that simulates the output of a complex high-fidelity model (Asher et al., 2015, Banda and Kumarasamy, 2020b). Undoubtedly, the success of the surrogate WQI and its advantages will ultimately intensify regular water resource monitoring in South Africa. In the same context, thirteen variables applicable to UWQI have been subjected to multivariate statistical analysis to select the most meaningful proxy variables for the surrogate WQI.

Based on the study results, surrogate WQI(a) which includes SO_4 as an input variable, struggles to assess water quality datasets with excessive parameter concentration levels. In this regard, pH performed much better than SO_4, hence the inclusion of pH among the model input variables. Subsequently, chlorophyll-a, electrical conductivity, pondus Hydrogenium and turbidity are the final four proxy parameters.

Minimising the input parameters can significantly reduce time, effort and cost required to evaluate water resources, thereby making the process more feasible and economically viable (Bhosekar and Ierapetritou, 2018, Tripathi and Singal, 2019b, Jahin et al., 2020, Banda and Kumarasamy, 2020b). It is then vital for water quality scientists to consider the application of surrogate WQIs, to reduce parameter input demand, thereby lowering resources required for water quality monitoring activities. Despite that, the suggested proxy WQI is developed for surface water pollution control and river basin planning functions, the application range of surrogate WQIs matches that of high-fidelity models. It can extend to any other water body and serve a diverse range of water uses. In this study, the terms "low-fidelity model," "surrogate model," and "proxy model" bear the same meaning and are used interchangeably.

1.3.4 Index classification system

WQI scores from the proposed WQIs are classified using as five-class categorisation schema. The ranking mechanism follows an increasing scale identical to the standard percentage hierarchy. Thus, offering a better understanding of water classification scale, especially to non-technical individuals (Banda and Kumarasamy, 2020c). Similar to the methods used by Abrahão et al. (2007), Rabee et al. (2011), Rubio-Arias et al. (2012), Sutadian et al. (2018), appropriate mathematical functions with logical linguistic descriptors such as "less than," "equal to" and "greater than" have been assigned to each categorisation class. By so doing, the categorisation schema can accommodate all possible index scores regardless of the decimal value. More importantly, the established categorisation schema aids in closing gaps identified in the literature and present a progressive approach that will contribute significantly towards water quality indices development. Such an academic contribution reflects on the models' efficiency and attributes to the success of the current study.

1.3.5 Microsoft Excel-based water quality variability model (WQVM)

Typically, most water quality (WQIs) are documented as scientific equations that are somewhat difficult to comprehend and generally problematic to implement (Banda, 2015). Therefore, to overcome such trends, the proposed WQIs are merged and presented in a more useful and acceptable manner; a format that is user-friendly and convenient to most people, even non-technical individuals. Considering that Microsoft Excel is a commonplace and straightforward (Varma and Khan, 2014, Avdic, 2018), the proposed water quality variability model (WQVM) utilises Excel software as an operating platform. The software integrates three WQIs using multiple logistical functions coded to handle thirteen predefined water quality variables and the algorithms of each particular water quality index (WQI). Selecting Microsoft Excel program was motivated by the functionality and computational power bestowed by Excel. Even more importantly, Excel being a familiar interface, the study has an opportunity to benefit on acceptability more than introducing completely new software to operate the WQVM.

1.4 Research data and study area

Water quality data from Umgeni Water Board (UWB) was used to achieve specific objectives of the current study. The study utilised water quality samples tested weekly for a period of six and half years spanning from January 2012 to July 2018. All the water quality variables were sampled following standard methods prescribed by the Department of Water and Sanitation (DWS), and further analysed according to international standards in an ISO 9001 accredited laboratory owned and operated by UWB (Namugize et al., 2018). The research dataset from UWB satisfactorily provided all the required thirteen water quality variables, and these are, ammonia (NH_3), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), electrical conductivity (EC), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), pondus Hydrogenium (pH), sulphate (SO_4) and turbidity (Turb).

Water quality data provided by Umgeni Water Board originates from six sampling stations falling under the jurisdiction of four different catchment areas. The sampling sites are as follows:

- three stations situated in Umgeni River catchment (U20) and located at Henley, Inyanda and Midmar Dams respectively;
- one station at Hazelmere Dam located within Umdloti River catchment (U30);
- one station at Nungwane Dam under Nungwane River catchment (U70); and
- one station at Umzinto Dam found in Umzinto/uMuziwezinto River catchment (U80).

At least one or more stations were considered for each of the four drainage basins applicable to the study. Testing the model with data from these four river catchments supports the objective of establishing a water quality index (WQI) appropriate to serve the greater part of South Africa, if not the whole country. Over and above the availability of data from UWB, the economic significance of KwaZulu-Natal Province (Shoko, 2014, Hughes et al., 2018), the distinctiveness of its inter-basin arrangements, the scope of the transfer schemes involved and extensive water demand (Umgeni Water, 2018, 2019a, 2019b); all these, uniquely encouraged the choice of the study area, which falls under Pongola-Mtamvuna water management area (WMA) (Republic of South Africa, 2012, Chiluwe, 2014). The research dataset was sufficient to examine the models and accomplish the primary objective of developing nationally acceptable water quality monitoring tools.

1.5 Purpose and significance of the study

The current study attempts to provide significant contribution and simplify water resource monitoring across all the nine provinces of South Africa, through the development of a flexible and much easier, but scientifically justifiable water quality index applicable to most distinct, if not all the South African river catchments. Such an essential tool can be decisive in evaluating the current water affairs and predicting future trends; which becomes helpful towards water resource allocation and prioritisation of water conservation programmes. Consequently, the developed universal water quality index (UWQI) has been structured to integrate with the proposed water quality variability model (WQVM) and represents quality variability among various water use locations.

These models are virtual tools capable of providing realisable water classification, thereby attaching the actual value of surface water depended upon contamination level. Thus, ultimately intensifying the effectiveness and proficiency of water resource management systems, which enables greater economic efficiency and proper environmental protection strategies. Even more importantly, the models have the potential to balance water resource allocation, through optimisation of water uses based on water quality, which technically translates pollution-based water management.

1.6 Research question

How capable is the proposed development of water quality index and water quality variability model using artificial neural network (ANN) to analyse and monitor water quality status for South African rivers?

The study created a multi-layered feed-forward backpropagated artificial neural network (ANN) model to address the research question. The capabilities of artificial neural networks towards evaluating water quality trends have been demonstrated, and the ANN model proved to be a useful alternative to conventional methods of developing water quality indices. Between artificial intelligence (AI) and conventional techniques; the AI-based models are more direct and flexible than traditional methods. AI involves less prior knowledge of WQIs and offers the opportunity to minimise analytical errors, time and effort required to monitor water resources.

1.7 Study objectives

The study suggests the following set of objectives, which were prescribed primarily to accomplish specific study goals and particularly to substantiate the research hypothesis.

1.7.1 Main objective

Unlike most existing water quality indices (WQIs) which are confined to specific application boundaries; the primary objective of the current study involves developing nationally applicable water quality monitoring tools that are founded on different fundamentals.

1.7.2 Specific objectives

The specific objectives of this doctoral work are framed towards obtaining the primary goal, which is centred on establishing practical and sustainable water quality evaluation mechanisms. The study objectives are then defined as follows:

(1) To develop a universal water quality index (UWQI) suitable for use across the catchment areas in South Africa;

(2) To adopt artificial intelligence (AI) using artificial neural network (ANN) model to compute WQI and analyse spatial and temporal variability, and then to compare with traditional proposed UWQI;

(3) To develop a surrogate water quality index model that can operate with four key determinants as a proxy to the unbridged UWQI;

(4) To establish a list of water quality parameters for the UWQI, develop a standard ranking scale and assigning weights to the selected parameters;

(5) To establish four proxy determinants for the surrogate WQI and assign relative coefficients for the model;

(6) To produce water classification grading and water categorisation schema suitable for the proposed water quality indices and water quality variability model; and

(7) To transform the proposed water quality indices (WQIs) into a water quality variability model (WQVM) that can produce water quality classification grading based on a specific water categorisation schema. That is creating a practical tool appropriate for regular water resource monitoring.

The methods applied to fulfil the specific objectives are summarised in the following section and are discussed further in Chapter Three of the study.

1.7.3 Methodological approach

Monthly observed water quality data spanning for four years from 2014 to 2018 has been used towards fulfilling the primary objective of the study. The dataset emanates from six sampling stations located within four different river catchment areas managed by Umgeni Water Board (UWB) in KwaZulu-Natal, a coastal province in South Africa. The research data was adequate to complement the objective of establishing nationally acceptable water quality tools.

Objectives (1) and (4): The Rand Corporation's Delphi Technique popularly known as the Delphi method, was used implemented to attain objective one and four. The technique utilises expert opinion to define the most significant parameters, assigning of relative weight coefficients, setting out the corresponding rating curves and sub-index functions. These attributes allow the most imparted parameters to impart the most significant effect on the index score, offering a hierarchical structure of influence.

Objective (2) and research question: A feed-forward backpropagated artificial neural network (ANN) model was developed to satisfy objective two. The model is founded on artificial intelligence (AI) algorithm similar to the biological neural system with a multi-layered set of neurons responsible for accepting input variables, analysing the parameter composition and eventually producing an index score. The AI-based network uses the same set of parameters considered for the UWQI.

Objectives (3) and (5): Multivariate statistical methods which include principal component analysis (PCA), hierarchical cluster analysis (HCA) and multiple linear regression (MLR) were collectively employed to address the requirements of objectives three and five. PCA and HCA assisted in defining four proxy determinants for the surrogate WQI, whereas MLR produced the parameter coefficients and the linear-based aggregation equation.

Objective (6): An increasing scale index was established to achieve objective six and simplified the interpretation of WQI scores, primarily to accommodate non-technical personnel. The classification system follows the typical percentage hierarchy, which is better understood by the general public.

Objective (7): Lastly, the water quality variability model defined in objective seven was built by combining three diversified water quality indices (WQIs); which are founded on distinctive indexing methods. The three WQIs are (a) UWQI defined by objectives one and four, (b) ANN model under objective two, and (c) surrogate WQI from objective three and five.

Although the methodologies and techniques were successfully implemented, it is worth noting the following limitations and assumptions.

1.8 Limitations and assumptions

The suggested limitations and assumptions are technically formulated to ensure appropriate application of the proposed tools, and they do not devalue the significance of the study. The limitations and assumptions are defined as follows:

- The universal water quality index (UWQI) was developed entirely independently from any water quality data or particular drainage region; hence the application of such a model is not restricted to specific boundaries. The dataset from the four river catchments was only used to attest the UWQI rather than the development phase;
- Although the surrogate WQI and ANN model are designed based upon specific water quality dataset, their application can stretch beyond the four different watersheds considering that the depended (target) variable used were generated form a nationally acceptable index system, which is the UWQI;
- Assume that water boards are using the same set of water quality variables to define contamination levels within river catchments. Therefore, index scores may vary when a different set of parameters are used as input variables. In order to achieve a composite evaluation, all the prescribed variables should be considered;
- The proposed water quality variability model (WQVM) was built using Microsoft Excel software, thus limiting the application of the WQVM to the use of Microsoft Office Suite;
- Both UWQI and ANN models are restricted to thirteen water quality parameters (NH_3, Ca, Cl, Chl-a, EC, F, $CaCO_3$, Mg, Mn, pH, SO_4 and turbidity), whereas the Proxy WQI is limited to only four explanatory variables (Chl-a, EC, pH and turbidity); and
- The proposed models (UWQI, ANN and Proxy WQI) uses predetermined weighted coefficients, limiting the model to specific parameter input range. Inputting of different variables other than the defined is prohibited since the models rely only on predetermined coefficients. If different variables are desired, then new coefficients must be generated.

Beyond achieving the specific objectives of the study, the limitations and assumptions mentioned above simplifies the models and minimise data requirements while exploiting on their efficiency. Therefore, these restrictions do not disadvantage the purpose of the research; instead, they add value to the effectiveness and possible application of the models developed under this study.

The specified limitations and assumptions provided are related to the methodologies applied, in cognisance the gaps and flaws identified from existing literature. Chapter Two contains details of existing water quality indices and water quality variability models reviewed under the study.

CHAPTER 2

2. LITERATURE REVIEW

2.1 Overview of the literature review

A comprehensive evaluation and monitoring of South Africa's water resources are vital towards implementing appropriate management and long-term sustainability of the scares water resources. Such practices are done using a significant amount of data, and such information needs to be analysed and applied using methods, tools and or models that are capable of deducing such amount of information into usable datasets and structured formats.

Proper design and formation of such tools is a pivotal step in assessing our water resources and in cognisance of such, this study endeavours to develop a water quality-monitoring tool that applies to distinct catchments in South Africa. This tool should analyse and integrate the significance of physical, chemical and biological constituents of surface water and be able to present them in a simple, but yet technically justifiable method.

In order to properly compile and develop a better model, one has to evaluate, review and consider the flaws and limitations of the current and previously developed models of similar nature. Henceforth, Chapter Two focuses on reviewing the literature relevant to the study, incognisance of the specific objectives described in Chapter One. This chapter concentrates more on aspects relating to the development of the water quality indices (WQIs) and water quality variability models (WQVMs).

2.2 Definition and uses of raw water

2.2.1 Raw water

Raw water signifies water found naturally in the environment, without any treatment, and this includes rainwater, groundwater and surface water found in the form of dams, lakes and rivers. Raw water can be abstracted directly from its source without treatment to support activities which include but not limited to agricultural, mining, and construction. Furthermore, raw can be extracted for purification to meet a variety of purposes, such as medical, industrial and domestic applications (Banda, 2015). However, the objectives of this study are centred on raw surface water found in South African river catchments.

2.2.2 River water quantity and quality

Rivers are complex large natural flowing watercourses which are typically fed by converging tributaries, and they usually contain freshwaters flowing towards another waterbody. In order to establish the suitability and sustainability of any river, both the quantity and quality of the river water has to be considered. The two, can assist in describing the inherent potential of a river, establish whether its condition is stable, ascertain its capacity for self-repair when unsettled and the extent of management support required (Karr et al., 1986, Norris and Thoms, 1999).

River water quantity is considered to be the volumetric measure of water resources available for abstraction without depleting the environmental reserve. Thus, the surplus water available after taking into account the amount of water sufficient enough to cater for the aqua-life and river health as a whole. In contrast, river water quality describes the biological, chemical and physical characteristics of river water (Davies-Colley, 2013, Banda, 2015). River water quality is naturally variable but usually comprises of significant contaminants in the form of dissolved ions, particles and living organisms. Features and details of the pollutants vary depending on the degree of development along the river, size of the river, human activities as well as physical and hydrological catchment characteristics (Chapman, 1996, Alberta, 2011).

Since the efforts by Horton (1965) of developing water quality analysis tools, our proficiencies to measure and analyse water quality data has evolved over the past decades, expanding our knowledge base and understanding of water quality (Bhargava, 1985, House, 1986, 1989, 1990, Smith, 1987, 1990, Dojlido et al., 1994, Nagels et al., 2001, CCME, 2002, Boyacioğlu, 2007, Thi Minh Hanh et al., 2011, Banda, 2015, AL-Sabah, 2016, Gitau et al., 2016, Ewaid and Abed, 2017a, Shah and Joshi, 2017, Trikoilidou et al., 2017). Regardless of such growth, it is still difficult to provide a simple definition of water quality. It is very complicated to comprehend the combined effect of several complex factors used to describe water quality and the challenges of identifying the most significant variables used to evaluate the status of water resources in the quantitative terms (Chapman, 1996).

Considering the review work by Lumb et al. (2011a), Poonam et al. (2015) and Sutadian et al. (2016), it is noted that various water quality analysis tools have been developed, with the effort to measure and quantify the extent at which water resource quality can vary. Such useful mathematical tools deduce complex water quality data sets and provide a single classifying value that grades water quality based on the degree of pollution. The single grading value is commonly known as water quality index (see Khan et al., 2004, Alberta, 2011, Lumb et al., 2011b, Abdel-Satar et al., 2017, Ewaid and Abed, 2017b).

In the same context, this study aims to develop a common water quality index (WQI) model that works with various river catchments in South Africa. The specific objectives of this study are framed towards achieving a practical and sustainable water quality-monitoring system that will provide a holistic approach in solving water quality problems in South Africa. The tool will provide an essential platform to measure whether specific water resources need to be restored and to what degree. Thus, assisting in the prioritisation of water quality activities.

2.3 Objectives of establishing water quality monitoring tools

The world-over has experienced a continuous growth on socio-economic activities; however, such progression has been accompanied by accelerated growth in water contamination, causing pollution stress on the aquatic environment (Chapman, 1996, Palanisami, 2009). Undoubtedly, this evolution of water pollution has led to the birth of numerous water quality indices (WQIs) as water quality monitoring tools (Poonam et al., 2015). The development of such tools can be based on either (i) a single-objective monitoring process, whereby it addresses a specific single problem area or (ii) a multi-objective monitoring process, which covers various water applications and provides data for more than one assessment programme (Chapman, 1996).

According to World Health Organisation (1991), global water quality monitoring objectives are defined to address the public, government institutions, scientific and research community, water economists and policymakers on matters relating to water quality assessment. The specific objectives of water quality monitoring programmes are modelled specifically:

- To define the water quality status and assist in identifying the most favourable action, relative to human and aquatic ecosystem health;
- To describe water quality trends, thereby providing a platform to outline crisis stages;
- To delineate the source of water quality trends and dominant circumstances;
- To identify and cluster the types of water quality problems experienced in specific catchment areas; and
- To provide the water quality assessment information in a structured format that can be easily understood by water resource management and regulatory agencies when evaluating alternatives and making necessary decisions.

Given the context of water quality monitoring objectives, water quality index is, therefore, a useful statistical tool. Its ability to interpret complex water quality information and deduce it into a single numeric value makes it a vital model necessary to achieve global water quality objectives.

Thus, validating the purpose of this study, which is to develop a universal water quality index appropriate for application across various catchment areas in South Africa.

2.4 Water quality indices (WQIs)

Water quality indices (WQIs) have been recognised as significant environmental performance indicators, and the concept of expressing water quality using a numerical value has been readily appreciated, leading to the suggestion of various indexing models. Henceforth, this section of the study reviews the formulation of several WQIs and document both the favourable and unfavourable elements of most of the existing models.

Specific water quality indices were identified as most significant, based on their wider application and are discussed in detail under this section of the study. Nevertheless, the rest of the reviewed indices are documented towards the end of this thesis as Annexure A: Details of reviewed water quality indices (WQIs).

2.4.1 Historical background and definition of WQIs

The idea of describing water quality based on the degree of cleanliness or contamination level started as early as 1848 in Germany (Lumb et al., 2011a, Medeiros et al., 2017). Subsequently, during the 19th century, Kolkwitz and Marsson (1909) developed the "saprobic system" as a biological concept of determining water quality. The system provides a saprobic index value based on the organic degradable composition of the water resources (Sládeček, 1973, Cairns, 1974, Lindegaard, 1995, Hawkes, 1998, Rolauffs et al., 2004, Medeiros et al., 2017). The saprobic indexing system relied on the distribution pattern and the relative abundance of various biological aquatic species and such a non-chemical analysis, cannot address the modern challenges relating to water quality. However, the presence of certain species in water ensures that certain minimal water quality conditions have been met, which is why the saprobic system has been accepted by the public and remains as a traditional method of assessing the suitability of water for several applications (Cairns, 1974, Rolauffs et al., 2004).

More than a century after the birth of the saprobic index, Horton (1965) established the first parameter based numerical indexing system. This approach utilises a mathematical model to rate and aggregate the combined implication of selected biological, chemical and physical water parameters and present them in a simple, but scientifically justifiable method (Kannel et al., 2007, Lumb et al., 2011a, Effendi, 2016, Sutadian et al., 2016). After Horton (1965) suggested the first water quality index (WQI), subsequently, many other indices were developed to improve the original concept (Ewaid and Abed, 2017b). Parameters of consideration, mathematical formation, indexing scale (also known as the categorisation schema) and application boundaries are the significant aspects being targeted with each improvement. And, the objectives of this study are aiming to address the same, thereby developing a universal water quality index applicable to various river catchments in South Africa.

Water quality is defined by pollutants, which can be grouped as physical, chemical and biological properties of the water. These variables can collectively be integrated into a systematically structured indexing scale, commonly known as water quality index (WQI). It is capable of converting a large quantity of water pollution data into a single dimensionless index value, which represents the level of contamination of the water resources (Boyacioğlu, 2007, Darapu et al., 2011, Kalyani et al., 2016, Ewaid et al., 2018). Considering such ability to integrate a pool of water quality variables into a simple easily understood number, WQI is, therefore, regarded as a handy and significant communication tool for water managers and policymakers (Zandbergen and Hall, 1998, Khan et al., 2005, Kankal et al., 2012).

Water quality indices (WQIs) are used to simplify and streamline what would otherwise be impractical assignments, thus justifying the efforts of developing such WQIs.

2.4.2 Classification of water quality indices

Poonam et al. (2015) classified water quality indices (WQIs) into four main categories, the first three are grouped according to their application, and the fourth one is based on the formation technique rather than the purpose of establishment. Statistical approaches are formulation techniques, aimed at substituting the Delphi method on establishing parameters, sub-indices and weights. It is therefore subjective to consider design method when classifying WQIs. This being that, under this study; categorisation of water quality indices is based on the purpose of establishment and the groups are as follows:

(i) **General indices:** created for general water quality assessment and basically, their evaluation process is independent of the purpose and application of the water reserve. A practical example being the National Sanitation Foundation Water Quality Index (Brown et al., 1970).

(ii) **Specific indices:** developed for one particular application, and practical examples include drinking, irrigation, industrial and ecosystem preservation. The Vaal Water Quality Index (WQI) developed by Banda (2015) is an example of a specific index created to evaluate the status of raw surface water intended for treatment to portable standards. Another example is from Argentina, whereby, Almeida et al. (2012) developed a water quality index, particularly for the assessment of recreational water resources.

(iii) **Planning indices:** these are water evaluation tools, purposefully designed to assist water managers and policymakers in substantiating their decisions regarding water quality. The United States of America developed such an index for routine stream monitoring (Hallock, 2002, Banda and Kumarasamy, 2020e).

Generally, WQIs are not designed for broad application, they are customarily developed for a specific watershed and or region, unless otherwise if different basins share the same water quality monitoring objectives and test the same range of water quality variables. The choice and selection of water quality variables to be incorporated in an index is governed by the proposed uses of the water quality index. The combined effect of such technicalities eventually demarcates the application boundaries of the indexing model (Banda, 2015, Banda and Kumarasamy, 2020e).

Expanding index application boundaries is, perhaps, the most demanding scientific need; that is, the development of a unified water quality index, that works with most, if not all the watersheds in South Africa. An index not limited to specific application boundaries, and thus the aim of this study.

2.4.3 The basic procedure of developing water quality indices

A considerable number of indices have been developed since the primary index by Horton (1965); however, regardless of such efforts, there is still no globally acceptable manner in which water quality indices are developed (Sutadian et al., 2016, Banda and Kumarasamy, 2020e). Nonetheless, there is an inevitable and realisable trend, which is distinguished by the following common steps (Abbasi and Abbasi, 2012b, Fu and Wang, 2012, Walsh and Wheeler, 2012, Tyagi et al., 2013, Poonam et al., 2015, Paun et al., 2016, Unda-Calvo et al., 2019):

(i) **Selection of parameters:** identifying and choosing the most critical variables suitable enough to provide a practical sense to the water quality index. Proficiency is required to establish just enough parameters, not too few or too many. Parameter selection can be performed by either expert opinion (whether individually or as a group) or through statistical techniques.

(ii) **Formation of sub-index values:** considering that various water quality parameters have different scientific units, it becomes necessary to transform them into a single common scale, and this task is achieved by generating sub-indices.

(iii) **Establishing weights:** parameter weightage coefficients are assigned based on the level of importance of each variable, and they are established through evaluating the potential impact of each input variable, especially when parameter concentration levels are outside the permissible limits. Though Delphi is a tedious process, the method will minimise subjectivity in establishing weights and enhance the credibility of the index.

(iv) **Aggregation of sub-indices:** thus regarded as the final step towards obtaining an absolute index value. In cognisance of the assigned weights, mathematical models are used to combine all the sub-indices into one index number. They are various aggregation methods available, but there are three fundamental models commonly used. These are additive, multiplicative and logical functions.

Of lately, several attempts have been made to explore the structure and relationship of water quality variables using statistical approaches like cluster analysis, discriminant analysis, factor analysis and principal component analysis (see Mahapatra et al., 2012, Zhao et al., 2012, Wan et al., 2013). Even the application of artificial intelligence methods, which includes fuzzy logic and artificial neural networks has been tested, to reduce prejudice and improve on the reliability of the water quality index models (Lermontov et al., 2009, Singh et al., 2009, Gazzaz et al., 2012, Scannapieco et al., 2012, Cordoba et al., 2014, Poonam et al., 2015). The current study will also examine the capabilities of artificial neural network (ANN) to analyse and monitor water quality status for South African rivers.

Further details regarding the steps and procedures of developing water quality indices (WQIs) are discussed at length in the subsequent sections of this chapter.

2.4.4 Selection of water quality parameters

Water quality variables are the most important constituents of any water quality index; they are the basis at which the index value is generated. Consequently, the selection of such parameters becomes an essential step in the establishment of an index. The selection process is done in cognisance of the hazard and risk posed by different pollutants. With special attention being given to water quality variables which have more impact in disturbing the environmental and human health, whenever their concentration levels exceed the tolerable limits. (European Union, 1995, CCME, 2001a, World Health Organization, 2003a, 2003b, 2011a, EFSA, 2012).

In order to critically ascertain the influence of each variable; one has to establish the intended use of the water body since acceptability and level of impact differ with each application. Therefore, it is equally important to note that; the selection of parameters used to evaluate water quality depends mainly on the envisioned use of the water body (Srebotnjak et al., 2012, Banda and Kumarasamy, 2020e). Accordingly, the parameter selection process becomes apprehensive with uncertainty and subjectivity, as it is aligned to the usefulness of the water quality index. It then becomes crucial to exercise enormous care and sound judgement, in order to reduce the ambiguity and ensure that the most representative parameters are included in a WQI (Abbasi and Abbasi, 2012b).

According to Sutadian et al. (2016), there are three systems applicable to the parameter selection process, and the three categories are defined as follows:

(a) **Fixed system:** in this case, WQI application is restricted to a limited set of parameters, which are selected by the WQI developer as the most suitable set of variables, necessary for the calculation of the final index value. Although using a fixed set of parameters allows index users to analyse and compare water quality status among different sites appropriately, the system is considered rigid; which is a common problem with most of the water quality indices. Even if it becomes necessary and vital to include additional variables in the index, a fixed system cannot accommodate the addition of new parameters, hence the term rigid.

(b) **Open system:** a more flexible approach that permits index users to incorporate parameters of their choice. Though such water quality indices (WQIs) are flexible and eliminates rigidity, they pose critical problems in comparing results from different monitoring sites. Unless otherwise, the users enforce the usage of identical parameters, it is then inappropriate to apply such indices (open system) as comparison tools; especially when generating priority matrixes based on pollution status and water quality classification.

(c) **Mixed system:** a combination of the fixed and open approach. The design consists of a primary definite set of parameters that are compulsory for calculating the index value, as well as additional parameters that can be inputted based on the users' discretion.

Although the hybrid system is the best fit between the fixed and open system, the mixed system still suffers from the same problem with the open system, though with a reduced margin of error. Given the advantages and disadvantages of the three methods, the fixed index structure is designed to analyse and compare water quality from different water bodies. Henceforth, making it the most appropriate system, suitable for the development of a unified WQI, that can be functional in most, if not all the catchments in South Africa, which is the main aim of the study.

Parameter selection for a fixed system requires enormous care, attention, experience and proficiency, to ensure that the most significant variables are incorporated in the WQI. Expertise is necessary to delineate what is regarded as too few or too many variables; the ability to optimise the ideal number of parameters needed or just enough to calculate a meaningful water quality index value. The selection procedure can be performed using an expert opinion (either as a group or individually), or through statistical methods (Banda and Kumarasamy, 2020e).

Due to human influence, the expert opinion method can be subjective and uncertain. In an attempt to reduce the subjectivity in parameter selection, statistical tools have been developed and widely adopted as standard practice (Liu et al., 2011, Shyu et al., 2011, Abbasi and Abbasi, 2012b, Zhao et al., 2012, Sun et al., 2016a). Hypothetically, this might be the most objective method; however, the human influence is paramount on selecting the dataset should be statistically analysed, hence compromising the accuracy of the procedure (Sutadian et al., 2016). Nevertheless, through the use of pattern recognition; statistical methods, remain as the most powerful technique for interpreting the variance between a large number of variables and convert them into smaller groups of independent variables (Liu et al., 2011, Sun et al., 2016a).

Water quality parameters are measured in different scientific units, and these units have to be transformed into a common scale. The conversion process translates and aligns their influence on the single-unitless index value. Henceforth, the application of mathematical sub-indices is necessary to achieve the transformation process.

2.4.5 Formation of sub-indices

Considering that water quality variables are measured in various units; sub-indices are mathematical tools utilised to transform the scientific units into a common non-dimensional scale. Most of the traditional WQIs can only aggregate parameters with a common scale; hence the process of standardising and rescaling parameter values is necessary. However, a few water quality indices do not have such functionality. Instead, the actual measured parameter values are used to calculate the final index value (Sutadian et al., 2016). For example; CCME (2001a) established a multivariate statistical formula to aggregate the original parameter values without the application of sub-indices. In a similar case, Said et al. (2004) developed a mathematical equation that calculates the final index value without standardising the actual measured parameter values.

Depending on the aggregation technique being employed, variables can be considered directly as sub-indices and aggregated into a single index value. Whereas in some instances, the primary parameter sub-indices can be further grouped and aggregated into a bigger secondary group of sub-indices, which are then later aggregated into the final index value. Such are often composite or aggregated sub-indices, and a practical example is Bhargava (1985), which have four different composite sub-indices in the form of organic and inorganic, coliforms, heavy metals and physical sub-indices (Sutadian et al., 2016).

The mathematical relationships between the measured parameter values and the sub-index values are referred to as, the sub-index functions. The actual parameters values can be translated to sub-index through sub-index functions, which can be presented graphically as rating curves (parameter values plotted to the corresponding sub-index values). There are three standard methods used to develop sub-index functions, that is; (1) expert judgement or opinion, which can be done either individually or as a group, (2) use of water quality standards or regulations, and lastly (3) statistical methods (Sutadian et al., 2016, Banda and Kumarasamy, 2020e).

2.4.5.1 Expert judgement

Similar to the selection of water quality parameters, either individual or group expertise and skills are utilised to establish sub-index functions. In this method, critical points of the rating curves are established from personal opinion and plotted graphically to represent the impact of each parameter at different concertation levels. The process can be done individually, but involving several experts minimise partiality and ambiguity. If several water experts are involved, then the Delphi method can be employed, whereby questionnaires are used to collect the relevant data required for the formation of sub-index functions. Collectively, the set of information from the experts' opinion is converged into rating curves which are further converted into linear or non-linear sub-index functions.

Since its inception in 1970, the Rand Corporation's Delphi Technique has been widely adopted in the establishment of various water quality indices. Indices which includes the National Sanitation Foundation (NSF) Index, Scottish Research Development Department (SRDD) Index, Ross's Index, Oregon Index, House's Index, Smith Index and Almeida's Index (see Brown et al., 1970, SRDD, 1976, Ross, 1977, Dunnette, 1979, House, 1986, Smith, 1987, Almeida et al., 2012).

2.4.5.2 Use of water quality standards

The second method involves the use of water quality legislative standards to establish sub-index functions. Permissible parameter concentration levels are used to derive the rating curves, which can eventually be transformed to sub-index functions. Unlike the Delphi method, the critical points of the rating curves are obtained using the permissible limits for each particular parameter, incognisance of the intended use of the water body. Actual measured water quality parameter values can be translated to sub-index values using three methods, namely, linear interpolation rescaling, categorical scaling and comparison with permissible limits. The first technique known as linear interpolation rescaling, relays on an identical range of sub-index values, normally between zero to hundred (0-100) or zero to one (0-1).

Similarly, the establishment of water quality classification follows a sequential order, which can be, Class 1, Class 2, …, Class 5. After that, using the permissible limits from the minimum to the maximum, each limit corresponding to the relevant water quality classification is assigned to the corresponding sub-index number (Sutadian et al., 2016, Banda and Kumarasamy, 2020e). For example; considering permissible limits of 20, 30, 40, 80 and 120 mg/ℓ, and sub-index range of 100, 75, 50, 25 and 1; then the pairing of the key points can observe the following sequence; Class 1 (20:100), Class 2 (30:75), …, Class 5 (120:1). These paired set of data are the key points of the rating curve and are the basis at which sub-index functions are developed. If the actual parameter value falls between two classes, the linear interpolation method is used to obtain the real sub-index value. The following general equations are applicable to this particular approach (Sutadian et al., 2016):

$$s_i = s_1 - \left[(s_1 - s_2) \left(\frac{x_i - x_1}{x_2 - x_1} \right) \right] \qquad \text{Eq. 2.1}$$

$$s_i = s_1 - \left[(s_1 - s_2) \left(\frac{x_1 - x_i}{x_1 - x_2} \right) \right] \qquad \text{Eq. 2.2}$$

where: s_i is the i^{th} sub-index value;

s_1 and s_2 are the sub-index values for the upper and lower class, respectively;

x_i is the i^{th} parameter value; and

x_1 and x_2 are values of permissible limits for upper and lower class.

In the case that a parameter decreases the level of water quality with an increase in parameter value, then Equation 2.1 is applicable. Otherwise, Equation 2.2 can be adopted when a parameter increases the level of water quality with an increase in parameter value (Sutadian et al., 2016).

The second technique is the categorical scaling method; actual parameter values are transformed to sub-indices using constant values of either zero (0) or one (1). The sub-index value of zero (0) is assigned to a parameter with concentration levels exceeding the acceptable limit; whereas the sub-index value of one (1) is assigned to a parameter with concentration levels below the permissible limits (Sutadian et al., 2016). The following two mathematical functions are used for this technique:

$s_i = 0$; if x_i is well above the permissible limits Eq. 2.3

$s_i = 1$; if x_i is well below the permissible limits Eq. 2.4

where: s_i is the i^{th} sub-index value; and

x_i is the i^{th} actual parameter value.

The third and last approach involves comparing the actual measured parameter values with the legislative standards. In cognisance of the permissible limits, sub-indices are generated according to the degree of water quality form the worst quality to the highest quality; and the sub-index values ranges from zero to one. The sub-index values are computed using Equation 2.5 below:

$$s_i = \frac{x_i}{x_{\max}} \qquad \text{Eq. 2.5}$$

where: s_i is the i^{th} sub-index value;

x_i is the i^{th} actual parameter value (mg/ℓ); and

$x_{\max}$ is the maximum value of the permissible limit (mg/ℓ).

2.4.5.3 Statistical Methods

In this approach, the critical points of the rating curves are developed through statistical analysis of historical parameter data. This technique relays on the statistical characteristics like the mean values and various quantiles of the parameters measured over a long period. Different water quality index developers have successfully used this method; developers like Dunnette (1979), Bhargava (1985) and Hallock (2002).

Upon establishment of sub-index functions, the sub-index value has to be factored into the final index; this procedure can be achieved by multiplying the sub-index values with assigned parameter weightage. Establishment of such parameter weights is discussed in the subsequent section of this chapter.

2.4.6 Establishing weights

Each parameter has a different effect on water classification; hence weighting factors are used to reflect the influence of each parameter on the index model. These mathematical tools are assigned to each water quality variable based on the level of significance and their impact on the overall index value (Sharma et al., 2014, Sutadian et al., 2016). In general, weighting factors are established as either equal or unequal weights. Equal weights are practical if all the water quality parameters are regarded as equally important; whereas, unequal weights are useful where some parameters are considered as more or less influential than the others (Sutadian et al., 2016).

A limited number of index developers adopted the use of equal weights because of the possibilities of unfairness in assigning the weighting factors. Besides, if due diligence is not exercised; unequal weights could promote sensitivity of the index model, favouring the heavily weighted water quality variables (Sutadian et al., 2016). Such biasness brings about the element of doubt towards the application of unequal weights. This being said, appropriate measures should be taken in selecting the most suitable technique of developing unequal weights, and the method should minimise prejudice and ratify the integrity of the index model.

Similar to the selection of parameters and development of sub-indices, there are also participatory based methods available for establishing weights, and the commonly used are the Analytical Hierarchy Process (AHP) and the Rand Corporation's Delphi Technique (Delphi Method). The two procedures are discussed next:

(i) **Analytical Hierarchy Process (AHP):** a mature and easy concept which has been broadly employed in many other different fields, other than water quality index development. The idea allows the incorporation of both quantitative and qualitative aspects in the decision-making process. Expert opinion is gathered through "pairwise comparison matrices," in which the experts are required to present their preference by comparing numerous alternatives. AHP is a beneficial method of establishing weights for either individual or aggregated water quality variables. Ocampo-Duque et al. (2006) and Gazzaz et al. (2012) have both implemented AHP to generate weights for calculating water quality index.

(ii) **Rand Corporation's Delphi Technique (Delphi Method):** using questionnaires, water specialists compare relative water quality parameters using a scale of one (highest) to five (lowest). All the expert's ratings are combined, and arithmetic mean values are calculated, which are later converted to weight ratings between zero (lowest impact weight) to one (most influential parameter). The procedure was introduced by Horton (1965), later improved by Brown et al. (1970). Since then, Delphi method has been widely employed in various water quality indices to produce relative weights of the selected parameters.

Notably, for most water quality indices; the total weight, which is the summation of all the weights of the selected parameters adds up to unity (1). The reason being that the combined effect of the water quality parameters should not exceed a hundred per cent (Banda, 2015). Otherwise, aggregation of sub-indices will be compromised, and deem the water quality index dysfunctional.

2.4.7 Aggregation of sub-indices

Aggregation of sub-indices is performed by mathematical functions. These equations integrate sub-index values of selected critical parameters in relation to the assigned weights; and obtain the overall water quality status, which is generally presented as a unit-less number. Application of aggregation formula is governed by the degree of accuracy required and whether the parameter weights are either equally or unequally defined. Aggregation process may occur in sequential phases depending on whether an index has aggregated sub-indices or not. Though there are various aggregation techniques available, the common aggregation methods are the additive (arithmetic) and multiplicative (geometric) methods (Sutadian et al., 2016).

The following sub-sections of the study attempts to discuss only the commonly used aggregation methods and state their mathematical structures. Nevertheless, the rest of the reviewed aggregation techniques, including their mathematical structures, are documented towards the end of this thesis as Annexure B: Aggregation formulation of the reviewed WQIs.

2.4.7.1 Additive method

The additive method has been broadly used for aggregation of sub-indices of various water quality indices (see Brown et al., 1970, Prati et al., 1971, Walski and Parker, 1974, SRDD, 1976, Ross, 1977, Stoner, 1978, Martínez de Bascarón, 1979, Dunnette, 1979, House, 1989, Sargaonkar and Deshpande, 2003, Štambuk-Giljanović, 2003, Liou et al., 2004, Boyacioğlu, 2007, Shuhaimi-Othman et al., 2007, Thi Minh Hanh et al., 2011, Banda, 2015, García-Ávila et al., 2018). A simple technique, wherein, the overall index number calculated by adding the weighted sub-indices. The following Equation 2.6 and Equation 2.7 apply to parameters with equal weights and unequal weights, respectively:

$$\text{WQI} = \sum_{i=1}^{n} s_i \qquad \text{Eq. 2.6}$$

$$\text{WQI} = \sum_{i=1}^{n} s_i w_i \qquad \text{Eq. 2.7}$$

where: WQI is the aggregated index value;

n is the number of sub-indices;

s_i is the i^{th} sub-index value; and

w_i is the i^{th} weight value.

Note that, on Equation 2.7 for unequally weighted sub-indices; the weight (w_i) indicate the relative importance of each sub-index (s_i).

2.4.7.2 Modified additive method

Research work such as House (1989), Tyson and House (1989), SRDD (1976), Bordalo et al. (2001), Bordalo et al. (2006) and Carvalho et al. (2011) have applied the modified additive methods; such that, the mathematical model becomes a squared function and divided by 100. The modified additive functions are represented as Equation 2.8 and Equation 2.9 for equally weighted parameters and unequally weighted parameters, respectively:

$$\text{WQI} = \frac{1}{100}\left(\sum_{i=1}^{n} s_i\right)^2 \qquad \text{Eq. 2.8}$$

$$\text{WQI} = \frac{1}{100}\left(\sum_{i=1}^{n} s_i w_i\right)^2 \qquad \text{Eq. 2.9}$$

where: WQI is the aggregated index value;

n is the number of sub-indices;

s_i is the i^{th} sub-index value; and

w_i is the i^{th} weight value.

Similar to Equation 2.7 for unequally weighted sub-indices; the weight (w_i) in Equation 2.9 indicates the relative importance of each sub-index (s_i).

Another version of the modified additive aggregation function was developed by Martínez de Bascarón (1979). In this particular version, the final index value is achieved by dividing the total sum of the aggregated sub-indices by the total sum of the parameter weights, as indicated in Equation 2.22. With continued growth in the application of water quality indices, the Martínez de Bascarón (1979) version has been adopted and modified further in various water quality indices (see Pesce and Wunderlin, 2000, Debels et al., 2005, Abrahão et al., 2007, Sánchez et al., 2007, Koçer and Sevgili, 2014).

According to Smith (1990), the additive model would never register zero as a final water quality index value, even if one of the sub-index value is zero. Furthermore, following the review by Lumb et al. (2011a), it was found that the additive method lacked sensitivity regarding the impact of the low-value parameter. The mathematical formula actually "hides" the effects of variables with unacceptable levels and this challenge is commonly known as the eclipsing problem. In this aspect, the lowly weighted sub-indices might be dominated by highly weighted sub-indices or vice versa; and this ultimately compromises the overall water quality rating (Swamee and Tyagi, 2007, 2000, Bharti and Katyal, 2011, Juwana, 2012, Juwana et al., 2012).

2.4.7.3 Multiplicative method

In an attempt to rectify the eclipsing problem, Brown et al. (1973) proposed a multiplicative function as an amendment of the National Sanitation Foundation WQI. Subsequent studies show that experts agreed more to the multiplicative formula than they did with the additive method, which explains the widespread application of the multiplicative function. However, the additive function has equally being used (Lumb et al., 2011a, Abbasi and Abbasi, 2012b). Practical examples of multiplicative aggregation indices include Walski and Parker (1974), Bhargava (1985), Dinius (1987), Štambuk-Giljanović (1999, 2003), Almeida et al. (2012), Ponsadailakshmi et al. (2018), and Sutadian et al. (2018). The multiplicative functions for equally weighted and unequally weighted parameters are shown as Equation and Equation2.10, respectively:

$$\mathrm{WQI} = \prod_{i=1}^{n} \mathrm{S}_i^{\left(\frac{1}{n}\right)} \qquad \text{Eq. 2.10}$$

$$\mathrm{WQI} = \prod_{i=1}^{n} \mathrm{S}_i^{wi} \qquad \text{Eq. 2.11}$$

where: WQI is the aggregated index value;

n is the number of sub-indices;

s_i is the i^{th} sub-index value; and

w_i is the i^{th} weight value and $w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equation 2.11.

For unequally weighted sub-indices; the weight (w_i) in Equation indicates the relative importance of each sub-index (s_i). When the parameter weights (w_i) are equal, then the function takes the form represented in Equation 2.11, which is commonly known as the geometric mean of sub-indices (Abbasi and Abbasi, 2012b). As with all the multiplicative aggregation functions, a water quality index value of zero is attained if any one of the sub-indices value is zero. Under such circumstances, the eclipsing problem will not exist, because if one particular sub-index demonstrates poor water quality, the overall water quality index will respond accordingly and presents poor water quality (Abbasi and Abbasi, 2012b).

2.4.7.4 Minimum operator method

The minimum operator method was suggested by Ott (1978) and significantly applied by Smith (1987, 1990). Equation 2.12 represents the general form of the minimum operator function:

$$\mathrm{I}_{min} = \sum \min\left(\mathrm{I}_{sub1}, \mathrm{I}_{sub2}, \ldots, \mathrm{I}_{subn}\right) \qquad \text{Eq. 2.12}$$

where: I_{min} is the lowest sub-index value;

I_{sub1} is the sub-index value of the first parameter (1, 2, …, n); and

I_{subn} is the sub-index value of the last parameter (1, 2, …, n).

Although the minimum operator method is free from the eclipsing and ambiguity problems, the operator function fails to provide a composite representation of the overall water quality. Since any change, other than the lowest quality variable is not reflected by Equation 2.12; consequently, it becomes inappropriate to aggregate sub-indices using such an insensitive model (Swamee and

Tyagi, 2000, Abbasi and Abbasi, 2012b). That is, the operator cannot be effectively employed to monitor water quality; hence the application of this method has been limited to few indices such as Oudin et al. (1999) and Hèbert (2005). These challenges promoted the birth of yet another aggregation method, namely the harmonic mean of squares method.

2.4.7.5 The harmonic mean of squares method

With an attempt to resolve the eclipsing problem by improving both the arithmetic mean formula and the geometric mean method, Dojlido et al. (1994) proposed the harmonic mean of squares method in the following form:

$$\mathrm{WQI} = \left[\frac{n}{\sum_{i=1}^{n}\left(\frac{1}{s_i^2}\right)}\right]^{0.5} \qquad \text{Eq. 2.13}$$

where: WQI is the aggregated index value;

n is the number of sub-indices; and

s_i is the i^{th} sub-index value.

If $s_i \neq 0$ for each i^{th} sub-index, then Equation 2.13 applies, but if $s_i = 0$ for any i^{th} sub-index, then the water quality index value will be zero (WQI = 0).

According to Cude (2001), the harmonic mean squares method allows the low-quality variables to influence the overall water quality index and further acknowledged that the technique significantly tolerates water quality variability with the change in parameter values. Regardless of such attributes, Swamee and Tyagi (2000) stated that the harmonic method has ambiguity problems. Such a situation occurs where the sub-indices are acceptable, but yet the overall index is not. In this case, the water might be of satisfactory quality, but the aggregation index declares it unacceptable (Sutadian et al., 2016).

With the continuous efforts of improving the aggregation techniques, Liou et al. (2004) proposed the combination of the additive and multiplicative methods.

2.4.7.6 Mixed aggregation method (a combination of additive and multiplicative methods)

Aiming to minimise the eclipsing and ambiguity problems, Liou et al. (2004) proposed a different approach, whereby water quality variables are grouped into three categories depending on their correlation characteristics. The clustered parameters are aggregated into group sub-indices using the additive method, and further of which, the group sub-indices are aggregated using the multiplicative method in the form of geometric mean model. Besides, the aggregated index is multiplied by three prefixed scaling coefficients, addressing the effects of temperature, pondus

Hydrogenium (pH) and toxic substances. The following is the general form of the combined aggregation method (Sutadian et al., 2016):

$$\mathrm{WQI} = c_{temp}c_{pH}c_{tox}\left[\left(\sum_{i=1}^{n}\mathrm{I}_i w_i\right)\left(\sum_{j=1}^{n}\mathrm{I}_j w_j\right)\left(\sum_{k=1}^{n}\mathrm{I}_k w_k\right)\right]^{\frac{1}{3}} \quad \text{Eq. 2.14}$$

where: WQI is the aggregated index value;

n is the number of sub-indices;

w_i is the i^{th} weight value for organic parameters;

w_j is the j^{th} weight value for particulate parameters;

w_k is the k^{th} weight value for faecal coliform;

I_i is the i^{th} sub-index value for organic parameters;

I_j is the j^{th} sub-index value for particulate parameters;

I_k is the sub-index value for faecal coliform;

c_{temp}, c_{pH} and c_{tox} are temperature, pondus Hydrogenium (pH) and toxic substance coefficients respectively.

Though with some modifications, Thi Minh Hanh et al. (2011) applied a similar hybrid summation method to aggregate the sub-indices of the Basic Water Quality Index (WQI_B). Furthermore, the same author multiplied the hybrid aggregation method with a geometric mean function to form a model, namely the Overall Water Quality Index (WQI_O).

Another useful technique was introduced in the development of the Canadian Council of Ministers of the Environment (CCME) WQI. A unique but simple method of calculating the final water quality index using the compliance objectives as established in the national water quality standards.

2.4.7.7 CCME method

Conceptually, the Canadian Council of Ministers of the Environment (CCME) method consists of three factors, namely, scope (F_1), frequency (F_2) and amplitude (F_3). The first factor, scope (F_1) institutes the number of parameters that are not complying with the water quality standards. Whereas, the second factor, frequency (F_2) defines the number of occasions with which the objectives are not met. Finally, the third factor, amplitude (F_3) describes the magnitude of deviation; that is, the amount by which the targeted goals are not met (CCME, 2001a, 2001b, Lumb et al., 2011a, Sutadian et al., 2016). Further details regarding this method are documented under Section 2.4.8 of this study. The following formula represents the CCME aggregation function:

$$\mathrm{WQI} = 100 - \left(\frac{\sqrt{F_1^2 + F_2^2 + F_3^2}}{1.732} \right) \quad \text{Eq. 2.15}$$

where: WQI is the final index value;

F_1 is the scope ("failed variables");

F_2 is the frequency ("failed tests");

F_3 is the amplitude (magnitude of failed tests"); and

1.732 is a factor to normalise the WQI to a maximum value of 100.

Even though Tyagi et al. (2013) have mentioned that the first factor (F_1) does not work correctly when too few variables are considered or when too much covariance exists among them, the CCME method has gathered widespread and applied in various water quality indices (that is, Khan et al., 2003, Davies, 2006, Boyacioğlu, 2007, Tobin et al., 2007, de Rosemond et al., 2009, Terrado et al., 2010, Lumb et al., 2011b, Nikoo et al., 2011, Sharma and Kansal, 2011, Espejo et al., 2012, Hurley et al., 2012, Damo and Icka, 2013, Mostafaei, 2014).

Each aggregation method has its problems; therefore, the developer has to decide on the most appropriate and relevant approach, preferably with minimum issues that might negatively impact on the final water quality index. Otherwise, the selection of the best aggregation method is close to impossible. Since there is no one straightforward and favourable method of developing WQIs, several tools have been developed for specific regions, using different water quality variables and distinctive analytical techniques.

And for the same reasons, there is continuing interest to develop accurate water quality indices. Such vital tools provide a simple and concise method of expressing water quality, and their significance is readily appreciated. The most significant water quality indices (WQIs) are discussed in the following section.

2.4.8 Existing water quality indices (WQIs)

Since Horton (1965), suggested the first numerical water quality index (WQI), there have been several more water quality indices developed (Bharti and Katyal, 2011). However, most of such WQIs are founded on similar structures and principles; the only realisable distinctions are the application boundaries and parameters involved. In general, "conventional" water quality indices are based on comparing observed parameter values with the existing local normative standards (Debels et al., 2005, Sun et al., 2016b).

There are two commonly used methods to develop water quality indices, with subsequent modifications. First, the weighted sum method, whereby the index score is generated using sub-indices which are combined further to become an overall WQI value. Sub-indices are value functions used to convert the different units of water quality variables to a mutual scale (Boyacioğlu, 2007, Banda, 2015). Second, the amplitude technique (objective-based), where overall water quality index value is founded through quantifying the extent at which water quality variables deviate from the objectives (CCME, 2001a, Khan et al., 2005, Radwn, 2005, Mostafaei, 2014). Both methods can further be deduced into various mathematical models, though with the same scope and outcomes.

Although the study investigated forty water quality indices (WQIs), only fifteen WQIs are discussed in the following sub-sections. Covering all the existing WQIs in this study is out of reach, hence commonly used and perceived as important WQIs are discussed in detail. Nonetheless, the rest of the reviewed WQIs are presented in summary under Annexure A of this study.

2.4.8.1 Horton model of water quality index (United States of America)

Horton (1965) established a simple mathematical technique of calculating water quality index, based on eight water quality variables, as indicated in Table 2.1. Rating scales between zero and hundred were assigned for each variable, and a weighting factor ranging from one to four was given to each parameter depending on its relative impact on the final index value. Weight factor of four was designated to parameters of high significance, whereas those of minimum impact were assigned a weight factor of one. The overall water quality index values ranged from zero to hundred, with lower scores representing poor water quality and vice versa (Debels et al., 2005, Lumb et al., 2011a, Lumb et al., 2011b). Equation 2.16 represents the mathematical formula suggested by Horton (1965):

$$\mathrm{WQI} = \left[\frac{w_1 s_1 + w_2 s_2 + w_3 s_3 + \ldots + w_n s_n}{w_1 + w_2 + w_3 + \ldots + w_n} \right] m_1 m_2 \qquad \text{Eq. 2.16}$$

where: WQI is the aggregated index value;

n is the number of water quality variables used to evaluate the WQI value;

s_n is the n^{th} sub-index value, which represents the rating number assigned to each variable ranging from zero to hundred;

w_n is the n^{th} weight factor ranging from one to four;

m_1 is the temperature correction factor; and

m_2 is the pollution correction factor.

In this case, the total number of water quality variables (n) is eight and the temperature correction factor (m_1) is regarded as 0.5 when the temperature is less than 34°C, otherwise 1. Whereas, the pollution correction factor (m_1) is either 0.5 or 1 depending on the degree of pollution which created colour or odour nuisance and this included the formation of sludge, deposits, presence of oil, debris, foam, etc. (Lumb et al., 2011a).

Table 2.1: Water quality variables for Horton's WQI

ID	Water quality variables		ID	Water quality variables	
	Description	Weight		Description	Weight
1	Alkalinity	1.0000	5	Dissolved oxygen	4.0000
2	Carbon chloroform extract	1.0000	6	pondus Hydrogenium (pH)	4.0000
3	Chlorides	1.0000	7	Sewage treatment	4.0000
4	Coliform density	1.0000	8	Specific conductance	1.0000

Source: Bhargava (1983), Lumb et al. (2011a)

Notes: Two other variables, namely temperature and obvious pollution appeared in the form of multiplicative factors, rather than observed parameter values; hence not considered as input parameters.

Bhargava (1983) pointed out that, the arithmetic weighted mean used by Horton (1965) lacked sensitivity to the effect of lowering the values of some of the water quality parameters and this drawback is commonly known as the eclipsing problem. Furthermore, according to Lumb et al. (2011b), one of the significant difficulties in Horton's concept was the arbitrariness in the selection of the index parameters, which led to the improvements suggested by Brown et al. (1970), as well as Deininger and Maciunas (1971).

2.4.8.2 National Sanitation Foundation WQI (United States of America)

Targeting to improve Horton's water quality model, Brown et al. (1970) established a more comprehensive and widely used water quality index. The National Sanitation Foundation (NSF) of the United States of America (USA) supported the development and application of the model; hence the water quality index is commonly referred to as NFS WQI. Although the NFS WQI is similar to Horton's Index, Brown et al. (1970) employed more rigorous attention and high precision in parameter selection, development of the rating curves and assigning of parameter weights. The National Sanitation Foundation water quality model comprises of eleven water quality variables (Brown et al., 1970, Low et al., 2016).

A team consisting of 142 water experts assisted in establishing the list of significant parameters, developing a standard ranking scale and assigning weights to the selected water quality variables. Brown et al. (1970) floated questionnaires based on a technique commonly known as the Rand Corporation's Delphi method. With it, expert opinion rating curves were developed to attribute the degree of water quality variation caused by different level of concentration of each chosen parameter (Wills and Irvine, 1996, Bharti and Katyal, 2011, Banda, 2015, Poonam et al., 2015). Utilising the established quality rating curves and associated parameter weights which are listed in Table 2.2, and the original NSF WQI is in the form of the additive model as represented in Equation 2.17 (Brown et al., 1972, Abbasi and Abbasi, 2012b):

$$\mathrm{WQI} = \sum_{i=1}^{n} w_i T_i(\rho_i) = \sum_{i=1}^{n} w_i q_i \qquad \text{Eq. 2.17}$$

where: WQI is the aggregated index value;

n is the number of sub-indices;

ρ_i is the measured value of the i^{th} parameter;

T_i is the quality rating transformation curve of the i^{th} parameter;

q_i is the individual parameter quality rating ($T_i \rho_i = q_i$); and

w_i is the i^{th} weight value such that $w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equation 2.17.

Table 2.2: Water quality variables for NSF WQI

ID	Water quality variables			ID	Water quality variables		
	Description	Impact	Weight		Description	Impact	Weight
1	Biochemical oxygen demand	0.6000	0.1100	**7**	Phosphates	0.6000	0.1000
2	Dissolved oxygen	1.0000	0.1700	**8**	Temperature	0.6000	0.1000
3	Faecal coliform density	0.9000	0.1600	**9**	Total solids	0.4000	0.0700
4	Nitrates	0.6000	0.1000	**10**	Turbidity	0.5000	0.0800
5	Pesticides	N/A	N/A	**11**	Toxic elements	N/A	N/A
6	pondus Hydrogenium (pH)	0.7000	0.1100				

Source: Brown et al. (1972), Abbasi and Abbasi (2012b), Low et al. (2016)

Notes: The total sum of weights of ALL the nine weighted parameters is equal to 1. Pesticides and toxic elements are not weighted and do not form part of the mathematical expression by Brown et al. (1970), (Brown et al., 1972). Instead, it was considered that if the total contents of detected pesticides or toxic elements (of all types) exceed 0.10 mg/ℓ, the overall water quality index value automatically registers zero.

The most obvious limitation of this technique is that it was developed for particular water quality variables; therefore, it does not recognise and describe specific water functions. Any alteration on the parameter listings, thus inclusion or exclusion of any water quality variable necessitates restarting the whole tedious process again. Although simple to comprehend, the weighted arithmetic formulation lacked sensitivity and fails to capture the effect of a single bad parameter value towards the overall WQI (Banda, 2015, Low et al., 2016).

2.4.8.3 Modified NSF WQI (United States of America)

Considering the flaws of the original National Sanitation Foundation (NSF) water quality index developed by Brown et al. (1970), subsequently, Brown et al. (1973) proposed the weighted geometric mean (multiplicative) function as a modification of the original NSF WQI. The multiplicative model was successfully adopted and considered more appropriate than the original additive model. However, both models have continued to be in use, regardless of the variation in prediction accuracy. The modified water quality index is expressed as follows (Bharti and Katyal, 2011, Lumb et al., 2011a, Abbasi and Abbasi, 2012b, Poonam et al., 2015):

$$\text{WQI} = \prod_{i=1}^{n} \text{S}_i^{wi} \qquad \text{Eq. 2.18}$$

where: WQI is the aggregated index value;

n is the number of sub-indices;

s_i is the i^{th} sub-index value; and

w_i is the i^{th} weight value and $w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equation 2.18.

Poonam et al. (2015), suggested that unweighted harmonic square mean formula can be employed to improve the weighted geometric mean formula. The inclusion of the harmonic procedure allows the most impaired parameter to impart the greatest influence on the WQI, hence offering the significance of different variables on overall water quality at different times and locations. The modified NSF WQI used the same water quality variables as the original NSF WQI, and they are presented in Table 2.2.

2.4.8.4 Scottish Research Development Department WQI (Scotland)

Similar to the National Sanitation Foundation (NSF) water quality index developed by Brown et al. (1970), the Engineering Division of Scottish Research Development Department (SRDD) developed a water quality index based on the Delphi method (SRDD, 1976). The index is commonly known as the Scottish water quality index (Scottish WQI) and operates with ten water quality indicators established using the Delphi technique. Sub-indices and individual parameter weights were developed through a convergence of water quality experts (Sutadian et al., 2016).

The ten water quality indicators and their respective weights are indicated in Table 2.3. The final modified weighted arithmetic function (modified additive), which is the result of squaring the sum of the products of parameter values (q_i), and of the individual variable weightings (w_i), divided by one hundred as demonstrated with the following Equation 2.19 (Bordalo et al., 2001, Bordalo et al., 2006, Dadolahi-Sohrab et al., 2012):

$$\text{WQI} = \frac{1}{100}\left(\sum_{i=1}^{n} q_i w_i\right)^2 \qquad \text{Eq. 2.19}$$

where: WQI is the aggregated index value;

n is the number of sub-indices;

q_i is the i^{th} sub-index value; and

w_i is the i^{th} weight value and $w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equation 2.19.

Table 2.3: Water quality variables for Scottish WQI

ID	Water quality variables		ID	Water quality variables	
	Description	Weight		Description	Weight
1	Ammonia (free and saline ammonia)	0.1200	**6**	Phosphates	0.0800
2	Biochemical oxygen demand (BOD_5)	0.1500	**7**	pondus Hydrogenium (pH)	0.0900
3	Conductivity	0.0600	**8**	Suspended solids	0.0700
4	Dissolved oxygen	0.1800	**9**	Temperature	0.0500
5	Escherichia coli (E. coli)	0.1200	**10**	Total oxidised nitrogen	0.0800

Source: Sutadian et al. (2016)

Notes: Parameters are listed according to alphabetic, other than the order of importance. The total sum of all weights is equal to one whole number.

Regardless of the Scottish WQI being developed for monitoring the water quality in Scotland watersheds, several researchers have modified this particular index and applied it in various countries, which includes Spain, Portugal, and Iran (see Bordalo et al., 2001, Bordalo et al., 2006, Carvalho et al., 2011, Dadolahi-Sohrab et al., 2012). Such widespread explains its appropriateness as a water quality monitoring tool.

2.4.8.5 Oregon water quality index (United States of America)

The Oregon water quality index (OWQI) was suggested by Dunnette (1979) and the index required enormous resources to calculate and produce the final index value which resulted in the index being discontinued in 1983 (Sutadian et al., 2016). Subsequently, Cude (2001) modified the original OWQI by adding two more variables (temperature and phosphorus), refining the sub-indices and improving the aggregation technique.

The original OWQI was modelled after the National Sanitation Foundation (NSF) water quality index, which applied the Delphi method for selecting the most significant parameters. Both Oregon water quality indices (as suggested by Dunnette, 1979, and Cude, 2001), utilised the logarithmic transform to covert water quality indicators into sub-indices. The advantage of this method is that a change in magnitude at lower levels of impairment has more significant impact than an equal shift in concentration at higher levels of impairment (Cude, 2001, Poonam et al., 2015). The original OWQI used the weighted arithmetic mean (additive) method and the modified index used the unweighted harmonic square mean function as shown by Equation 2.20 and Equation 2.21 respectively (Cude, 2001, Sarkar and Abbasi, 2006, Poonam et al., 2015):

$$\mathrm{WQI} = \sum_{i=1}^{n} \mathrm{SI}_i w_i \quad \text{Eq. 2.20}$$

$$\mathrm{WQI} = \sqrt{\frac{n}{\sum_{i=1}^{n} \frac{1}{\mathrm{SI}_i^2}}}$$ Eq. 2.21

where: WQI is the aggregated index value;

n is the number of sub-indices;

SI_i is the i^{th} sub-index value; and

w_i is the i^{th} weight value and $w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equation 2.20.

Table 2.4: Water quality variables for Oregon WQI

ID	Water quality variables	Dunnette (1979) OWQI		Cude (2001) OWQI	
		Include	Weight	Include	Weight
1	Biochemical oxygen demand (Unfiltered BOD_5)	Yes	0.1000	Yes	0.1250
2	Dissolved oxygen	Yes	0.4000	Yes	0.1250
3	Faecal coliform density	Yes	0.2000	Yes	0.1250
4	Nitrate + ammonia	Yes	0.1000	Yes	0.1250
5	Phosphorus	N/A	N/A	Yes	0.1250
6	pondus Hydrogenium (pH)	Yes	0.1000	Yes	0.1250
7	Temperature	N/A	N/A	Yes	0.1250
8	Total solids	Yes	0.1000	Yes	0.1250

Source: Dunnette (1979), Sutadian et al. (2016)

Notes: Parameters are listed according to alphabetic, other than the order of importance. The total sum of all weights is equal to one whole number.

Cude (2001) claimed that unequal weights are only applicable to water quality indices that are developed for a specific application, rather than general uses, where other parameters might contribute more to the index value than the others. Consequently, Cude (2001) employed an equal-weighted function for the modified OWQI (Sutadian et al., 2016).

2.4.8.6 Martínez de Bascarón water quality index (Spain)

Martínez de Bascarón (1979) suggested a twenty-six-parameter based water quality index specifically for Spain, and the index has been modified and applied in various studies for countries such as Argentina, Chile, Brazil, India, Spain and Turkey (refer to; Pesce and Wunderlin, 2000, Debels et al., 2005, Abrahão et al., 2007, Kannel et al., 2007, Sánchez et al., 2007, Koçer and Sevgili, 2014). Although Martínez de Bascarón (1979) recommended twenty-six variables, the index can easily allow the inclusion and exclusion of water quality indicators; hence it is regarded as a flexible water quality index (Abrahão et al., 2007, Sutadian et al., 2016). Originally, Martínez de Bascarón (1979), suggested the subjective water quality index (WQI_{sub}); whereby, the water quality index value is multiplied with a subjective constant representing the visual impression of the river contamination. WQI_{sub} is expressed as Equation 2.22 (Pesce and Wunderlin, 2000, Abrahão et al., 2007, Kannel et al., 2007, Sánchez et al., 2007, Poonam et al., 2015):

$$\text{WQI}_{sub} = k\frac{\sum_{i=1}^{n} C_i P_i}{\sum_{i=1}^{n} P_i} \quad \text{Eq. 2.22}$$

Such an equation overestimates the contamination level due to the application of the subjective constant, which is not necessarily correlated to the measured parameter values (Pesce and Wunderlin, 2000). Therefore, a modified version known as the objective water quality index (WQI_{obj}) was suggested and documented in the existing literature. In this case, the constant (k) is considered as one (k=1), thereby allowing the water quality index to represent only the variations caused by measured parameter values, without the influence of human judgement in the form of "visual impressions." The WQI_{obj} is expressed as Equation 2.23 (Debels et al., 2005, Abrahão et al., 2007, Kannel et al., 2007, Lumb et al., 2011a, Koçer and Sevgili, 2014):

$$\text{WQI}_{obj} = \frac{\sum_{i=1}^{n} C_i P_i}{\sum_{i=1}^{n} P_i} \quad \text{Eq. 2.23}$$

A selected few variables, mostly regarded as the crucially important water quality parameters, may be used to calculate the minimum water quality index (WQI_{min}). The WQImin method could be useful for routine monitoring exercises that require less precision. The WQI_{min} can be worked out using Equation 2.24 (Kannel et al., 2007, Koçer and Sevgili, 2014):

$$\text{WQI}_{\min} = \frac{\sum_{i=1}^{n} C_i P_i}{n} \quad \text{Eq. 2.24}$$

where: WQI_{sub} is the subjective water quality index value;
WQI_{obj} is the objective water quality index value;
WQI_{min} is the minimum water quality index value;
n is the number of sub-indices;
k is the subjective constant representing the visual impression of river contamination;
C_i is the value assigned to parameter i^{th} after normalisation; and
P_i is the relative weight assigned to the i^{th} parameter and ranges from 1 to 4 as highest.

The parameters applicable for WQI_{min} varies with the author, purpose of the evaluation, constantly available parameter readings, and desired level of accuracy. Nevertheless, the twenty-six variables, as suggested by Martínez de Bascarón (1979), together with their weighting factors, are indicated in Table 2.5.

Table 2.5: Water quality variables for Martínez de Bascarón WQI

ID	Water quality variables		ID	Water quality variables	
	Description	Weight		Description	Weight
1	Ammonia nitrogen	3.0000	**14**	Magnesium	1.0000
2	Apparent aspect	N/A	**15**	Nitrates	2.0000
3	Biochemical oxygen demand (BOD_5)	3.0000	**16**	Nitrites	2.0000
4	Calcium	1.0000	**17**	Oil and grease	2.0000
5	Chlorides	1.0000	**18**	Permanganate reduction	3.0000
6	Colour	2.0000	**19**	Pesticides	2.0000
7	Conductivity	4.0000	**20**	Phosphorus	1.0000
8	Cyanides	2.0000	**21**	pondus Hydrogenium (pH)	1.0000
9	Detergents	4.0000	**22**	Sodium	1.0000
10	Dissolved oxygen	4.0000	**23**	Sulphates	2.0000
11	Dissolved oxygen saturation percent	2.0000	**24**	Temperature	1.0000
12	Free carbon dioxide	3.0000	**25**	Total coliform	3.0000
13	Hardness	1.0000	**26**	Turbidity	4.0000

Source: Sutadian et al. (2016)

Notes: Parameters are listed according to alphabetic, other than the order of importance. The total sum of all weights is equal to fifty-five. Apparent aspect does not have any weighting.

Over the past years, several European studies have adopted and applied the Martínez de Bascarón (1979) water quality index (Lumb et al., 2011a), such widely spread use exhibits the flexibility of the index and its ability to be used with minimum water quality indicators (Abrahão et al., 2007). The challenge with the subjective water quality index (WQI_{sub}), is that; an individual without environmental or water quality background might exaggerate the subjective constant (k) that represents the "visual impression" of the river contamination which may lead to the presentation of distorted index values (Pesce and Wunderlin, 2000).

2.4.8.7 Bhargava's water quality index (India)

One of the first Asian based water quality index (Abbasi and Abbasi, 2012b), derived exclusively for the classification of water quality for drinking purposes (Lumb et al., 2011a). Unlike most indices, where sub-indices and weighting factors are considered separately; Bhargava (1983, 1985) developed sensitivity functions which account for both parameter concentrations and their weightage coefficients which are related to their level of importance towards the overall index calculation process (Al-Ani et al., 1987, Avvannavar and Shrihari, 2008, Lumb et al., 2011a, Abbasi and Abbasi, 2012b). Therefore, based on an approach where the significance of each water quality parameter is included within the sensitivity function, Bhargava (1983, 1985), suggested a simplified and rational model for calculating water quality index value as expressed by Equation 2.25:

$$\mathrm{WQI} = \left[\prod_{i=1}^{n} f_i(P_i)\right]^{\frac{1}{n}} \qquad \text{Eq. 2.25}$$

where: WQI is the water quality index value;

n is the number of variables considered more relevant; and

$f_i(P_i)$ is the sensitivity function of the i^{th} parameter, which includes the effects of the weighting of the i^{th} parameter.

Bhargava (1985) identified four-parameter groupings which included (1) coliform organisms, (2) toxicants, heavy metals, etc., (3) indicators that cause physical effects, that is, odour, turbidity, colour, etc., and (4) inorganic and organic, nontoxic substances such as chloride, sulphate, total dissolved solids, etc. The index sensitivity functions assumed values of 1.0, 0.8, 0.5, 0.2 and 0.1; which related to water quality index values of 100, 80, 50, 20 and 1 (almost zero), thus aligning to water class one to five respectively (Bhargava, 1983).

Bhargava (1985), argued that Brown et al. (1970) arithmetic mean (additive) index was not significantly sensitive to changes in the values of the water quality parameters, hence, he suggested a model in the multiplicative form. The multiplicative models are designed to eliminate the eclipsing problem since they respond well when sub-indices value almost reaches or equals to zero; the index will react accordingly and register a lower index value (Bhargava, 1983, Abbasi and Abbasi, 2012b). The parameter groupings sensitivity functions assumed Bhargava (1985) are indicated in Table 2.6.

Table 2.6: Water quality variables for Bhargava WQI

ID	Water quality variables Description	Sensitivity function
1	**Parameter Group I** Coliform organism, (coliform bacteria, etc.)	$f_i = \exp[-16(C-1)]$
2	**Parameter Group II** Heavy metals, other toxicants (chromium, lead, silver, etc.)	$f_i = \exp[-4(C-1)]$
3	**Parameter Group III** Physical variables (turbidity, colour, odour, etc.)	$f_i = \exp[-2(C-1)]$
4	**Parameter Group IV** Organic and inorganic nontoxic substances (chloride, sulphate, TDS, etc.)	$f_i = \exp[-2(C-1)]$

Source: Bhargava (1985), Abbasi and Abbasi (2012b), Poonam et al. (2015)

Notes: No particular weighting factors assigned to the variables; instead, the sensitivity functions are built to include the effect of the concentration and weight of the water quality parameter. Variable Group III and IV have similar sensitivity functions.

2.4.8.8 House's water quality index (United Kingdom)

In the United Kingdom (UK), House (1986, 1989, 1990) established four water quality indices. First, the general water quality index (WQI) for evaluating river health for regular monitoring programs. Second, the potable water supply index (PWSI) for assessing the quality and suitability of the potable water supply. Third, the aquatic toxicity index (ATI) developed to monitor the toxicity in the aquatic environment, and lastly; the fourth WQI, which was suggested for evaluating water quality for the wildlife population and the index is commonly known as the potable sapidity index (PSI). These four indices can be used separately or in combination, depending on the required outcome and level of accuracy desired (Sutadian et al., 2016). Nevertheless, this study focuses on the initially developed general water quality index; which is then referred to as House's water quality index (House's WQI).

The House's WQI was conceptually developed in the same manner as the National Sanitation Foundation water quality index (NSF WQI) of United States of America (Lumb et al., 2011a), where the nine water quality parameters and their weights are established using the Delphi method. Table 2.7 represents the nine water quality parameters and their relative weights as suggested by House (1986, 1989, 1990), and the aggregation formula is expressed as Equation 2.26.

$$\mathrm{WQI} = \frac{1}{100}\left(\sum_{i=1}^{n} q_i w_i\right)^2 \qquad \text{Eq. 2.26}$$

where: WQI is the aggregated index value;

n is the number of sub-indices;

q_i is the i^{th} sub-index value; and

w_i is the i^{th} weight value and $w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equation 2.26.

Table 2.7: Water quality variables for House's WQI

ID	Water quality variables		ID	Water quality variables	
	Description	Weight		Description	Weight
1	Ammoniacal nitrogen	0.1600	**6**	pondus Hydrogenium (pH)	0.0900
2	Biochemical oxygen demand (BOD_5)	0.1800	**7**	Suspended solids	0.1100
3	Chlorides	0.0400	**8**	Temperature	0.0200
4	Dissolved oxygen	0.2000	**9**	Total coliforms	0.1100
5	Nitrates	0.0900			

Source: House (1986, 1989), Tyson and House (1989), House (1990), Sutadian et al. (2016)

Notes: Parameters are listed according to alphabetic, other than the order of importance. The total sum of all weights is equal to one whole number. The PWSI, ATI and PSI water quality parameters are not listed, refer to House (1990).

Index values produced by various aggregation methods were tested and authenticated to select the most feasible aggregation technique. Accordingly, the modified arithmetic formula suggested by SRDD (1976) in the development of the Scottish WQI was found more suitable and adopted as the WQI for river management by House (1989). The WQI developed by House (1986, 1989) can be applied objectively and produces results which are reproducible and repeatable manner, both temporally and spatially (House, 1989). Thereby allowing a structured comparison of various data sets, providing a precise picture of water quality variability and facilitating the development of best management practices (House, 1990).

2.4.8.9 Smith's water quality index for river systems (New Zealand)

Water quality index (WQI) developed by Smith (1987, 1990) is a hybrid of two standard practices available for water quality indices formation; that is, the application of both water quality standards and the Rand Corporation's Delphi method. The Delphi procedure was used to establish significant parameters, develop sub-indices and to assign relative parameter weight coefficients. Eventually, Smith (1987, 1990) applied the minimum operator technique to calculate the final index scores and the model is expressed in Equation 2.27 (Smith, 1987, 1990, CCME, 2001a, Bharti and Katyal, 2011, Poonam et al., 2015):

$$\mathrm{I}_{min} = \sum \min\left(\mathrm{I}_{sub1}, \mathrm{I}_{sub2}, \ldots, \mathrm{I}_{subn}\right) \qquad \text{Eq. 2.27}$$

where: I_{min} is the lowest sub-index value;

I_{sub1} is the sub-index value of the first parameter (1, 2, …, n); and

I_{subn} is the sub-index value of the last parameter (1, 2, …, n).

Smith's WQI was developed for four water applications, which are bathing, water supply, fish spawning (salmonids) and general uses. The index comprises of a maximum of eight water quality variables, grouped differently for each particular application, with specific weighting factors relevant to specific water use. However, the relative weights are redundant since Smith (1987) eventually omitted the application of the multiplicative indexing model. The eight water quality variables are included in Table 2.8 and Table 2.9.

Table 2.8: Water quality variables for Smith's WQI (water supply & fish spawning)

ID	Water quality variables	Water supply use			Fish spawning use		
		Include	Impact	Weight	Include	Impact	Weight
1	Ammonia	Yes	2.59	0.1600			
2	Biochemical oxygen demand (Unfiltered BOD_5)	Yes	N/A	N/A	Yes	2.48	0.1400
3	Dissolved oxygen	Yes	2.38	0.1800	Yes	1.00	0.3400
4	Faecal coliform density	Yes	1.78	0.2400			
5	pondus Hydrogenium (pH)	Yes	2.79	0.1500	Yes	2.81	0.1200
6	Suspended materials	Yes	2.82	0.1500	Yes	2.41	0.1400
7	Temperature	Yes	3.59	0.1200	Yes	1.35	0.2600
8	Turbidity	Yes	N/A	N/A			

Source: Smith (1987, 1990), and Sutadian et al. (2016)

Notes: The water supply index used all the nine parameters, whereas the fish spawning index only used five out of the nine listed variables. The biochemical oxygen demand (unfiltered BOD_5) and turbidity were not included in the initially proposed multiplicative model, but later included in the minimum operator index for water supply uses; hence their weights and impact rating is not available.

Table 2.9: Water quality variables for Smith's WQI (bathing & general use)

ID	Water quality variables	Bathing use			General use		
		Include	Impact	Weight	Include	Impact	Weight
1	Ammonia						
2	Biochemical oxygen demand (Unfiltered BOD_5)	Yes	2.23	0.1500	Yes	2.20	0.1800
3	Dissolved oxygen	Yes	2.15	0.1500	Yes	1.33	0.3000
4	Faecal coliform density	Yes	1.00	0.3200	Yes	3.18	0.1200
5	pondus Hydrogenium (pH)	Yes	3.10	0.1000	Yes	3.13	0.1300
6	Suspended materials	Yes	1.73	0.1900	Yes	2.57	0.1500
7	Temperature	Yes	3.78	0.0900	Yes	3.15	0.1200
8	Turbidity	Yes	N/A	N/A	Yes	N/A	N/A

Source: Smith (1987, 1990), and Sutadian et al. (2016)

Notes: Both bathing and general use indices utilise seven similar parameters, and both WQI tools exclude ammonia in their indexing model. Turbidity was not included in the initially proposed multiplicative model, but later included in the minimum operator index for both bathing and general uses; hence its weight and impact rating is not available.

The simplicity and flexibility of the minimum operator index make it easier to implement, without ambiguity or eclipsing problems. However, the accuracy of Smith's water quality index (WQI) is questionable, since the model can only retain the minimum sub-index value, without considering the effects of the rest of the sub-indices. The problem implies that the composite picture of water quality is compromised; since any change, other than the minimum sub-index value is not reflected in the overall WQI. Such an insensitive operator is unsuitable for aggregation; that is, it can work for neither a single source monitoring nor for comparing two different sources (Swamee and Tyagi, 2000, Abbasi and Abbasi, 2012b). The situations elaborate on why the application of the minimum operator technique has been limited to a few water quality indices (see Oudin et al., 1999, Hèbert, 2005).

2.4.8.10 British Columbia WQI (Canada)

In 1995, the Canadian government, under the guidance of the Ministry of Environment, Lands and Parks established water quality index (WQI) for the British Columbia Province (Zandbergen and Hall, 1998, Bharti and Katyal, 2011). The BCWQI is an objective-based index similar to the Canadian Council of Ministers of the Environment (CCME) WQI. However, one of the factors is not considered in any of the other indices, which factor is the percentage of water quality guidelines exceeded (F_1). The following mathematical expression is used for British Columbia WQI (Zandbergen and Hall, 1998, CCME, 2001a, Bharti and Katyal, 2011):

$$\mathrm{WQI} = \left(\frac{\sqrt{F_1^2 + F_2^2 + \left(F3/3\right)^2}}{1.453} \right) \qquad \text{Eq. 2.28}$$

where: WQI is the overall water quality index value;

F_1 is the percentage of water quality guidelines exceeded;

F_2 is the frequency with which objectives not met as a percentage of objectives checked;

F_3 is the maximum by which any of the guidelines were exceeded; and

1.453 is the factor to normalise the WQI to a maximum value of 100.

Two factors are comparable to other water quality indices (WQIs). The index factor two (F_2) is similar to the Alberta index, whereas, factor three (F_3) corresponds to Centre St Laurent index. Whilst factor one (F_1) does not appear in any of the other WQIs. It was found that BCWQI is exceptionally sensitive to sampling design and highly dependent on the specific application of water quality objectives. Furthermore, the British Columbia index in its original form has serious limitations for comparing water bodies and for establishing management priorities (Zandbergen and Hall, 1998, Said et al., 2004). However, comparable to the Council of Ministers of the Environment water quality index (CCME WQI), the British Columbia WQI is flexible and adaptive to various applications (CCME, 2001a).

2.4.8.11 Canadian Council of Ministers of the Environment WQI (Canada)

The CCME water quality index (CCME WQI) is a modification of the British Columbia water quality index (BCWQI). Similar to the British Columbia index, the CCME WQI comprises of three factors regarded as, (i) scope, (ii) frequency and (iii) amplitude (CCME, 2001a, Khan et al., 2005, Radwn, 2005, Alberta, 2008, 2011, Abbasi and Abbasi, 2012b). The composition of the CCME index and the three factors are discussed as follows:

(i) **Factor 1 - Scope (F_1):** This factor quantifies the water quality variables that do not meet water quality objectives; which explains the extent of water quality non-compliance over a specific period of concern (percentage of parameters that do not meet objectives). Factor 1 is calculated using the following Equation 2.29.

$$F_1 = \frac{\text{number of failed variables}}{\text{total number of variables}} \times 100 \qquad \text{Eq. 2.29}$$

(ii) **Factor 2 - Frequency (F_2):** This factor describes how frequently does measurement not meet water quality objectives. The factor is the percentage of individual tests that fail to meet objectives (“failed tests”), and test refers to an individual parameter value per observation. Equation 2.30 is applied to calculate frequency.

$$F_2 = \frac{\text{number of failed tests}}{\text{total number of tests}} \times 100 \qquad \text{Eq. 2.30}$$

(iii) **Factor 3 - Amplitude (F_3):** This factor represents how much do measurements not meet objectives. Which is the amount by which failed test values do not meet their objectives. Unlike the scope and frequency factors, the amplitude factor is calculated in three steps. The first step involves the calculation of the excursion, which is the number of times by which an individual variable is greater than or less than the water quality objective, and is defined in two ways. Scenario A, represented by Equation 2.31, that is ideal when the test value must not exceed water quality objective and Equation 2.32, applies to Scenario B, whereby the test value must not fall below water quality objective.

$$\text{excursion}_i = \left(\frac{\text{failed test value}_i}{\text{objective}_j}\right) - 1 \qquad \text{Eq. 2.31}$$

$$\text{excursion}_i = \left(\frac{\text{objective}_j}{\text{failed test value}_i}\right) - 1 \qquad \text{Eq. 2.32}$$

The second step involves the calculation of the normalised sum of excursions (*nse*). That is, the collective amount by which individual tests are out of compliance is calculated by summing the excursion of individual tests from their objectives and dividing by the total number of tests. The normalised sum of excursions (*nse*) is denoted by the following Equation 2.33.

$$nse = \frac{\sum_{i=1}^{n} \text{excursion}_i}{\text{total number of tests}} \qquad \text{Eq. 2.33}$$

Upon that, the third step can be performed, which covers the calculation of the amplitude factor. Amplitude is derived by an asymptotic function that scales the normalised sum of excursion (*nse*) from water quality objectives to yield a value ranging from zero to a hundred. The following Equation 2.34 is applicable when calculating the amplitude factor.

$$F_3 = \left(\frac{nse}{0.01nse + 0.01}\right) \qquad \text{Eq. 2.34}$$

Finally, using the scope factor (F_1), frequency factor (F_2) and amplitude factor (F_3); the overall water quality index is obtained using Equation 2.35 as follows (Nikoo et al., 2011, Hurley et al., 2012):

$$\mathrm{WQI} = 100 - \left(\frac{\sqrt{F_1^2 + F_2^2 + F_3^2}}{1.732} \right) \quad \text{Eq. 2.35}$$

where: WQI is the final index value;

nse is the normalised sum of excursions;

n is the total number of the excursions;

F_1 is the scope (“failed variables”);

F_2 is the frequency (“failed tests”);

F_3 is the amplitude (magnitude of failed tests”); and

1.732 is a factor to normalise the WQI to a maximum value of 100.

Since each of the three factors values can reach as high as hundred, it means that the vector length $(100^2 + 100^2 + 100^2)^{0.5}$ can reach 173.2, hence the factor 1.732 was introduced into the index model to contain the index values not to exceed a maximum of hundred (Lumb et al., 2006).

Considering that the CCME technique does not require statistically defined data to function, it is beneficial in the sense that, it provides leverage to alter the selection of water quality variables. Because of this, the CCME WQI is a flexible tool adaptable to accommodate various water quality parameters, as long as the appropriate pollution limits are adequately defined. These attributes explain the widespread and application of the Canadian Council of Ministers of the Environment water quality index (refer to, Khan et al., 2003, Davies, 2006, Boyacioğlu, 2007, Tobin et al., 2007, de Rosemond et al., 2009, Terrado et al., 2010, Lumb et al., 2011b, Nikoo et al., 2011, Sharma and Kansal, 2011, Espejo et al., 2012, Hurley et al., 2012, Damo and Icka, 2013, Mostafaei, 2014).

2.4.8.12 Liou’s water quality index (Taiwan)

Liou et al. (2004), employed a distinctive river status index (RSI) for monitoring Keya River in Taiwan. The index is a hybrid of the additive and multiplicative model, which relay on six water quality variables as listed in Table 2.10. Based on the principal component analysis (PCA), the water quality variables are categorised into three groups, namely organics, particulates and microorganisms. The overall index consists of three phases. Firstly, an additive model employed to aggregate the grouped variables into group sub-indices. Secondly, the multiplicative function used to aggregate the three group sub-indices and further multiplied by three prefixed coefficients which address the effects of temperature, pondus Hydrogenium (pH) and toxic substances (Liou et al., 2004, Sutadian et al., 2016). The index proposed by Liou et al. (2004) is defined as follows:

$$\mathrm{RSI} = C_{temp} C_{pH} C_{tox} \left[\left(\sum_{i=1}^{3} \mathrm{I}_i w_i \right) \left(\sum_{j=1}^{2} \mathrm{I}_j w_j \right) \left(\sum_{k=1}^{1} \mathrm{I}_k w_k \right) \right]^{\frac{1}{3}} \qquad \text{Eq. 2.36}$$

Equal weights are assigned for the variables associated in the same category, that is, organic variables are assigned a weighting factor of 0.33. In contrast, particulates are given a coefficient of 0.50 and microorganisms retain factor of 1.00 since only one variable is associated with this group. Thus, satisfying the following:

$$\sum_{i=1}^{n} w_i = 1; \sum_{j=1}^{n} w_j = 1; \text{and} \sum_{k=1}^{n} w_k = 1 \qquad \text{Eq. 2.37}$$

where: RSI is the aggregated index value;

n is the number of sub-indices;

w_i is the i^{th} weight value for organic parameters;

w_j is the j^{th} weight value for particulate parameters;

w_k is the k^{th} weight value for microorganisms;

I_i is the i^{th} sub-index value for organic parameters;

I_j is the j^{th} sub-index value for particulate parameters;

I_k is the sub-index value for microorganisms; and

c_{temp}, c_{pH} and c_{tox} are temperature, pondus Hydrogenium (pH) and toxic substance coefficients respectively.

Table 2.10: Water quality variables for Liou's WQI

ID	Water quality variables			ID	Water quality variables		
	Description	Group	Weight		Description	Group	Weight
1	Ammonia nitrogen	A	0.33	**4**	Suspended solids	B	0.50
2	Biochemical oxygen demand	A	0.33	**5**	Temperature	B	0.50
3	Dissolved oxygen	A	0.33	**6**	Facial coliforms	C	1.00

Source: Liou et al. (2004)

Notes: Three other variables, namely pondus Hydrogen (pH), temperature and toxicity, appeared in the form of multiplicative factors, rather than observed parameter values; hence not considered as input parameters. Group A is the organics; Group B is the particulates, and Group C is the microorganisms. The sum of all the group weighting is 1 per each category as defined in Equation 2.37.

The concern of eclipsing and ambiguity occurring from aggregation and or a large number of water quality variables was minimised through categorisation of parameters and assigning appropriate mathematical functions. From the proposed hybrid function; if any of the parameters approach zero value, the overall index responds accordingly lowering the river status index value towards zero (Liou et al., 2004).

2.4.8.13 Fuzzy-based water quality index (Spain)

Fuzzy-based water quality index (FWQI) is one of the most useful tools developed by Ocampo-Duque et al. (2006) for assessing the water quality of the Ebro river in Spain. FWQI is a rule-based fuzzy model that deals with non-linear, but ill-defined, mapping of input variables to appropriate outputs (Nikoo et al., 2011). That is, a linguistic description is assigned to each fuzzy set, and then, the rule-sets are named based on a perceived degree of quality ranging from poor to excellent (Lermontov et al., 2009). Fuzzy logic data sets allow the inclusion of the qualitative aspects of human knowledge and reasoning process, through qualitative conditional expressions with verbal meaning, without employing precise quantitative analysis (Nikoo et al., 2011).

The method of modelling using intrinsically vague linguistic knowledge is based on the mathematics of fuzzy sets originally suggested by Zadeh (1965) and further explored by various water scientists including Ocampo-Duque et al. (2006), Lermontov et al. (2009), Nikoo et al. (2011), Ocampo-Duque et al. (2013), and Wardhany et al. (2018) The FWQI for Ebro river in Spain uses a comprehensive set of twenty-seven water quality variables, divided into five parameters groupings as indicated in Table 2.11.

Table 2.11: Water quality variables for Fuzzy-based WQI

ID	Water quality variables		ID	Water quality variables	
	Description	Indicator Group		Description	Indicator Group
1	Conductivity	Primary	**15**	Phosphates	Anions (cont.)
2	Dissolved oxygen		**16**	Sulphates	
3	pondus Hydrogenium (pH)		**17**	Arsenic	Priority element
4	Suspended solids		**18**	Atrazine	
5	Biochemical oxygen demand	Organic matter	**19**	Benzene (BTEX)*	
6	Total organic carbon		**20**	Chromium	
7	Faecal coliform	Microbiology	**21**	Hexachlorbutadiene	
8	Faecal streptococcus		**22**	Lead	
9	Salmonellas		**23**	Mercury	
10	Total coliforms		**24**	Nickel	
11	Ammonia	Anions	**25**	Polycyclic aromatic hydrocarbons	
12	Chlorides		**26**	Simazine	
13	Fluorides		**27**	Trichlorobenzenes	
14	Nitrates				

Source: Ocampo-Duque et al. (2006), Abbasi and Abbasi (2012a)

Notes: *Benzene-toluene-ethylbenzene-xylenes (BTEX). Ninety-six rules were enunciated in the following order, three for each indicator, and three for each partial score into groups. Each rule had only one antecedent to facilitate the weight assignment.

The index operates with ninety-six linguistic data rules, three for each parameter and three for each partial group score. Ocampo-Duque et al. (2006) used trapezoidal membership functions to represent the various fuzzy sets, and the rule-sets are derived from Equation 2.38. Whereas the final index score is achieved by Equation 2.39:

$$\mu(x;a,b,c,d) = \max\left(\min\left(\frac{x-a}{b-a},1,\frac{d-x}{d-c}\right),0\right) \qquad \text{Eq. 2.38}$$

$$\text{FWQI} = \frac{\int \mu(z) \bullet z\mathrm{d}z}{\int \mu(z) z\mathrm{d}z} \qquad \text{Eq. 2.39}$$

where: FWQI is the fuzzy-based water quality index value (between 0 and 100);

z is the independent variable of the fuzzy output set in each rule; and

a, b, c, and d are membership function parameters as summarised in Table 2.11.

Though regarded as less accurate than the traditional numerical indices, water quality models based on fuzzy rules are perceived as adequate tools to represent uncertainties and inaccuracies in knowledge and data. The advantages brought by the simplicity, flexibility and computational speed of fuzzy-based models, may successively compensate for the loss in accuracy (Lermontov et al., 2009). Hence the choice on applicable methodologies depends on whether the index developer is concerned with precision, or simplicity and computational capabilities. Of which, the debate is biased towards the purpose of the water quality index.

2.4.8.14 Universal water quality index – Boyacioğlu index (Turkey)

An index that describes the appropriateness of surface water for drinking purposes was developed by Boyacioğlu (2007) and the model is commonly known as the universal water quality index (UWQI). The indexing tool utilises twelve water quality variables to describe the quality of drinking water and the parameters are listed in Table 2.12.

Table 2.12: Water quality variables for universal water quality index (UWQI)

ID	Water quality variables			ID	Water quality variables		
	Description	Impact	Weight		Description	Impact	Weight
1	Arsenic	4	0.113	**7**	Mercury	3	0.086
2	Biochemical oxygen demand	2	0.057	**8**	Nitrate - Nitrogen	3	0.086
3	Cadmium	3	0.086	**9**	pondus Hydrogenium (pH)	1	0.029
4	Cyanide	3	0.086	**10**	Selenium	3	0.086
5	Dissolved oxygen	4	0.114	**11**	Total coliform	4	0.114
6	Fluoride	3	0.086	**12**	Total phosphorus	2	0.057

Source: Boyacioğlu (2007), Abbasi and Abbasi (2012b), Boyacioğlu and Gündoğdu (2013), Sutadian et al. (2016)

Notes: Higher weightage was assigned to parameters related to health matters, whereas chemical parameters were assigned lower weighting than microbiological parameters.

Temporary weights ranging from one to four on a basic scale of importance were assigned to the water quality parameters. After that, provisional weights were divided by the sum of all the initial impact factors to establish the final weighting coefficients. The UWQI uses the weighted sum method to aggregate the twelve sub-indices, and the formula is as follows (Boyacioğlu, 2007, Abbasi and Abbasi, 2012b, Boyacioğlu and Gündoğdu, 2013):

$$\mathrm{WQI} = \sum_{i=1}^{n} w_i \mathrm{I}_i \qquad \text{Eq. 2.40}$$

where: WQI is the universal water quality index value;

w_i is the weighted coefficient for the i^{th} water parameter;

I_i sub-index for the i^{th} water parameter; and

n total number of the ranked water parameters.

The universal water quality index (UWQI) is based on permissible limits of relevant water quality standards set by the Council of European Communities and the Turkish water pollution control regulations. Unlike most of the existing indices which are based on particular national water quality standards, UWQI was developed by considering multi-national standards, thus ultimately extending its application boundaries. Similar to Boyacioğlu (2007) study, the purpose of this study includes the development of a universal water quality index suitable for use across various catchment areas in South Africa, which may be distinct in their characteristics. By so doing, we ascertain the functionality of the WQI, improve simplicity and expand the application boundaries of the model.

2.4.8.15 Vaal water quality index (South Africa)

Banda (2015) developed an index for evaluating surface waters, particularly for the Vaal Basin in South Africa, hence the term Vaal water quality index (Vaal WQI). The index comprises of fifteen critical water quality parameters as indicated in Table 2.13.

Table 2.13: Water quality variables for Vaal WQI

ID	Water quality variables			ID	Water quality variables		
	Description	Impact	Weight		Description	Impact	Weight
1	Ammonia/Ammonium	5	0.0962	**9**	Manganese	5	0.0962
2	Calcium	2	0.0385	**10**	Nitrate/Nitrite	5	0.0962
3	Chloride	3	0.0577	**11**	Orthophosphate	4	0.0769
4	Chlorophyll 665	1	0.0192	**12**	pondus Hydrogenium (pH)	5	0.0962
5	Electrical conductivity	3	0.0577	**13**	Sulphate	3	0.0577
6	Fluoride	5	0.0962	**14**	Total alkalinity	3	0.0577
7	Hardness	3	0.0577	**15**	Turbidity	3	0.0577
8	Magnesium	2	0.0385				

Source: Banda (2015)

Notes: The ranking coefficients are depended on the toxic effects of the pollutant. Death due to short term exposure being the highest in the order of the impact is therefore ranked five. Whereas death because of long term exposes ranked four. Ranking three and two represents debilitating effects due to immediate exposure and long-term exposure, respectively—whilst a minimum score of one express the hierarchy of water quality variable with effects of slightest significance.

A ranking criterion with five levels was adopted for the Vaal WQI, whereby the maximum score of five being the highest order and minimum score of one expressing the ranking of variables with effects of the slightest significance. The rankings were assigned separately for human and environmental health effects and later combined to form single aggregated ranking value; thus, selecting the highest of both the human and environmental impact. The final weight coefficients were then formulated using Equation 2.41 and the overall classification of water quality is achieved through the weighted sum method (additive) as represented by Equation 2.42 (Banda, 2015).

$$w_i = \frac{b_i}{\sum_{i=1}^{n} b_i} \qquad \text{Eq. 2.41}$$

$$\text{WQI} = \sum_{i=1}^{n} w_i \mathrm{I}_i \qquad \text{Eq. 2.42}$$

where: WQI is the universal water quality index value;

b_i is the assigned ranking of the i^{th} water parameter (1 minimum and maximum of 5);

w_i is the weighted coefficient for the i^{th} water parameter (decimal value);

I_i sub-index for the i^{th} water parameter; and

n total number of the ranked water parameters.

The coefficients are represented as decimal numbers, and the sum of all coefficients is one, thereby guaranteeing that the overall index value does not exceed hundred per cent ($w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equations 2.41 and 2.42).

The Vaal WQI is specific to the Vaal Basin, hence restrict its application boundaries. And this study attempts to break such barriers, through the development of a universal index that applies to most river catchments in South Africa. Thereby promoting a standardised way of monitoring and comparing water quality of various watersheds in South Africa, which eventually assist in the prioritisation of water resources across all the nine provinces of South Africa.

The fifteen water quality indices (WQIs) discussed under Chapter Two, Section 2.4.8 are summarised in Annexure A: Details of reviewed water quality indices (WQIs) and Annexure B: Aggregation formulation of the reviewed WQIs. The summaries include application boundaries, water quality parameters, type of sub-indices and aggregation method used in the formulation of the index score. For comparison and benchmarking purposes, it is common practice that water quality index values be presented and described as classes. The categories and details of each index rank are discussed in the following section.

2.4.9 Water classification and index scores

Water quality index scores can be classified in two different ways. The first approach is whereby the index value increases with the decrease in contamination level. This approach is referred to as the increasing scale indices. The second approach is where the index value decreases with the degree of pollution. This approach is referred to as the decreasing scale indices. Nevertheless, the purpose of scaling is the same; both indices reflect water quality based on pollution levels (Banda, 2015). The assignment of water quality index values to classes of water quality is termed "categorisation" or "classification" and indicates an imperative but somewhat subjective process. The classification should be based on the best available information, expert judgment, and the general public's expectations of water quality (CCME, 2001a).

Typically, water quality index values are between zero and one hundred (0 to 100) and classified in categories ranging from class 1 to class 5. The meaning of the index values and classes depends on whether the model is an increasing or decreasing scale index and typical examples are included in Table 2.14 and Table 2.15, for increasing scale indices and decreasing scale indices respectively.

Table 2.14: Typical WQI classification for increasing scale index

Class	**Increasing scale water quality indices**					
	House, Bordalo & Carvalho WQI		CCME WQI		Universal & Vaal WQI	
	Rank	Index score	Rank	Index score	Rank	Index score
Class 1	Very good	91 to 100	Excellent	95 to 100	Excellent	95 to 100
Class 2	Good	71 to 90	Good	80 to 94	Good	75 to 94
Class 3	Reasonable	51 to 70	Fair	65 to 79	Fair	50 to 74
Class 4	Polluted	26 to 50	Marginal	45 to 64	Marginal	25 to 49
Class 5	Badly polluted	10 to 25	Poor	0 to 44	Poor	0 to 24

Source: CCME (2001a), Bordalo et al. (2006), Boyacioğlu (2007), Carvalho et al. (2011), Banda (2015)

Notes: House WQI: House's water quality index (United Kingdom), Bordalo WQI: Bordalo et al water quality index (Iberian Peninsula: Portuguese-Spanish Border), Carvalho WQI: Carvalho et al water quality index (Portugal), CCME WQI: Canadian Council of Ministers of the Environment WQI (Canada), Universal WQI: Universal water quality index – Boyacioğlu index (Turkey) and Vaal WQI: Vaal water quality index (South Africa).

A significant gap identified in most of the water quality classification scales is that not all possible index scores are accommodated in various WQ classification systems reviewed under this study. For instances, considering a classification schema by Rao et al. (2010), index score values between 25-26; 50-51; and 75-76 cannot be categorised, unless otherwise, the final index score is rounded off to a whole number, which is not the case with most of the research work investigated under this chapter. Some of the water quality indices with similar challenges include Kannel et al. (2007), Ramakrishnaiah et al. (2009), Al Obaidy et al. (2010), Yadav et al. (2010), Khanna et al. (2013), Rao and Nageswararao (2013), Bhadra et al. (2014), Sharma et al. (2014), Banda (2015), Meher et al. (2015), AL-Sabah (2016), Sudha et al. (2016), Wanda et al. (2016), Abdel-Satar et al. (2017), and Ewaid and Abed (2017b).

Table 2.15: Typical WQI classification for decreasing scale index

Class	Decreasing scale water quality indices					
	BCWQI		Rao, Vatkar & Vasanthavigar WQI		Rao et al WQI	
	Rank	Index score	Rank	Index score	Rank	Index score
Class 1	Excellent	0 to 3	Excellent	< 50	Excellent	0 to 25
Class 2	Good	4 to 17	Good	50.1 to 100	Good	26 to 50
Class 3	Fair	18 to 43	Poor	100.1 to 74	Bad	51 to 75
Class 4	Borderline	44 to 59	Very poor	25 to 49	Very bad	76 to 100
Class 5	Poor	60 to 100	Unsuitable	> 300	Unfit	100 and above

Source: Zandbergen and Hall (1998), Rao et al. (2010), Vasanthavigar et al. (2010), Rao and Nageswararao (2013), Vatkar et al. (2016)

Notes: BCWQI: British Columbia water quality index (Canada), Rao WQI: Rao and Nageswararao water quality index (India), Vatkar WQI: Vatkar et al water quality index (India), Vasanthavigar WQI: Vasanthavigar et al water quality index (India) and Rao et al WQI: Rao et al water quality index (India).

Table 2.16: Index score classification for Martínez de Bascarón WQI

ID	Water quality classification	
	Description of rank and classification	Index score
1	**Class I – Good water quality** Water quality is protected with a virtual absence of threat or impairment; conditions very close to natural or pristine levels	91 ≤ Index ≤ 100
2	**Class II – Acceptable water quality** Water quality is usually protected with only a minor degree of threat or impairment; conditions rarely depart from natural or desirable levels	61 ≤ Index < 91
3	**Class III – Regular water quality** Water quality is usually protected but occasionally threatened or impaired; conditions sometimes depart from natural or desirable levels	31 ≤ Index < 61
4	**Class IV – Bad water quality** Water quality is frequently threatened or impaired; conditions often depart from natural or desirable levels	16 ≤ Index < 31
5	**Class V – Very bad water quality** Water quality is almost always threatened or impaired; conditions usually depart from natural or desirable levels	0 ≤ Index < 16

Source: Abrahão et al. (2007)

Notes: Class 1 index values (excellent) can only be obtained if all measurements are within objectives virtually all of the time.

In some instances, possible index scores fall within two categories; for example, index scores of 25; 50; 70 and 90 in a scale of ‘very bad’ (0-25), ‘bad’ (25-50), ‘medium’ (50-70), ‘good’ (70-90) and ‘excellent’ (90-100). Index score 25 falls within the ‘very bad’ and ‘bad’ categories, whereas index score 50 falls within the ‘bad’ as well as the ‘medium’ categories, and so forth. Practical examples of this scenario are water classification scales developed by Hamid et al.

(2013), Vatkar et al. (2013), Kalyani et al. (2016), Luzati and Jaupaj (2016), Guettaf et al. (2017), and Shah and Joshi (2017).

Zhao et al. (2012), and Al-Janabi et al. (2015), Abtahi et al. (2015), Al Obaidy et al. (2015), and García-Ávila et al. (2018), attempted to resolve the problem by minimising the difference between classes to a decimal fraction. Though the problem has been minimised, the fact remains, the categorisation schema does not accommodate all the achievable index scores. It is then crucial that the use of logical linguistic descriptions like, "less than", "equal to" and "greater than," be adopted to allow the inclusion of all possible index values. Abrahão et al. (2007), Rabee et al. (2011), Rubio-Arias et al. (2012), and Sutadian et al. (2018), are good examples of water categorisation schema with appropriate mathematical functions that encompass all the possible index values.

Water quality indices (WQIs) are essential instruments capable of minimising a significant volume of data and simplifies the expression of the water quality status. They are useful tools designed to compare different water bodies through the evaluation of spatial and temporal changes in water quality. Water quality index (WQI) is a single unit-less score that describes water quality in a simple but structured way, through the aggregation of scientific measurements from a list of multiple water quality variables. Since the inception of mathematically based water quality indices in 1965, various water quality scientists and experts have been formulating, and they continue to develop much more straightforward, but scientifically sound water quality models. Such attempts have brought more understanding in the field of water quality science, providing much easier, flexible, accurate and efficient water quality indices.

This being that, water quality indices have become a pivotal component of water resource management, making them important and popular tools in water quality monitoring initiatives; especially in surface water resources management. Water resource monitoring provides basic, but yet decisive information, relevant to water authorities for detecting current water affairs and future trends. The use of water quality indices ultimately promotes effective water resource management and effective prioritisation of decisions and resources among various water management agents (WMAs). Hence the need for a more integrated approach in water quality monitoring.

Considering all this, the current study aims to provide a significant contribution towards water quality monitoring in South African river catchments, through developing a simple and easily understandable WQI that is applicable across many, if not all the river catchments in South Africa. A universal water quality index that is not confined to specific regional demographics. Though not fully comprehensive, the study is a step towards a more integrated water resource management approach, which consequently creates a more rational water monitoring system.

Water quality indices can be modelled into tools for assessing contaminants in a water resource, freshwater in particular. Such tools are called water quality variability models (WQVMs), and they are discussed in the subsequent section.

2.5 Water quality variability models (WQVMs)

A Water Quality Variability Model (WQVM), is a simplified mathematical tool that converts a range of multidimensional water quality data into information that is more understandable and practically applicable. It provides a single figure or grading that describes the overall water quality based on water quality parameters. (Kankal et al., 2012, Boyacioğlu, 2007, Banda, 2015). There is a variety in the type and complexity of WQVMs, and they are generally categorised into three (3) groups based on their uniqueness and purpose. That is; empirical, mechanistic and computer simulation models and these categories outline the theoretical origins and format of the water quality variability model (Riecken, 1995, Banda, 2015).

The models discussed in this review are generally mathematical models with a set of equations that describe input parameters and variables to quantified outputs, based on specific assumptions (Riecken, 1995, Banda, 2015). The following sections contain definitions and overview of the various types of models.

2.6.1 Types of water quality variability models

2.6.1.1 Empirical and mechanistic models

Empirical models are established primarily from analysis of data rather than theoretical principles. They are based more on fitting a set of data, whereas mechanistic models are intended to be a mathematical description of the theoretical tenets. It should be noted that better functional models usually have both empirical and mechanistic features (Riecken, 1995). A practical example of a mechanistic model is AQUATOX (Park and Clough, 2012). The model is considered as a general ecological risk assessment tool that presents the combined environmental fate and effects of conventional pollutants, such as sediments and toxic chemicals in the aquatic ecosystem (Park and Clough, 2012, Banda, 2015).

In South Africa, Water Quality 2000 Model (WQ2000) was developed to assess the catchment salinity for naturalised and human-altered conditions. It is an interface that links the user to an extensive water resource database. The database contains seventy (70) year monthly time series rainfall data, naturalised infiltration and urban catchment runoff and calibrated water quality-total dissolved solids (WQT) hydro-salinity model parameter values (Herold and le Roux, 2004, Banda, 2015).

2.6.1.2 Simulation and optimisation models

Simulation models are imitation tools designed to describe the function of a system. Optimisation models are developed to find the most suitable solution in some sense. Thus, the best fit, whether of minimum or maximum effect, is often subject to constraints such as cost and environmental quality. Considering the computational requirements, many of the simulation models are computer-based programs that provide an interface between the user and the model. The nature and degree of complexity of the model depend on the developer. Some models are user friendly, and some are sophisticated knowledge programs.

A practical example of the simulation and optimisation model being the EUTROMOD (lake eutrophication) model which is reasonably simple to use (Hession et al., 2001). Whilst Branched Lagrangian Transport Model (BLTM) (stream transport), requires programming background to operate, especially when inputting data (Riecken, 1995, Banda, 2015).

2.6.1.3 Static and dynamic models

Static, also known as the steady-state models, describe behaviour that is constant over time (time-independent models). At the same time, dynamic models entail action that varies with time (time-dependent models) (Riecken, 1995). The Cornell mixing zone expert system (CORMIX) model is a practical example of the steady-state model (Jirka et al., 1996), designed for analysing, predicting of aqueous toxic or conventional pollutant discharge into the water bodies (Jirka et al., 1996, Banda, 2015).

2.6.1.4 Lumped and distributed parameter models

Lumped parameter models are developed based on the assumption that there are uniform conditions throughout the system; hence they are zero-dimensional in space. Conversely so, distributed-parameter models describe techniques with variable conditions in one or more spatial dimension. The simplest model is a one-dimensional model that simulate either the vertical or longitudinal behaviour of a water body. Two-dimensional models simulate longitudinal and either transverse behaviour or depth of a water body. The most complex models being the three-dimensional models, which attempt to simulate all the three types of behaviours (Riecken, 1995, Banda, 2015). Water Quality Analysis Simulation Program (WASP) is an example of a model which can be applied in one, two and three dimensions. WASP is a mass balance framework for modelling contaminant fate and transport in surface waters (Ambrose and Wool, 2009).

An example of a comprehensive and versatile one-dimensional stream water quality model is the Enhanced Stream Water Quality Model (QUAL2). It is a water planning tool designed to determine total maximum daily loads (TMDLs), and identify the magnitude and quality characteristics of non-point pollution sources (Birgand, 2004, Hadgu et al., 2014, Banda, 2015).

2.6.1.5 Deterministic and stochastic models

Models that use expected values, with no real data for all the parameters and variables and output predictions that are also expected values are called deterministic models. Whilst stochastic models incorporate variability, and possibly an error in probability density functions for selected parameters, resulting in a probability density function for the prediction (Riecken, 1995, Banda, 2015).

2.6.2 Water quality variability models (WQVMs) application

The extent to which a model can be applied relies on the purpose of the modelling exercise, data requirements, suitability and computational capability of the chosen model, hardware requirements and the ability of the user to interpret the data. Nevertheless, WQVMs are used for water quality variability modelling, which includes determining and analysing the environmental impact of existing and potential loadings. Furthermore, they are used to understand the complex relationships among the biotic and abiotic components of water systems (Riecken, 1995, Banda, 2015).

With an attempt to extend the application boundaries of water quality variability models and keeping to the study objectives, a more straightforward but effective model would be most appropriate. That is; self-oriented, requiring fewer input data, with minimum computational memory requirements and having output results that are easily understood. The choice of the model type usually depends on the data available, and the objective to be achieved.

2.6 Summary of the review

Forty water quality indices (WQIs) were reviewed, and only fifteen significant WQIs were discussed in detail under Chapter Two, essentially to establish the existing knowledge and provide background information to the current study. Consequently, the review was guidance towards selecting the most appropriate research methods and ensuring that objectives set for the research study are attained, which becomes a logical basis (rationale) for evaluating more existing WQIs. Hence the purpose of Chapter Two, in particular, was to provide further information on existing WQIs and enables the researcher to anticipate the most appropriate methods. This chapter also provides a theoretical framework to justify the outcome of the study and substantiate the choices made. There are numerous water quality indices developed since the 19^{th} century, and it is extensive work and beyond reach to attempt discussing all of them under this review. Therefore, only forty WQIs were investigated, and supplementary information is attached at the back of the thesis as Annexures.

The main objective of WQIs is to convert multiple parameter data into information that is understandable by both technical and non-technical personnel. The ability of WQIs to synthesis complex scientific data into simple and easily understood formats makes them the most fundamental and indispensable elements of water quality monitoring agenda. Hence, they are universally acknowledged as "lifeline" for water quality studies, and their development continues as an on-going affair. Various methods and procedures are considered when developing water quality indices, but the traditionally applied approach involves, (i) selection of the significant water quality parameters; (ii) formation of sub-indices; (iii) establishing relative parameters weights; (iv) aggregation of the sub-indices; and (v) assigning index scores to a water classification schema.

Each step in the development of water quality indices has alternative methods to consider; it is then critically important to select the most appropriate of each alternative. Despite having scientific knowhow of water quality models, WQIs developers should apply due diligence, avoid subjective judgements and biasness in the process of developing water quality indices. Otherwise, the water quality index will inherit such problems and be deemed dysfunctional. Hence, proper design and formation of water quality indices are then a pivotal step in assessing our water resources and in cognisance of such, this study endeavours to develop a water quality monitoring tool that applies to distinct catchments in South Africa. This tool should analyse and integrate the significance of physical and chemical constituents of surface water and be able to present them in a simple, but yet technically justifiable method.

Typically, WQIs are not designed for broad application, but they are customarily developed to accommodate specific water quality parameter, only those regarded as the most significant water quality variables. Therefore, WQIs cannot evaluate the quality of water for all the applications; neither can they outline all the water quality hazards, nor can they deliver a complete and comprehensive analysis of water quality. Instead, they can only provide a quick holistic guide necessary to evaluate water quality trends. However, the most challenging aspect is that water quality indices are developed for a particular region and source-specific; there is no single water quality index that has been globally accepted. Which then, perhaps becomes the ultimate goal, to explore and delineate the possibilities of breaking such limitations, and witness the birth of a robust water quality index that can be applied across various watersheds.

CHAPTER 3

3. METHODOLOGY

3.1 Overview

Chapter Three outlines the methods and procedures applied to accomplish the objectives of the study. The discussion and synopsis of this chapter follow the specific goals of the research, as discussed in Chapter One. The discussion herein Chapter Three focuses on research data, parameter selection, universal water quality index (UWQI) model, artificial neural network (ANN) model, surrogate WQI model, index categorisation schema, water quality variability model (WQVM), constraints and assumptions of the study. Furthermore, the justification of the techniques used to develop the proposed water quality monitoring tools are presented under this chapter. Given the practical nature of this study, a comprehensive explanation of the methodologies applied might not be feasible in this chapter. Henceforth, chapter three provides an overview of the methods used, whilst an in-depth presentation is being accorded in Chapter Five of the thesis.

The study involves the development of a universal water quality index (UWQI) which computes and reports on the degree of pollution and substantiate the healthiness of water resources in relation to individual parameter concentrations. The UWQI model is based on the conventional method of developing WQIs. The computation process involves the use of weighted sum (additive) method to aggregate the compound influence of thirteen preselected water quality variables, with unequally weighted coefficients and sub-indices comprising of sixty-two sub-index linear functions. The model provides a single-digit score that can be compared and assigned to a specific class describing the quality of water. The WQI score is non-dimensional, easy to comprehend and most importantly, it is scientifically justifiable.

In an attempt to answer the research question, the study scientifically demonstrated the application of artificial neural networks (ANNs). The correlation between the results of the UWQI and that of ANN model validated the use of ANNs to analyse and monitor water quality status for South African river catchments. The artificial neural network (ANN) model utilises the same thirteen water quality variables from UWQI model as input descriptors. Further to this, the ANN model contains nineteen neuro-nodes which transforms the water quality variables and aggregates them into a single non-dimensional index rating. The ANN model consists of multiple layers presented as (i) the input layer responsible for receiving external datasets, (ii) the output layer that produces the ultimate result, and (ii) the hidden layers (zero layers) located in-between the input and out layer. The methods used in this study are represented in Figure 3.1.

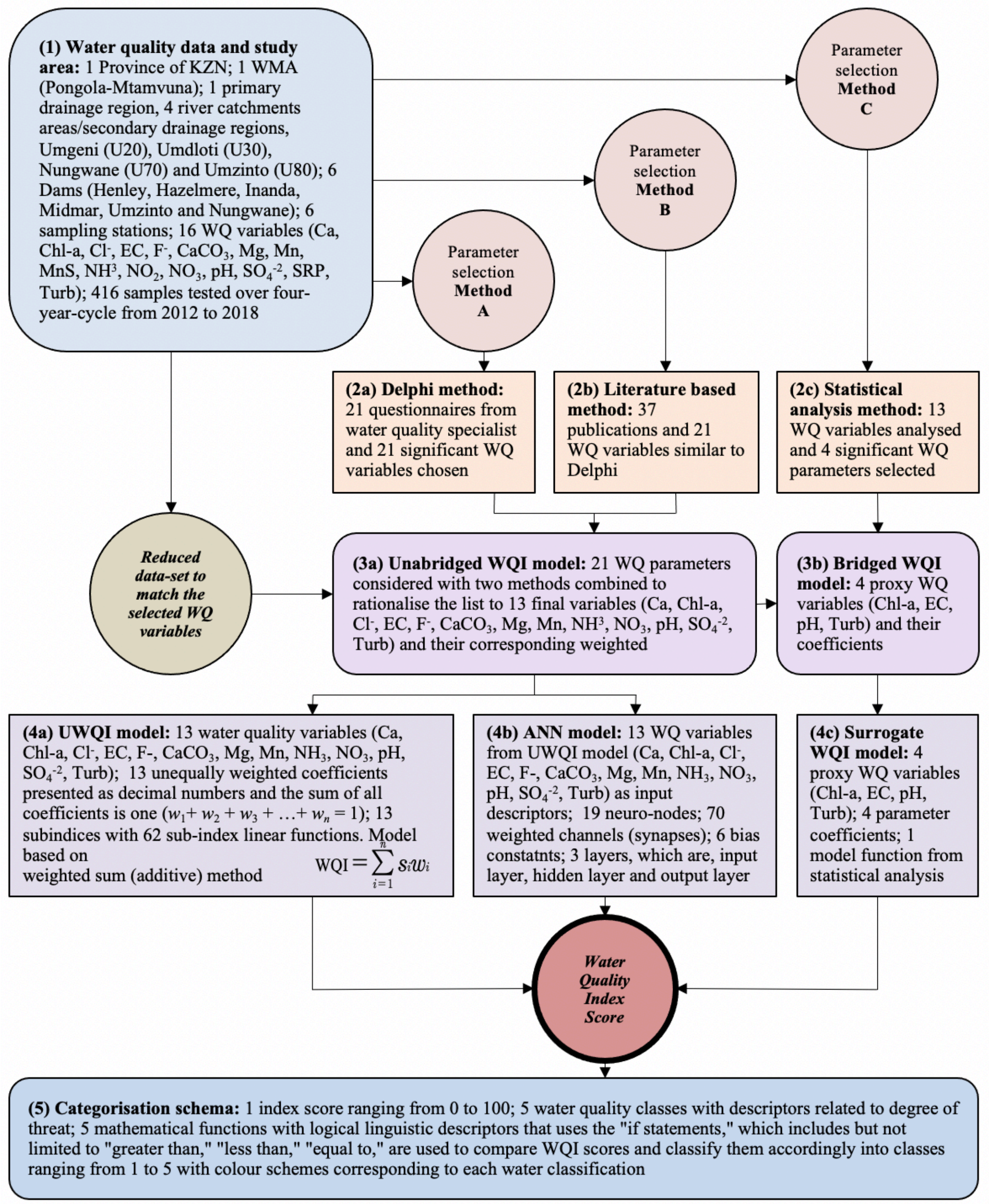


Figure 3.1: Flow diagram illustrating the research methods applied in the development of the water quality indices and outcomes achieved

Source: Authors diagram produced for the current study.

Notes: The flow diagram summaries the processes and techniques adopted in the development of the universal water quality index (UWQI). Although the Umgeni Water Board (UWB) has more water quality monitoring stations, only six water quality monitoring stations are considered in the development of the UWQI model.

With an effort to provide a quick water quality evaluation, especially in the absence of a full set of parameters, the study also developed a surrogate water quality index model which functions with only four water quality variables selected using statistical analysis. The four parameters are chlorophyll-a (Chl-a), electrical conductivity (EC), pondus Hydrogenium (pH) and turbidity (Turb). The model is based on a mathematical function with fixed unequal coefficients relative to the influence of each of the four selected parameters. The output index value is similar and comparable to that of UWQI and ANN models. For comparison and benchmarking purposes, the index scores from all the three WQI models are classified using a standard categorisation schema with five classes distinguished by mathematical functions with logical linguistic descriptors used to compare WQI scores and rank them accordingly.

Although the study attempts to provide water quality tools that are applicable across all river catchments in South Africa, it is beyond reach and improbable to consider data from all the Water Service Authorities (WSAs) in South Africa. Therefore, a considerable number of catchments have been considered for testing the functionality of the models. The selection of these catchments does not devalue the objectives of the study; instead, it marks the first step towards justifying that the developed models work with most drainage regions in South Africa. Full details about the research data and study area are discussed in the following section.

3.2 Research data and study area

Water quality data from Umgeni Water Board (UWB) was used to achieve specific objectives of the current study. The study utilised 416 samples tested monthly for a period extending to four years spanning from 2014 to July 2018. All water quality variables were sampled following standard methods prescribed by the Department of Water and Sanitation (DWS), and further analysed according to international standards in an ISO 9001 accredited laboratory owned and operated by UWB (Namugize et al., 2018). The research dataset from UWB satisfactorily provided all the required thirteen water quality variables. These are, ammonia (NH_3), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), electrical conductivity (EC), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), pondus Hydrogenium (pH), sulphate (SO_4) and turbidity (Turb).

The study observed some inconsistency in the frequency of sampling, with a more significant effect on calcium (Ca), fluoride (F), hardness ($CaCO_3$) and magnesium (Mg); some variables were tested on varying intervals of weekly, monthly and quarterly basis. Where possible, estimation of missing data was done using interpolation, with a back-and-forward filling of the data gaps. Approximation of the missing data in-between measured intervals was achieved by linear interpolation using the available last set of measurements before and after the data gaps. Whilst missing data at the end or beginning of the period were back or forward filled (Schullehner et al., 2017).

Water quality data provided by Umgeni Water Board is for six sampling stations which fall under the jurisdiction of four different catchment areas. That is, three stations situated in Umgeni River catchment (U20) and located at Henley, Inyanda and Midmar Dams respectively; one station at Hazelmere Dam located within Umdloti River catchment (U30); one station at Nungwane Dam under Nungwane River catchment (U70); and lastly one station at Minto Dam found in Minto/Umuziwezinto River catchment (U80).

Testing the model with data from these four river catchments support the objective of establishing a universal water quality index (UWQI) applicable to the greater part of the country, if not the whole of South Africa. Over and above the availability of data from UWB, the economic significance of KwaZulu-Natal Province (Shoko, 2014, Hughes et al., 2018), the distinctiveness of its inter-basin arrangements, the scope of the transfer schemes involved and extensive water demand (Umgeni Water, 2018, 2019a, 2019b). All these attributes uniquely encouraged the choice of the study area, which falls under Pongola-Mtamvuna water management area (WMA) (Republic of South Africa, 2012, Chiluwe, 2014). The project data was adequate to examine the model and complement the objective of developing a universally acceptable water quality model.

3.3 Water quality index (WQI)

There are various techniques applied when establishing water quality indices (WQIs), and these are usually governed by the degree of accuracy required and application boundaries (Sutadian et al., 2016). Nonetheless, the current study adopted only three methods in the development of three different, but interlinked WQI models. The first model is based on conventional techniques, the second model uses artificial intelligence (AI) in the form of artificial neural networks (ANNs), and lastly, as a proxy to the unbridged UWQI, the surrogate water quality index is based on statistical techniques. The first two models use thirteen water quality parameters, whereas the proxy model uses only four variables. Developing various WQI models presented a platform to test each model against similar functioning tools and advocated the readiness of each model. The methods used to create the three WQI models are discussed in the following subsections and further detailed in Chapter Five.

3.3.1 UWQI using the conventional method

With the endeavour to accomplish objective one of the study, UWQI was formulated using the conventional method of establishing water quality indices. And such a technique involved four common steps, which are (1) selection of water quality variables, (2) setting relative weightage coefficients (3) formation of sub-index rating curves and sub-index functions, and (4) deriving of the appropriate aggregation or indexing model (Abbasi and Abbasi, 2012b, Fu and Wang, 2012, Walsh and Wheeler, 2012, Tyagi et al., 2013, Poonam et al., 2015, Paun et al., 2016).

The methods employed for the development of the UWQI are selected based on a couple of reasons. Firstly, they eliminate individual biasness through the incorporation of objective and subjective opinion from water quality scientists through appraisal questionnaires. Secondly, comparing to other available techniques, the chosen methods are both practical, convenient and easy to implement in electing variables and generating weightage coefficients (Sutadian et al., 2018). Lastly, the methods are proven and have been performed in WQI studies that include, Horton (1965), Brown et al. (1970), Brown et al. (1973), SRDD (1976), Ross (1977), House (1986, 1989, 1990), Dinius (1987), Smith (1987, 1990), Tyson and House (1989), Nagels et al. (2001), Kumar and Alappat (2009), and Almeida et al. (2012).

3.3.1.1 Selection of water quality variables

These steps and procedures were performed cautiously with cognisance of the fact that the model should widen its application boundaries and target to become a nationally accepted water quality monitoring tool. Reasoning from this fact, a fixed set of parameters were established using expert opinion. The advantage of a fixed set of variables is that the model can be applied in various catchments without the possibility of altering the structure and functionality of the model (Sutadian et al., 2016). Thereby permitting stakeholders to fairly compare the water quality of different sites and develop a more informed national prioritisation schedule without prejudice. Moreover, expert opinion has the advantage of promoting the acceptability of the model; in the sense that, most of the experts engaged are also the targeted end-users of the model. The idea of being involved in the process of developing the UWQI might facilitate acceptance through a sense of ownership.

Nevertheless, this alone does not warrant the usefulness of the model; the author exercised enormous care and great attention to ensure that the most significant variables are incorporated in the UWQI. Of great importance, the author had to optimise the ideal number of parameters necessary to provide a meaningful water quality index value.

Following the Rand Corporation’s Delphi Technique, a panel of thirty water specialists from government parastatals, private sector and academia were established. Delphi Questionnaires were circulated to the participants and were asked to consider twenty-one water quality parameters for their possible inclusion in the UWQI. The panellists were instructed to designate each variable as: “Include” and “Exclude” and further assign a relative significance rating against each variable elected as “Include.” The rating scale ranged from one to five, whereby “scale 1” denoted the uppermost significance and "scale 5" represented a comparatively low significance. In addition to the prescribed twenty-one parameters, the experts were allowed to add at most five more variables if desired. A total of twenty-one questionnaires were returned out of the thirty questionnaires circulated. The Rand Corporation's Delphi Technique is described in detail by Horton (1965), Brown et al. (1970), Linstone and Turoff (1975, 2002) and applied in several studies which include Kumar and Alappat (2009), Nagels et al. (2001), Almeida et al. (2012).

Complementary to that, existing literature on WQIs was used to select the most significantly used water quality variables. thirty-seven studies were considered, and each variable was designated as "Include" if it corresponded to the twenty-one parameters considered for the Delphi Questionnaires; else, it was designated as "Not Included." Furthermore, the formerly assigned significance rating was adopted as the relative significance rating for each parameter that was "Included" in the study in question. The rating was based on a scale ranging from one to five; with "scale 1" representing the lowest significance and "scale 5" for relatively high importance. If a different significance rating scale was used in the existing studies, the original rating values were equivalently transformed to match the preferred rating scale.

Finally, a holistic ranking order was derived from a combined effect of the two methods, as mentioned earlier. Upon which, rejection rationale was employed to eliminate redundant variables which are not commonly monitored across South African river catchments (Sutadian et al., 2018). Accordingly, the thirteen most appropriate variables consider for inclusion in the UWQI are, ammonia (NH_3), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), electrical conductivity (EC), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), pondus Hydrogenium (pH), sulphate (SO_4) and turbidity (Turb). Methods used for deducing the weightage coefficients are discussed in the subsequent section.

3.3.1.2 Establishing relative weightage coefficients

Considering that in this current study, water quality parameters are viewed to have different influence towards the overall classification of water, some variables are considered more significant than the others; therefore, weights were established to reflect the diversity of each parameter appropriately. The comparative scale used is biased towards the level of influence and significance towards the overall index value (Sharma et al., 2014, Sutadian et al., 2016). Since some parameters are regarded as less important than the others, a standard scale of influence, ranging from one (lowly rated) to five (highly rated) was adopted for the current study. Similar to the selection of parameters, assigning of weights was achieved through participatory based Delphi method and extraction from existing literature on water quality studies. The weight ratings from the two procedures were merged to portray one holistic rating for each variable.

The relative weightage coefficients are directly proportional to the weight ratings, and they were established by dividing the parameter weight rating value by the sum of all weight ratings. The index coefficients are represented as a decimal number with a sum equal to one. In principle, this theory governs the model from computing index values above one hundred per cent. Otherwise, the aggregation process will be compromised and jeopardise the scientific steadiness of the model (Banda, 2015). Upon this, the sub-index rating curves and sub-index functions were formulated as discussed in the following Subsection.

3.3.1.3 Formation of sub-index rating curves and sub-index functions

Given the fact that model input variables are assessed using different units of measure, sub-indices were employed to transform the measurement units into a common unitless scale. Moreover, the indexing model can only aggregate parameters with a standard scale, which became more necessary to harmonise the parameter values using a standardised non-dimensional scale. Using the permissible water quality parameter concentrations prescribe by DWAF (1996a, 1996b, 1996c), fixed key points of the rating curves were established and converged with straight-line graphs. After that, the linear equations associated with the straight-line graphs were collectively transformed into linear sub-index functions. The advantage of this technique is that sub-index functions can interpolate index values laying between water classification categories using the linear regression method. The final sub-index curves and sub-index functions are included in Chapter Five.

3.3.1.4 Deriving of the appropriate indexing model

Various aggregation methods are documented in the existing literature, and amongst them, there is no one distinctive method regarded as the supreme and favourable method. Each aggregation method has considerable problems, and some are even unavoidable. Bearing that in mind, the author tried and tested three different aggregation techniques. These are (i) weighted sum (additive) method, (ii) modified weighted sum method, and (iii) weighted multiplicative method. The three aggregation equations are represented in Chapter Five. Using the selected thirteen water quality variables, parameter weightage coefficients and sub-indices; the modified weighted sum method demonstrated better predictive capabilities. Henceforth, the technique has been considered as the most appropriate and relevant method to develop the UWQI targeted for assessing water quality within South African river catchments. Upon conducting scenario-based analysis, the modified weighted sum equation has been further improved to align with local conditions and specific requirements of the UWQI. The final model responded steadily to the variation in parameter values and managed to indicate spatial and temporal changes in water quality for the four catchment areas considered for the study.

Hypothetically, this advocates the readiness of the UWQI model and deem the study a success. Such a milestone fulfils the aim of the research, and more importantly, it provides a tool that can be adopted across the country and solve challenges being experienced by water quality professionals. The structure of the universal water quality index model is represented as Figure 3.2 below.

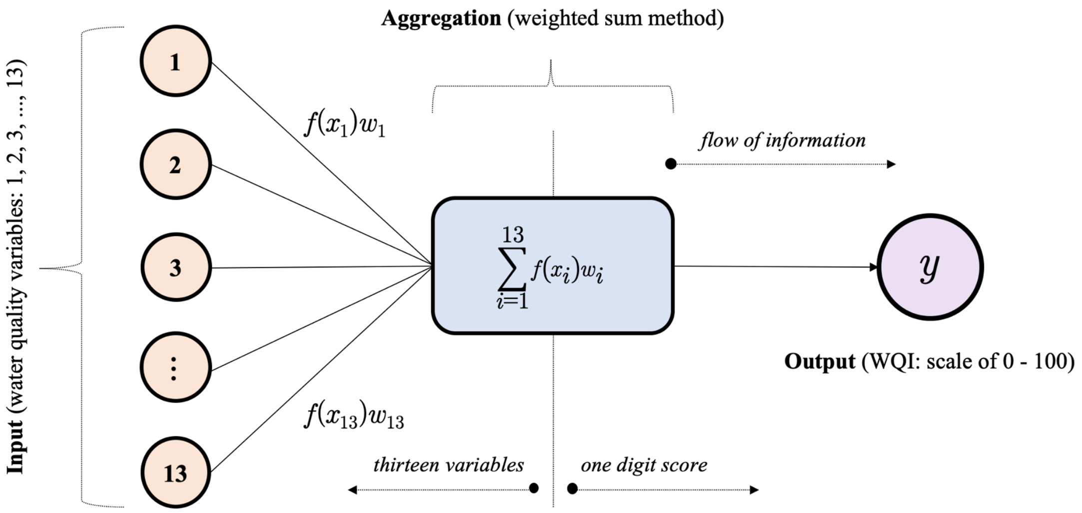


Figure 3.2: Design diagram indicating the framework and concept considered for the establishment of the universal water quality index (UWQI) model

Source: Authors diagram documented in Banda and Kumarasamy (2020c).

Notes: A model framework showing the link between following: (i) thirteen water quality input variables x_1, x_2, x_3, …, x_{13}; (ii) corresponding parameter weights w_1 to w_{13}, (iii) parameter sub-index functions $f(x_1)$ to $f(x_{13})$, and (iv) the aggregation function $\sum f(x_i)w_i$ applied to sum the weighted influence of the input variables.

With success, the whole of Section 3.3.1 satisfies the requirements of objectives one and four of the study; in particular, Part 3.3.1.1 to Part 3.3.1.3 addresses objective four, whereas Part 3.3.1.4 fulfils the specifics of objective one. The methods used to achieve objective two are discussed in the forthcoming section.

3.3.2 Artificial neural network (ANN) model

Corresponding to the universal water quality index (UWQI), the study designed an artificial neural network (ANN) model based on a similar set of input variables as considered for the UWQI. Accordingly, the thirteen input descriptors are analysed and processed by predefined multidimensional parameter relationships in the form of mathematical coding. The mechanism employed is identical to the pattern and functionality of the natural human brains (Singh et al., 2009, Khalil et al., 2011, Huo et al., 2013, Seo et al., 2016, Qaderi and Babanezhad, 2017, Salari et al., 2018, Bansal and Ganesan, 2019, Isiyaka et al., 2019, Kadam et al., 2019, Ramasubramanian and Singh, 2019, Soro et al., 2020). Whereby, layers of neurons are interconnected in a web-like structure and communicate from one layer to the other depending on the data received and the desired output. Similarly, the ANN model consists of nineteen neuro-nodes and seventy synapses commonly known as the "channels," which together transforms multiple water quality parameters and combine them into one non-dimensional digit score that describes the quality of water resources. The basic structure of the ANN model is represented as Figure 3.3.

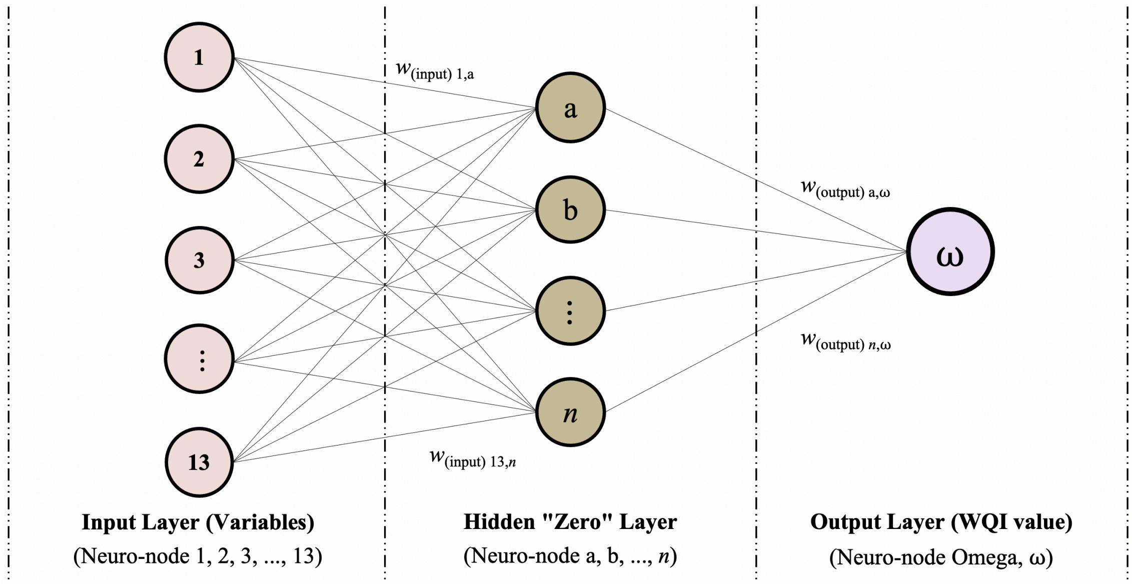


Figure 3.3: Basic structure considered for the development of the artificial neural network (ANN) model

Source: Authors diagram showing the basic structure of an artificial neural network (ANN). The graphical model was adopted from the following literature: Singh et al. (2009), Huo et al. (2013), Cordoba et al. (2014), Sarkar and Pandey (2015), Seo et al. (2016), Yilma et al. (2018), García-Alba et al. (2019), Haldorai et al. (2019), and Kim et al. (2019b).

Notes: The input layer represents the thirteen water quality variables (1, 2, 3, …, 13). Depending on the problem being investigated; the number of hidden or "zero" layers may vary and can be more than one, but for presentation purposes, they are combined and included as one layer in Figure 3.3 above. The output layer contains the final water quality index score (ω).

The developed ANN model comprises of several layers that are connected by links with varying weights. These layers are structured as, (1) the input layer that functions to receive external data, (2) hidden or "zero" layers which attempt to analyse the input information and filter to the relevant neurons, and lastly (3) the output layer that integrate data and produce a consolidated output report. The hidden layers are located in-between the input and the output layers (Sarkar and Pandey, 2015). ANN models are regarded as "black-box models," as a consequence of providing minimal insight towards the contribution of each variable towards the final index value (Kim and Seo, 2015, Salari et al., 2018). However, neural networks are undoubtedly powerful and reasonably simple non-linear statistical models that enhance artificial intelligence (AI) and solve improbable problems. Hence they are popularly known as "universal function approximators" (Kim and Seo, 2015, Bansal and Ganesan, 2019, Kim et al., 2019b, Li and Liu, 2019, Ramasubramanian and Singh, 2019, Tiyasha et al., 2020).

The learning process of the neural network was performed using backpropagation algorithm (Isiyaka et al., 2019, Rajaee et al., 2020). And research data samples were randomly portioned to achieve training (70 %), testing (15 %) and validation (15 %) data subsets (Lucio et al., 2007, Shanthi et al., 2009, Banerjee et al., 2011, Safavi and Malek Ahmadi, 2015, Qaderi and Babanezhad, 2017, Gebler et al., 2018, Ahamad et al., 2019, García-Alba et al., 2019, Kadam et al., 2019, Rajaee et al., 2020). Data splitting is performed to ensure that the model utilises different dataset per each learning process. Training data was applied during pattern recognition, selection of neuron activation functions and optimisation of hidden layer neurons, channel weights together with bias constants. Whereas the generalisation ability of the model was assessed using the testing data subset, whilst validation data evaluated the predictive performance of the neural network (Isiyaka et al., 2019). The learning process was controlled and terminated using predefined stopping guidelines implemented to avoid over-fitting (Singh et al., 2009, Khalil et al., 2011, Sarkar and Pandey, 2015, Qaderi and Babanezhad, 2017).

Parameter measurement units were standardised, forming a standard non-dimensional scale ranging from zero to one. This approach eliminates the effects of varying measurement scales and prohibits particular parameters from erratically dominating the prediction process (Gazzaz et al., 2012, Huo et al., 2013, Rajaee et al., 2020). Quantitative statistics which includes correlation coefficient (R), coefficient of determination (R^2) and root mean squared error (RMSE) were measured to evaluate the predictive performance of the neural network. Global and pointwise sensitivity analysis examined further the appropriateness of the proposed ANN model.

For time preservative and cost-effective measure, the ANN model was developed using TIBCO Statistica Automated Neural Networks (SANN) software (TIBCO Software Inc., 2020). This program provides an efficient way of configuring the architecture of the artificial neural networks (ANNs) and optimising the number of neurons required for the model to function appropriately without compromise (Kim et al., 2019b). The development of this ANN model conferred the successful implementation of objective two and considered an essential milestone of the study

The development of this ANN model conferred the successful implementation of objective two and considered an essential milestone of the study. Besides the UWQI and ANN models, the study also developed a surrogate water quality index model that works as a proxy WQI in the absence of a full dataset. The formation of the proxy WQI is an attempt to achieve objective three of the research.

3.3.3 Surrogate water quality index model

For this particular model, water quality parameters were defined using a two-stage screening process. The procedure included the following (i) Delphi method conducted for the universal water quality index (UWQI), where twenty-one parameters were deduced to thirteen variables, then (ii) further reduced the parameters to four proxy variables using statistical assessment. Figure 3.4 illustrates the model architecture applied in the development of the surrogate water quality index model. During parameter selection procedure, principal component analysis (PCA) was used for pattern recognition and explaining the structure of the underlying dataset (Wold et al., 1987, Bouza-Deaño et al., 2008). It aided in identifying intercorrelated parameters and provided crucial statistical information on the most significant parameters that are regarded as proxy variables.

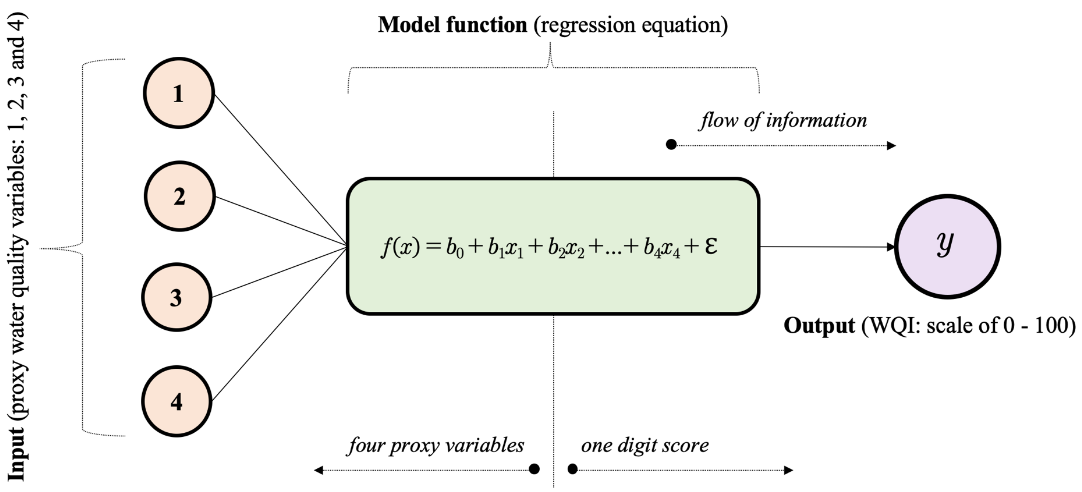


Figure 3.4: Model architecture applied in the development of the surrogate water quality index model using four proxy water quality variables

Source: Authors diagram documented in Banda and Kumarasamy (2020b).

Notes: A model outline displaying the structure of the surrogate WQI with four input variables x_1, x_2, x_3 and x_4; their corresponding coefficients b_1 to b_4, intercept term b_0, error term for the regression model symbolised as $\mathcal{E}$, and the regression model function $f(x) = b_0 + b_1x_1 + b_2x_2 + ... + b_4x_4 + \mathcal{E}$ as the proxy or surrogate WQI.

Further to this, hierarchical cluster analysis (HCA) was performed to provide instinctive similarity relationships that exist among water quality parameters and in the process, HCA yielded a dendrogram (tree diagram) that illustrated the cluster arrangement and parameter proximity to one another (Zhao et al., 2012, Khalil et al., 2014). After that, multivariate regression analysis was adopted to estimate the relationship between WQI (dependent variable) and independent variables (predictors/covariates) which are the final four proxy parameters. The resulting regression equation and coefficients represent the surrogate WQI model.

The advantage of this method is that optimum selected parameters can still describe water quality in the absence of the entire dataset (Zhao et al., 2012, Karamizadeh et al., 2013). It provides an essential quick-guide identical to the outcome of the high-fidelity model (UWQI) and conforms to the requirements of objective three. All the statistical computations were performed using IBM SPSS Statistics Version 24 for Macintosh Operating System (macOS) (SPSS Inc., 2016).

3.4 Index categorisation schema

In the interest of simplifying the interpretation of water quality index (WQI) values, mostly to accommodate non-technical individuals, an index categorisation schema was established. The classification mechanism is based on an increasing scale index, and the advantage of this system is that it is identical to a typical percentage hierarchy (Banda, 2015, Banda and Kumarasamy, 2020c); therefore, the public can easily relate to its function and interpretation. Both models applicable to this study yields WQI values between zero and a hundred.

Accordingly, the WQI scores are categorised using classes ranging from one to five. With "Class 1" representing water of the highest degree of purity with a possible maximum score of hundred and vice versa, "Class 5" denotes water quality of the lowest degree with index scores nearing or equal to zero. With the aim of closing gaps identified in various existing classification scales (Banda and Kumarasamy, 2020e, Banda and Kumarasamy, 2020c), appropriate mathematical functions with logical linguistic descriptors which includes but not limited to, "greater than," "less than," "equal to," are used to appraise WQI scores and respectively assigned them to the corresponding category (Banda and Kumarasamy, 2020b, 2020c).

Studies such as Abrahão et al. (2007), Rabee et al. (2011), Rubio-Arias et al. (2012), and Sutadian et al. (2018), have incorporated similar approach, which authenticates the application of the method used for this particular study. Beyond doubt, the developed schema can accommodate all possible index scores regardless of the decimal value. And such proficiency essentially assists in closing the flaws identified in the existing literature and provides insight into the fundamentals of water quality index development. Figure 3.5 illustrates the principle and design mechanism adopted in formulating the classification tool.

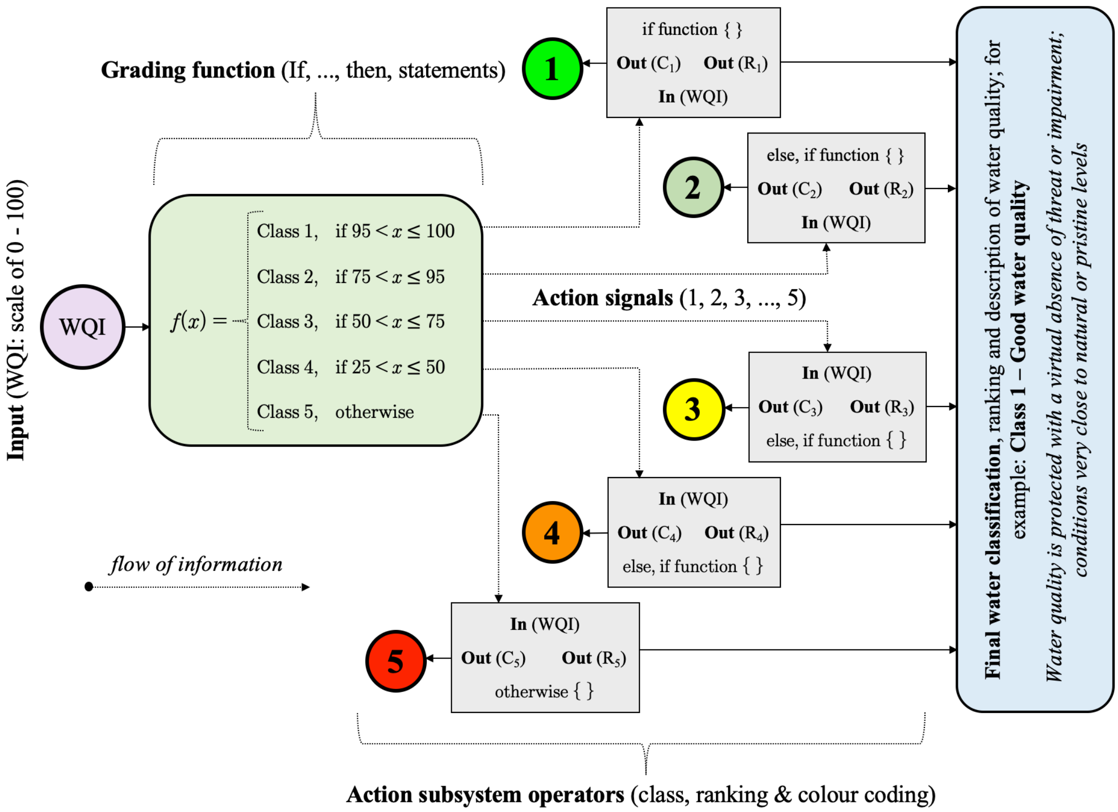


Figure 3.5: Water classification system containing subsystems and action blocks that are executed using logical linguistic descriptors

Source: Authors diagram derived from the classification system documented in Banda and Kumarasamy (2020b), and Banda and Kumarasamy (2020c). The schematic diagram represents a modified version of the water quality index (WQI) categorisation schema suggested by Banda (2015).

Notes: The highest classification rank representing class 1 index values (excellent) can only be obtained if all measurements are within objectives virtually all the time. The water quality categories assume the "green-yellow-red" colour gradient, corresponding to the relevant water quality classes from excellent (class 1) to worse (class 5).

The establishment of the categorisation schema corresponds with objective six of the study. It promotes the achievement of objective seven which involves the transformation of the suggested water quality indices (WQIs) into a water quality variability model (WQVM) that can produce water quality classification grading based on a specific water categorisation schema.

3.5 Microsoft Excel-based water quality variability model

The water quality variability model (WQVM) developed under this study is a combination of three diversified water quality indices (WQIs); which are all founded on distinctive indexing techniques. With full details being provided elsewhere in the study, the three indices are; (1) universal water quality index (UWQI), (2) artificial neural network (ANN) model, and (3) surrogate water quality index (WQI). In practice, most of the WQIs are presented as mathematical equations that are somewhat difficult to apply in the real world (Banda, 2015). To overcome such trends, Microsoft Excel 2016 Version 16.43 was used to combine the three WQI models into a practical tool.

With the aid of Excel, multiple logistical functions were used to explore water quality data and provide a status quo based on assigned analytical functions, which are coded to handle specific data sets and perform exclusive computational tasks. The choice of Excel is motivated by its computational abilities, usability and functionality. More so, Excel is a commonplace that is straightforward, convenient and user-friendly (Varma and Khan, 2014, Avdic, 2018). Being a familiar interface, Excel has the potential to elevate the degree of acceptance more than building entirely new software. The algorithms of the WQVM are clustered and bundled into an array of hidden calculation spreadsheets, with each sheet assigned and conforming to a particular WQI. Concealing of the calculation sheets minimise the risk of tempering and eliminate the challenge of navigating between spreadsheets, especially in light of non-technical end-users. Figure 3.6 explains the structure of the proposed WQVM.

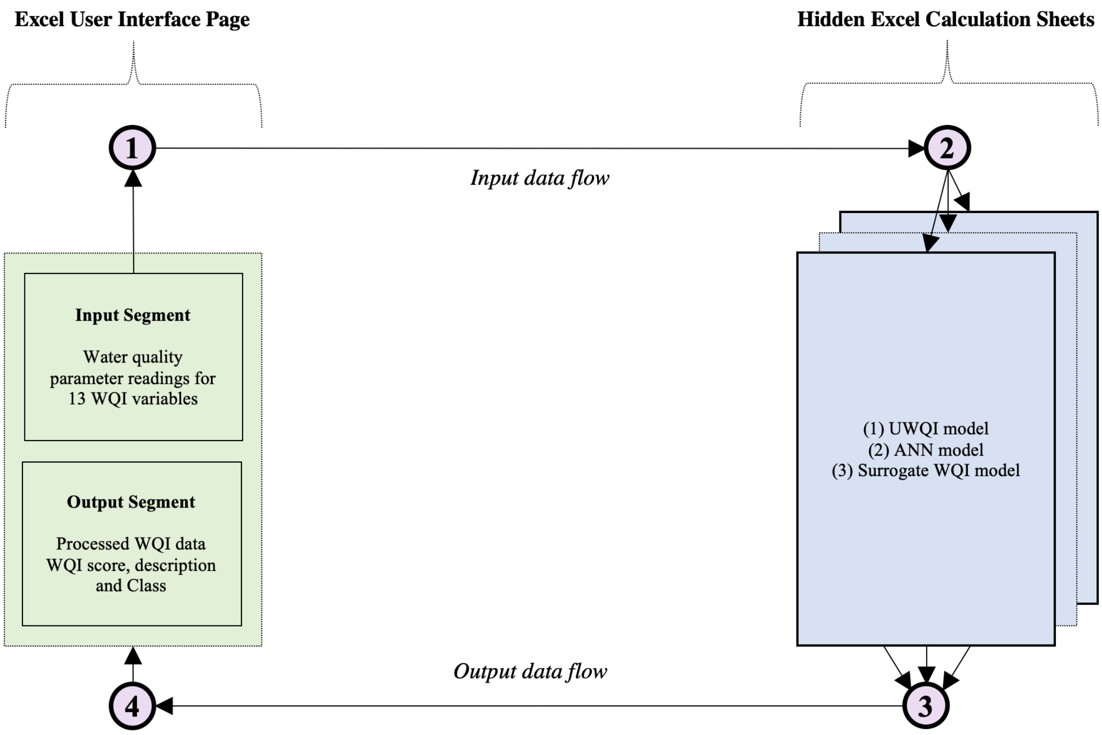


Figure 3.6: Model diagram illustrating the design principle used to combine the three water quality indices into a water quality variability model (WQVM)

Source: Authors diagram produced for the current study.

Notes: The model uses a maximum of thirteen predefined parameters, minimum of four proxy variables and three different water quality indices defined as (1) universal water quality index (UWQI) model $\sum f(x_i)w_i$ with thirteen unequal weights, (2) artificial neural network (ANN) model that uses seventy predetermined channel weight coefficients and six bias constants, and (3) surrogate or proxy WQI model in the form of $f(x) = b_0 + b_1x_1 + b_2x_2 + ... + b_4x_4 + \varepsilon$. The proxy WQI operates with four variables with fixed regression constants.

The WQVM is qualified to handle one thousand samples, which is approximately twenty years of weekly measured data. Regardless of the model preference, inputting of explanatory variables is done once for all the three WQIs. Both UWQI and ANN models require thirteen variables to produce a more accurate and reliable index score, whereas, the surrogate WQI requires only four proxy variables to function. The overall WQI grading is displayed in the numeric, graphical and descriptive formats. The numeric digit score is given as a ratio equivalent to the percentage, and the graphical presentation indicates the highs and lows of the calculated WQI. On the other hand, the descriptive format extracts information from the categorisation schema that consist of five classes compatible with the degree of cleanness. The five classes are; Class 1 (good quality), Class 2 (acceptable quality), Class 3 (regular quality), Class 4 (bad quality), and lastly Class 5 (very bad quality).

The successful implementation of WQVM is a significant step, not only for the author but the national community at large. The model allows South Africans the opportunity to work with a robust and steady toolkit, that is seemingly fast and reliable in providing water quality results. Needless to mention that, WQVM brings about a rationalised "yardstick" for water resource monitoring, thereby encouraging fairness in national prioritisation programs (Banda, 2015). The establishment of the WQVM is an important milestone that bundles all the seven objectives of the study and translates to the research topic. Which is defined as the "development of a universal water quality index and water quality variability model for South African river catchments."

The constraints and assumptions arising from the procedures as mentioned earlier and methodologies applied in the study are presented and discussed in the subsequent section.

3.6 Constraints and assumptions

The limits and conditions assumed for this research relate to the methods used and resources allocated towards the study. They are entrusted to uphold the functionality and effectiveness of the models. Their primitive role is to ascertain the accomplishment of the study objectives and ratify the integrity of the research work. Furthermore, the restrictions are set to exploit on the proficiency of the models through optimising data requirements, which eventually simplifies the models and promote their application. Therefore, they do not devalue the significance of the research work; instead, they add value to the effectiveness of the models developed under this study and attempt to widen their application boundaries.

Regular water quality sampling and analysis is a costly and demanding task, hence acquiring large volumes of water quality data is often a challenge and requires a significant amount of financial resources (Pegram and Görgens, 2001, Ochieng, 2007). Given that, the current studies could not gather its own samples; instead, water quality data from Umgeni Water Board (UWB) was used to achieve the objectives of the research and attest the functionality of the models. UWB dataset was collected from six stations which fall under the jurisdiction of four different catchment areas and contained over four hundred monthly samples extending to four years, ranging from 2014 to 2018. The research data provided by UWB was adequate and contributed significantly towards the success of the doctoral work.

All the WQIs developed uses preselected variables and fix coefficients, which limits the indices to operate with a specific parameter input range; otherwise, new coefficients must be generated if different variables are preferred. Such restrictions corroborate with the idea of standardising the model and have results comparable without prejudice. It is then more of a measure than constraint.

Finally, considering that most Water Boards and relevant stakeholders are utilising Microsoft applications, the WQVM was developed using Microsoft Excel, thus limiting the application of the toolkit to the use of Microsoft Office Suite.

All these constraints and limitations are specific to the objectives of the study and define the parameter input range. Application of water quality indices differs depending on the benefit they intend to bring and to whom. Therefore, the limits discussed herein might be an advantage to the next person, and constraints to the other. But for the current research, they are regarded as necessary measures implemented to achieve study objectives.

CHAPTER 4

4. AREA OF STUDY

4.1 Background and specific considerations

The subsequent increase in population and improper disposal of wastewater has a significant influence on the diminishing of water quality in rivers and other surface water reservoirs. As a consequence, routine water quality assessment and pollution control measures are necessary to preserve and restore the healthiness of surface water bodies (Low et al., 2016, Banda and Kumarasamy, 2020c). On the same basis, this study attempts to put forward a practical and standardised tool that can be used towards monitoring surface water quality across all South African river catchments.

Even though the current study is targeting all South African river catchments, specific data set from a distinct Water Service Authority (WSA) have been considered to ascertain the appropriateness of the proposed model. It is a far-reaching and considerable amount of work to test the model against water quality data from all the Water Boards (WBs) in South Africa. On that ground, water quality data form the Umgeni Water Board (UWB) was deemed fitting to establish the effectiveness of the developed water quality model. The selection of UWB does not devalue the purpose of the study; instead, it marks the beginning of a long-term undertaking to demonstrate that the developed model is indeed universal and applicable to most, if not all South African river catchments.

Umgeni Water Board is a Water Service Authority responsible for water and sanitation affairs of KwaZulu-Natal Province in the Republic of South Africa (Nozaic et al., 2001, Manickum et al., 2014). UWB falls under the jurisdiction of Pongola-Mtamvuna Water Management Area (WMA) which has four primary drainage regions labelled T, U, V and W. Amongst the four areas, primary drainage basin U was considered for the current study. Further to this, only four secondary drainage regions were selected, and these are Umgeni, Umdloti, Nungwane and Minto River catchments which are identified by the Department of Water and Sanitation (DWS) as U20, U30, U70 and U80 respectively. Umgeni River catchment is the major of the four; consequently, the drainage basin is regarded as the primary study area and considered more significant than the other three catchments.

Chapter Four presents basic information relating to the study area, and the forthcoming sections provide details about water service institutional arrangements in the Republic of South Africa; more attention being given to details describing Umgeni River catchment and Umgeni Water

Board (UWB). Considering the significance of the other three watersheds; then, only baseline information is provided for Umdloti, Nungwane and Minto River catchments.

4.2 Institutional arrangements

According to the National Water Act No. 36 of 1998 (Republic of South Africa, 1998), the Minister in charge of the Department of Water and Sanitation, formally the Department of Water Affairs, is empowered to act on behalf of the Nation with ultimate responsibility to fulfil particular mandates regarding access, allocation and protection of water resources. Through the departmental structures, the Minister is responsible for establishing Water Management Areas (WMAs), and these demarcations should be strategically and geographically positioned to manage at least one or more primary drainage regions. Furthermore, the Act instituted that WMAs be governed by Catchment Management Agencies (CMAs) with Water User Associations (WUAs) in subordinate positions. Both CMAs and WUAs are regarded as local level structures thereto undertake water-related activities at the catchment level (Republic of South Africa, 1998, Chiluwe, 2014).

However, since 1998, the establishment and functionality of CMAs have been a national challenge (Chiluwe, 2014). Therefore, in the year 2017, the DWS decided to establish a single Catchment Management Agency (CMA) to manage all water resources in the Republic of South Africa. The decision was aimed at decentralising water resource management as supported by Section 78(3) of the National Water Act (1998), National Water Resource Strategy (2002, 2013) and National Policy Positions on Water (2014). Under such developments, the new agency is referred to as the National Water Resource Management Agency (NWRMA), and its boundaries cover all the nine Water Management Areas (Republic of South Africa, 2017).

4.2.1 Water management areas (WMAs)

Previously there were nineteen Water Management Areas (WMAs) in South Africa. Through the revision of the National Water Strategy, it was then resolved to restructure the WMAs and reduced them to nine instead of the former nineteen Water Management Areas. This decision was reached amid efforts to improve the water resource management model for the current funding arrangements, available skills sets and expertise, institutional capacity and integrated management system. The nine newly formed WMAs are, (1) Limpopo, (2) Olifants, (3) Inkomati-Usuthu, (4) Pongola-Mtamvuna, (5) Vaal, (6) Orange, (7) Mzimvubu-Tsitsikamma, (8) Breede-Gouritz, and lastly (8) Berg-Olifants (Republic of South Africa, 2012, Chiluwe, 2014). The following Figure 4.1 is indicative of the new WMA boundaries.

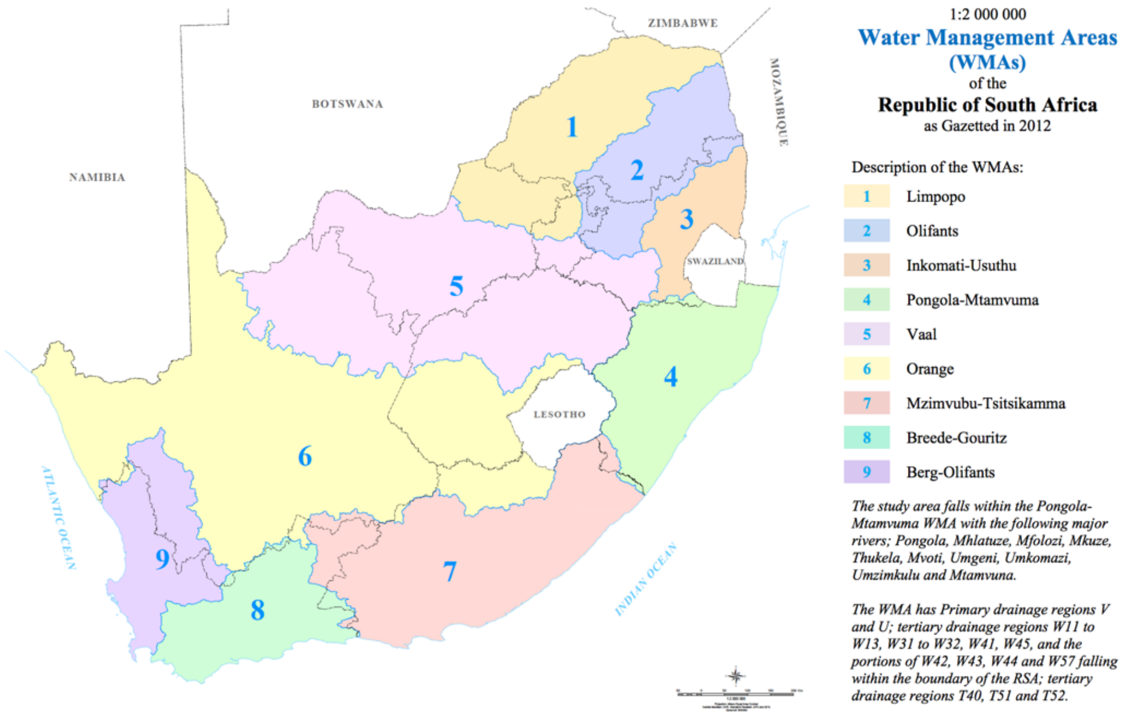


Figure 4.1: Map showing the new boundaries of Water Management Areas (WMAs) of the Republic of South Africa as Gazetted in 2012

Source: Authors diagram modified from the water management areas map (Republic of South Africa, 2012).

Notes: The boundaries of Water Management Areas (WMAs) do not follow the Provincial boundaries; instead, they are aligned to the drainage regions.

The naming of the WMAs is attributed to the major rivers associated with that particular WMA. Accordingly, the study area is within Pongola-Mtamvuna WMA, and the details of this specific WMA are discussed in the following subsection.

4.2.2 Pongola-Mtamvuna water management area (WMA)

Pongola-Mtamvuna Water Management Area (WMA) emerged following the combination of Mhlatze, Thukela and Mvoti-Umzimkulu WMAs as set-out in the former demarcations. This newly established WMA have major rivers flowing eastward into the Indian Ocean; and these include Pongola, Mhlatuze, Mfolozi, Mkuze, Thukela, Mvoti, Umgeni, Umkomazi, Umzimkulu and Mtamvuna. As mentioned earlier, Umgeni, Umdloti, Nungwane and Minto/Umuziwezinto River catchments are within Pongola-Mtamvuna WMA, with Umgeni Water Board serving as the leading Water Service Authority.

4.3 Umgeni River catchment

Umgeni River catchment is a sub-humid drainage basin located along the Indian Ocean coastline in KwaZulu-Natal Province in the Republic of South Africa (Warburton et al., 2012, Rangeti, 2015, Hughes et al., 2018). With Umgeni basin having a diversified land usage and multiple water supply systems, the watershed is regarded as one of the complex drainage regions in the country. The river basin is subdivided into twelve quaternary drainage regions, also known as quaternary catchments (QCs). Seven of the QCs are situated in the uppermost part of Umgeni basin, three are in the middle, and two are in the lower part of the secondary drainage region (Warburton et al., 2012, Namugize et al., 2018). Umgeni River catchment plays a significant role in the economic development of the country; it serves South Africa's biggest trading port and the second largest province in terms of population and economic sizes (Hughes et al., 2018). Such a pivotal role influence the perspective of why Umgeni is considered one of the most significant river catchments in the Republic of South Africa.

4.3.1 Significance of Umgeni River catchment

Umgeni Water Board (UWB) produces approximately 435.0 x 10^6 m^3/yr of potable water; of which 95.4 % (415.0 x 10^6 m^3/yr) is achieved using raw water abstracted from Umgeni basin (Umgeni Water, 2018). The river catchment supports a geographical coverage of 94 359.0 km^2, which habitats about 11.4 million people; that is basically 19.7 % of South Africa's total population (Rangeti, 2015, Umgeni Water, 2018, Stats SA, 2018b). Of great significance, the Umgeni basin addresses the water needs of the Durban-Pietermaritzburg business corridor. And act as the primary source of water supplied to the Port of Durban, which is the biggest trading port in Africa and contributes significantly to the Gross Domestic Product (GDP) of the Republic of South Africa (Shoko, 2014, Hughes et al., 2018). KwaZulu-Natal Province contributes approximately 16.0 % of the National GDP (Stats SA, 2018a), and employs almost 15.0 % of South Africa's employed population. The GDP and Population figures for the Republic of South Africa are presented in Figure 4.2.

Considering the social and economic activities in KwaZulu-Natal, the province is regarded to be a highly ecologically disturbed region (Namugize et al., 2018), and this describes the motivation for the adoption of Umgeni catchment as the main study area. The water demand of KwaZulu-Natal is expected to increase to 657.0 x 10^6 m^3/yr by the year 2044, resulting from further economic developments, increased population migration and improvements in the living standards (Hughes et al., 2018). The current activities and projected developments in Umgeni River catchment have extraordinary effects on the national water resources. Therefore, they require a comprehensive water management monitoring model that focuses on protecting the water reserves. It is then essential to develop a water quality index model that can be adopted to understand better the dynamics of water quality changes in Umgeni River catchment and South Africa as a whole. The model will provide institutional support in delineating water quality concerns across various river catchments and provide factual information to water technocrats and decision-makers.

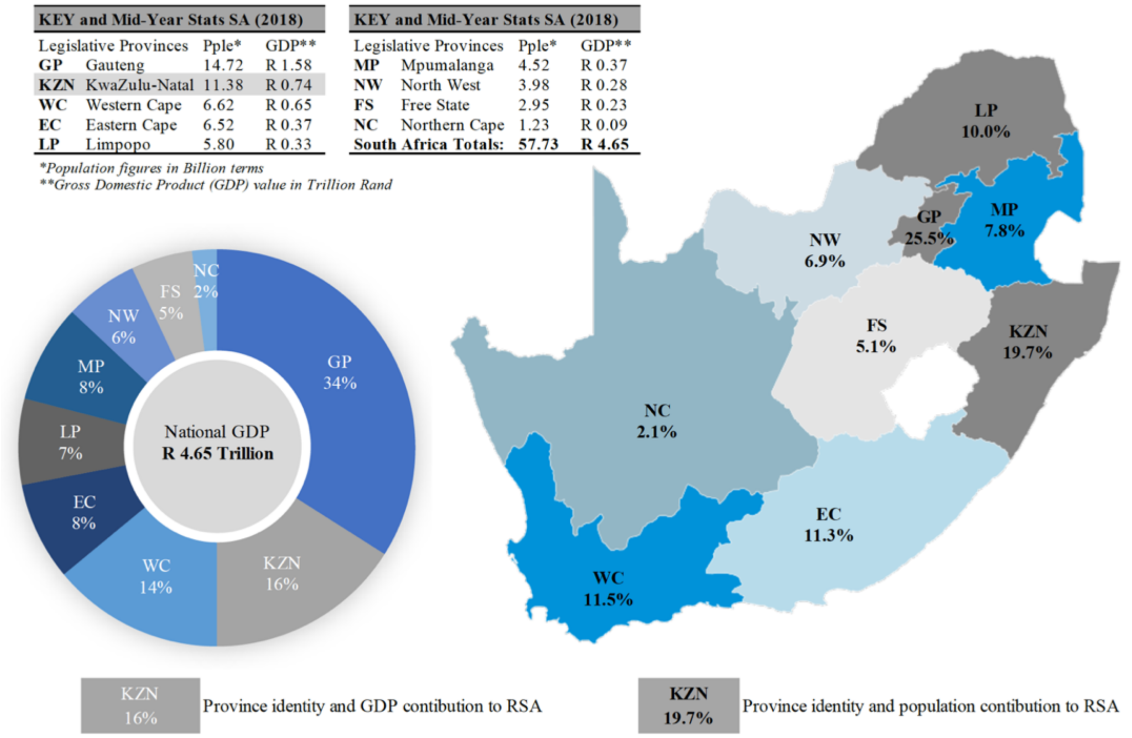


Figure 4.2: Gross Domestic Product (GDP) and Population details for the Republic of South Africa during the middle of the Year 2018

Source: Authors diagram that graphically represents statistical information documented in Stats SA (2018a, 2018b).

Notes: Population figures (PPle*) are presented in Billion terms and the Gross Domestic Product (GDP**) values are presented in Trillion Rand.

4.3.2 Catchment coverage and land use

Umgeni River catchment has surface area nearing 4 432.0 km^2, with Umgeni River as the primary water channel of the drainage basin (Chiluwe, 2014, Olaniran et al., 2014, Shoko, 2014, Singh and Lin, 2015, Namugize et al., 2018). The river originates from the Drakensberg mountains and flows eastwards towards the Indian Ocean. The 232-kilometre long Umgeni River has four main cardinal tributaries which are Lions, Karkloof, Impolweni and Umsunduzi Rivers (Chiluwe, 2014, Rangeti, 2015). Lions River is the most contributing tributary on the upstream of Midmar Dam, and it serves as the transfer channel conveying water resources from the adjacent Mooi River Catchment (Namugize et al., 2018). The basin land cover is characterised as heterogeneous mostly consisting of urban areas, natural forest, commercial sugarcane plantations, small-scale to commercial agricultural farms and the Port City of Durban (Warburton et al., 2012, Shoko, 2014, Hughes et al., 2018, Namugize et al., 2018). Notably, Umgeni River supports the livelihood of informal settlers residing along the river course. They rely on the river for various household activities, irrigation and livestock production (Gakuba et al., 2015).

4.3.3 The climate of Umgeni River catchment

The rainfall pattern of Umgeni basin is seasonal, with rains concentrated in the summer months (October to March). The amount of precipitation is highly variable, increasing from the western side to the eastern part of the river catchment. The highest rainfall occurs in coastal areas with a range of 1 000.0 mm/yr to 1 500.0 mm/yr (Shoko, 2014, Rangeti, 2015). The rainfall intensity is due to moisture-laden air from the warm Mozambique rainfall corridor. Occasionally, Umgeni basin experiences tropical cyclones, which are associated with devastating thunderstorms and flooding. The inland parts of Umgeni basin generally receive rainfall ranging from 800.0 mm/yr to 1 000.0 mm/yr (Warburton et al., 2012, Shoko, 2014, Namugize and Jewitt, 2018). According to Chiluwe (2014), groundwater recharge for Umgeni basin varies between 3.0 % and 7.0 % of the mean annual precipitation (MAP). The average annual temperature ranges from 12.0 ^{o}C to 22.0 ^{o}C; leading to evaporation rates between 1 567.0 mm/yr and 1 737.0 mm/yr (Namugize et al., 2018). The headwater of Umgeni River is located 1 760.0 meters above mean sea level (AMSL) in KwaZulu-Natal Midlands within the Drakensberg mountains; whereas, the river mouth is situated north of Durban's natural harbour, and discharging into the Indian Ocean at sea level (Namugize et al., 2018).

4.3.4 Surface water reservoirs

Four major dams are used to regulate and preserve the water resources within the Umgeni drainage region. These are, Midmar, Albert Falls, Nagle and Inanda; which were commissioned in 1965, 1976, 1950 and 1988 respectively (Namugize et al., 2018, Umgeni Water, 2019a). Midmar Dam (235.4 x 10^6 m^3) supplies Pietermaritzburg and some portions of Durban, whereas Albert Falls Dam (289.1 x 10^6 m^3), Nagle Dam (24.6 x 10^6 m^3) and Inanda Dam (251.6 x 10^6 m^3) cater for the greater part of Durban Metropolitan (Warburton et al., 2012, Chiluwe, 2014, Rangeti, 2015). In addition to the four major dams, there is Henley Dam (1.5 x 10^6 m^3) situated south of Midmar Dam along Msunduzi River, a tributary of Umgeni River. Henley Dam is no longer used for domestic supply purposes. Apart from that, there are about 300 farm dams utilised for irrigating nearly 185.0 km^2 of commercial farms in Umgeni catchment area (Warburton et al., 2012).

4.3.5 Inter-basin transfer schemes

With the focus of reducing the risk of limited or non-supply of water to Pietermaritzburg and Durban areas, Mooi-Mgeni Transfer Scheme was implemented to augment Umgeni drainage region. The transfer scheme abstracts water from Mearns Weir situated downstream of Springs

Grove Dam where Mooi and Little Mooi Rivers converge. From thereon, water is pumped through a 21.6 km long pipeline to an outflow structure located along Mpofana River, then flows into Lions River and subsequently into Umgeni River upstream of Midmar Dam. The first 13.3 km of the pumping main is Ø1.4 m and further reduced to Ø0.9 m for the remaining length of 8.3 km. The transfer scheme, formally known as Mearns Emergency Transfer Scheme, was initially implemented in 1983 as a drought relief project with an initial capacity of 1.3 m^3/s and decommissioned in 1993. Later in 2003, the augmentation scheme was upgraded and recommissioned as Mooi-Mgeni Transfer Scheme Phase 1 (MMTS1), with the capacity to deliver up to 3.2 m^3/s. Further, in 2016, Mooi-Mgeni Transfer Scheme Phase 2 (MMTS2) was completed to achieve a continuous supply of 4.5 m^3/s towards Umgeni System (Umgeni Water, 2019a).

Deliberations are underway to consider the implementation of Umkomazi-Mgeni Transfer Scheme to supplement the Umgeni System. Umkomazi River is the third-largest rivers in KwaZulu-Natal in terms of mean annual runoff (MAR), hence being contemplated as an alternative transfer scheme (Umgeni Water, 2019b).

4.4 Umdloti River catchment

Umdloti catchment is situated north-east of Umgeni basin, adjacent to Nagle and Inanda Dams. The catchment has an estimated area of 597.0 km^2 with Umdloti River as the main watercourse of the basin (Umgeni Water, 2019d). The river source is found in the Noodberg area, with an altitude of 823.0 m above means sea level (Govender, 2009). Umdloti River course stretches for nearly 88.0 km, flowing eastwards towards the Indian Ocean. The river estuary is approximately 25.0 km north-east of Durban Central (Govender, 2009, Olaniran et al., 2014). A considerable portion of the catchment is utilised for commercial farming, dominated by sugarcane and banana plantations with minimal of vegetable and citrus farming. Apart from these, other establishments include residential, Verulam Town, game reserves, Hazelmere Dam and Hazelmere wastewater treatment plant (Govender, 2009). Similar to Umgeni basin, the catchment experiences summer rainfall with mean annual precipitation ranging between 800 mm and 1 125 mm. Temperatures are varying from 9 ^oC in winter to 38 ^oC in summer (Govender, 2009). Hazelmere Dam is the primary water impoundment in Umdloti catchment, with an upgraded capacity of 37.1 x 10^6 m^3 (Umgeni Water, 2019d). The dam was established to service the domestic, industrial and agricultural needs of the Durban area, including the new Durban International Airport (Govender, 2009, Olaniran et al., 2014).

4.5 Nungwane River catchment

Located south-west of Umgeni drainage region, Nungwane River catchment has an average annual precipitation of 938.0 mm/yr and annual evaporation close to 1 200.0 mm/yr. The significant impoundment in the quaternary catchment is the Nungwane Dam situated along Nungwane River, which is a tributary of Lovu River (Umgeni Water, 2019c). The impoundment was built in 1977 with a catchment area of 58.0 km^2 and a volume of 2.2 x 10^6 m^3 at full supply level (FSL). Raw from Nungwane Dam is treated at Amazimtoti water treatment plant and supply eThekwini Municipality (Umgeni Water, 2019c).

4.6 Umzinto/Umuziwezinto River catchment

Umzinto River catchment also known as Umuziwezinto River catchment lies further south of Nungwane Dam. According to Umgeni Water (2019c), the river basin receives rainfall averaging 985 mm/yr, with an evaporation rate of 1 200.0 mm/yr. In 1983, Umzinto Dam was constructed along Umzinto/Umuziwezinto River with a capacity nearing 0.5 x 10^6 m^3 at FSL and catchment coverage of 51.6 km^2. Together with EJ Smith Dam, raw water from Umzinto Dam is treated at Umzinto water treatment plant (WTP) and distributed to Ugu District Municipality (Mwelase, 2016, Umgeni Water, 2019c).

Both dams, EJ Smith and Umzinto, provides approximately 0.083 m^3/s and 0.073 m^3/s respectively towards the operation of Umzinto WTP, with current utilisation of 13.6 Mℓ/day and design capacity of 22.0 Mℓ/day (Mwelase, 2016, Umgeni Water, 2019c). During the drought season of 2014/2015, the Mpambanyoni Emergency Scheme was established to augment Umzinto System with an additional supply of 8.0 Mℓ/day. The system was abstracting from Mpambanyoni River and later decommissioned in 2016 when both EJ Smith and Umzinto Dams reached FSL (Umgeni Water, 2019c).

4.7 Sampling locations

Umgeni Water Board (UWB) established water sampling stations to enhance water quality monitoring, and the stations are strategically positioned to provide a holistic understanding of water affairs within the service area of KwaZulu-Natal Province. Instead of establishing new research-based sampling stations, the current studies utilised water quality data collected by UWB.

The six identified sampling stations fall under four different catchment areas. These are Umgeni River catchment (U20) for Henley, Inanda and Midmar Dams; Umdloti River catchment (U30) for Hazelmere Dam; Nungwane River catchment (U70) for Nungwane Dam; and lastly Umzinto/Umuziwezinto River catchment (U80) for Umzinto Dam. Testing the model with data from various river catchments promote the objective of establishing a universal water quality index (UWQI) suitable for use across the catchment areas in South Africa.

At least one or more stations were considered for each of the four drainage basins as demonstrated by Figure 4.3, which illustrates the geographic positions of the six sampling stations. Further details of the selected sampling stations are included in the following Table 4.1.

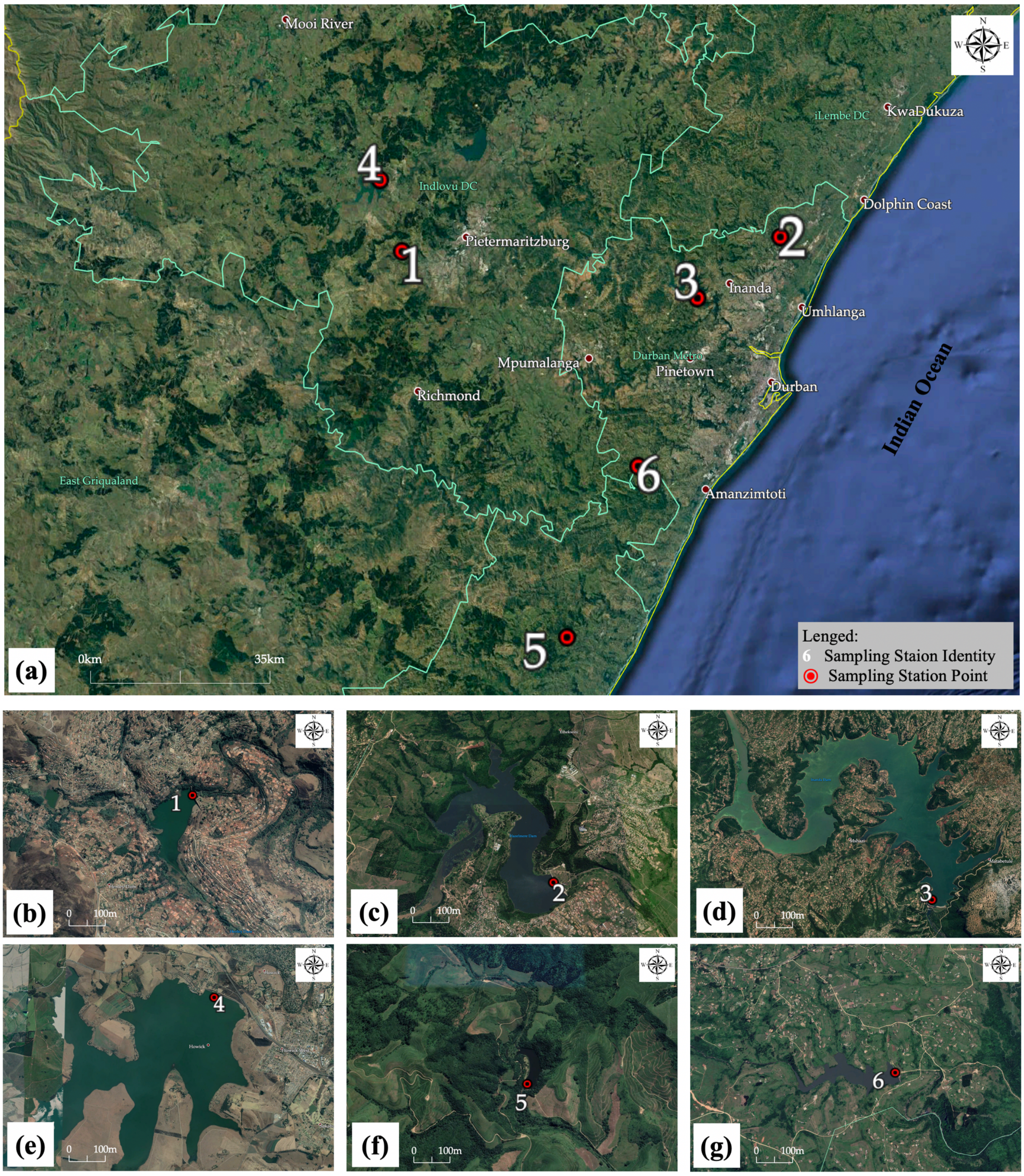


Figure 4.3: Locality map for sampling stations relevant to the study, (**a**) all six sampling stations, (**b**) Henley Dam, (**c**) Hazelemere Dam, (**d**) Inanda Dam, (**e**) Midmar Dam, (**f**) Umzinto Dam, and (**g**) Nungwane Dam

Source: Authors diagram (Banda and Kumarasamy, 2020b, 2020c). The underlying map used for the production of the locality map was downloaded from Google Earth, and station coordinates are from Umgeni Water Board (2014 to 2018 water quality data) presented in Table 4.1.

Notes: Sampling Stations identity (1) Henley Dam DHL003, (2) Hazelmere Dam DHM003, (3) Inanda Dam 0.3 km DIN003, (4) Midmar Dam DMM003, (5) Umzinto Dam DMZ009, and (6) Nungwane Dam DNW003.

Table 4.1: Details of sampling stations relevant to the study

ID	Description of the sampling station	Station identity No.	Catchment identity No.	Location coordinates (DMS)*	
				Latitude	Longitude
1	Henley Dam – Main basin integrated	DHL003	U20	S 29° 37' 25.734"	E 30° 14' 49.754"
2	Hazelmere Dam – Main basin integrated	DHM003	U30	S 29° 35' 53.722"	E 31° 02' 32.121"
3	Inanda Dam – Integrated 0.3 km from the dam wall	DIN003	U20	S 29° 42' 27.403"	E 30° 52' 03.352"
4	Midmar Dam – Main basin integrated	DMM003	U20	S 29° 29' 47.332"	E 30° 12' 05.655"
5	Umzinto Dam – Main basin integrated	DMZ009	U80	S 30° 18' 40.676"	E 30° 35' 34.580"
6	Nungwane Dam – Main basin integrated	DNW003	U70	S 30° 00' 24.473"	E 30° 44' 36.150"

Source: Umgeni Water Board (Banda and Kumarasamy, 2020b, 2020c).

Notes: *Location coordinates based on the World Geodetic System 84 (WGS 84) and DMS stands for Degrees, Minutes and Seconds. Although the Umgeni Water Board (UWB) has more water quality monitoring stations, Table 4.1 is an extract of only the eight water quality monitoring stations considered in the development of the universal water quality model.

The economic importance of the Umgeni Basin, the uniqueness of its inter-basin arrangements, the magnitude of the transfer schemes involved and extensive water demand; are vital elements leading to a comprehensive water resource management. All these distinctively motivated the identification and selection of the Umgeni River catchment as the main study area. Beyond that, they are three additional catchments incorporated into the study to examine the models further and complement the objective of developing universally acceptable water quality models.

CHAPTER 5

5. RESULTS AND DISCUSSION

5.1 Overview

Since water quality is a prime natural resource, it is then important to conduct regular water quality assessment that describes the degree of pollution and substantiate the healthiness of water resources. Of which water quality index (WQI) is an essential tool that can provide a quick initial guide necessary to evaluate the water quality status of a given water body. Water quality indices are beneficial for integrating significant physical, chemical and biological constituents of water and provide a simple, but yet scientifically justifiable water quality rating score. Such a valuable and unique rating comprehend the influence of various water quality variables and easily communicate water quality data to non-technical individuals and more importantly, the policy-makers. In order to obtain a WQI, sub-indices of water quality variables are employed to indicate water quality on a scale most probably from zero (worst quality) to unity (best quality). Furthermore, the sub-indices are aggregated to yield an overall WQI value usually between zero (poor quality) and hundred (excellent quality).

In this study, various water quality index models have been evaluated, outlining their advantages and disadvantages. Conclusions have been drawn about the similarities and dissimilarities existing among different models, and the findings lead to the suggestion of possible methods applicable in the development of a universal water quality index (UWQI) for South African river catchments. The UWQI model was developed using conventional methods and attested with an artificial neural network (ANN) model. Furthermore, a water quality variability model (WQVM) comprising of UWQI model, ANN model and surrogate WQI was established and tested.

Therefore, this chapter presents the results and discussion of water quality index development using conventional techniques and multivariate statistical methods. Chapter Five also aims to document important information relevant to the use of Artificial Intelligence (AI) in water quality science, through the application of artificial neural networks (ANNs).

5.2 Research data

Although the study is focusing on all South African river catchments, specific data set have been considered for testing the functionality of the models developed under this particular research. It is extensive work and time consuming to attempt testing water quality data from all the Water Boards (WBs) in South Africa. In this regard, water quality data obtained from Umgeni Water Board (UWB) has been utilised to achieve specific objectives of the study. The dataset comprises of 416 samples gathered monthly for over four years starting from 2014 until 2018. Table 5.1 documents the descriptive statistics for the research data.

Table 5.1: Descriptive statistics for Umgeni water quality data gathered monthly for over four years starting from 2014 until 2018

ID	Water quality variables	Unit	Statistical summary of the observed water quality data for Umgeni				
			Minimum	Average	Maximum	Standard deviation	Coefficient of variation
1	Ammonia	mg N/ℓ	0.040	0.107	0.990	0.072	66.973 %
2	Calcium	mg Ca/ℓ	1.000	9.457	30.500	5.719	60.477 %
3	Chloride	mg Cl/ℓ	1.821	26.843	79.000	14.560	54.244 %
4	Chlorophyll-a	µg/ℓ	0.140	5.057	92.220	7.986	157.917 %
5	Electrical Conductivity	µS/m	6.840	20.708	48.000	8.991	43.417 %
6	Fluoride	mg F/ℓ	0.100	0.140	0.544	0.053	37.423 %
7	Hardness	mg $CaCO_3$/ℓ	6.615	47.752	128.457	23.249	48.687 %
8	Magnesium	mg Mg/ℓ	1.000	5.857	14.600	2.448	41.793 %
9	Manganese	mg Mn/ℓ	0.010	0.051	1.210	0.105	207.381 %
10	Nitrate	mg N/ℓ	0.050	0.590	9.580	0.700	118.598 %
11	pondus Hydrogenium	Unit less	0.000	7.766	9.100	0.545	7.023 %
12	Sulphate	mg SO_4/ℓ	0.160	8.696	24.200	6.422	73.846 %
13	Turbidity	NTU	0.600	14.157	367.000	30.956	218.659 %

Source: Umgeni Water Board (Banda and Kumarasamy, 2020b, 2020c)

Notes: Parameters are listed according to alphabetic, other than the order of importance. Although the data received from Umgeni has more water quality variables, Table 5.1 is an extract of only the thirteen water quality parameters considered for the study. The UWB data consist of 416 samples measured from six sampling stations located within six different river catchments.

The total number of samples measured and recorded is 416, and none of the thirteen water quality variables has the maximum number of tests recorded; the closest being chlorophyll-a and turbidity with both parameters having approximately 97.7 % tests recorded. The degree of consistency in sampling is 63.1 % with a noticeable effect on calcium (Ca), hardness ($CaCO_3$), fluoride (F) and magnesium (Mg) having missing data equating to 61.5 %, 61.4 %, 94.3 % and 61.5 %, respectively. Where circumstances permitted, linear interpolation assisted in estimating missing data, especially data gaps lying in-between measured intervals. The back-and-forward filling approach was applied to calculate missing data at the start or end of the testing period (Schullehner et al., 2017, Banda and Kumarasamy, 2020b).

The UWB measured hardness ($CaCO_3$) quarterly and where possible, using the measured values of Ca and Mg, an approximation of $CaCO_3$ missing values were alternatively obtained using Equation 5.1. The method is a common practice and prescribed in various studies (see DWAF, 1996a, 1996b, Banda, 2015, Bogart et al., 2016, Beyene et al., 2019, Banda and Kumarasamy, 2020c).

$$CaCO_3 = 2.497Ca + 4.118Mg \qquad \text{Eq. 5.1}$$

Where: $CaCO_3$ is the calculated hardness concentration in milligrams per litre (mg/ℓ);

Ca is the observed calcium concentration in milligrams per litre (mg/ℓ); and

Mg is the observed magnesium concentration in milligrams per litre (mg/ℓ).

Regardless of the amount of missing data, the samples obtained from UWB were adequate and contributed significantly towards the success of the research studies. Umgeni water quality data has been considered based on availability, other than being a priority and limiting the number of WBs used for testing the models do not devalue the significance of the study. The rationale used in developing the universal water quality index is entirely independent of the data set used for testing the functionality of the model. Nevertheless, as an ongoing project and in support of the current studies, it is recommended that additional data from other WBs if not all, be considered and documented separately.

The subsequent thesis sections discuss the approach and processes employed to select the most significant thirteen water quality parameters. There are numerous methods involved in the development of water quality indices, but this study focuses on the application of the conventional technique, statistical approach and artificial neural networks (ANNs). The application of the three methods is also deliberated in the subsequent sections.

5.3 Universal water quality index (UWQI) using the conventional methods

Water quality is a multi-parameter attribute, that is assessed through combining the cumulative effects of a considerable amount of water quality variables. Accordingly, water quality indices provide a sensible solution in resolving lengthy, multi-parameter water analysis reports into a single-digit score (Sarkar and Abbasi, 2006, Banda and Kumarasamy, 2020a). Water quality index is a simple, but yet intelligible rating score that provides the composite influence of various water quality variables in a given water body (Luzati and Jaupaj, 2016, Wanda et al., 2016, Guettaf et al., 2017). The index number is generally measured against a relative scale to explain the quality of water resources based on categories ranging from zero to hundred, which is further classified from very poor to excellent (Paun et al., 2016).

Commonly, the development of water quality indices (WQIs) involves (i) selection of the significant water quality parameters; (ii) formation of sub-indices; (iii) establishing relative parameter weights; and (iv) aggregation of the sub-indices (Srebotnjak et al., 2012, Al-Mutairi et al., 2014, Paun et al., 2016, Sutadian et al., 2016, Shah and Joshi, 2017, Unda-Calvo et al., 2019, Banda and Kumarasamy, 2020a). Similarly, the current studies prescribe to the same procedure of developing WQIs, especially when using conventional methods. On that premise, the following sections of the thesis attempt to discuss the techniques applied during the development of the universal water quality index (UWQI) and present a comparative analysis of the most critical aspects of the UWQI.

5.3.1 Water quality parameters

As significant indicators of the aquatic-ecosystem health, water quality variables can be employed to quantify the degree of impairment of a given water body, which might be attributed to both natural and anthropogenic activities (EPA Victoria, 2003). The magnitude and extent of such damage can be measured against predefined water quality benchmarks, that is; the criteria, water quality objectives, prescribed targets, legislative standards, action levels and associated concertation limits. Such yardsticks are established explicitly for individual water quality variables to safeguard the aquatic environment and protect human users, considering what is regarded as non-toxic and risk-free. Water quality benchmarks have been established with a distinctive meaning, and for diverse applications, some are generic, and some are specific (CWT, 2004, Banda, 2015).

Individual parameter indicator values and limits are defined and governed by Water Quality Objectives (WQOs). Thus, the laws, legislative policies and regulations that factors in various fundamentals relevant to the establishment of pollution tolerance levels and associated effects, whether short term or long-term effects. As experts discover more about conservation requirements of the aquatic-ecosystem and evidence relating to the impact of each water quality parameter, then adjusting the tolerance limits becomes necessary and regarded as a continuous exercise. Such circumstances are the reason why WQOs are forever changing (CWT, 2004, Banda, 2015). Therefore, constant evaluation of water quality indices is of great importance, especially for water quality models that are built for sustainability and high precision. The process explains why the development and modification of water quality indices is forever growing and becoming a norm. Given this, regardless of the success of the suggested universal water quality index, the parameters and their associated limits need to be reviewed over a particular period time.

The succeeding sections of the thesis document and discuss the thirteen specific water quality parameters considered significant in the developing of a universal water quality index model for South African river catchments.

5.3.2 Selection of the significant water quality parameters

Selection of water quality parameters is the most critical element of establishing a water quality index. The index developer should identify and chose the most significant variables; not too few or too many, but just enough to provide a practical sense; in cognisance of the purpose of the index and the perceived degree of accuracy. The process requires proficiency, enormous care, experience and sound judgement since it can be apprehensive with uncertainty and subjectivity. Parameter selection can be achieved through the use of either statistical methods or expert opinion, which can be an individual or a group of professionals.

Accordingly, the current studies decided to involve expert opinion with a fixed set of parameters. Expert opinion has the advantage of engaging with stakeholders who are potentially the targeted end-users of the index model. The process eventually capacitates the acceptance of the index model through the sense of ownership, the idea that they are involved and henceforth acknowledging the index model as their own. The study purposefully considered the application boundaries of the proposed indexing model and decided to implement a fixed system as the most appropriate approach to evaluate the water quality status of various catchments. The procedure eliminates the possibility of altering the functionality of the model, thereby allowing a proper comparison of water quality status among different sites and promote prioritisation of national programmes without prejudice.

In respect to the expert opinion, three techniques were applied. Firstly, the Rand Corporation's Delphi Technique commonly known as the Delphi method (Linstone and Turoff, 1975, 2002), which involved a panel of water quality specialists communicating and responding through questionnaires (Nagels et al., 2001, Kumar and Alappat, 2009, Almeida et al., 2012). Secondly, the literature review method, whereby the author considers water quality parameters previously selected by similar research studies. Thirdly, the use of rejection rationale to produce a screened set of frequently monitored water quality variables. The methods are presented and discussed in the following sub-sections.

5.3.2.1 Selection of parameters by Rand Corporation's Delphi Technique (Delphi method)

A total of twenty-one water quality variables were selected for the inclusion into the Delphi Questionnaire, and the selection was influenced by the availability of published water quality objectives, guidelines, regulations and possible impact towards altering the quality of surface water. With a balanced selection of ten water quality specialists from each sector, a combined total of thirty panellists were identified from government parastatals, private sector and academia. Through existing relationships and referrals, the choice of the panel was reached based on their work positions, experience in water quality science and amount of peer-reviewed publications.

Similar to Nagels et al. (2001), and Almeida et al. (2012), Delphi questionnaires were circulated to the thirty prospect survey participants. They were asked to consider twenty-one water quality variables for their possible inclusion in the universal water quality index. Participants were instructed to designate each parameter as: "Include" and "Exclude" and further assign a relative significance rating against each parameter defined as "Include." The rating was based on a scale ranging from 1 to 5; with scale 1 representing the highest significance and scale 5 for relatively low significance. Beyond the twenty-one parameters listed in the questionnaire, panellists were permitted to add up to a maximum of five more variables if desired. Out of the thirty prospective participants, responses were received from twenty-one panellists, and the final significance ratings were calculated as tabulated in Table 5.2.

Table 5.2: Statistical analysis of Rand Corporation's Delphi Technique

ID	Water quality variables	Statistical summary of the Delphi Method									
		No answer	Exclude	Include	Significance						Final significance
					1	2	3	4	5	Average	
1	Ammonia	2	0	19	12	4	2	0	1	1.632	4.368
2	Biochemical Oxygen Demand	1	4	16	10	3	2	1	0	1.625	4.375
3	Calcium	1	1	19	2	11	3	1	2	2.474	3.526
4	Chloride	0	0	21	4	9	7	0	1	2.286	3.714
5	Chlorophyll-a	0	3	18	0	0	2	9	7	4.278	1.722
6	Dissolved Oxygen	0	0	21	14	1	3	3	0	1.762	4.238
7	Electrical Conductivity	1	1	19	0	5	11	0	3	3.053	2.947
8	Faecal Coliforms	6	2	13	1	2	5	1	4	3.385	2.615
9	Fluoride	0	5	16	3	7	5	1	0	2.250	3.750
10	Hardness	0	7	14	0	1	8	3	2	3.429	2.571
11	Magnesium	3	3	15	4	2	7	1	1	2.533	3.467
12	Manganese	0	5	16	7	5	1	0	3	2.188	3.813
13	Nitrate	0	0	21	5	11	3	2	0	2.095	3.905
14	Nitrite	0	0	21	6	9	4	1	1	2.143	3.857
15	Phosphate	2	4	15	2	7	5	1	0	2.333	3.667
16	pondus Hydrogenium	0	3	18	11	4	1	2	0	1.667	4.333
17	Sulphate	1	8	12	0	2	7	3	0	3.083	2.917
18	Temperature	3	6	12	0	1	9	1	1	3.167	2.833
19	Total Alkalinity	0	10	11	2	0	4	4	1	3.182	2.818
20	Total Dissolved Solids	1	7	13	0	1	5	5	2	3.615	2.385
21	Turbidity	0	3	18	0	3	10	1	4	3.333	2.667

Source: Twenty-one questionnaires from the water quality specialist considered for the Delphi exercise.

Notes: Parameters are listed according to alphabetic, other than the order of importance. A total of twenty-one questionnaires were captured in Table 5.2.

The same parameter list used for the Rand Corporation's Delphi Technique was considered for the selection of parameters using the literature review method.

5.3.2.2 Selection of parameters by literature review method

Complementing the Rand Corporation's Delphi Technique, the existing literature on the water quality indices (WQIs) was used to select the most significant variables. Thirty-seven studies were considered, and each parameter was designated as "Included" if it formed part of the identified research work and the predefined twenty-one parameters listed in Table 5.2; otherwise, it was designated as "Not Included." Furthermore, the originally assigned significance rating was recorded as the relative significance rating for each parameter that was "Included" in the study in question. The rating was based on a scale ranging from one to five; with "scale 1" representing the lowest significance and "scale 5" for relatively high significance. If a different significance rating scale was used in the existing studies, the original rating values were equivalently transformed to match the preferred rating scale using Equation 5.2 as follows (Banda and Kumarasamy, 2020c):

$$y = \mathrm{a} + (\mathrm{b} - \mathrm{a})(x_i - x_{min})/(x_{max} - x_{min}) \quad \text{Eq. 5.2}$$

where: y is the new rating; a, b, are minimum and maximum values of the targeted scale rating; x_{min}, x_{max}, are minimum and maximum possible ratings in the specified scale; and x_i is the i^{th} rating value of the specified scale.

The results of the statistical analysis of the literature review method are presented in Table 5.3.

Table 5.3: Statistical analysis of the literature review method

ID	Water quality variables	Statistical summary of the literature review method				
		Not included	Included	Maximum significance	Minimum significance	Average of the Significance
1	Ammonia	17	20	5.000	1.650	3.503
2	Biochemical Oxygen Demand	14	23	5.000	0.331	3.211
3	Calcium	22	15	5.000	0.989	1.996
4	Chloride	14	23	5.000	0.010	1.925
5	Chlorophyll-a	36	1	1.000	1.000	1.000
6	Dissolved Oxygen	10	27	5.000	1.650	4.214
7	Electrical Conductivity	18	19	5.000	0.002	2.314
8	Faecal Coliforms	14	23	5.000	1.780	3.574
9	Fluoride	29	8	5.000	2.000	3.462
10	Hardness	22	15	4.000	0.903	1.894
11	Magnesium	23	14	5.000	1.000	1.933
12	Manganese	31	6	5.000	1.500	3.109
13	Nitrate	6	31	5.000	0.176	3.007
14	Nitrite	25	12	5.000	0.110	2.572
15	Phosphate	17	20	5.000	1.000	2.535
16	pondus Hydrogenium	2	35	5.000	0.221	2.595
17	Sulphate	21	16	5.000	0.989	2.971
18	Temperature	16	21	5.000	0.500	2.053
19	Total Alkalinity	28	9	3.580	1.000	2.317
20	Total Dissolved Solids	10	27	5.000	0.079	2.959
21	Turbidity	23	14	4.920	0.397	2.623

Source: Horton (1965), Brown et al. (1970), Brown et al. (1973), SRDD (1976), Dunnette (1979), Martínez de Bascarón (1979), House (1986), Smith (1987), Tyson and House (1989), House (1990), Pesce and Wunderlin (2000), Cude (2001), Liou et al. (2004), Debels et al. (2005), Kannel et al. (2007), Boyacioğlu (2007), Sánchez et al. (2007), Kumar and Alappat (2009), Carvalho et al. (2011), Hamid et al. (2013), Koçer and Sevgili (2014), Sharma et al. (2014), Abtahi et al. (2015), Banda (2015), Singh et al. (2015), Ewaid (2016), Guettaf et al. (2017), Trikoilidou et al. (2017), Ewaid et al. (2018), García-Ávila et al. (2018), Ponsadailakshmi et al. (2018), Sutadian et al. (2018), Tiri et al. (2018), and Yousefi et al. (2018).

Notes: Parameters are similar to water quality variables listed in Table 5.2 employed on the Rand Corporation's Delphi Technique under Section 5.3.2; and they are listed according to alphabetic, other than the order of importance. A total of thirty-seven studies were captured in Table 5.3.

The results of the Rand Corporation's Delphi Technique and the literature review method were combined to designate the final list of the parameters included in the universal water quality index.

5.3.2.3 Final parameters considered for UWQI

Lessening the monitoring data requirements, governs the input parameter demand and reduce the bulkiness of the indexing model. In this way, it intensifies regular use of the index and promotes the application of the indexing model in most, if not all, the river catchments within South Africa. Which is in line with the primary objective of the study, and if achieved, then the current study will be considered successful. On the basis thereof, the twenty-one parameters were reduced to an optimum, just enough to ensure functional sense and scientific steadiness. The final water quality parameters considered for the index model are included in Table 5.4 below.

Table 5.4: Ranking of parameters according to significance ratings

Selection by Delphi method			Selection by literature review method			Combined Delphi and literature review method			Final water quality parameters considered		
Rank	Rating	Var.	Rank	Rating	Var.	Rank	Rating	Var.	Rank	Rating	Var.
1	4.375	BOD_5	**1**	4.214	DO	**1**	4.226	DO	**1**	3.936	NH_3
2	4.368	NH_3	**2**	3.574	CFU	**2**	3.936	NH_3	**2**	3.606	F
3	4.333	pH	**3**	3.503	NH_3	**3**	3.793	BOD_5	**3**	3.464	pH
4	4.238	DO	**4**	3.462	F	**4**	3.606	F	**4**	3.461	Mn
5	3.905	NO_3	**5**	3.211	BOD_5	**5**	3.464	pH	**5**	3.456	NO_3
6	3.857	NO_2	**6**	3.109	Mn	**6**	3.461	Mn	**6**	2.944	SO_4
7	3.813	Mn	**7**	3.007	NO_3	**7**	3.456	NO_3	**7**	2.820	Cl
8	3.750	F	**8**	2.971	SO_4	**8**	3.215	NO_2	**8**	2.761	Ca
9	3.714	Cl	**9**	2.959	TDS	**9**	3.101	PO_4	**9**	2.700	Mg
10	3.667	PO_4	**10**	2.623	Turb	**10**	3.094	CFU	**10**	2.645	Turb
11	3.526	Ca	**11**	2.595	pH	**11**	2.944	SO_4	**11**	2.630	EC
12	3.467	Mg	**12**	2.572	NO_2	**12**	2.820	Cl	**12**	2.233	$CaCO_3$
13	2.947	EC	**13**	2.535	PO_4	**13**	2.761	Ca	**13**	1.361	Chl-a
14	2.917	SO4	**14**	2.317	TA	**14**	2.700	Mg			
15	2.833	Temp	**15**	2.314	EC	**15**	2.672	TDS			
16	2.818	TA	**16**	2.053	Temp	**16**	2.645	TA			
17	2.667	Turb	**17**	1.996	Ca	**17**	2.630	Turb			
18	2.615	CFU	**18**	1.933	Mg	**18**	2.568	CFU			
19	2.571	$CaCO_3$	**19**	1.925	Cl	**19**	2.443	$CaCO_3$			
20	2.385	TDS	**20**	1.894	$CaCO_3$	**20**	2.233	TDS			
21	1.722	Chl-a	**21**	1.000	Chl-a	**21**	1.361	Chl-a			

Source: Extracted from Table 5.2 and Table 5.3 of the current study

Notes: Parameters are listed according to their significance rating scores in ascending order. "Var." denotes water quality variables. The chemical symbols are defined as follows: ammonia (NH_3), biochemical oxygen demand (BOD_5), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), dissolved oxygen (DO), electrical conductivity (EC), faecal coliforms (CFU), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), nitrite (NO_2), phosphate (PO_4), pondus Hydrogenium (pH), sulphate (SO_4), temperature (Temp), total alkalinity (TA), total dissolved solids (TDS), turbidity (Turb).

Rejection rationale was employed to eliminate seven water quality parameters which are not commonly monitored across the South African river catchments. The seven parameters omitted are: biochemical oxygen demand (BOD_5), dissolved oxygen (DO), faecal coliforms (CFU), phosphate (PO_4), temperature (Temp), total alkalinity (TA) and total dissolved solids (TDS). Another variable excluded was nitrite (NO_2), the reason being that; in most instances, nitrite and nitrates are considered as one, and reasoning from this fact, it was found more appropriate to eliminate nitrite (NO_2) with less aggregated significance rating.

Against this background, the final thirteen parameters considered for the development of the water quality index are ammonia (NH_3), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), electrical conductivity (EC), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), pondus Hydrogenium (pH), sulphate (SO_4) and turbidity (Turb). The relative weightage coefficients of the final thirteen parameters are deliberated in the following Section.

5.3.3 Establishing relative parameter weightage coefficients

For this study, water quality parameters are regarded as diverse, having a unique set of effects on the classification of water. Some are regarded as less or more imperative than the others. With an attempt to distinguish the influence of each variable, weighting coefficients are assigned to each parameter depending on the level of influence and significant towards the overall index value (Sharma et al., 2014, Sutadian et al., 2016, Banda and Kumarasamy, 2020e). The significance ratings obtained from the participatory based Delphi method are aggregated together with significance ratings extracted from literature to form final average ratings. The aggregated weight ratings use a basic scale of importance, ranging from one (lowest impact) to five (highest impact). Upon deriving the weight ratings, weight coefficients which are directly proportional to the weight ratings are then achieved by dividing the rating value by the sum of all ratings as denoted by Equation 5.3 (Banda, 2015).

$$w_i = \frac{b_i}{\sum_{i=1}^{n} b_i} \qquad \text{Eq. 5.3}$$

where: b_i is the assigned significance rating of the i^{th} water parameter (one being the lowest rating and five the highest rating);

w_i is the weighted coefficient for the i^{th} water parameter (decimal value); and

n total number of the rated water quality parameters.

The coefficients are represented as decimal numbers, and the sum of all coefficients is one, thereby guaranteeing that the overall index value does not exceed hundred per cent ($w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equations 5.3). Otherwise, aggregation of sub-indices will be compromised, and deem the index model dysfunctional. The weight coefficients and final parameters proposed for the development of a universal water quality index for South African river catchments are presented in Table 5.5.

Table 5.5: Parameters of consideration and their aggregated weightage coefficients

ID	Water quality variables	Symbol	Unit	Impact ratings and weightage coefficients			
				Significance from Delphi method	Significance from review method	Aggregated significance value	Aggregated weighted coefficients
1	Ammonia	NH_3	mg N/ℓ	4.368	3.503	3.936	0.103529
2	Calcium	Ca	mg Ca/ℓ	3.526	1.996	2.761	0.072631
3	Chloride	Cl	mg Cl/ℓ	3.714	1.925	2.820	0.074168
4	Chlorophyll-a	Chl-a	µg/ℓ	1.722	1.000	1.361	0.035803
5	Electrical Conductivity	EC	µS/m	2.947	2.314	2.630	0.069193
6	Fluoride	F	mg F/ℓ	3.750	3.462	3.606	0.094852
7	Hardness	$CaCO_3$	mg $CaCO_3$/ℓ	2.571	1.894	2.233	0.058734
8	Magnesium	Mg	mg Mg/ℓ	3.467	1.933	2.700	0.071022
9	Manganese	Mn	mg Mn/ℓ	3.813	3.109	3.461	0.091037
10	Nitrate	NO_3	mg N/ℓ	3.905	3.007	3.456	0.090907
11	pondus Hydrogenium	pH	Unit less	4.333	2.595	3.464	0.091121
12	Sulphate	SO_4	mg SO_4/ℓ	2.917	2.971	2.944	0.077438
13	Turbidity	Turb	NTU	2.667	2.623	2.645	0.069565
					Totals	**38.017**	**1.000000**

Source: Derived from Table 5.2 and Table 5.3 of the study (Banda and Kumarasamy, 2020b, 2020c).

Notes: The total sum of all weights is equal to one whole number. Parameters are listed according to alphabetic, other than the order of importance. Using aggregated weighted coefficients, the following order of importance is achieved: $NH_3 > F > pH > Mn > NO_3 > SO_4 > Cl > Ca > Mg > Turb > EC > CaCO_3 > Chl-a$.

Considering that water quality parameters are monitored in different scientific units; sub-indices are applied to convert different units of measure into a single standard non-dimensional scale. The standardisation of scientific units is a common practice, and the conventional method involves sub-index rating curves which are later transformed into mathematical functions commonly known as sub-indices. The sub-index rating curves and mathematical functions for the thirteen suggested parameters are presented in the following sections.

5.3.4 Formation of sub-index rating curves and mathematical functions

Development of sub-indices is highly subjective and mostly based on personal judgement (Banda, 2015), however, similar to the selection of parameters and assigning of weight ratings; expert opinion can be utilised to delineate rating curves and sub-index functions. The challenge is that fitting and optimising a series of hand-plotted graphs is a daunting task, unlike selections of parameters and weight coefficients which involves numbers only. In light of that, sub-index rating curves and sub-index functions were individually developed by the author. For practical purposes, fixed key points of the rating curves were graphically established with reference to the permissible concentration limits (see Table 5.6). Straight-line graphs were used to converge the plotted points and produce a series of linear graphs, which were further converted into linear sub-index functions. Target Water Quality Ranges (TWQRs) as prescribed by DWAF (1996a, 1996b, 1996c) were consulted in the process.

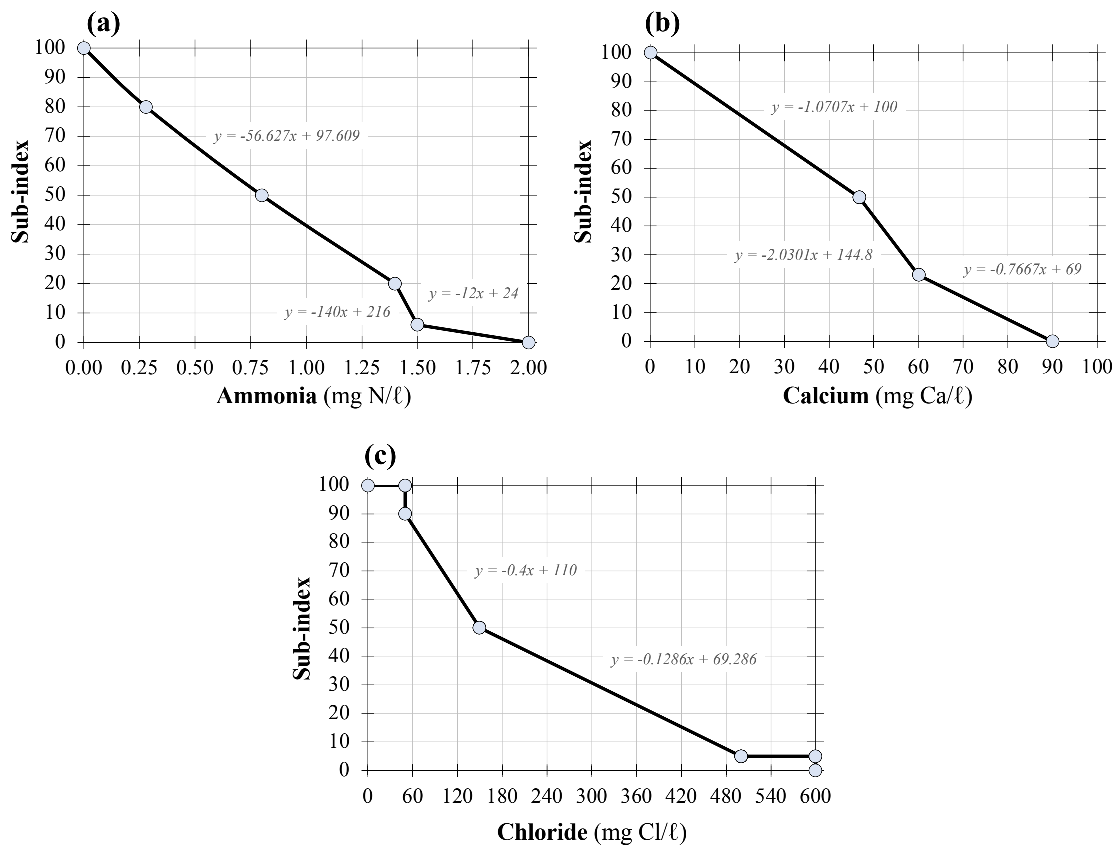
Table 5.6: Range of water quality parameters and their key points defined for establishing the sub-index rating curves

Variable		Key Points of the Sub-Index Graph ($SI_{0,\ldots,100}$ = Sub-Index zero to Sub-Index one hundred)										
		Class 5				Class 4		Class 3		Class 2		Class 1
		SI_0	SI_5	SI_{10}	SI_{25}	SI_{45}	SI_{50}	SI_{55}	SI_{75}	SI_{90}	SI_{95}	SI_{100}
1	NH_3	2.000	1.580	1.470	1.280	0.930	0.840	0.750	0.400	0.130	0.050	0.000
2	Ca	90.000	83.470	76.950	59.010	49.160	46.700	42.030	23.350	9.340	4.670	0.000
3	Cl	601.000	501.000	461.010	344.370	188.850	150.000	137.500	87.500	50.000	50.000	50.000
4	Chl-a	29.000	24.000	20.000	17.000	13.000	12.000	11.000	5.500	1.000	1.000	1.000
5	EC	492.860	471.440	450.000	385.770	300.000	278.580	257.150	171.450	70.000	70.000	70.000
6	F	1.510	1.380	1.270	0.920	0.460	0.350	0.330	0.270	0.050	0.050	0.050
7	$CaCO_3$	300.000	280.000	260.000	200.000	180.000	175.000	170.000	150.000	75.000	50.000	0.000
8	Mg	91.000	82.000	74.000	50.000	46.000	45.000	44.000	40.000	32.500	30.000	0.000
9	Mn	1.540	1.430	1.330	1.030	0.630	0.530	0.490	0.340	0.050	0.050	0.050
10	NO_3	2.000	1.750	1.500	0.950	0.750	0.700	0.650	0.370	0.070	0.030	0.000
11	pH^a	4.000	4.000	4.000	4.190	4.940	5.120	5.310	6.060	6.620	6.810	7.000
	pH^b	11.000	11.000	11.000	10.810	10.060	9.870	9.690	8.940	9.370	8.190	8.000
12	SO_4	350.000	310.000	270.000	150.000	113.980	104.990	95.990	60.000	37.500	30.000	0.000
13	Turb	45.000	27.500	10.000	8.750	7.080	6.670	6.250	4.600	3.400	3.000	0.000

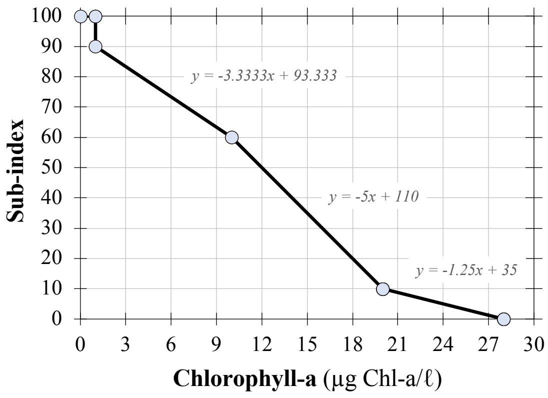
Source: The key points are based on Target Water Quality Ranges as prescribed by DWAF (1996a, 1996b, 1996c).

Notes: [a] pondus Hydrogenium lower limits (pH^a), [b] pondus Hydrogenium upper limits (pH^b).

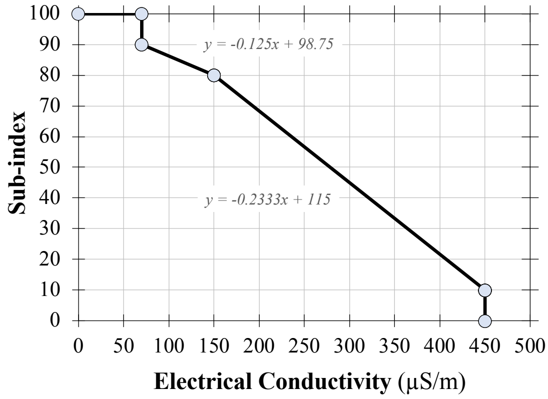
The sub-index curves for each variable are presented as Figure 5.1 and sub-index functions are Equation 5.4 to Equation 5.16.



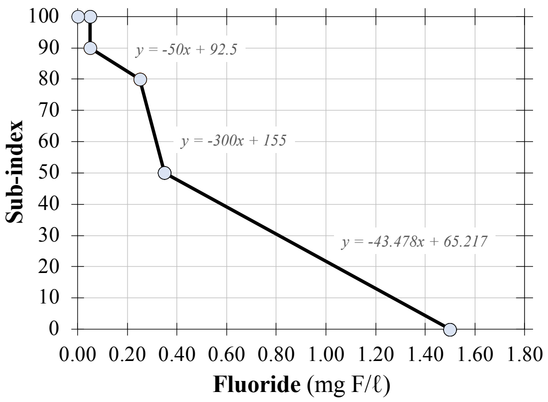
(d)


Sub-index
y = -3.3333x + 93.333
y = -5x + 110
y = -1.25x + 35
Chlorophyll-a (μg Chl-a/ℓ)

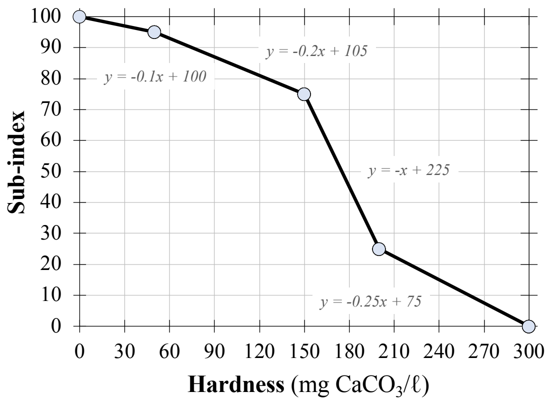
(e)


Sub-index
y = -0.125x + 98.75
y = -0.2333x + 115
Electrical Conductivity (μS/m)

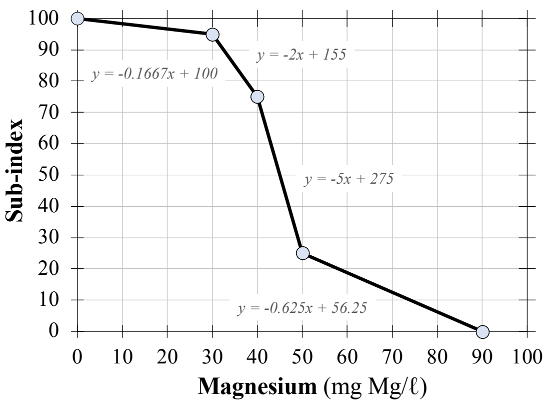
(f)


Sub-index
y = -50x + 92.5
y = -300x + 155
y = -43.478x + 65.217
Fluoride (mg F/ℓ)

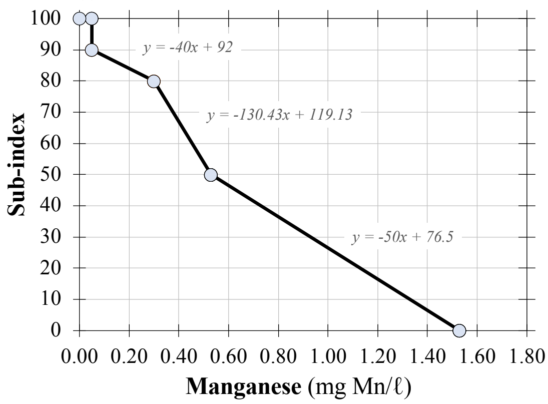
(g)


Sub-index
y = -0.2x + 105
y = -0.1x + 100
y = -x + 225
y = -0.25x + 75
Hardness (mg CaCO3/ℓ)

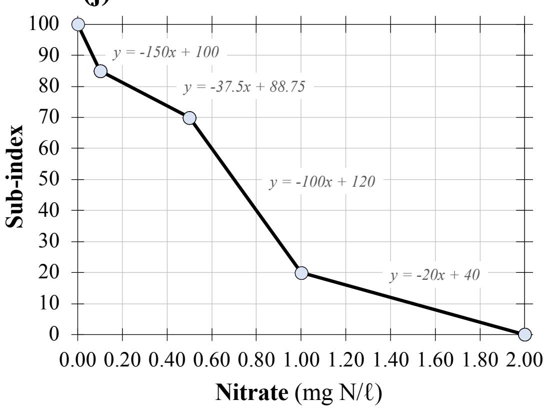
(h)


Sub-index
y = -2x + 155
y = -0.1667x + 100
y = -5x + 275
y = -0.625x + 56.25
Magnesium (mg Mg/ℓ)

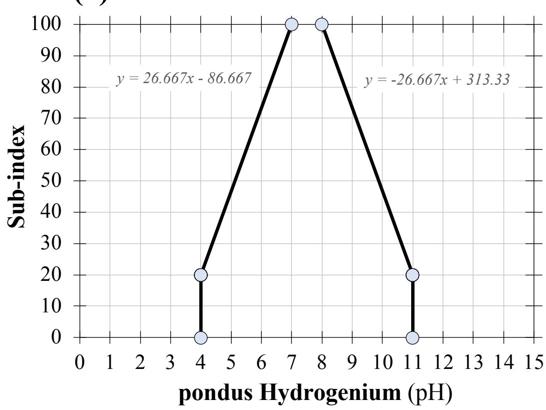
(i)


Sub-index
y = -40x + 92
y = -130.43x + 119.13
y = -50x + 76.5
Manganese (mg Mn/ℓ)

(j)


Sub-index
y = -150x + 100
y = -37.5x + 88.75
y = -100x + 120
y = -20x + 40
Nitrate (mg N/ℓ)

(k)


Sub-index
y = 26.667x - 86.667
y = -26.667x + 313.33
pondus Hydrogenium (pH)

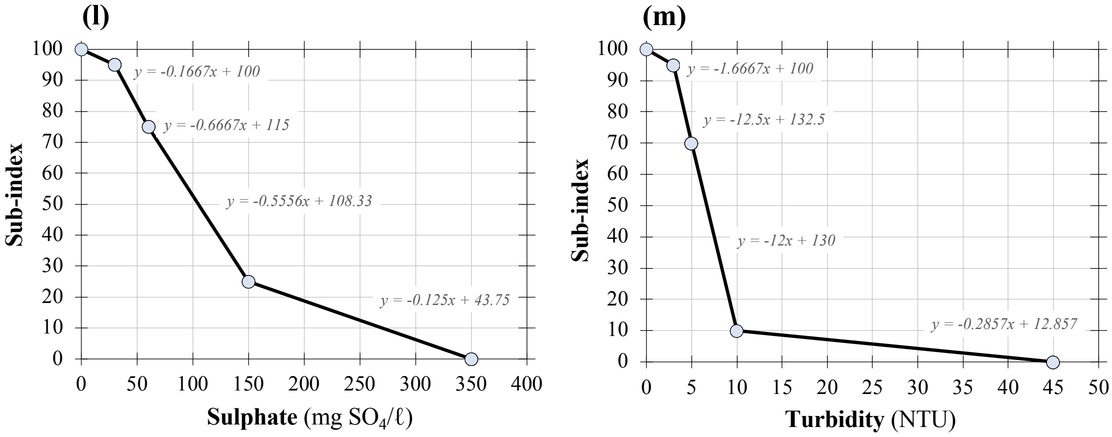


Figure 5.1: Graphical established sub-index rating curves for the selected water quality parameters (**a**) NH_3, (**b**) Ca, (**c**) Cl, (**d**) Chl-a, (**e**) EC (**f**) F, (**g**) $CaCO_3$, (**h**) Mg, (**i**) Mn, (**j**) NO_3, (**k**) pH, (**l**) SO_4 and (**m**) turbidity

Source: Authors' graphs produced for the current study (Banda and Kumarasamy, 2020b, 2020c).

Notes: Fixed key points of the rating curves were graphically established with reference to the permissible concentration limits known as the Target Water Quality Ranges (TWQRs) as prescribed by DWAF (1996a, 1996b, 1996c). Refer to Table 5.6.

The following are the model sub-index functions for the thirteen water quality parameters considered for developing a universal water quality index for South African river catchments.

$$\mathrm{SI}_a = \begin{cases} -56.627x_a + 97.609, & \text{if } x_a \leq 1.4 \\ -140x_a + 216, & \text{if } 1.4 < x_a \leq 1.5 \\ -12x_a + 24, & \text{if } 1.5 < x_a \leq 2.0 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.4}$$

$$\mathrm{SI}_b = \begin{cases} -1.0707x_b + 100, & \text{if } x_b \leq 46.70 \\ -2.0301x_b + 144.8, & \text{if } 46.70 < x_b \leq 60 \\ -0.7667x_b + 69, & \text{if } 60 < x_b \leq 90 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.5}$$

$$\mathrm{SI}_c = \begin{cases} 100, & \text{if } x_b \leq 50 \\ -0.4x_c + 110, & \text{if } 50 < x_c \leq 150 \\ -0.1286x_c + 69.286, & \text{if } 150 < x_c \leq 500 \\ 5, & \text{if } 500 < x_c \leq 600 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.6}$$

$$\mathrm{SI}_d = \begin{cases} 100, & \text{if } x_d \le 1 \\ -3.3333x_d + 93.333, & \text{if } 1 < x_d \le 10 \\ -5x_d + 110, & \text{if } 10 < x_d \le 20 \\ -1.25x_d + 35, & \text{if } 20 < x_d \le 28 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.7}$$

$$\mathrm{SI}_e = \begin{cases} 100, & \text{if } x_e \le 70 \\ -0.125x_e + 98.75, & \text{if } 70 < x_e \le 150 \\ -0.2333x_e + 115, & \text{if } 150 < x_e \le 450 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.8}$$

$$\mathrm{SI}_f = \begin{cases} 100, & \text{if } x_f \le 0.05 \\ -50x_f + 92.5, & \text{if } 0.05 < x_f \le 0.25 \\ -300x_f + 155, & \text{if } 0.25 < x_f \le 0.35 \\ -43.478x_f + 65.217, & \text{if } 0.35 < x_f \le 1.50 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.9}$$

$$\mathrm{SI}_g = \begin{cases} -0.1x_g + 100, & \text{if } x_g \le 50 \\ -0.2x_g + 105, & \text{if } 50 < x_g \le 150 \\ -1.0x_g + 225, & \text{if } 150 < x_g \le 200 \\ -0.25x_g + 75, & \text{if } 200 < x_g \le 300 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.10}$$

$$\mathrm{SI}_h = \begin{cases} -0.1667x_h + 100, & \text{if } x_h \le 30 \\ -2.0x_h + 155, & \text{if } 30 < x_h \le 40 \\ -5.0x_h + 275, & \text{if } 40 < x_h \le 50 \\ -0.625x_h + 56.25, & \text{if } 50 < x_h \le 90 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.11}$$

$$\mathrm{SI}_i = \begin{cases} 100, & \text{if } x_i \le 0.05 \\ -40x_i + 92, & \text{if } 0.05 < x_i \le 0.30 \\ -130.43x_i + 119.13, & \text{if } 0.30 < x_i \le 0.53 \\ -50x_i + 76.50, & \text{if } 0.53 < x_i \le 1.53 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.12}$$

$$\mathrm{SI}_j = \begin{cases} -150x_j + 100, & \text{if } x_j \le 0.1 \\ -37.5x_j + 88.75, & \text{if } 0.1 < x_j \le 0.5 \\ -100x_j + 120, & \text{if } 0.5 < x_j \le 1.0 \\ -20x_j + 40, & \text{if } 1.0 < x_j \le 2.0 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.13}$$

$$\mathrm{SI}_k = \begin{cases} 0, & \text{if } x_k \le 4 \\ 26.667x_k - 86.667, & \text{if } 4 < x_k < 7 \\ 100, & \text{if } 7 \le x_k \le 8 \\ -26.667x_k + 313.33, & \text{if } 8 < x_k \le 11 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.14}$$

$$\mathrm{SI}_l = \begin{cases} -0.1667x_l + 100, & \text{if } x_l \le 30 \\ -0.6667x_l + 115, & \text{if } 30 < x_l \le 60 \\ -0.5556x_l + 108.33, & \text{if } 60 < x_l \le 150 \\ -0.125x_l + 43.75, & \text{if } 150 < x_l \le 350 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.15}$$

$$\mathrm{SI}_m = \begin{cases} -1.6667x_m + 100, & \text{if } x_m \le 3 \\ -12.5x_m + 132.5, & \text{if } 3 < x_m \le 5 \\ -12.0x_m + 130, & \text{if } 5 < x_m \le 10 \\ -0.2857x_m + 12.857, & \text{if } 10 < x_m \le 45 \\ 0, & \text{otherwise} \end{cases} \qquad \text{Eq. 5.16}$$

where: $\mathrm{SI}_{a,b,\ldots,m}$ sub-index for the following thirteen water quality parameters, (a) NH_3, (b) Ca, (c) Cl, (d) Chl-a, (e) EC, (f) F, (g) $CaCO_3$, (h) Mg, (i) Mn, (j) NO_3, (k) pH, (l) SO_4 and (m) turbidity; and

$x_{a,b,\ldots,m}$ is the observed water quality reading of the respective water quality parameter.

In respect to the weight coefficients in Table 5.5 and sub-index functions Equation 5.4 to Equation 5.16, weighted sub-indices were calculated and summarised in Figure 5.2. Annexure E bears the weighted sub-index values for each parameter per given data set.

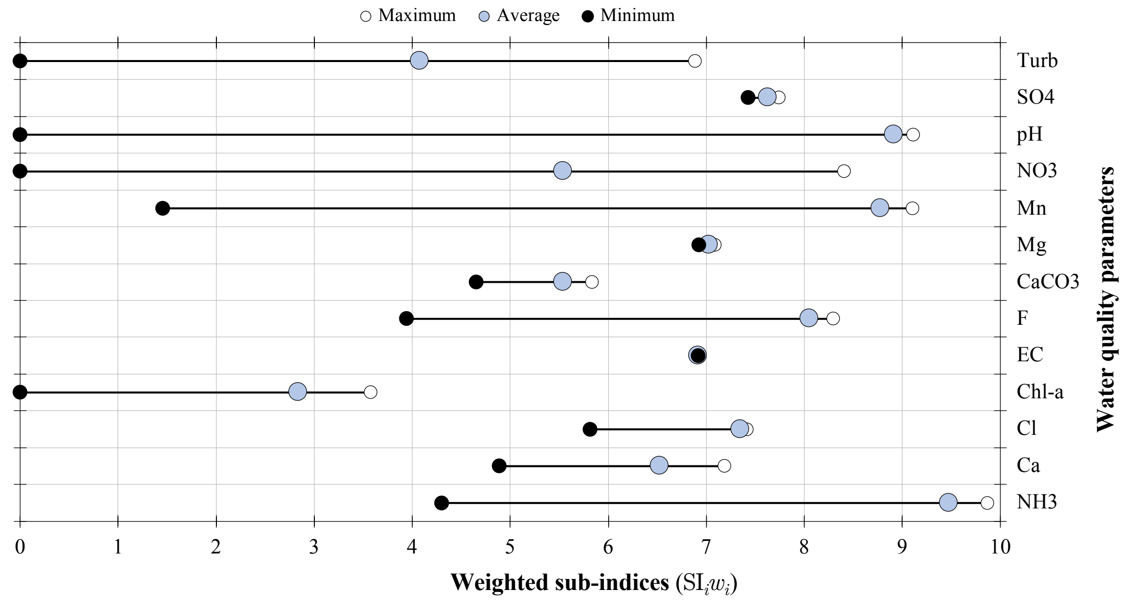


Figure 5.2: Statistical summary of the weighted sub-indices ($\mathrm{SI}_i w_i$) calculated using Umgeni water quality data gathered monthly for four years starting from 2014 until 2018

Source: Authors' graph and the sub-index values are extracts from the water quality variability model (WQVM).

Notes: Parameters are abbreviated as follows: ammonia (NH_3), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), electrical conductivity (EC), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), pondus Hydrogenium (pH), sulphate (SO_4) and turbidity (Turb).

In the process of establishing a rational water quality model, professional judgement and expert opinion techniques were adopted to determine the number and determinants most adequate to define and summarise water quality based on the degree of pollution. The rationale for the thirteen parameters of relevance is presented in the following subsection.

5.3.5 The rationale on selected water quality parameters

The discussion of the thirteen chosen water quality determinants is done so in the alphabetical order and not in order of preference. With more attention being given to the meaning, sources of such pollutants, their health effects on both humans and aquatic organisms, as well as the treatment options available to minimise the contamination levels to desirable limits.

5.3.5.1 Ammonia (NH_3)

Ammonia (NH_3) is endogenously produced toxicant with a biochemical reaction that is directly influenced by the ionic composition, pH levels and temperature of a given water body. An increase in pH level instantaneously worsens the toxicity effects of NH_3 (USEPA, 1999, CCME, 2010). According to DWAF (1996a), the ammonia toxicity level is exceptionally high under alkaline conditions and generally low under acidic conditions. Which substantiate why water bodies free from carbon-based wastes have low ammonia nitrogen concentrations typically less than 0.2 mg N/ℓ whereas, concentrations exceeding 10.0 mg N/ℓ are associated with wastewater pollution (World Health Organization, 2003a, 2011a). Commonly, unpleasant odour and taste problems may be detectable at concentrations between 1.00 and 2.00 mg N/ℓ (SEPA, 2006). The presence of NH_3 in concentrations exceeding 2.00 mg N/ℓ compromises water chlorination process, decreases disinfection efficiency of water, and promotes the formation of nitrite in water distribution networks; which eventually cause taste and odour problems (Zhang et al., 2018, Tian et al., 2019).

Nitrite is toxic to fish, and aquatic invertebrates at levels as low as 0.10 mg N/ℓ (Francis-Floyd et al., 2012) and more importantly, nitrite is possibly fatal, especially to infants (Shah and Joshi, 2017). Consequently, NH_3 levels permitting the nitrification process should then be monitored and controlled as a primary measure of this effect (Banda, 2015). According to EFSA (2012), NH_3 can react with other substances to form salts such as ammonium chloride, ammonium sulphate and ammonium nitrate. Furthermore, the World Health Organization (2011a) confirms that NH_3 reacts with chlorine and reduces free chlorine, which affects water boards (WBs) treating water to potable standards. Ammonia corrosive action damages zinc and copper alloy-based metals (Cherchi et al., 2019). Treatment of NH_3 in water can be achieved through cation alteration using hydrogen zeolite, de-aeration, membrane filtration and chlorination. Whereby, commercial ion exchange resins which have a spontaneous affinity for ammonia can be used for the total removal of ammonia in water (DWAF, 1996a, Tian et al., 2019).

5.3.5.2 Calcium (Ca)

Calcium (Ca) is the most abundant alkaline mineral of the earth (MacAdam and Jarvis, 2015). Fortunately, calcium has no adverse short term physiological problems in the human system (Sudha et al., 2016); however, in the long-term, continuous consumption of calcium at excessive concentration might cause kidney stones (Rolence et al., 2014). Calcium concentration levels of 100.00 mg Ca/ℓ and beyond are capable of forming scales in water distribution pipes and household appliances (Sudha et al., 2016, Al-Ghouti et al., 2019). Tang et al. (2019), stated that water softening technologies which include lime softening, pallet softening, ion exchange and membrane filtration, are used to reduce the effects of calcium in potable water.

5.3.5.3 Chloride (Cl)

Chloride-containing compounds are a common constituent in water and generally found in the form of inorganic salts such as sodium chloride (NaCI), potassium chloride (KCI), calcium chloride ($CaCI_2$) and magnesium chloride ($MgCl_2$). They are highly soluble in water and regarded as the principal-agents contributing to the variation of water salinity (Oswald et al., 2019). Chlorides accumulate in solution form with constituents originating from natural and anthropogenic sources including weathering material, atmospheric precipitation, saline intrusion, leaching from contaminated soils, wastewater effluent, industrial effluent, and road/overland runoff (Medalie, 2013, Corsi et al., 2015, Oswald et al., 2019). Although high chloride concentrations are unpleasant, they are necessary for human health, and they can be consumed at appropriate quantities to assist the kidneys, nervous system and for nutrition purposes (Government of Saskatchewan, 2010). Conversely, excessive intake of chloride is associated with kidney failure and hypertension leading to, ischaemic heart disease and stroke (EFSA, 2005).

High chloride concentrations tend to accelerate the rate of corrosion in the distribution systems and household appliances (Ng and Lin, 2016, Stets et al., 2018, Venâncio et al., 2018). The recommended corrosive thresholds are, 50.00 mg Cl/ℓ for distribution systems and 200.00 mg Cl/ℓ for household appliances. Although aesthetic thresholds are dependent on the associated cation, approximately 200.00 mg Cl/ℓ gives a salty taste that becomes very distinctive when chloride levels reach 400.00 mg Cl/ℓ and intolerable with concentrations beyond 600.00 mg Cl/ℓ. In excess of 2,000.00 mg Cl/ℓ, nausea problems are evident, and concentration level of 10,000.00

mg Cl/ℓ have a tendency of causing dehydration and vomiting (DWAF, 1996a, World Health Organization, 2011a). The recommended threshold for both drinking water and aquatic life is 25.0 mg Cl/ℓ. Severely elevated chloride concentrations are detrimental to aquatic organisms and responsible for a phenomenon called meromixis (stratification) resulting in oxygen depletion and ultimately limiting the survival of aquatic life (CCME, 2011, Oswald et al., 2019). Chlorides are effectively removed by ion exchange and desalination techniques (Banda, 2015).

5.3.5.4 Chlorophyll-a (Chl-a)

Chlorophyll (Chl-a) is an essential indicator of photosynthetic organisms in surface water, and Chl-a is generally associated with the presence of phytoplankton and or algae (González-García et al., 2018, Nhiwatiwa et al., 2019). In clear surface water, Chl-a concentration levels are approximately less than 1.00 µg Chl-a/ℓ, and in severe nuisance conditions, concentrations can surpass 50.00 µg Chl-a/ℓ. Though considered as rare scenarios, extreme concentrations above 1,000.00 µg Chl-a/ℓ have been recorded (DWAF, 1996a). Soluble nutrients, especially phosphorus and nitrogen, are the key determinants promoting algae blooms (eutrophication), which contribute significantly towards increased levels of chlorophyll-a (Ajmal et al., 2018, Sadeghian et al., 2018, Afridi et al., 2019, Andrade et al., 2019, Hashim et al., 2019, Liu et al., 2019). Such enriching nutrients often originates from anthropogenic activities which include septic system leakages, malfunctioning wastewater treatment plants and fertiliser runoff (Banda, 2015, Omwene and Kobya, 2018, Omwene et al., 2018, Rankinen et al., 2019).

Numerous phytoplankton species exist, some are the source of oxygen and food for herbivorous grazers (Kovács et al., 2017), but some are harmful. The most unfavourable algal blooms (i.e., cyanobacteria) are burdensome because of their toxicity and the ability to adapt to the most extreme environmental conditions (Kim et al., 2019b). Blue-green algae might cause severe gastroenteritis, vomiting and liver function impairment in humans. Whereas, in mammals, toxic algal might cause neurotoxic poisoning and respiratory arrest (DWAF, 1996a). Furthermore, algal gives rise to undesirable tastes and odours, which ultimately causes water to be less acceptable, especially for domestic uses. The presents of algal cells in water distribution systems causes potential bacterial regrowth and turn treated water into a greenish colour (Jones and Lee, 1982, DWAF, 1996a). Although effective removal of algae solely depends on the species involved; treatment processes such as coagulation, flocculation, sedimentation and chlorination are among the techniques employed to sufficiently eliminate the effects of chlorophyll causing plants. However, chlorination may produce potentially toxic by-products (DWAF, 1996a, Banda, 2015).

5.3.5.5 Electrical conductivity (EC)

Electrical conductivity (EC), trustily affected by the presence of inorganic dissolved solids such as bicarbonate, carbonate, chloride, nitrate, sulphate, phosphate, sodium, magnesium, calcium, iron, potassium and aluminium cations (World Health Organization, 2003d, 2011a). Accordingly, EC of water is directly proportional to total dissolved solids (TDS) concentration in water; and depending on the accuracy desired, EC and TDS measurements can be used interchangeably to indicate an approximate concentration of the other (Rhoades et al., 1999, Payment et al., 2003). Although not precisely equivalent, EC and TDS are directly related, and for most purposes, they are comparable in their meaning and both used to represent the salinity of surface water (USEPA, 1986, Piccolo and Marini, 2004, Banda, 2015). Nevertheless, EC is commonly used as compared to TDS because, it is easier faster and inexpensive to measure EC of water rather than TDS concentration (DWAF, 1996a, 1996c, World Health Organization, 2003d, Wozniak, 2011).

Fundamentally, TDS (mg/ℓ) can be achieved from multiplying EC (μmhos/cm) with an experimentally derived coefficient value ranging from 0.55 to 0.90 with 0.65 being the most favourable value as suggested by the following conversion equation (DWAF, 1996a, 1996b, 1996c, Narsimha and Sudarshan, 2018):

$$TDS = 6.5EC \qquad \text{Eq. 5.17}$$

Where: TDS total dissolved solids concentration in milligram per litre (mg/ℓ); and

EC is the electrical conductivity concentration in micro Siemens per meter (µS/m).

Notably, EC is also affected by temperature, and for the same reason, EC measurements are standardised at twenty-five degrees Celsius (25 °C). EC of water increases with the increase in temperature (DWAF, 1996c, CWT, 2004). Since sewage contains chloride, phosphates, nitrates, etc., pollution by wastewater effluent will automatically increase the EC of water; but conversely so, oil spillages will significantly reduce electrical conductivity (Banda, 2015).

EC related cations, in particular, calcium and magnesium salts have substantial nutritional value when consumed at low concentrations, typically less than 45.00 µS/m. In contrast, high concentrations cause an unpleasant taste to water and may adversely affect the kidneys. Besides, laxative and neurotoxic effects are associated with intake of salts at high concentrations; especially sodium sulphate and magnesium sulphate. (DWAF, 1996a). Extremely low salt concentrations may be objectionable because they cause water to have a bland, watery taste. Whereas, an increase in dissolved salts escalates hardness of water, which causes soap to lather poorly and skin dryness if used for bathing and washing purposes (World Health Organization, 2003d, Wilson, 2013).

Scaling and corrosion tendencies triggered by a high concentration of salts, mostly relating to EC have a severe effect on durability and functionality of industrial, plumbing and household appliances (World Health Organization, 2003d, 2011a, Madarász et al., 2014). Depending on the difficultness and complexity of the primary salts to be removed, EC and or TDS can be treated with simple processes such as pH balancing, chemical precipitation, and to some extent, with costly and sophisticated technologies such as reverse osmosis (DWAF, 1996a, 1996b).

5.3.5.6 Fluoride (F)

Considerably in appropriate concentrations, fluoride (F) is regarded as a critical factor to human health, beneficial to both dental and bone development. Concentrations of less than 1.0 mg F/ℓ are deemed as reasonably safe, ideal for strengthening the bone structure and providing a tooth-enamel surface that prevents dental decay (Walia et al., 2017, Zhang et al., 2017, Abiye et al., 2018, Narsimha and Sudarshan, 2018, Barathi et al., 2019). While fluoride is considered an essential trace element in human health, excessive expose is harmful to human beings. Excessive concentrations give rise to a series of adverse health effects that damages the osseous tissues (teeth and bone) and soft tissues (liver, kidney, brain, etc.) (Yang et al., 2018). High concentrations exceeding 2.00 mg F/ℓ results in permanently mottled teeth, commonly known as dental fluorosis (Ncube and Schutte, 2005, Thiessen, 2010, Azhdarpoor et al., 2018, Buckley et al., 2018, Barathi et al., 2019); whereas concentrations above 4.00 mg F/ℓ are associated with severe skeletal fluorosis and extreme bone deformity (Vani and Reddy, 2000, World Health Organization, 2004a, 2005, Thiessen, 2010, Abiye et al., 2018, Singh et al., 2018, Li et al., 2019).

Studies also suggest that prolonged intake of high fluoride might cause brain damage, increased rate of urolithiasis (kidney stones), impaired intelligence development in children (Narsimha and Sudarshan, 2018), digestive and nervous disorder (Banda, 2015, Barathi et al., 2019). Worse still, the chronic effects of high doses might attack the kidneys of the foetus (unborn babies) and that of the suckling mammals (Yang et al., 2018). Increasing water temperature increases the toxic effects of fluoride, whilst increasing water hardness reduces the harmful effects (DWAF, 1996c).

Fluoride-bearing minerals are generally associated with local igneous and metamorphic rocks, and these minerals can undergo dissolution leading to a significant rise of fluoride in water (Zhang et al., 2017, Abiye et al., 2018, Buckley et al., 2018). Other fluoride-contaminants are dispersed by wastewater and industrial effluents, with fertiliser, toothpaste, insecticide aluminium and steel manufacturing plants being the most contributing agents (Barathi et al., 2019). Solely for health benefits, fluoride (F) is frequently added in potable water to achieve the desired concentration of about 1.00 mg F/ℓ; which concentration level is regarded as relatively safe and beneficial to human consumption (National Research Council, 2007, Tiemann, 2013, Yang et al., 2018, Barathi et al., 2019).

Different reports and studies (DWAF, 1996a, Fawell and Bailey, 2006, Buckley et al., 2018), have shown that; technologies employed for the treatment of fluoride in water are relatively expensive, both in the capital and operational costs. More so, they are sophisticated, requiring high levels of skill during design, operation and maintenance of the treatment plants. The purification process is influenced by the proportion of the fluoride ions and the solubility of such ions (Webber, 2009). In most cases, because fluoride is a relatively stable anion; it is difficult to reduce fluoride to desirable concentration levels. Nevertheless, precipitation, adsorption, ion exchange, membrane filtration, electrodialysis and reverse osmosis forms part of the treatment methods available for the removal of fluorides in water (Lennon et al., 2004, World Health Organization, 2011a, Singh et al., 2018, Barathi et al., 2019).

5.3.5.7 Hardness ($CaCO_3$)

Hardness, customarily expressed as calcium carbonate ($CaCO_3$) is an inverse solubility salt, with calcium (Ca) and magnesium (Mg) as primary cations (World Health Organization, 2011b, Sepehr et al., 2013). $CaCO_3$ is prompted by a change in water temperature, water pressure and pondus Hydrogenium (pH) levels, mainly due to reduction of carbon dioxide (CO_2) from the solution. Calcium carbonate is perhaps, the most frequently encountered deposit formulated in water systems and the resulting scale might range from an easily removable, small-thin coating to a very hard and widespread encrustation (MacAdam and Jarvis, 2015). Most commonly, water bodies with hardness levels exceeding 200.00 mg $CaCO_3$/ℓ, but less than 300.00 mg $CaCO_3$/ℓ are considered marginal and tolerated, whilst values exceeding 300.00 mg $CaCO_3$/ℓ are not acceptable for most domestic applications (Tirkey et al., 2017, Hailu et al., 2019).

Hardness is categorised in two forms; that is, (i) temporary hardness which is associated with the presence of bicarbonates of calcium (Ca) and magnesium (Mg), and (ii) permanent hardness that is attributed to non-bicarbonate minerals (salts) such as chloride (Cl), sulphate (SO_4) and nitrate (NO_3). In the absence of observed hardness concentration values, and given the concentrations of Ca and Mg, then hardness values can be alternatively obtained using the following Equation 5.18 (DWAF, 1996a, 1996b, Banda, 2015, Bogart et al., 2016, Beyene et al., 2019):

$$CaCO_3 = 2.497Ca + 4.118Mg \qquad \text{Eq. 5.18}$$

Where: $CaCO_3$ is the calculated hardness concentration in milligrams per litre (mg/ℓ);

Ca is the observed calcium concentration in milligrams per litre (mg/ℓ); and

Mg is the observed magnesium concentration in milligrams per litre (mg/ℓ).

Hard water is formed when water becomes in contact with carbonate-bearing rock, particularly limestone deposits and chalk-containing minerals (MacAdam and Jarvis, 2015). The health effects of hardness are directly associated with the major cations involved; for instances, hypercalcaemia and milk-alkali syndrome are primarily caused by excessive calcium intake (World Health Organization, 2011b). Whereas increased consumption of magnesium salts may cause a temporary adaptable change in bowel habits (diarrhoea), and occasionally causes hypomagnesaemia. Furthermore, a high concentration of Mg and SO_4 might trigger laxative effects (World Health Organization, 2011b, Banda, 2015).

Excessively hard water has corrosion tendencies and reduces the lathering capabilities of cleaning detergents and washing soaps. It also causes scum formation in heat exchange surfaces, which eventually develops anaesthetic marking of enamel surfaces (Kocher et al., 2003, Sepehr et al., 2013, Wilson, 2013). Furthermore, if such deposits build in thickness, the coating surfaces act like insulation and compromise the efficiency of heat transfer (Skipton, 2009, Madarász et al., 2014). In cases of water transfer pipes, the service diameter will be reduced, affecting the delivery capacity of such.

Historically, the most commonly used water softening process, especially at a household level is water boiling, and it is most effective were bicarbonate salts responsible for temporary hardness are involved. Otherwise, antiscalants and softening agencies are employed to address hardness and reduce scaling potential (Cherchi et al., 2019). Depending on the level of cations involved, electro deionisation, electrodialysis, adsorption, chemical precipitation (lime soda), ultrafiltration, nano-filtration, microbial desalination, reserve osmosis and ion exchange are some of the technologies used to address hardness (refer to Bob and Walker, 2006, Apell and Boyer, 2010, Brastad and He, 2013, Rolence et al., 2014, Madarász et al., 2014, Zhang and Chen, 2016, Sellami et al., 2017). Amongst all these methods, ion exchange has been reported as the most convenient and economical without sludge generation (Vaaramaa and Lehto, 2003, Sepehr et al., 2013, Hailu et al., 2019).

5.3.5.8 Magnesium (Mg)

Magnesium (Mg), together with calcium (Ca), is responsible for water hardness (Yang et al., 2006, Leurs et al., 2010, Brenner et al., 2015, Kousa, 2015, Jiang et al., 2016, Rosen et al., 2018). Magnesium is an essential nutritional element of the human body, involved in various enzymatic reactions, and also necessary for several vital physiological functions (World Health Organization, 2009, Rosanoff, 2013, Avni et al., 2013, Maraver et al., 2015, Al Alawi et al., 2018). Therefore, appropriate intake of Mg in water have potential health benefits (Stevanovic et al., 2017) and the recommended dietary intake is approximately 250.00 mg Mg/day (DWAF, 1996a, Maraver et al., 2015). Assuming water consumption between 3.00 to 5.00 ℓ/capita/day, the corresponding Mg concentration range of 50.00 to 83.00 mg Mg/ℓ is still within the dietary intake limits. Nevertheless, 70.00 mg Mg/ℓ is the threshold for potable water (DWAF, 1996a).

Evidence suggests that inadequate intake of Mg results in magnesium disorders (hypomagnesemia) that are associated with several adverse health outcomes (see World Health Organization, 2009, Jiang et al., 2016, Koren et al., 2017, Al Alawi et al., 2018, Rosen et al., 2018). On the other hand, water with excessively high levels of Mg is aesthetically unacceptable, with a bitter taste and potentially cause diarrhoea (DWAF, 1996a). Similar to calcium and hardness, Mg inhibits the lathering of washing detergents and contributes to scaling problems (Sepehr et al., 2013, Brenner et al., 2015).

Furthermore, Mg is also a cofactor to photosynthesis and protein synthesis operations of the aqua plants, low-magnesium-content water results in a decreased leaf magnesium with ultimately affect the chlorophyll content of the plants (Avni et al., 2013). In addition to the dissolution of carbonate rocks (Kousa, 2015)and seawater intrusion, pollution of surface water with high concentrations of Mg is typically from municipal and industrial wastewater discharge (Qadir et al., 2018). Although adsorption has been widely accepted, most probably due to low cost and high treatment efficiency, other treatment techniques such as membrane filtration, chemical precipitation and ion exchange have been employed in the treatment of water containing high concentrations of magnesium (DWAF, 1996a).

5.3.5.9 Manganese (Mn)

As a naturally occurring element, manganese (Mn) is relatively abundant in the earth’s crust (WRA, 2013, Neculita and Rosa, 2019, Pietrelli et al., 2019), and commonly found in water through weathering of manganese-bearing rocks (Banda, 2015, Gerke et al., 2016). Among other pollution sources, industrial effluent, acid-mine drainage, wastewater discharge, landfill leachate, borehole equipment (i.e., casing, piping, pump components, etc.) and underground storage tanks; they all significantly contribute towards the presence of Mn in water (Shu et al., 2019, Pietrelli et al., 2019, Neculita and Rosa, 2019). Most of the existing concentration limits of Mn in water are explicitly derived for aesthetic affairs other than health concerns. The human health effects are only relevant at significantly elevated concentrations, most probably at levels approximately ten times high than the recommended consumption limit of 0.05 mg Mn/ℓ (DWAF, 1996a, Gerke et al., 2016).

Nevertheless, considering such extreme exposure, manganese has been associated with neurological disorders and intellectual impairment (Ong et al., 2007, Hoyland et al., 2014, Gerke et al., 2016, Iyare, 2019, Neculita and Rosa, 2019, Shu et al., 2019), with symptoms such as headache, agitation, deafness, rigidity and tremor (Alvarez-Bastida et al., 2013, Pietrelli et al., 2019). Children have a higher tendency of being affected because of their immature manganese homeostatic mechanism (Iyare, 2019). At high levels, Mn results in the formation of dark-brown precipitates responsible for altering turbidity (colour) of water, imparting unpleasant taste and giving rise to odour (smell) and scaling problems (WRA, 2013, Alvarez-Bastida et al., 2013, Hoyland et al., 2014, Gerke et al., 2016). Furthermore, the deposits might break off as black particles, which ultimately causes the unpleasant appearance of water, clog delivery pipes, stain plumbing fixtures and laundry (World Health Organization, 2011c, Abu Hasan et al., 2014, Dvorak and Skipton, 2014).

Rust flakes might also be produced, risking the possibility of unwanted bacteria growth and contamination of already treated water in cases of water distribution systems (Banda, 2015, Scholz, 2016). The effectiveness of the available treatment techniques depends on the parameter's relative concentration, type of Mn involved and pH level of water. Nonetheless, effective treatment methods for reducing manganese levels in drinking water include, aeration followed by filtration, adsorption systems, chemical precipitation, greensand filtration, ion exchange, oxidising filters and reverse osmosis (refer to; World Health Organization, 2011c, Dvorak and Skipton, 2014, Scholz, 2016, Vries et al., 2017, Hoslett et al., 2018, Neculita and Rosa, 2019, Pietrelli et al., 2019).

5.3.5.10 Nitrate (NO_3)

Nitrate (NO_3) is a naturally occurring ion (Gupta et al., 2000, Grosse et al., 2006, Fan, 2011, World Health Organization, 2011d, Serio et al., 2018), which is widespread and regarded as the most significant contaminant in water (Espejo-Herrera et al., 2015, Sadler et al., 2016). Usually, under anaerobic conditions; nitrate reduces to nitrite (denitrification process), and through oxidation, nitrites transform rapidly to nitrate (nitrification process) (DWAF, 1996a, 1996c, Banda, 2015). The processes are governed by water pH levels, temperature and availability of oxygen. Due to their co-occurrence and rapid inter-conversion, the two (nitrate and nitrite) are normally considered and measured simultaneously for water quality assessment procedures (DWAF, 1996a, 1996c, Banda, 2015).

Nitrates can contaminate surface waters via geological formations containing nitrogen compounds, agricultural fertilisers, septic tank runoff, wastewater effluent, airborne nitrogen compounds emitted by the industry and automobiles, decaying plant and animal excrement from areas of high-density animal confinement (Terblanche, 1991, Weyer et al., 2001, World Health Organization, 2011d, Fan, 2011, ODEQ, 2014, Sadler et al., 2016, Moore and Bringolf, 2018, Radfard et al., 2018, Serio et al., 2018, Ward and Brender, 2018, Biddau et al., 2019, Kawagoshi et al., 2019). Nitrate itself is a low-toxic compound, but when endogenously converted to nitrite (NO_2), it becomes toxic to human health and the aquatic environment (Fan, 2011, Moore and Bringolf, 2018, Serio et al., 2018).

Excessive exposure to nitrate/nitrite has been associated to several human health conditions, primarily amongst those are, (i) its tendency to interfere with the oxygen-carrying capacity of the red blood cells, leading to infant methaemoglobinaemia which is an acute health condition that causes the skin to turn a bluish colour; hence the term "blue baby syndrome" (Sadler et al., 2016, Radfard et al., 2018, Ward and Brender, 2018, Uzun and Debik, 2019); (ii) reacts readily with nitrosatable compounds in the stomach and generate N-nitroso compounds which potentially causes cancers of the digestive tract in adults (Weyer et al., 2001, Grosse et al., 2006, Espejo-Herrera et al., 2015, Sadler et al., 2016, Schullehner et al., 2017, Uzun and Debik, 2019); and (iii) adverse pregnancy outcomes which include spontaneous abortion, foetal deaths (stillbirths), prematurity (delivery before thirty-seven weeks gestation) as well as infant mortality (Sadler et al., 2016, Ward and Brender, 2018).

Other consequences of high nitrate ingestion are recurrent stomatitis and diarrhoea (Gupta et al., 2000, Banda, 2015). In addition to human health effects, especially when combined with phosphates, high level of nitrate stimulates aqua-plant growth and contribute to eutrophication in surface waters (DWAF, 1996a, ODEQ, 2014, Uzun and Debik, 2019). Though the scientific community argue about the appropriateness of the current limits set for nitrates in potable water (Fan, 2011, Ward and Brender, 2018), 50.00 mg N/ℓ is the norm (Fan, 2011, Espejo-Herrera et al., 2015, Sadler et al., 2016, Radfard et al., 2018, Biddau et al., 2019). therefore, to achieve such standards, treatment techniques such as water softening (anion exchange), distillation, reverse osmosis, nano-filtration and electrodialysis apply to the removal of nitrates in water (DWAF, 1996a, Gupta et al., 2000, NHDES, 2010, Uzun and Debik, 2019). The limitations in volumetric capacity and high cost of operation governs the application of these treatment processes (Gupta et al., 2000, Banda, 2015).

5.3.5.11 Pondus Hydrogenium (pH)

pH is a master variable, an essential property of the aqueous solution since it influences chemical reactions, equilibrium conditions and biological toxicity of an aqueous medium (Marion et al., 2011, Karastogianni et al., 2016, Salvo et al., 2018, Anes et al., 2019). In surface water, pH is the measure of acid-base equilibrium of the water body (World Health Organization, 2003c, CANSE, 2008a). pH is governed by the number of free hydrogen ions (H^+), hence the term "pondus Hydrogenium" referring to "potential Hydrogen" (CANSE, 2008b, Banda, 2015, Salvo et al., 2018). The parameter is notionally defined as the negative decimal logarithm of the hydrogen ion activity (DWAF, 1996a, 1996b, Buck et al., 2002, Camões and Anes, 2015, Qin et al., 2015, Karastogianni et al., 2016). Usually, pH values range from 0 to 14.00; at pH level 7.00, the water is regarded as neutral. Whereas acidic conditions are indicated by pH values below 7.00 and pH levels greater than the neutral mark (pH>7.00), signifies alkaline (basic) conditions (CCME, 1999, USEPA, 2006, Wilson, 2011, Qin et al., 2015, Karastogianni et al., 2016, Wardhany et al., 2018).

pH levels in water are primarily influenced by acid mine drainage, acid rain (resultant of industrial pollution), solid waste in the landfills, industrial effluent discharge particularly from chemical processing institutions, seawater intrusion, geology and geochemical composition of the underlying rocks (DWAF, 1996b, CCME, 1999, Qin et al., 2015, Karastogianni et al., 2016). If not carefully monitored and controlled, some of the water treatment chemicals and or processes might significantly affect the pH levels of both treated and de-sludging water, which might eventually lead into freshwater bodies (CANSE, 2008b, Banda, 2015, Qin et al., 2015).

It is difficult and close to impossible to establish direct human health effects of pH, given that, pH effects are closely associated with a variety of other water quality variables. Nevertheless, abnormal pH values are associated with gastrointestinal irritation (Qin et al., 2015), eye irritation and exacerbation of skin disorder (Avvannavar and Shrihari, 2008). The variation of water pH levels might negatively affect the disinfection efficiency of chlorine and eventually promote the toxicity of other water quality variables (DWAF, 1996a). PH levels may influence the aesthetic condition of water; for example, under acidic conditions (pH<4.00), water may taste sour; whilst under alkaline conditions (pH>9.00), water test bitter and soapy (DWAF, 1996a, Avvannavar and Shrihari, 2008). Corrosion problems escalate with water having pH levels less than 6.50 (CANSE, 2008b, NHDES, 2009, Qin et al., 2015), and scaling in plumbing pipes and fixtures may be evident at pH levels exceeding 8.50 (CANSE, 2008a, 2008b, Banda, 2015). The adjustment of pH in water achieved by the addition of alkaline or acid reagent. The commonly used alkaline reagents are sodium carbonate, sodium hydroxide and lime; whereas acidic reagents include carbon dioxide, hydrochloric and sulphuric acids (DWAF, 1996a, 1996b). Because alkalis and acids are hazardous substances, pH adjustment processes require special precautions and trained personnel (DWAF, 1996a, Banda, 2015).

5.3.5.12 Sulphate (SO_4)

Sulphate (SO_4) is a common constituent of water that is regarded as non-toxic and usually coexist with calcium (Ca) and magnesium (Mg) pollutants in both, freshwaters and wastewaters (Dou et al., 2017). Contamination of water with sulphate often originates from natural activities which include, saltwater intrusion, dissolution of sulphate-bearing minerals, acid rock drainage, atmospheric deposition and decomposing organic matter (see, World Health Organization, 2011a, Meays et al., 2013, Li et al., 2015, Pessoa-Lopes et al., 2016, Burke et al., 2018, Fernando et al., 2018). Besides, unregulated disposal of sulphates from human activities can artificially raise the concentration levels of sulphate in water. Example of such anthropogenic influences includes industrial discharge, acid mine drainage, wastewater effluent, burning of fossil fuels and agricultural runoff (refer to, World Health Organization, 2004b, Davies, 2007, Szynkiewicz et al., 2011, Meays et al., 2013, Kabdaşli et al., 2016, Dou et al., 2017).

Sulphate concentration levels below 200.00 mg SO_4/ℓ have no health or aesthetic effects. Depending on the cation involved, sulphates beyond 400.00 mg SO_4/ℓ may cause water to taste bitter and or salty (DWAF, 1996a, Nariyan et al., 2018), immediate intestinal discomfort, cause diarrhoea and subsequently dehydration (Banda, 2015, Venâncio et al., 2018). The extent of such a tendency is related to the cations involved; for example, magnesium will trigger diarrhoea, whereas sodium will not induce diarrhoea (DWAF, 1996a, Banda, 2015). The laxative effects may be temporary and may cease once accustomed and adaptive to high sulphate concentrations (DWAF, 1996a, Government of Saskatchewan, 2007). Further to this, high concentration of SO_4 triggers an increased rate of corrosion of concrete-made hydro-structures, plumbing pipes and fixtures (World Health Organization, 2004b, 2011a, Ng and Lin, 2016, Dou et al., 2017, Nariyan et al., 2018). As a result of the corrosion effect, metal oxides, and dark slime may be evident in the distribution system (CANSE, 2008c, Banda, 2015).

According to EPA (2001), even with minimum dissolved oxygen availability, sulphate can readily convert to sulphide and cause water to have noxious odours which smell like rotten eggs. Numerous technologies are available for the treatment of sulphate in water; and these include, ion exchange/adsorption, chemical precipitation, electrodialysis, distillation and reverse osmosis (as explained by, DWAF, 1996a, 1996b, De Los Santos et al., 2015, Kabdaşli et al., 2016, Dou et al., 2017, Fernando et al., 2018, Nariyan et al., 2018). The suitability and effectiveness of each specific treatment method depend on the volume of water to be treated, the concentration of the sulphate in water, the presence of other chemical parameters and whether bacterial contamination is of paramount concern (CANSE, 2008c, Banda, 2015, Fernando et al., 2018).

5.3.5.13 Turbidity (Turb)

Turbidity is not a contaminant concentration, but a dependant variable representing the collective measure of optical properties of other water contaminants responsible for causing light to be scattered and absorbed rather than transmitted in straight lines through a water sample (Wilde et al., 1998, Slaets et al., 2014, Castaño and Higuita, 2016, Robert et al., 2016, Miljojkovic et al., 2019). Consequently, it is known to be the "cloudiness" that represents the degree of water clarity (Birtwell et al., 2008, Constantin et al., 2016, World Health Organization, 2017, Stevenson and Bravo, 2019). They are numerous units of turbidity, which are considered virtually equivalent and sometimes used interchangeably (EPA, 2001). Nonetheless, the Nephelometric Turbidity Units (NTU) are the most commonly used in South Africa, hence adopted for this study. Turbidity is dynamic and somewhat inevitable; its stable state is significantly linked to environmental phenomena and operational activities (Miljojkovic et al., 2019, Stevenson and Bravo, 2019).

Nevertheless, the principal contributors to turbidity are, sediments, finely divided organic and inorganic matter, soluble coloured organic compounds and microscopic organisms, among others (Wilde et al., 1998, CANSE, 2008a, World Health Organization, 2011a). Sources of such suspended matter are diverse and include, but not limited to, reservoir drawdown-flushing, algal blooms (eutrophication), wastewater discharge, industrial effluent, exceptional rainfall events, soil erosion and decomposition of organic matter (Johnson et al., 2007, MPCA, 2008, Kjelland et al., 2015, Constantin et al., 2016, Robert et al., 2016, World Health Organization, 2017, Suzuki et al., 2018, Uncles et al., 2018). Turbidity might not directly present human health hazards (World Health Organization, 2017, Stevenson and Bravo, 2019); however, turbid water have a negative impact on consumer acceptability due to the visible cloudiness (World Health Organization, 2011a, Banda, 2015).

Direct human health threat depends exclusively on the exact composition of the turbidity causing particles (EPA, 2001, World Health Organization, 2017). As noted by DWAF (1996a), turbid water readily adsorbs viruses and bacteria, which have a significant effect on the microbiological quality of water. In the case of disease-causing organisms (bacteria, viruses, parasites, etc.); problems such as nausea, cramps, headaches and diarrhoea might arise (CANSE, 2008a, 2009, Robert et al., 2016). Turbidity levels exceeding 5.00 NTU may strongly affect the aesthetic properties of water, causing undesirable taste, smell (odour) and colour (DWAF, 1996a, CANSE, 2009, Banda, 2015). Turbid water is reported to cause evasive behaviour, gill clogging, physiological effects, and even death of aquatic organisms, especially less-mobile species (Kjelland et al., 2015, Suzuki et al., 2018)

In addition, the particles forming turbidity may seriously interfere with the treatability of water, and in the case of the disinfection process, the consequences might be severe. Turbid water tends to harbour pathogenic microorganisms and impair disinfection (Obi et al., 2008, CANSE, 2009, World Health Organization, 2017). Thus, increasing potential health effects and compromising the wellbeing of the end-users. Given this, turbidity acts as an indicator of possible microbial contamination (World Health Organization, 2011a). Treatment of turbidity depends on the primary contributor, for instance; iron and manganese require ion exchange processes, other than that; sedimentation of particulate matter through coagulation followed by filtration and disinfection is the common practice (Banda, 2015, World Health Organization, 2017, Nishat Ashraf et al., 2018).

Conclusively, the selection of the maximum allowable variables that can effectively classify and describe the degree of water quality is not always straightforward. Nonetheless, the above thirteen water quality parameters are the definite key contaminants regarded as the most frequently monitored variables in South Africa, with concentrated pollution effects, and the most dangerous variables with obdurate legal restrictions in water quality regulations. Accordingly, they have significant effects on water quality, which justify their inclusion as input parameters towards the proposed water quality model. The concept of using water quality indices (WQIs) is grounded on the comparison of individual water quality variables through the integration of sub-indices in relation with assigned weight coefficients of each parameter. Aggregation of sub-indices is accomplished through the use of mathematical functions commonly known as indexing models.

5.3.6 Weighted indexing model

The mathematical structures and application of indexing models are generally governed by the degree of accuracy perceived and the type of weightage coefficients, which might be equally or unequally defined. Various aggregation methods exist, and each technique has its formidable challenges; hence the index developer has to decisively select the most appropriate and relevant indexing model, preferably with fewer complications that might adversely influence the final index value. Otherwise, defining the best and absolute aggregation model is close to impossible. Since there is no supreme and favourable technique of formulating water quality indices (WQIs), various aggregation methods were tried and tested. Modified weighted sum (additive) method, was found to be the most appropriate for the development of a universal water quality index for monitoring South African watersheds. The modified weighted sum method is represented as Equation 5.19.

$$\mathrm{WQI} = \frac{1}{100}\left(\sum_{i=1}^{n} s_i w_i\right)^2 \qquad \text{Eq. 5.19}$$

The scenario-based analysis was used to modified and align the model with local conditions to developed the final universal water quality index (UWQI), which is an improved version of the weighted sum method. The model equation integrates sub-index values of selected parameters with relation to assigned parameter weights; and obtain the overall water quality status, which is presented as a unit-less number ranging from 0 to 100. The rationale employed is based on solving multiple systems of equations (Wang et al., 2019), where key-points of the rating curves were used to generate series of *m* equations, with two unknown variables (*x*, *z*) and *n* water quality parameters in the form:

$$WQI_1 = (1/x_1)(SI_{11}w_1 + SI_{12}w_2 + SI_{13}w_3 + \ldots + SI_{1n}w_n)^{z_1}$$

$$WQI_2 = (1/x_2)(SI_{21}w_1 + SI_{22}w_2 + SI_{23}w_3 + \ldots + SI_{2n}w_n)^{z_2}$$

Eq. 5.20

…

$$WQI_m = (1/x_m)(SI_{m1}w_1 + SI_{m2}w_2 + SI_{m3}w_3 + \ldots + SI_{mn}w_n)^{z_m}$$

where: $WQI_{1,\ldots,m}$ are the ideal water quality index values corresponding to the key-points of the rating curves;

$x_{1,\ldots,m}$ are the equation denominators (first unknown variable); $SI_{m1,\ldots,mn}$ are the corresponding sub-indices;

$w_{1,\ldots,n}$ are relative weight coefficients for the thirteen water quality parameters; and

$z_{1,\ldots,m}$ are the equation exponentials (second unknown variable).

The first part was to find the optimum values of *x* and *z*; thereafter, the closest *x-value* was rounded off and substituted into the same set of equations to find the corresponding optimum *z-value*, which become the final exponential factor of the UWQI. Equation 5.21 represents the final universal water quality (UWQI) model:

$$UWQI = \frac{2}{3}\left(\sum_{i=1}^{n} s_i w_i\right)^{1.0880563}$$ Eq. 5.21

where: UWQI is the aggregated index value ranging from zero to hundred, with zero representing water of poor quality and hundred denoting water of the highest quality;

s_i is the sub-index value of the i^{th} water quality parameter obtained from the sub-index linear functions, and the values range from zero to hundred, similar to WQI values; and

w_i is the weight coefficient value for the i^{th} parameter represented as decimal number and the sum of all coefficients is one, ($w_1 + w_2 + w_3 + \ldots + w_n = 1$); and

n is the total number of sub-indices and in this case $n = 13$.

5.3.7 Scenario-based analysis (UWQI)

The scenario-based analysis helps identify potential data-processing gaps, which in turn enlighten on the necessary precautions imperative to minimise the impact, or perhaps eliminate the problem. To determine such, ideal sets of predictive variables have been established under a variety of scenarios to calculate specific water quality variables. Considering increments of five scores, eleven probable scenarios have been examined to demonstrate the model's ability to predict scores of all ranges, from class one (excellent) to class five (worse). The eleven forecasts are founded on three-level-grading, which comprise of (i) worst-case scenario, $0 \leq \text{Index} \leq 25$; (ii) base-case scenario, $45 \leq \text{Index} \leq 55$; and lastly (iii) best-case scenario, $75 \leq \text{Index} \leq 100$.

Purposefully, the groupings provided a complete change of circumstances with each scenario, thereby widening the range of analysis and include a considerable array of possibilities. With reference to permissible concentration limits and developed linear sub-index functions (Figure 5.1), definite assumptions about all eleven cases have been carefully considered. Accordingly, parameter values corresponding to each scenario have been established and applied to perform the analysis. The results of the scenario-based analysis are presented in Table 5.7 and Figure 5.3.

Table 5.7: Comparison of modified weighted arithmetic water quality index (WQI) and the developed universal water quality index (UWQI) using the scenario-based analysis to establish the functionality and predictive capacity of the models

Sample identity	**Water quality index results from the scenario-based analysis**					
	Ideal WQI results		Modified weighted WQI results		Developed UWQI results	
	Index score	WQI class	Index score	WQI class	Index score	WQI class
Max.	100.000	1	99.506	1.0	99.736	1
Avg.	50.000	4	37.571	4.0	48.406	4
1	0.000	5	0.000	5.0	0.000	5
2	5.000	5	0.177	5.0	3.179	5
3	10.000	5	0.827	5.0	7.364	5
4	25.000	5	6.250	5.0	22.127	5
5	45.000	4	20.254	5.0	41.951	4
6	50.000	4	25.027	4.0	47.069	4
7	55.000	3	30.269	4.0	52.200	3
8	75.000	3	56.250	3.0	73.127	3
9	90.000	2	80.976	2.0	89.159	2
10	95.000	2	93.749	2.0	96.554	1
11	100.000	1	99.506	1.0	99.736	1

Source: Ideal WQI values are generated using sub-index key points, modified weighted WQI scores are produced using House (1986, 1989, 1990) and UWQI results are extracts from the WQVM (Banda and Kumarasamy, 2020b, 2020c).

Notes: Samples used for the scenario-based analysis are predictive values ideal for establishing a specific set of results as demonstrated with the ideal WQI results columns. With increments of five scores, eleven probable scenarios have been considered to illustrate the model's ability to predict scores of all ranges, from Class 1 (good) to Class 5 (very bad).

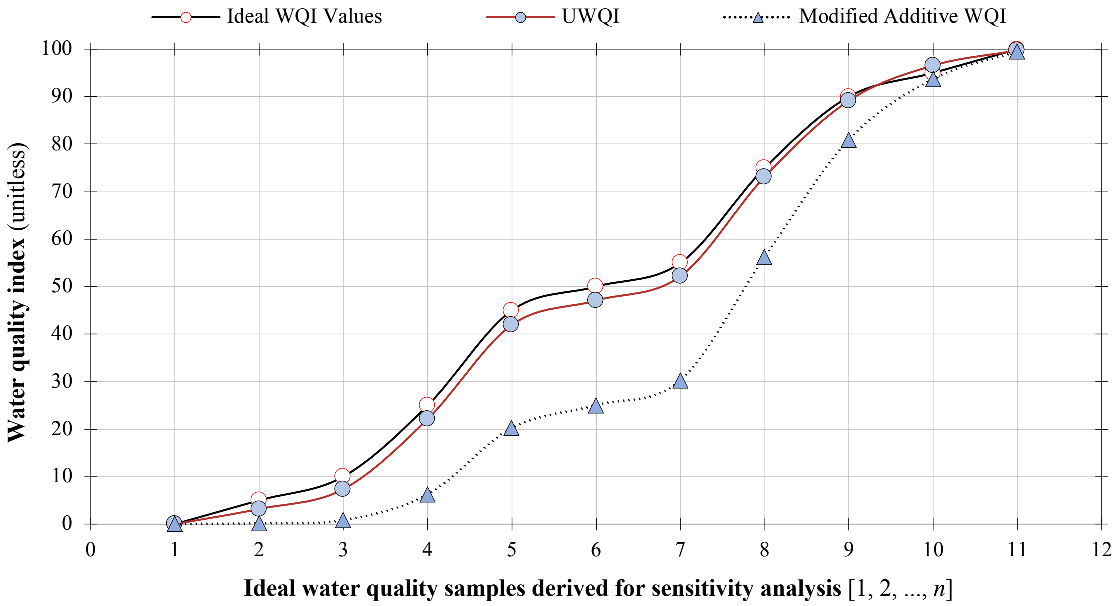


Figure 5.3: Plot diagram showing the results of the scenario-based analysis of the developed universal water quality index (UWQI) model and the modified additive water quality model (House, 1986, 1989, 1990) against ideal water quality values derived from eleven probable scenarios

Source: Ideal WQI values are generated using sub-index key points, modified weighted WQI scores are produced using equation suggested by House (1986, 1989, 1990) and UWQI results are extracts from the WQVM (Banda and Kumarasamy, 2020b, 2020c).

Notes: The eleven cases represented as samples 1, 2, …, n, which corresponds respectively to water quality (WQI) values of 0, 5, 10, 25 (worst-cases); 45, 50, 55 (base cases); and 75, 90, 95, 100 (best cases).

Not to devalue the efforts by House (1986, 1989, 1990), the modified weighted arithmetic model could not sufficiently satisfy the expected analytical results. Although the predictive pattern is recommendable, there is a significant lag between the calculated results and the ideal case, especially with the base-case scenarios (45 ≤ Index ≤ 55). Henceforth, the model was further improved to suit our local conditions. In view of the analysis results, it is evident that the proposed UWQI is robust and technically stable.

The degree of variation from the ideal values is negligible, better off; the prediction pattern followed the ideal graph with corresponding values on both WQI scores and classification. Which therefore pronounce the competence of the UWQI to be used as an evaluation tool for monitoring South African river catchments. With an attempt to pilot the initiative, Umgeni water quality data have been evaluated using sub-indices Equations 5.4 to 5.16, weight coefficients in Table 5.5 and the proposed universal water quality index (UWQI) model documented as Equation 5.21. The WQI results are summarised in Figure 5.4 and presented in detail as Annexure E.

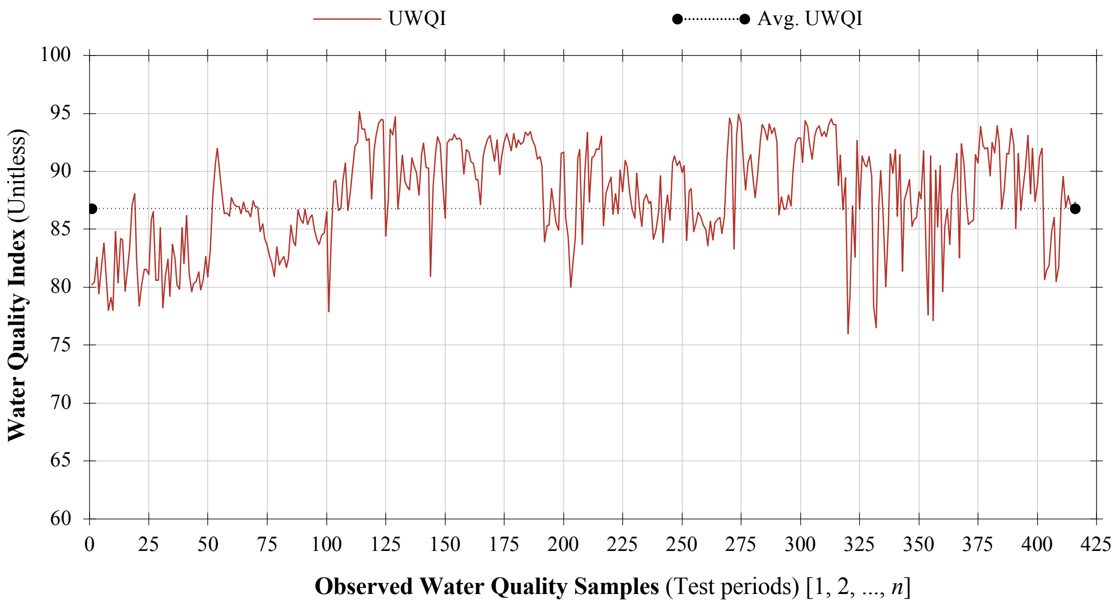


Figure 5.4: Water quality index results calculated using the developed universal water quality index (UWQI) for Umgeni water quality data gathered monthly for four years starting from 2014 until 2018

Source: UWQI results are extracts from the WQVM (Banda and Kumarasamy, 2020b, 2020c).

Notes: The Umgeni water quality data is from eight sampling stations which fall under four different catchment areas. The catchments include Umgeni River catchment (U20) for Henley, Inanda and Midmar Dams; Umdloti River catchment (U30) for Hazelmere Dam; Nungwane River catchment (U70) for Nungwane Dam; and lastly Umzinto/Umuziwezinto River catchment (U80) for Umzinto Dam. Testing the model with data from various river catchments promote the objective of establishing a universal water quality index suitable for use across the catchment areas in South Africa. The catchment identity codes in parentheses (); are unique codes drafted by the Department of Water and Sanitation to identify river catchments.

The spatial and temporal changes in water quality for Umgeni Water Board are evident over a period extending to four years. The varying sequence is very narrow and comprises of index scores as high as 95.154 (class one), an average of 87.780 (class two) and the lowest score of 75.985 (borderline of class two).

5.3.8 Evaluation of spatial and temporal trends using UWQI

Umgeni water quality data have been evaluated using the proposed universal water quality index (UWQI) model documented as Equation 5.21. Based on the UWQI, Table 5.8 and Figure 5.4 indicates spatial and temporal water quality variations among the six sampling sites. The results show that water quality in the region can be categorised as "acceptable water quality," with the lowest WQI score of 75.985 (class two) recorded at station 5 (Umzinto Dam). In this case, Turb and Mn are the main contributors to the deterioration of the water quality, having concentration levels of 13.20 NTU and 1.05 mg/ℓ, respectively. Sampling station 2 recorded the highest surface water quality with an index of 95.154 (class one) during the summer of 2017. NO_3 is the principal pollutant factor responsible for the minimum WQI scores for station 2, 3, 4 and 6 with NO_3 concentrations of 0.99, 1.31, 4.50 and 1.77 mg/ℓ respectively.

Table 5.8: Water quality index matrix for the six sampling stations

Year	Month	Sampling Stations					
		Station 1	Station 2	Station 3	Station 4	Station 5	Station 6
2014	July	80.454	91.972	88.398	91.205	89.422	90.709
	October	83.799	86.983	90.320	83.299	87.035	85.620
	Seasonal Average [1]	82.126	89.478	89.359	87.252	88.229	88.165
	Annual Average [2]	80.937	87.489	89.628	91.417	84.780	88.353
2015	January	79.093	84.188	92.351	94.918	86.730	90.699
	April	80.403	82.485	92.888	90.794	90.379	92.198
	July	79.684	84.039	87.125	87.718	78.318	89.607
	October	87.127	84.697	91.752	94.053	90.043	93.946
	Seasonal Average [1]	81.577	83.852	91.029	91.871	86.368	91.613
	Annual Average [2]	82.735	83.991	91.322	90.990	86.477	91.603
2016	January	78.382	84.365	93.280	94.079	85.265	88.383
	April	81.525	86.613	93.451	92.544	91.893	93.684
	July	86.512	90.727	83.930	86.759	81.372	91.553
	October	85.123	90.072	91.647	86.995	89.275	90.266
	Seasonal Average [1]	82.885	87.944	90.577	90.094	86.951	90.971
	Annual Average [2]	81.722	88.799	89.203	89.879	87.797	90.033
2017	January	82.434	95.154	83.685	92.857	86.034	92.016
	April	82.422	92.628	91.914	94.349	91.792	91.212
	July	85.156	91.868	86.296	91.048	91.310	81.898
	October	81.209	94.462	90.945	93.905	85.208	86.032
	Seasonal Average [1]	82.805	93.528	88.210	93.040	88.586	87.789
	Annual Average [2]	81.862	92.322	88.731	92.926	85.659	85.720
2018	January	80.474	87.497	84.115	92.964	85.161	87.465
	April	80.630	94.708	90.520	94.061	87.997	87.905
	July	83.139	91.396	84.653	91.407	82.548	87.348
	Seasonal Average [1]	81.415	91.200	86.429	92.811	85.235	87.570
	Annual Average [2]	81.259	90.804	86.758	92.830	86.709	87.580
Station Minimum WQI [3]		77.983	77.873	80.007	83.299	75.985	80.482
Station Maximum WQI [4]		88.083	95.154	93.451	94.918	92.639	93.946
Station Average WQI [5]		81.807	87.390	89.054	91.514	86.392	88.739

Source: UWQI results are extracts from the WQVM (Banda and Kumarasamy, 2020b, 2020c)

Notes: [1] Seasonal average considering WQI scores for January, April, July and October only, [2] Annual average considering WQI values for the entire year from January to December, and [3, 4, 5] Overall station WQI scores taking into account the whole period of water quality evaluation; that is, from June 2014 to July 2018.

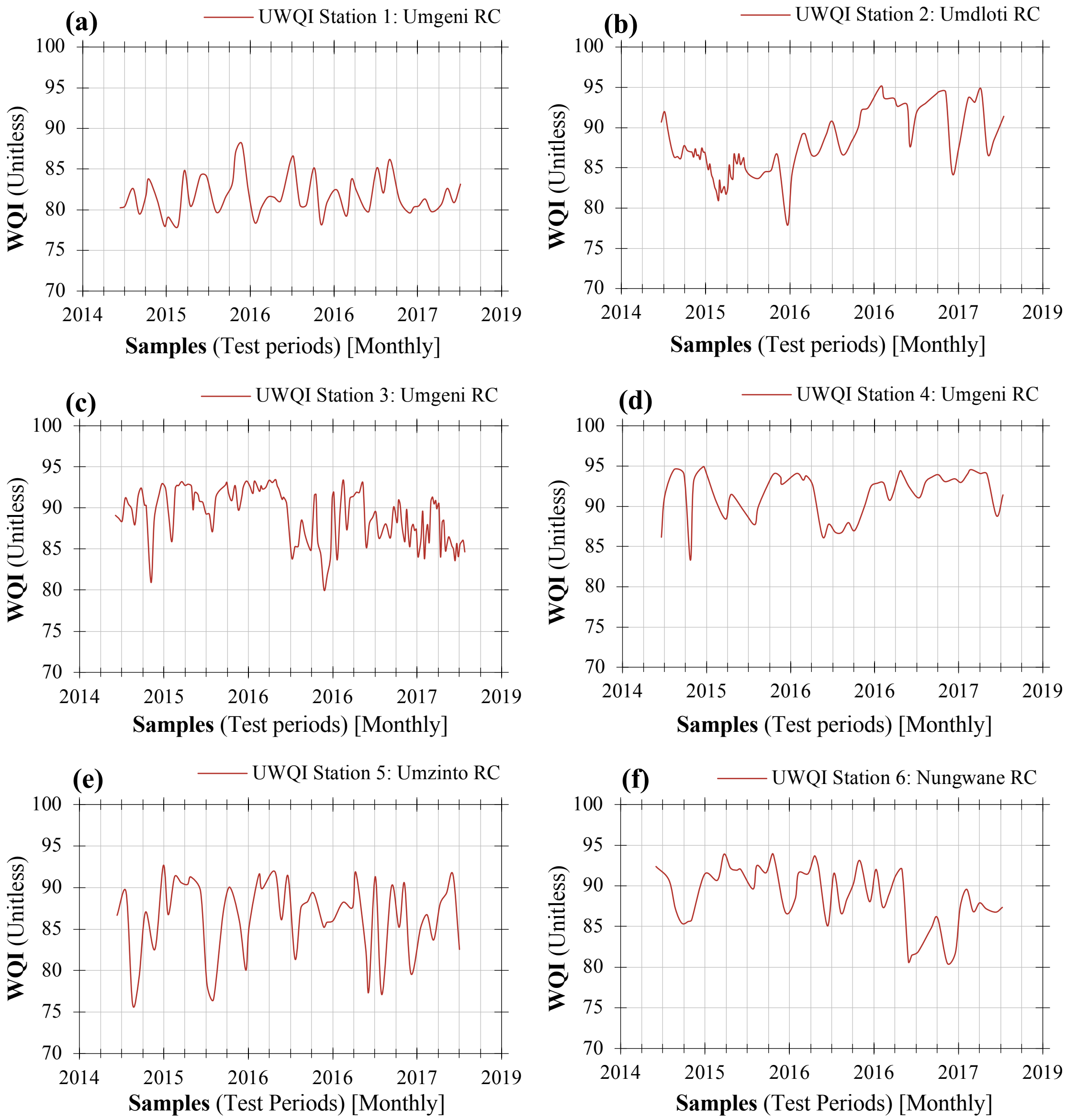


Figure 5.5: Water quality index results calculated using the developed universal water quality index (UWQI) for Umgeni water quality data for a period of four years from June 2014 to July 2018 (**a**) Umgeni River catchment for Henley Dams, (**b**) Umdloti River catchment for Hazelmere Dam, (**c**) Umgeni River catchment for Inanda Dams, (**d**) Umgeni River catchment for Midmar Dam, (**e**) Umzinto/Umuziwezinto River catchment for Umzinto Dam, and (**f**) Nungwane River catchment for Nungwane Dam

Source: Authors' graphs and UWQI results are extracts from the WQVM (Banda and Kumarasamy, 2020b, 2020c).

Notes: The water quality data is from six sampling stations observed monthly for a period extending to four years ranging from June 2014 until July 2018.

The high values of NO_3 are recorded during the summer periods and considering the socio-economic developments surrounding the sampling stations (Figure 4.3), the source of contamination might be anthropogenic activities, especially wastewater discharge among others.

NO_3 is a naturally occurring ion (Fan, 2011, Serio et al., 2018), which is widespread and regarded as the most significant contaminant in water (Espejo-Herrera et al., 2015, Sadler et al., 2016). Nitrate itself is a low-toxic compound, but when endogenously converted to nitrite (NO_2), it becomes toxic to human health and the aquatic environment (Fan, 2011, Serio et al., 2018). Hence the need for regular water quality monitoring to identify water quality trends over time and space (Shah and Joshi, 2017).

High levels of turbidity are evident during the summer seasons on stations 1, 2, 5 and 6 with corresponding values of 97.20, 66.70, 13.20 and 13.30 NTU. Together with NO_3, turbidity contributes significantly towards the deterioration of water quality among these sites. Sources of turbidity are diverse and include, but not limited to, reservoir drawdown-flushing, algal blooms (eutrophication), wastewater discharge, industrial effluent, exceptional rainfall events, soil erosion and decomposition of organic matter (Robert et al., 2016, Uncles et al., 2018). Chl-a concentrations at station 2 and 3 exceed targeted water quality levels in summer with values of 20.49 and 19.50 µg/ℓ respectively. Soluble nutrients, especially phosphorus and nitrogen, are the key determinants promoting algae blooms (eutrophication), which contribute significantly towards increased levels of chlorophyll-a (Andrade et al., 2019, Hashim et al., 2019). Such enriching nutrients often originates from anthropogenic activities which include wastewater discharge and fertiliser runoff (Banda, 2015, Omwene et al., 2018, Rankinen et al., 2019).

Marginal variations of WQI are observed for stations 1 (77.983 - 88.083) and station 4 (83.299 - 94.918). The two stations are located upstream of the catchment, and the rest of the sampling sites are situated downstream of the drainage region towards Durban-Pietermaritzburg business corridor. WQI results indicate that surface water quality varies more with the increase in socio-economic activities along the river water-course, with station 2 having the most considerable variation (77.873 - 95.154).

Testing the model with data from various river catchments promote the objective of establishing a universal water quality index suitable for use across the catchment areas in South Africa. Noticeably, the UWQI model responded steadily to the highs and lows of each water quality parameter value, with the index output graphs confirming to the variations. Such performances advocate the readiness of the UWQI to interpret water quality data and provide a simple non-dimensional score that is justifiable and in a repeatable manner. Such success fulfils the objective of developing a universal WQI and more importantly presents a "yardstick" that can be applied in most, if not all the distinct watersheds in South Africa. This accomplishment is a critical milestone, not only to the authors but to most of the stakeholders directly or indirectly involved in water quality science.

In an effort to confirm the capability of Artificial Intelligence (AI) in water quality science, an additional WQI was developed through the application of artificial neural networks (ANNs), and the following sections attempt to address the research question:

> *"How capable is the proposed development of water quality index and water quality variability model using artificial neural network (ANN) to analyse and monitor water quality status for South African rivers?"*

An ANN uses a highly nonlinear mapping process with predefined multidimensional parameter relationships in the form of mathematical coding. The application of ANNs has its respective advantages and disadvantages; however, immediate attention should be drawn towards its ability to understand and relate to variable dependency, which provides a unique benefit over the conventional way of developing water quality indices (Li and Liu, 2019).

5.4 Water quality index using artificial neural networks (ANNs)

Artificial neural networks (ANNs) are robust data-driven "black-box" models competent of analysing and outlining both linear and complex non-linear relationships between the target variable and the independent variables. Over the years, neural networks have demonstrated their efficiency as powerful computational algorithms for developing artificial intelligence-based models earmarked for simulating, predicting and forecasting spatio-temporal changes in water science. Hence, they have received more attention and become an acceptable substitute for conventional methods for hydro-chemical modelling. ANNs are the most commonly applied artificial intelligence (AI) algorithms for surface water quality models. Due to such large-scale acceptance, their robustness, flexibility and precision, the current study adopts an artificial neural network (ANN) technique and develop an alternative water quality index model applicable to South African watersheds.

The feed-forward, back-propagated multilayer perceptron model consists of three neuron layers in a parallel-distributed architecture with seventy weighted synapses oriented from left to right. First, the input layer comprises of thirteen nodes representing thirteen independent water quality parameters namely NH_3, Ca, Cl, Chl-a, EC, F $CaCO_3$, Mg, Mn, NO_3, pH, SO_4, and turbidity (NTU). Second, the hidden layer with eleven neurons responsible for predictive assignments. Third, is the output layer containing one perceptron accountable for transmitting network results through a one-digit water quality index score. The index ranges from zero to hundred, with zero being poor water quality and a hundred signifying excellent water quality.

The learning process of the AI-based model has been performed using water quality data from six sampling stations located in four drainage catchment areas under the jurisdiction of Umgeni

Water Board in KwaZulu-Natal Province, South Africa. The dataset consisting of 416 sample cases have been randomly partitioned using a split-ratio of 70:15:15% for training, testing and validation processes, respectively. The study applied the Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm to perform backpropagation training and optimising channel weights. The target variables are index values generated by the universal water quality index (UWQI) model established for South African river catchments.

The neural network indicated an increased performance with an overall correlation coefficient of 0.985, and specific performance ratings of 0.987, 0.992, and 0.977 for training, testing, and validation, respectively. Sensitivity analysis further authenticated the readiness and computational capabilities of the neural network. Having an average target to output error margins of ±0.242; the model has sufficient predictive capacity providing output values identical to the target UWQI, recording minimum and maximum model index scores of 75.995 and 94.420 respectively. Therefore, the three-layer ANN model is regarded as scientifically stable, with index scores and water quality grading matching the UWQI results. The following subsections attempt to document the procedures implemented and record the results achieved.

5.4.1 ANN architecture and rationale

An artificial neural network (ANN) uses a highly non-linear mapping process with predefined multidimensional parameter relationships in the form of mathematical coding (Singh et al., 2009, Khalil et al., 2011, Kim and Seo, 2015, Sarkar and Pandey, 2015, Salari et al., 2018, Ramasubramanian and Singh, 2019, Sousa et al., 2019). The application of artificial neural network (ANNs) has its respective advantages and disadvantages. Still, immediate attention should be drawn towards its ability to understand and relate to variable dependency, which provides a unique benefit over the conventional way of developing water quality indices (Li and Liu, 2019). The study developed a feed-forward, back-propagated multilayer perceptron model consisting of three neuron layers in a parallel-distributed architecture with seventy weighted synapses oriented from left to right.

First, the input layer comprises of thirteen nodes representing thirteen independent water quality parameters namely NH_3, Ca, Cl, Chl-a, EC, F $CaCO_3$, Mg, Mn, NO_3, pH, SO_4, and turbidity (NTU). Second, the hidden layer with five neurons responsible for predictive assignments. Third, is the output layer containing one perceptron accountable for transmitting network results through a one-digit water quality index score. The first set of neuro-nodes (input layer) accepts the water quality parameters, whereas the second set of perceptron (hidden layer) analyse the hydrochemistry. Finally, the third layer (output neuron) generates a single-digit index score describing the spatial and temporal variations of surface water quality. The ANN architecture is graphically illustrated in Figure 5.6.

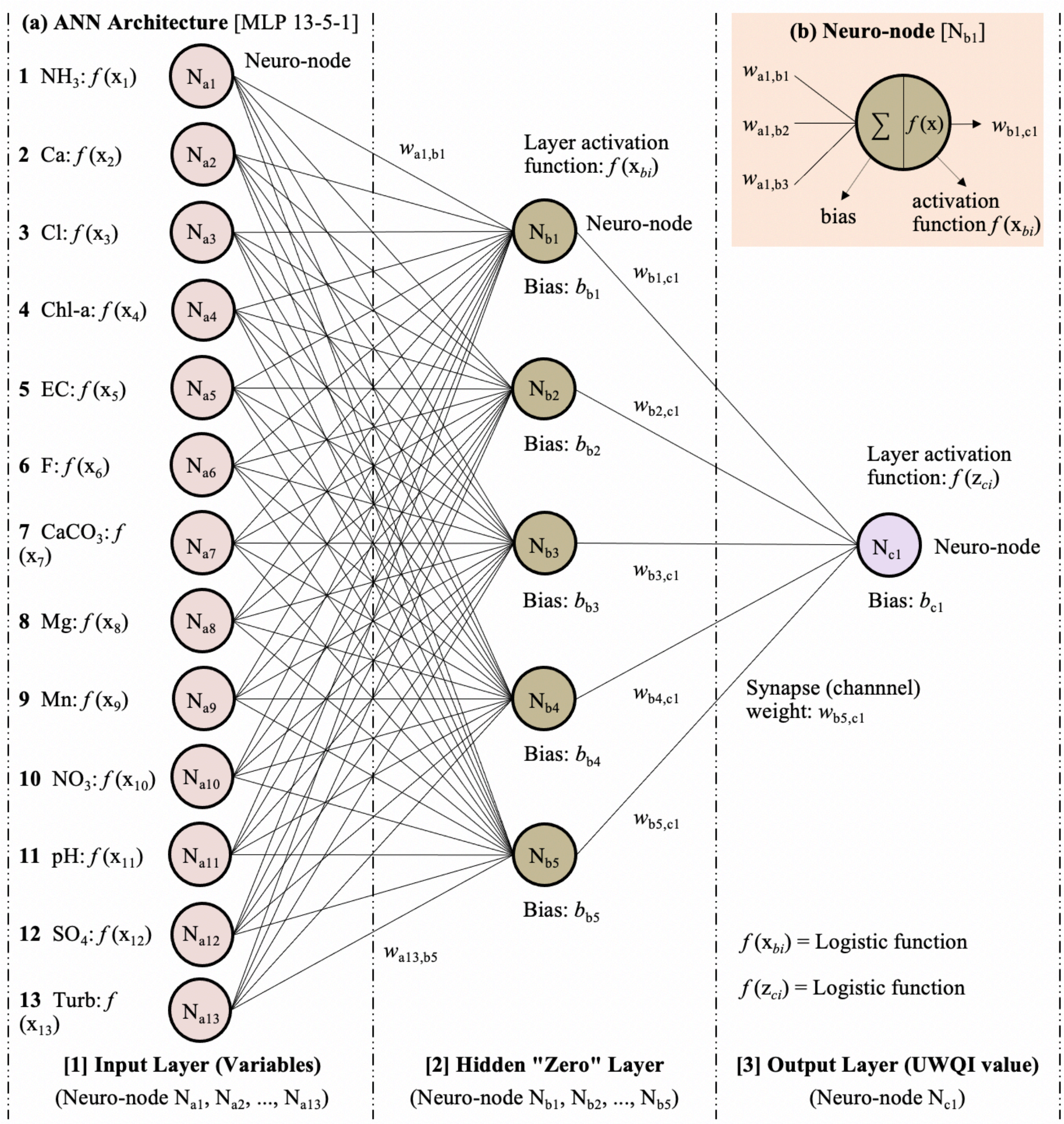


Figure 5.6: Schematic diagram representing the final optimum three-layered feed-forward artificial neural network with thirteen neuro-nodes in the input layer, five perceptron in the hidden layer, one output neuron, and seventy synapses oriented from left to right.

Source: Authors diagram illustrating the optimum architecture considered for the development of the artificial neural network (ANN) model was adopted from the following literature: Singh et al. (2009), Huo et al. (2013), Cordoba et al. (2014), Sarkar and Pandey (2015), Seo et al. (2016), Yilma et al. (2018), García-Alba et al. (2019), Haldorai et al. (2019), Kim et al. (2019b).

Notes: The artificial neural network structure was optimised using TIBCO Statistica Automated Neural Networks Software, TIBCO Software Inc. (2020).

5.4.1.1 Forward propagation process

Given that $f(x_i)$ represents the input parameter, w_i is the weight of each channel (synapse) and b_{ij} denotes the bias of each neuron, then the feed-forward process is described as follows (Singh et al., 2009, Khalil et al., 2011, Huo et al., 2013, Seo et al., 2016, Salari et al., 2018, Charulatha et al., 2017, Bansal and Ganesan, 2019, García-Alba et al., 2019, Rajaee et al., 2020, Ye et al., 2020):

(a) **Step 1 - inputting:** $f(x_i)$ admitted as input to each neuro-node of the first layer of the artificial neural network ($x_1, x_2, \ldots, x_n$).
(b) **Step 2 - transmission of data:** Feed through channels to the proceeding layer of neurons, and the synapses are assigned with relative coefficient known as weight (w_{ij}).
(c) **Step 3 - application of weightage coefficients:** Inputs from the first layer are multiplied by the corresponding numeric weight coefficients and processed as input to the subsequent later of neurons in the hidden layer ($x_1w_1+x_2x_2+\ldots+x_nw_n$) = ($\sum x_iw_i$).
(d) **Step 4 - application of bias constants and activation functions:** Each hidden layer neuron is associated with a numeric constant value known as bias ($b_1, b_2, \ldots, b_n$), which is added to the input sum ($\sum x_iw_i+b_i$). After that, it passes through a threshold function called the activation function, which determines whether the neuron particular neuron gets activated or not. The activated neuron transmits information further to the next set of neurons; and in this systematic manner, water quality data is forward propagated through the network from left to right.

5.4.1.2 Backward propagation of errors

Backpropagation is a popular optimisation method for performing automatic differentiation of complex nested functions. The procedure is applied to train multilayer artificial neural networks in an attempt to optimise the network error, using an error function; backpropagation calculates the gradient of the error function with respect to the channel weight (Singh et al., 2009, Huo et al., 2013, Kim and Seo, 2015). The optimisation technique proceeds backwards through the network, from right to left in a reverse-order approach. Backward propagation of errors allows efficient optimisation rather than the naive process of adjusting weights and biases of each layer separately (Rajaee et al., 2020). Even more importantly, the backpropagation algorithm allows artificial neural networks to be considered for a much wider field of problems that were previously off-limits due to computational demands.

Each iteration of feed-forward and backpropagation updates weight parameters and bias constants of the model, and the learning process is repeated with numerous cycles until an optimum neural network is achieved. The feed-forward and backpropagation process is illustrated graphically in Figure 5.7 and 5.8.

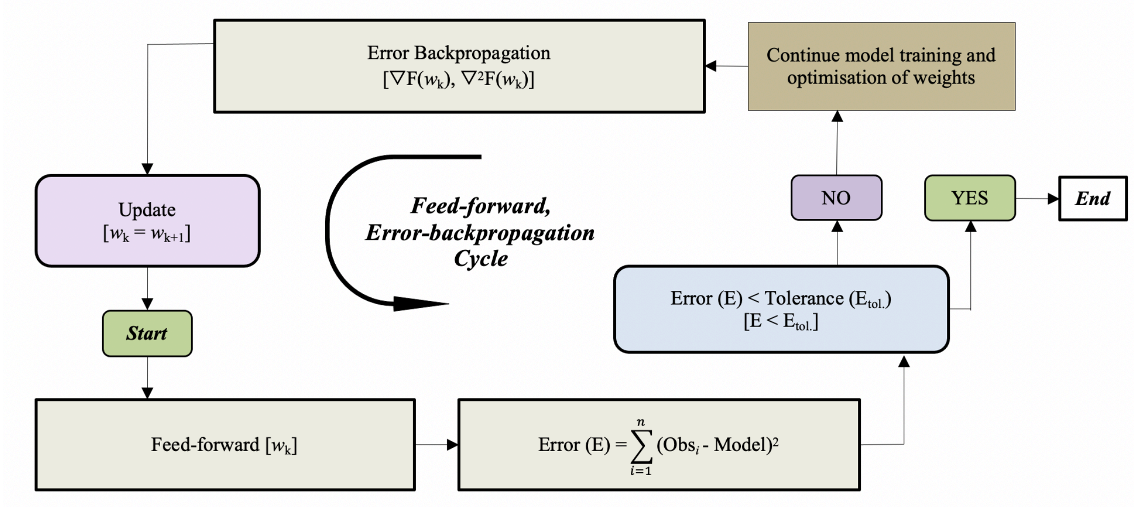


Figure 5.7: Graphical presentation of the feed-forward and error-backpropagation cycle for an artificial neural network model (ANN)

Source: Authors' diagram modified from concept documented by Kim and Seo (2015).

Notes: Feed-forward propagated information through the network from left to right, whereas backward propagation of errors proceeds backwards through the network, from right to left in a reverse-order approach.

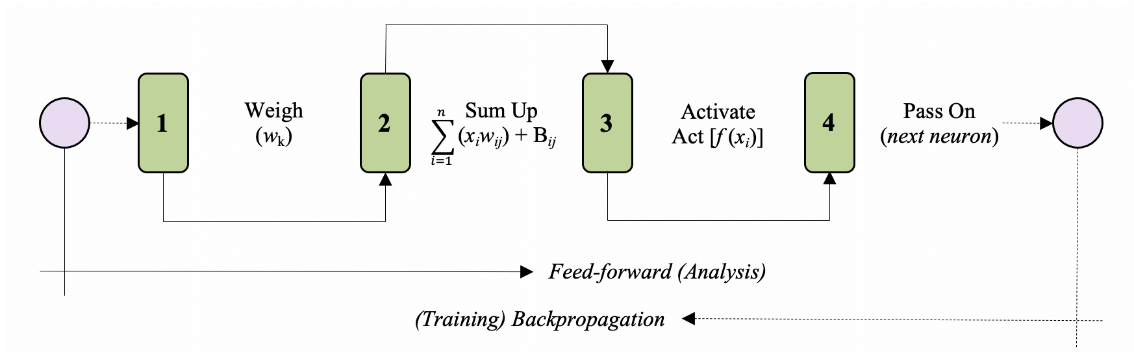


Figure 5.8: Illustration of the neuro-node operational cycle and feed-forward sequence

Source: Authors diagram formulated from the neuron processing cycle.

Notes: Feed-forward process, (1) $f(x_i)$ admitted as input by the first set of neurons (x_1, x_2, …, x_n), (2) feedthrough channels and proceed to the next set of neurons, (3) apply relative weight coefficients and processed as input to the hidden layer ($x_1w_1+x_2x_2+\ldots+x_nw_n$) = ($\sum x_iw_i$), (4) add bias constant to the input sum ($\sum x_iw_i+b_i$) and then passes through a threshold activation function, which determines whether the neuron particular neuron gets activated or not. Thereafter, transmit the data to the last set of neurons referred to as the output layer.

5.4.2 Optimisation and performance analysis

There is no specific procedure for determining the optimum number of layers and neuro-nodes; instead, the configuration is influenced by a different set of conditions (Qaderi and Babanezhad, 2017). According to the literature (Khalil et al., 2011, Qaderi and Babanezhad, 2017, Gazzaz et al., 2012, Sarkar and Pandey, 2015), neural networks with too many layers are associated with "over-fitting" problems and seldomly demonstrate optimal prediction performance. Therefore, the study considered three-layered artificial neural network; thus input, hidden and output layer. The number of neuro-nodes depends upon the problem being investigated (Singh et al., 2009, Sarkar and Pandey, 2015). Whereby input and output neurons are commonly fixed based on the number of input variables being considered and the model desired output. Neurons in the hidden layer are the core processing units of the neural network and optimising the number of such neurons is critical towards the models' overall performance. Restricting the neuro-nodes might limit the network from learning successfully, whereas an excessive number of hidden nodes may prolong the training process causing data "over-fitting" (Singh et al., 2009, Khalil et al., 2011, Sarkar and Pandey, 2015, Qaderi and Babanezhad, 2017).

Fletcher and Goss (1993) suggested that hidden layer neurons (H_{nod}) range from $2(I_{nod})^{0.5} + O_{nod}$ to $2I_{nod} + 1$; where I_{nod} and O_{nod} denote the number of input and output neuro-nodes respectively (Singh et al., 2009, Sarkar and Pandey, 2015). However, Alyuda Research Inc. (2003) argued that the H_{nod} range should be between $0.5I_{nod}$ and $4I_{nod}$. Furthermore, Palani et al. (2008) submitted that H_{nod} may range from I_{nod} to $2I_{nod} + 1$, but should not fall beneath $0.333I_{nod}$ and O_{nod} (Gazzaz et al., 2012). Even more recently, García-Alba et al. (2019) recommended that hidden layer nodes (H_{nod}) should be less than twice the input nodes (I_{nod}) and proposed the following Equation 5.22 (García-Alba et al., 2019):

$$0.5I_{nod} - 2 \leq H_{nod} \leq 2I_{nod} + 2 \qquad \text{Eq. 5.22}$$

Having thirteen fixed input nodes corresponding to water quality input variables and one output node representing; the study confined the number of hidden neuro-nodes to $5 \leq H_{nod} \leq 28$ following parameters set in Equation 5.22. Through trial and error approach, and using the whole spectrum of possibilities from 5 to 28 hidden neurons, five potential neural networks were developed as summarised in Table 5.9.

Accordingly, the finest ANN architecture (network two on Table 5.9) consists of a multilayer perceptron model having nineteen inter-connected neuro-nodes (13-5-1), six bias constants and seventy weighted synapses operating in a feed-forward manner from left to right (Figure 5.6). Activation functions are responsible for activating the perceptron based on higher weight. Four activation functions have been examined, thus (a) tanh, (b) exponential (c), logistic-sigmoidal, and (d) identity function. Subsequently, the logistic function, also known as the sigmoid activation function, worked better with the proposed neural network for both the hidden and output layers.

Table 5.9: Summary of the five potential artificial neural networks (ANNs) developed

Item	Description	Details of the Five Potential Artificial Neural Networks (ANNs) Developed				
		1	2	3	4	5
1	Network structure	MLP 13-16-1	MLP 13-5-1	MLP 13-12-1	MLP 13-28-1	MLP 13-8-1
2	Training R-value	0.974	0.987	0.980	0.962	0.981
3	Test R-value	0.970	0.992	0.967	0.905	0.978
4	Validation R-value	0.949	0.977	0.961	0.938	0.959
5	Overall R-value	0.964	0.985	0.969	0.935	0.973
6	Training error	0.491	0.238	0.375	0.708	0.350
7	Test error	0.601	0.174	0.658	1.815	0.435
8	Validation error	0.812	0.315	0.630	0.850	0.729
9	Overall error	0.634	0.242	0.554	1.124	0.505
10	Training algorithm	BFGS 58	BFGS 284	BFGS 105	BFGS 53	BFGS 97
11	Error function	SOS	SOS	SOS	SOS	SOS
12	Hidden activation	Tanh	Logistic	Logistic	Tanh	Logistic
13	Output activation	Exponential	Logistic	Logistic	Identity	Logistic

Source: ANN results from TIBCO Statistica Automated Neural Networks Software, TIBCO Software Inc. (2020).

Notes: The ANN software suggested twenty possible networks, but only five best models are extracted and represented in Table 5.9 above. Performance R-value represents the statistical correlation coefficient (R).

The sigmoid function activates the neuro-node when the sum of weights plus bias ($\sum x_i w_i + b_i$) is greater than or equal to 0.500; otherwise, the neuron is not activated. Values < 0.500 are converted to zero, and the neuron remains unactivated, but values ≥ 0.500 are transformed to one, and the neuron is activated to send through the information. The logistic function is further expressed as Figure 5.9 and Equation 5.23 (Palani et al., 2008, Huo et al., 2013, García-Alba et al., 2019).

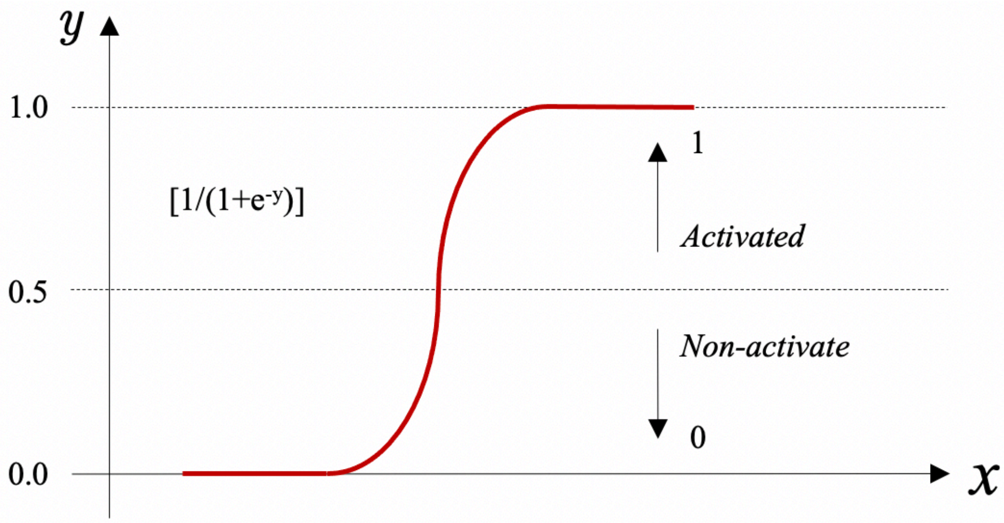


Figure 5.9: Logistic-sigmoidal activation function

Source: Authors' diagram generated from Equation 5.23 as documented by Palani et al. (2008), Huo et al. (2013), García-Alba et al. (2019).

Notes: The diagram represents the logistic-sigmoidal activation function used for the developed artificaila nueral networks as documented in Table 5.9 (Model 2 – MLP 13-5-1).

sigmoid function: $f(z) = \left[\dfrac{1}{1 + \mathrm{e}^{-z}} \right]$ Eq. 5.23

where: $z = \sum_{i=1}^{n} w_i x_i + b_i$ Eq. 5.24

The sigmoid function is traditionally popular activation function for neural networks with a general problem of saturation. Thus, higher sigmoidal values snap to one, whilst small digits snap to zero. Furthermore, the sigmoid activated function is sensitive to changes around the mid-point of the input. Nonetheless, the logistic-sigmoidal function proved to be the most favourable activation function for the developed artificial neural network.

Empirical datasets are generally associated with variables having different measurements units, which is quite burdensome and might lead to measurement errors, noise and or interference (Gazzaz et al., 2012, Huo et al., 2013, Kadam et al., 2019). Such effects may relay negative inputs during network training process since some ANN training algorithms are not compatible with diversified data units. For this reason, the study considered standardising the actual water quality measurements to match the logistic-sigmoidal units ranging from zero to one. The process prohibits parameters from randomly dominating the neural network operations (Gazzaz et al., 2012, Huo et al., 2013, Rajaee et al., 2020).

Practically, neural network training is performed to establish an optimum neural network with the best approximation capacity measurable through various statistical attributes. The training process should be guided and terminated using a predetermined stopping criterion which prevents overtraining and improves generalisation (Singh et al., 2009). Four stopping procedures were prescribed for the study, and these are:

(a) Terminate the training cycle when cross-validation subset stops changing or begins to increase (Gazzaz et al., 2012, Mitrović et al., 2019);
(b) Minimum improvement in the error corresponding to 0.0000001 (Gazzaz et al., 2012);
(c) Mean-Squared error (MSE) value on the training set of 0.010 (Gazzaz et al., 2012); and
(d) Maximum of ten thousand iterations (Gazzaz et al., 2012).

The study applied, Broyden-Fletcher–Goldfarb-Shanno (BFGS) algorithm (Mitrović et al., 2019, García-Alba et al., 2019, Shanthi et al., 2009) to perform network training and optimising the channel weights together with bias constants which are included under Table 5.11 and 5.10, respectively. The identity and connections listed on these two tables correspond to the labels provided in Figure 5.6.

Table 5.10: Channel relative weightage coefficients for the proposed multi-layered feed-forward perceptron model

Code	Weightage Coefficients for the Final ANN Model			Code	Weightage Coefficients for the Final ANN Model		
	Identity	Connection	Weight Coefficient		Identity	Connection	Weight Coefficient
1	w_{a1b1}	NH_3: N_{a1} - N_{b1}	-1.736787	**36**	w_{a8b1}	Mg: N_{a8} - N_{b1}	-3.214513
2	w_{a1b2}	NH_3: N_{a1} - N_{b2}	5.504801	**37**	w_{a8b2}	Mg: N_{a8} - N_{b2}	1.744056
3	w_{a1b3}	NH_3: N_{a1} - N_{b3}	1.188668	**38**	w_{a8b3}	Mg: N_{a8} - N_{b3}	-4.429081
4	w_{a1b4}	NH_3: N_{a1} - N_{b4}	-1.692601	**39**	w_{a8b4}	Mg: N_{a8} - N_{b4}	0.279011
5	w_{a1b5}	NH_3: N_{a1} - N_{b5}	-0.001097	**40**	w_{a8b5}	Mg: N_{a8} - N_{b5}	1.944368
6	w_{a2b1}	Ca: N_{a2} - N_{b1}	3.468499	**41**	w_{a9b1}	Mn: N_{a9} - N_{b1}	-7.983205
7	w_{a2b2}	Ca: N_{a2} - N_{b2}	2.115498	**42**	w_{a9b2}	Mn: N_{a9} - N_{b2}	6.424076
8	w_{a2b3}	Ca: N_{a2} - N_{b3}	1.106156	**43**	w_{a9b3}	Mn: N_{a9} - N_{b3}	-5.471109
9	w_{a2b4}	Ca: N_{a2} - N_{b4}	0.220185	**44**	w_{a9b4}	Mn: N_{a9} - N_{b4}	-0.342985
10	w_{a2b5}	Ca: N_{a2} - N_{b5}	-1.346809	**45**	w_{a9b5}	Mn: N_{a9} - N_{b5}	-0.484034
11	w_{a3b1}	Cl: N_{a3} - N_{b1}	-3.556672	**46**	w_{a10b1}	NO_3: N_{a10} - N_{b1}	-16.055562
12	w_{a3b2}	Cl: N_{a3} - N_{b2}	0.457860	**47**	w_{a10b2}	NO_3: N_{a10} - N_{b2}	-23.849729
13	w_{a3b3}	Cl: N_{a3} - N_{b3}	-1.580444	**48**	w_{a10b3}	NO_3: N_{a10} - N_{b3}	6.729461
14	w_{a3b4}	Cl: N_{a3} - N_{b4}	0.374732	**49**	w_{a10b4}	NO_3: N_{a10} - N_{b4}	-8.960559
15	w_{a3b5}	Cl: N_{a3} - N_{b5}	-0.404492	**50**	w_{a10b5}	NO_3: N_{a10} - N_{b5}	-0.338867
16	w_{a4b1}	Chl-a: N_{a4} - N_{b1}	1.377876	**51**	w_{a11b1}	pH: N_{a11} - N_{b1}	-15.304164
17	w_{a4b2}	Chl-a: N_{a4} - N_{b2}	-3.330414	**52**	w_{a11b2}	pH: N_{a11} - N_{b2}	3.871621
18	w_{a4b3}	Chl-a: N_{a4} - N_{b3}	-7.024330	**53**	w_{a11b3}	pH: N_{a11} - N_{b3}	-8.330722
19	w_{a4b4}	Chl-a: N_{a4} - N_{b4}	-0.022393	**54**	w_{a11b4}	pH: N_{a11} - N_{b4}	0.954006
20	w_{a4b5}	Chl-a: N_{a4} - N_{b5}	0.693426	**55**	w_{a11b5}	pH: N_{a11} - N_{b5}	1.730046
21	w_{a5b1}	EC: N_{a5} - N_{b1}	1.885811	**56**	w_{a12b1}	SO_4: N_{a12} - N_{b1}	4.874266
22	w_{a5b2}	EC: N_{a5} - N_{b2}	0.005186	**57**	w_{a12b2}	SO_4: N_{a12} - N_{b2}	-9.213797
23	w_{a5b3}	EC: N_{a5} - N_{b3}	5.441349	**58**	w_{a12b3}	SO_4: N_{a12} - N_{b3}	-0.854192
24	w_{a5b4}	EC: N_{a5} - N_{b4}	-1.280430	**59**	w_{a12b4}	SO_4: N_{a12} - N_{b4}	0.483610
25	w_{a5b5}	EC: N_{a5} - N_{b5}	-0.245986	**60**	w_{a12b5}	SO_4: N_{a12} - N_{b5}	-0.429851
26	w_{a6b1}	F: N_{a6} - N_{b1}	-5.420631	**61**	w_{a13b1}	Turb: N_{a13} - N_{b1}	5.242365
27	w_{a6b2}	F: N_{a6} - N_{b2}	15.774371	**62**	w_{a13b2}	Turb: N_{a13} - N_{b2}	2.942964
28	w_{a6b3}	F: N_{a6} - N_{b3}	2.011805	**63**	w_{a13b3}	Turb: N_{a13} - N_{b3}	-1.860321
29	w_{a6b4}	F: N_{a6} - N_{b4}	-1.672389	**64**	w_{a13b4}	Turb: N_{a13} - N_{b4}	0.832442
30	w_{a6b5}	F: N_{a6} - N_{b5}	-0.553722	**65**	w_{a13b5}	Turb: N_{a13} - N_{b5}	-88.813790
31	w_{a7b1}	$CaCO_3$: N_{a7} - N_{b1}	0.660897	**66**	w_{b1c1}	N_{b1} - N_{c1}: UWQI	-13.400521
32	w_{a7b2}	$CaCO_3$: N_{a7} - N_{b2}	2.067450	**67**	w_{b2c1}	N_{b2} - N_{c1}: UWQI	-0.727691
33	w_{a7b3}	$CaCO_3$: N_{a7} - N_{b3}	-1.458696	**68**	w_{b3c1}	N_{b3} - N_{c1}: UWQI	2.101400
34	w_{a7b4}	$CaCO_3$: N_{a7} - N_{b4}	0.449066	**69**	w_{b4c1}	N_{b4} - N_{c1}: UWQI	4.811822
35	w_{a7b5}	$CaCO_3$: N_{a7} - N_{b5}	-0.678565	**70**	w_{b5c1}	N_{b5} - N_{c1}: UWQI	11.009187

Source: ANN results from TIBCO Statistica Automated Neural Networks Software, TIBCO Software Inc. (2020).

Notes: The synapses weights and neuro-nodes correspond with the schematic diagram presented in Figure 5.6. The weights are rounded off to six decimal places for presentation only.

Though requiring high computational memory owing to Hassian matrix, BFGS is a robust second-order training algorithm with high-speed convergence rate. The technique offers general-purpose optimisation based on Nelder-Mead; quasi-Newton simulated annealing, and conjugate-gradient algorithms with an option for box-constrained optimisation. BFGS algorithm uses only function values and works well for non-differentiable functions.

Table 5.11: Proposed bias constants for the three-layered artificial neural network model

Code	Bias constants for the Final ANN Model			Code	Bias constants for the Final ANN Model		
	Identity	Connection	Bias constant		Identity	Connection	Bias constant
1	b_{b1}	B_{in} - N_{b1}	-4.408752	**4**	b_{b4}	B_{in} - N_{b4}	0.359861
2	b_{b2}	B_{in} - N_{b2}	4.751969	**5**	b_{b5}	B_{in} - N_{b5}	-2.506008
3	b_{b3}	B_{in} - N_{b3}	8.234114	**6**	b_{c1}	B_{out} - UWQI	-3.452418

Source: ANN results from TIBCO Statistica Automated Neural Networks Software, TIBCO Software Inc. (2020).

Notes: The bias constants correspond with the schematic diagram presented in Figure 5.6. The constant values are rounded off to six decimal places for presentation only.

A dataset comprising of 416 samples has been randomly portioned using data split-ratio of 70:15:15% for network training, testing and validation processes, respectively (Shanthi et al., 2009). As documented in Table 5.12, various split-ratios are suggested in the literature (Lischeid, 2001, Lucio et al., 2007, Mas and Ahlfeld, 2007, Olszewski et al., 2008, May and Sivakumar, 2009, Amiri and Nakane, 2009, Oliveira Souza da Costa et al., 2009, Shanthi et al., 2009, Singh et al., 2009, Banerjee et al., 2011, Gazzaz et al., 2012, Cordoba et al., 2014, Safavi and Malek Ahmadi, 2015, Seo et al., 2016, Qaderi and Babanezhad, 2017, Gebler et al., 2018, García-Alba et al., 2019, Isiyaka et al., 2019, Kadam et al., 2019, Rajaee et al., 2020, Soro et al., 2020). However, the study adopted the default ratio supported by Statistica Automated Neural Networks software developer TIBCO Software Inc. (2020).

Table 5.12: Documented data splitting schemes for developing artificial neural networks

Scheme	Data split-ratio (%)			Reference
	Training	Validation	Testing	
1	80.000 %	10.000 %	10.000 %	(Palani et al., 2008, Gazzaz et al., 2012, Seo et al., 2016, García-Alba et al., 2019)
2	75.000 %	10.000 %	15.000 %	(Gazzaz et al., 2012)
3	70.000 %	10.000 %	20.000 %	(May and Sivakumar, 2009)
4	70.000 %	15.000 %	15.000 %	(Lucio et al., 2007, Shanthi et al., 2009, Banerjee et al., 2011, Safavi and Malek Ahmadi, 2015, Qaderi and Babanezhad, 2017, Gebler et al., 2018, Ahamad et al., 2019, Kadam et al., 2019, García-Alba et al., 2019, Rajaee et al., 2020)
5	65.000 %	15.000 %	20.000 %	(Mas and Ahlfeld, 2007)
6	60.000 %	20.000 %	20.000 %	(Singh et al., 2009, García-Alba et al., 2019, Isiyaka et al., 2019)
7	60.000 %	15.000 %	25.000 %	(Amiri and Nakane, 2009)
5	50.000 %	25.000 %	25.000 %	(Lischeid, 2001, Olszewski et al., 2008, Oliveira Souza da Costa et al., 2009, Cordoba et al., 2014, Soro et al., 2020)

Source: Gazzaz et al. (2012) and particular studies as cited in Table 5.12.

Notes: The above-listed figures represent the percentage equivalent to the split ratios applied for each particular study to create data subsets for training, validation and testing procedures.

The training dataset is utilised during the learning process; whilst validation samples are used for cross-validation, thus establishing when to stop network training before over-fitting happens. Testing dataset assists in performing a reliable out-of-sample assessment and establishing an accurate network predictive error. After that, statistical performance evaluators are deployed to measure the usefulness of artificial neural network the AI-based model.

In order to evaluate the performance of the neural networks and identifying the best optimum model, six different quantitative statistical attributes are considered. These include correlation coefficient (R), coefficient of determination (R^2), Nash-Sutcliffe efficiency (NSE) mean absolute error (MAE), root mean squared error (RMSE) and mean absolute percentage error (MAPE) (Palani et al., 2008, Singh et al., 2009, Gazzaz et al., 2012, Huo et al., 2013, Kim and Seo, 2015, Sarkar and Pandey, 2015, Seo et al., 2016, Qaderi and Babanezhad, 2017, Gebler et al., 2018, Salari et al., 2018, Yilma et al., 2018, Azimi et al., 2019, Kadam et al., 2019, Mitrović et al., 2019, Rajaee et al., 2020, Tiyasha et al., 2020). Networks with the lowest regression error and highest performance rate for classification are retained (Gazzaz et al., 2012). Correspondingly, twenty models were trained, and training was terminated upon satisfying the prescribed stopping options. Thereupon, five networks with the lowest prediction error and the highest classification rate were retained. The statistics are indicated in Table 5.13, and the corresponding equations are documented from Equation 5.25 to 5.29.

Table 5.13: Performance statistics for the MLP 13-5-1 model

Item	Performance Statistics	
	Metrics	Ratings
1	Mean absolute error (MAE)	0.521
2	Root mean squared error (RMSE)	0.692
3	Nash-Sutcliffe efficiency (NSE)	0.974
4	Mean absolute percentage error (MAPE)	0.600%
5	The correlation coefficient (R)	0.985
6	Coefficient of determination (R2)	0.970
7	Mean squared error (MSE)	0.479

Source: ANN results from TIBCO Statistica Automated Neural Networks Software, TIBCO Software Inc. (2020).

Notes: The ratings are categorised as follows (Gazzaz et al., 2012, Charulatha et al., 2017, García-Alba et al., 2019, Lu et al., 2019, Mitrović et al., 2019, Rajaee et al., 2020): MAPE ≤ 10.0 % (highly accurate), 10.0 MAPE < MAPE ≤ 20.0 % (good), 20.0 < MAPE ≤ 50.0 % (reasonable), MAPE > 50.0 % (inaccurate); 0.75 < NSE ≤ 1 (very good), 0.650 < NSE ≤ 0.750 (good), 0.500 < NSE ≤ 0.650 (satisfactory), NSE ≤ 0.500 (unsatisfactory); and R^2 > 0.500 (acceptable).

Equations 5.25 to Equation 5.29 are documented in the following studies: Palani et al. (2008), Singh et al. (2009), Khalil et al. (2011), Safavi and Malek Ahmadi (2015), Qaderi and Babanezhad (2017), Gebler et al. (2018), Yilma et al. (2018), García-Alba et al. (2019), Lu et al. (2019), Mitrović et al. (2019), Isiyaka et al. (2019), Ye et al. (2020).

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n} | y_o - y_i | \qquad \text{Eq. 5.25}$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(y_{o} - y_{i}\right)^{2}} \qquad \text{Eq. 5.26}$$

$$\mathrm{R}^2 \text{ or NSE} = 1 - \frac{\sum\left(y_{o} - y_{i}\right)^{2}}{\sum\left(y_{o} - y_{m}\right)^{2}} \qquad \text{Eq. 5.27}$$

$$\mathrm{MAPE} = \frac{100\%}{n}\sum_{i=1}^{n}\frac{\left|y_{o} - y_{i}\right|}{y_{o}} \qquad \text{Eq. 5.28}$$

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(y_{o} - y_{i}\right)^{2} \qquad \text{Eq. 5.29}$$

where: y_o is the target value,

y_i is the predicted model value, and

y_m is the target mean value as

The artificial neural network model expressed a significantly high degree of accuracy registering an overall correlation coefficient (R) of 0.985 ($p < 0.010$) with specific R-values of 0.987, 0.992 and 0.977 for training, testing and validation, respectively. The correlation coefficient describes the predictive performance of the model with values greater than 0.500 being satisfactory and values close to 1.000, explaining a highly accurate model (Rajaee et al., 2020). Consequently, the R-values achieved are satisfactory, indicating an increased performance and well-specified neural network.

The goodness-of-fit is further explained using the coefficient of determination (R^2) which is equivalent to Nash-Sutcliffe efficiency (NSE) (Palani et al., 2008). Whereby the best optimum model is selected based on the highest value of R^2 ranging from zero to one, where the greater the value and closer to one, the better (Gazzaz et al., 2012, Safavi and Malek Ahmadi, 2015, Charulatha et al., 2017, Qaderi and Babanezhad, 2017, Rajaee et al., 2020). However, the coefficient of determination value greater than 0.500 is regarded as satisfactory. The proposed neural network has an NSE/R^2 value of 0.970, meaning that the neural network explains approximately 97.0 % variations in the measured WQI values. The ANN model has an average target to output error margins of $\pm$ 0.242; implying that the model has sufficient predictive capacity providing output values identical to the target UWQI, recording minimum and maximum model index scores of 75.995 and 94.420 respectively. Figure 5.10 and 5.11 explain the relationship between the target UWQI and ANN output WQI. A summary of the UWQI scores is presented in Figure 5.12.

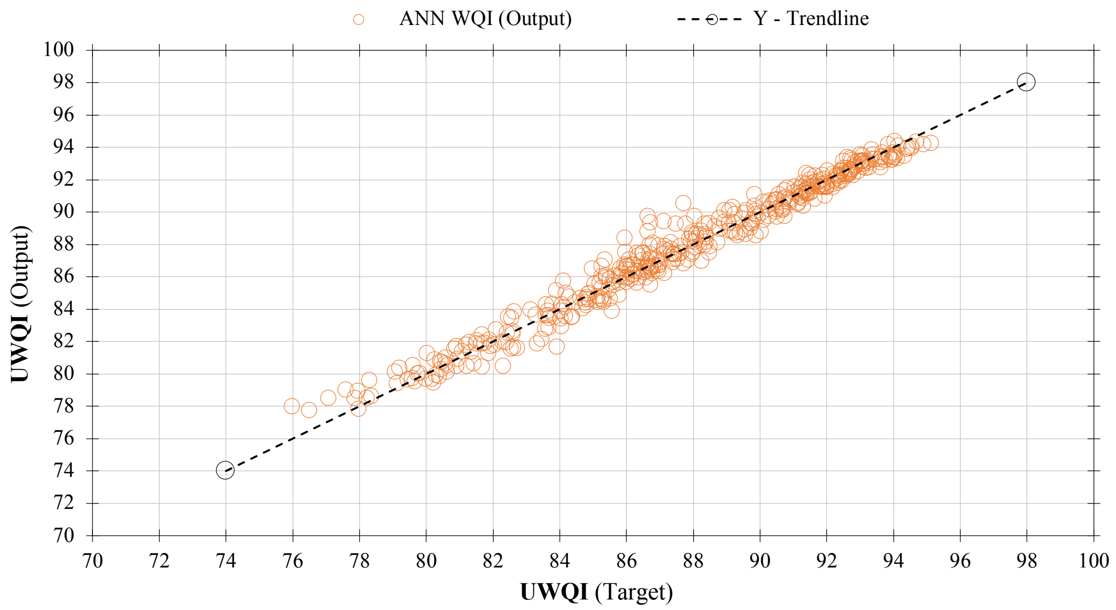


Figure 5.10: Results of ANN model validation showing a scatter plot of the relationship between the target UWQI values and their corresponding ANN model predictions. The plot demonstrates that a reasonable approximation was made by the ANN model across the spectrum of the UWQI values.

Source: ANN results from TIBCO Statistica Automated Neural Networks Software, TIBCO Software Inc. (2020).

Notes: The overall agreement between the measured (target variable) and simulated (output) WQI values was very satisfactory (R = 0.985, $p < 0.010$; $R^2 = 97.0$ %; NSE = 0.970, RMSE = 0.692, MAPE = 0.6 % and $n = 416$).

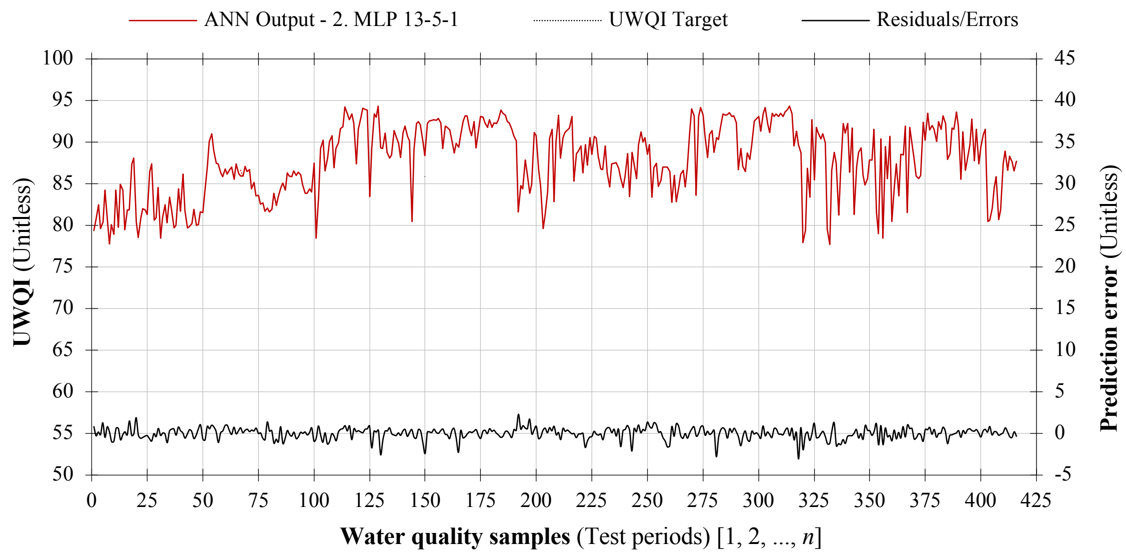


Figure 5.11: Comparison between the artificial neural network WQI scores (ANN Output) and the universal water index values (UWQI Target) with prediction error values

Source: ANN results from TIBCO Statistica Automated Neural Networks Software, TIBCO Software Inc. (2020).

Notes: The artificial neural network model has an average target to output error margins of ±0.242, which confirms the appropriateness of the neural network.

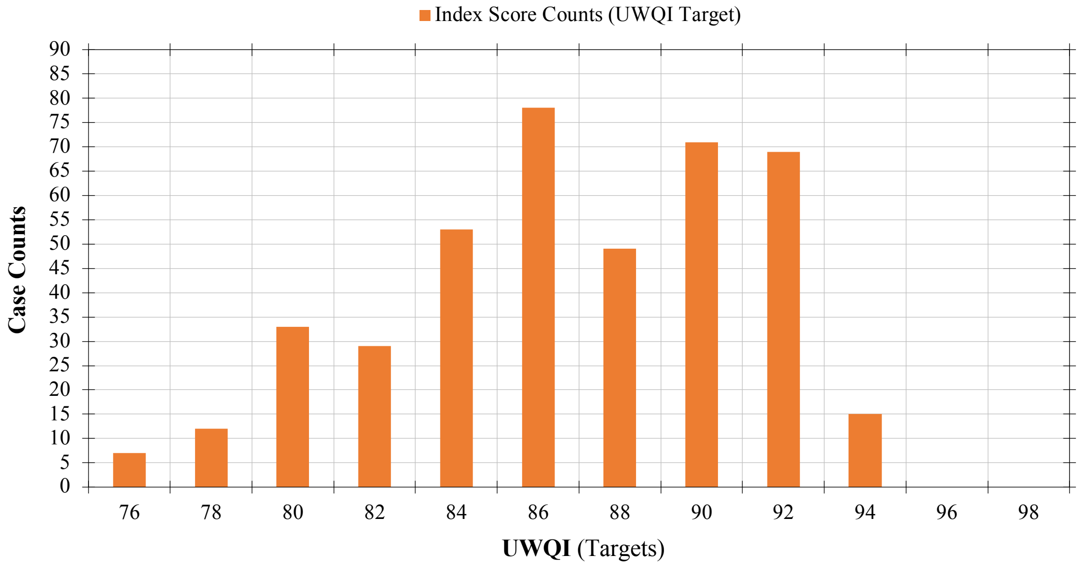


Figure 5.12: Index score counts for the universal water index values (UWQI Target)

Source: UWQI results extracted from Banda and Kumarasamy (2020c). Graph generated from TIBCO Statistica Automated Neural Networks Software, TIBCO Software Inc. (2020).

Notes: The water quality data used for calculating the UWQI scores is from six sampling stations observed monthly for a period extending to four years ranging from June 2014 until July 2018.

Beyond that, mean absolute error (MAE) and root mean squared error (RMSE) were observed with values of 0.521 and 0.693, respectively. Both MAE and RMSE are common quantitative statistics applied to measure the predictive capacity of the model, and the matrices range from zero to infinite number. They are negatively-oriented figures meaning that lower values are better (Safavi and Malek Ahmadi, 2015, Rajaee et al., 2020). A mean absolute percentage error (MAPE) of 0.6 % was recorded, signifying that the proposed neural network is highly accurate (refer to scale ratings in Table 5.13). MAPE expresses accuracy as a percentage and zero explains a perfect fit; however, MAPE has no upper limit, but models with MAPE values beyond 50.0 % are considered inaccurate (Rajaee et al., 2020). In light of these performance indicators, the proposed artificial neural network is regarded as robust and computationally stable.

5.4.3 Sensitivity analysis

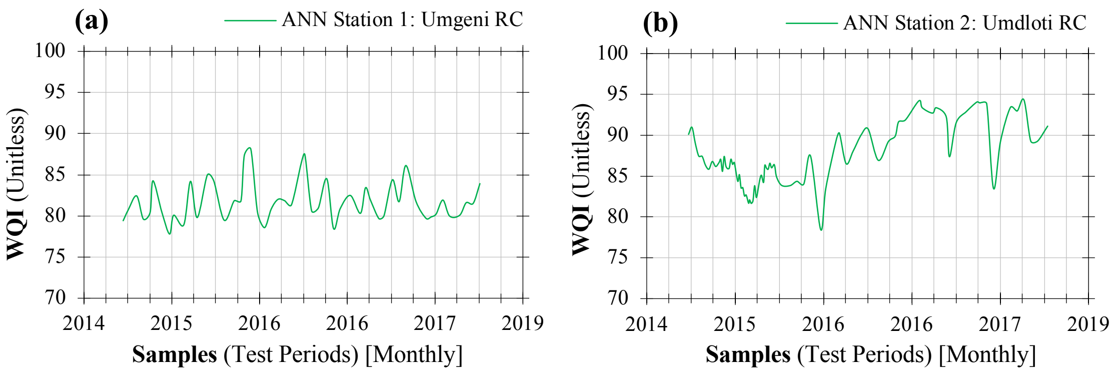
Sensitivity analysis is viewed as a powerful method for evaluating essential factors that contribute to output and comprehending the interrelationship among variables in multivariable datasets (Guo et al., 2011, Huo et al., 2013). Sensitivity analysis allows to properly apportion the uncertainty in outputs to the variability of the input parameters over their entire range of interest. SA determines the most contributing input variable towards a particular output behaviour.

Global sensitivity analysis involves input factors being varied simultaneously, whilst sensitivity is assessed over the whole range of each input factor. The process quantifies the impact of network input and their interactions with respect to the network output (Zhou et al., 2008). The method is more appropriate for a non-linear input-output relationship, even more importantly, the technique is more realistic considering applicability since the process enables all input parameters to be performed concurrently without difficulties (Zhou et al., 2008, Huo et al., 2013). There are various global sensitivity methods which include Fourier amplitude sensitivity test (FAST), Monte-Carlo-based regression-correlation indices and Sobol's sensitivity estimates. In this case, the study employed Fourier amplitude sensitivity test (FAST), and the SA results indicate that the proposed artificial neural network is computationally robust and scientifically stable.

The novel pointwise sensitivity analysis has been employed to investigate further the local patterns and sensitivity at individual data points; which outlines links between a focal point and neighbours (Guo et al., 2011). To better understand the usefulness of pointwise analysis, the method assisted to outline how water quality index scores are influenced by a particular input variable, either positively or negatively. Furthermore, the analysis describes the variables with a more significant effect on water quality indexing (Guo et al., 2011). The rationale is that; given the correlation between WQI scores (y-variables) and water quality parameters (x_1, x_2, …, x_3), sensitivity analysis explains the change rate of y-variables as x_i fluctuate (Guo et al., 2011). Each x-variable is adjusted using an outlier factor to establish anomalous local patterns that cannot conform with the global pattern. Pointwise sensitivity analysis authenticated the robust and analytical aptitude of the suggested ANN model.

5.4.4 Evaluation of spatial and temporal trends using ANN

Water quality data from Umgeni Water Board (UWB) have been assessed to substantiate spatial and temporal trends between six sampling sites. The spatiotemporal water quality variations are presented in Figure 5.11, 5.13 and 5.14.



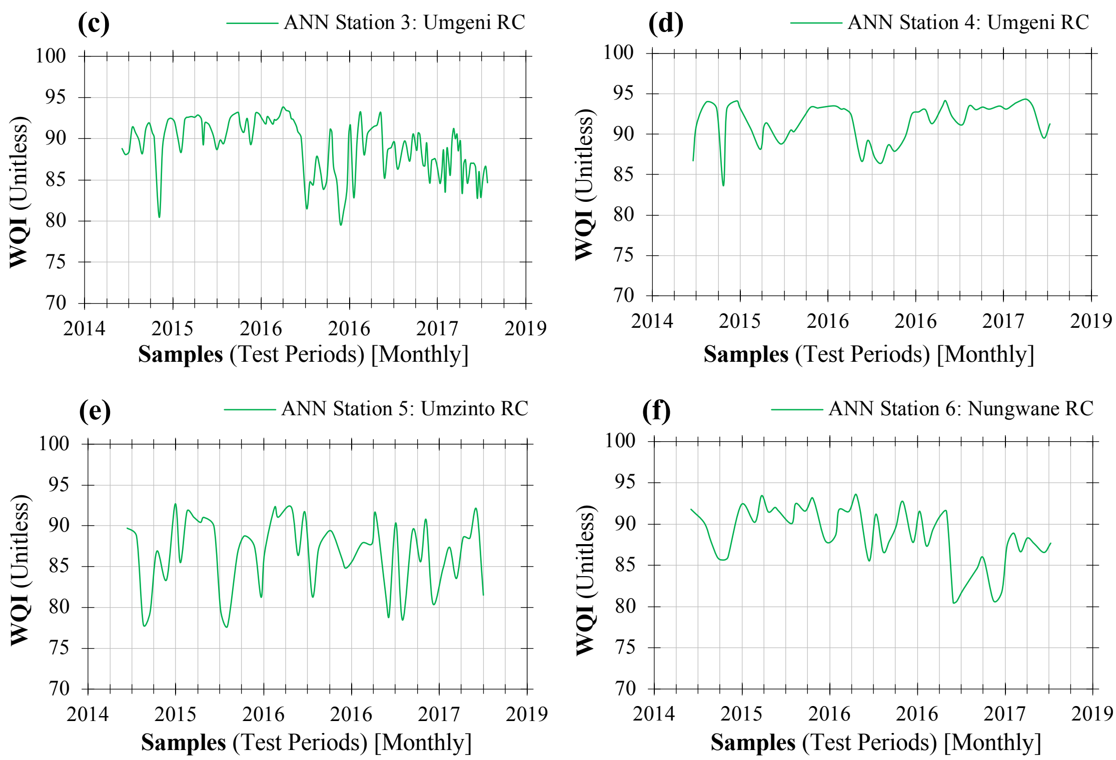
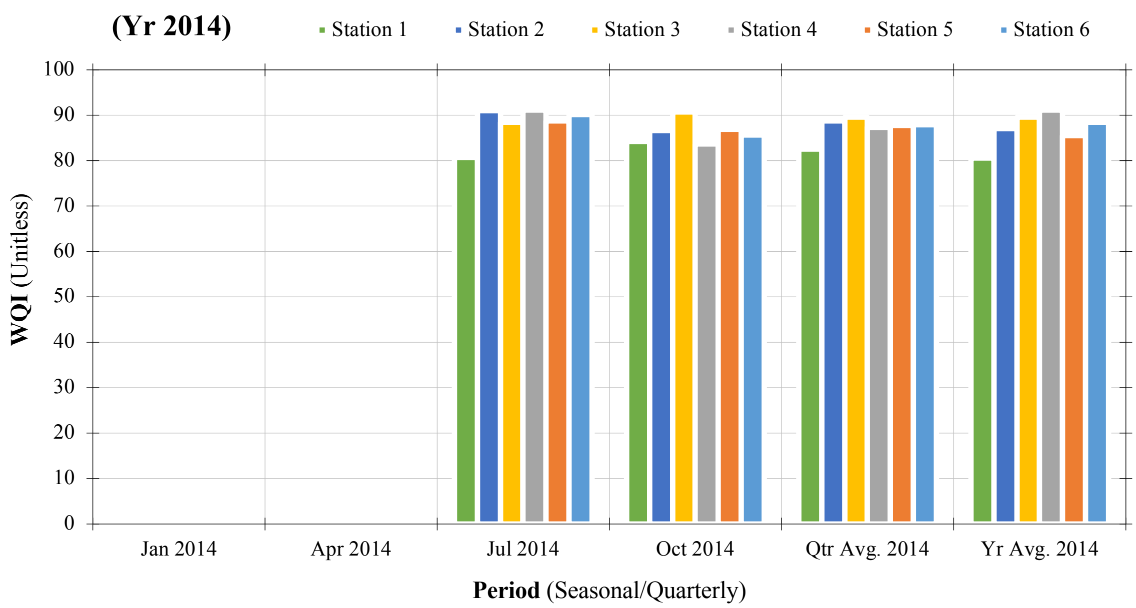
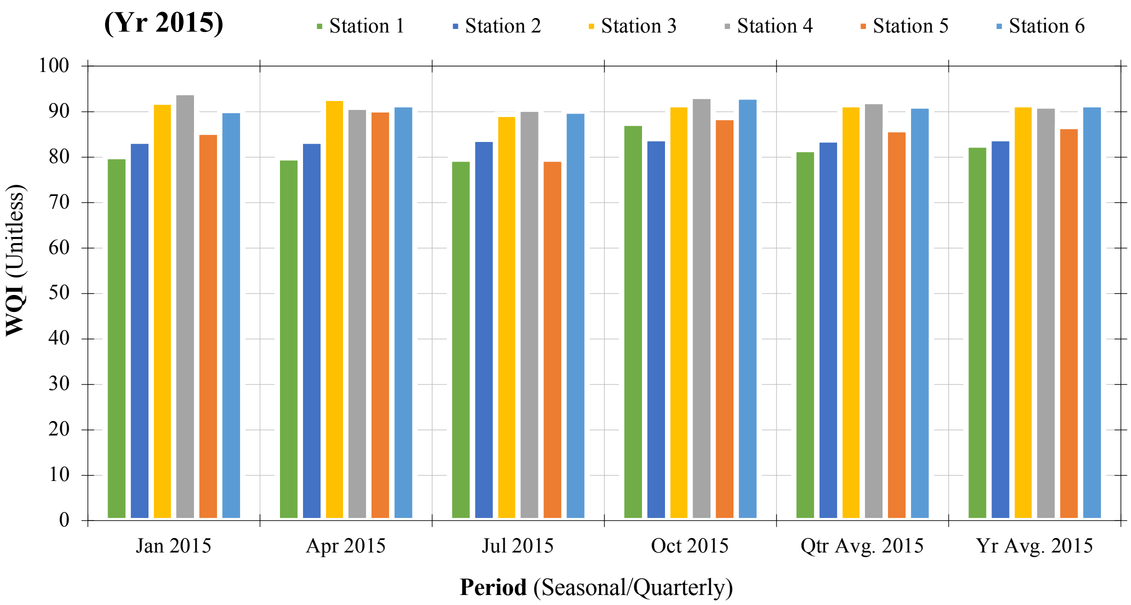


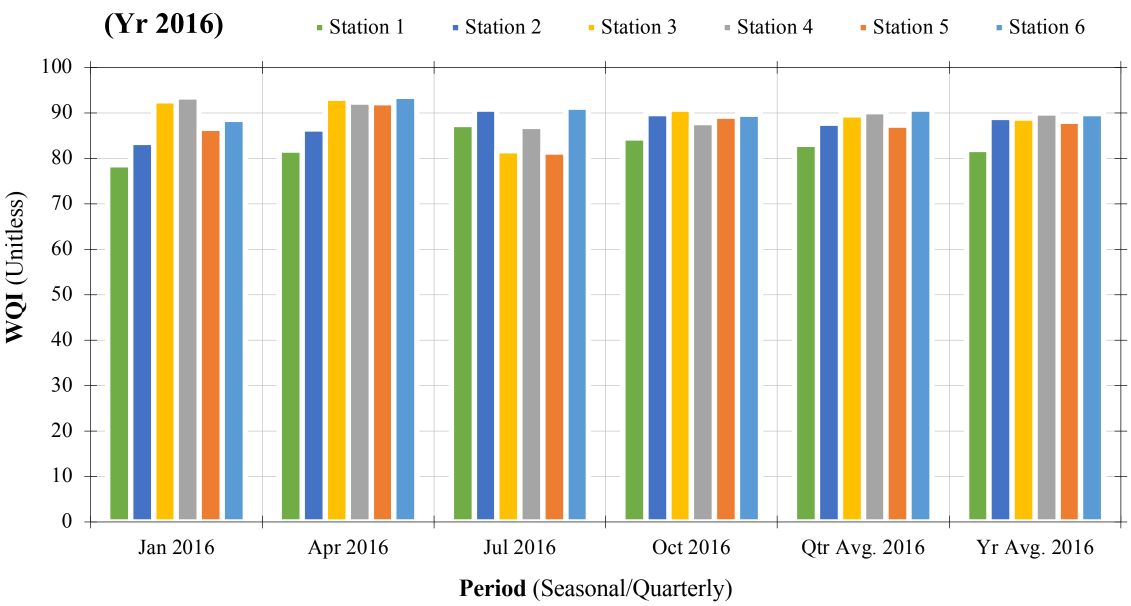
Figure 5.13: WQI results calculated using the ANN model for Umgeni water quality data from 2014 to 2018 (**a**) Umgeni Basin for Henley Dams, (**b**) Umdloti Basin for Hazelmere Dam, (**c**) Umgeni Basin for Inanda Dams, (**d**) Umgeni Basin for Midmar Dam, (**e**) Umzinto/Umuziwezinto Basin for Umzinto Dam, and (**f**) Nungwane Basin for Nungwane Dam

Source: ANN results from TIBCO Statistica Automated Neural Networks Software, TIBCO Software Inc. (2020).

Notes: The water quality data is from six sampling stations observed monthly for a period extending to four years ranging from June 2014 until July 2018




(Yr 2015)
Station 1
Station 2
Station 3
Station 4
Station 5
Station 6
WQI (Unitless)
100
90
80
70
60
50
40
30
20
10
0
Jan 2015
Apr 2015
Jul 2015
Oct 2015
Qtr Avg. 2015
Yr Avg. 2015
Period (Seasonal/Quarterly)


(Yr 2016)
Station 1
Station 2
Station 3
Station 4
Station 5
Station 6
WQI (Unitless)
100
90
80
70
60
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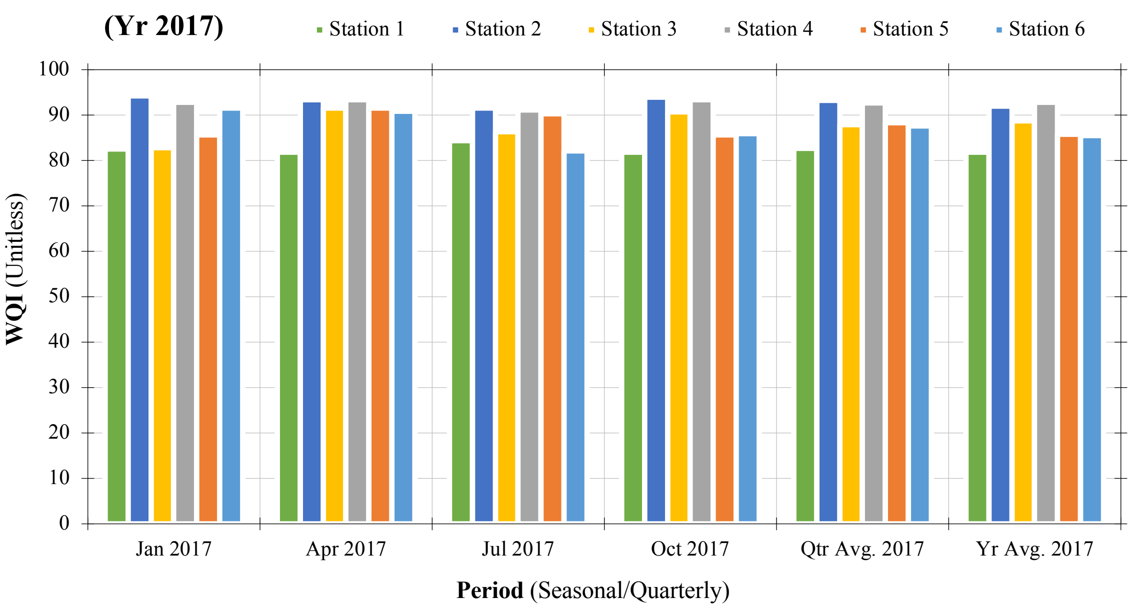
Jan 2016
Apr 2016
Jul 2016
Oct 2016
Qtr Avg. 2016
Yr Avg. 2016
Period (Seasonal/Quarterly)


(Yr 2017)
Station 1
Station 2
Station 3
Station 4
Station 5
Station 6
WQI (Unitless)
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Jan 2017
Apr 2017
Jul 2017
Oct 2017
Qtr Avg. 2017
Yr Avg. 2017
Period (Seasonal/Quarterly)

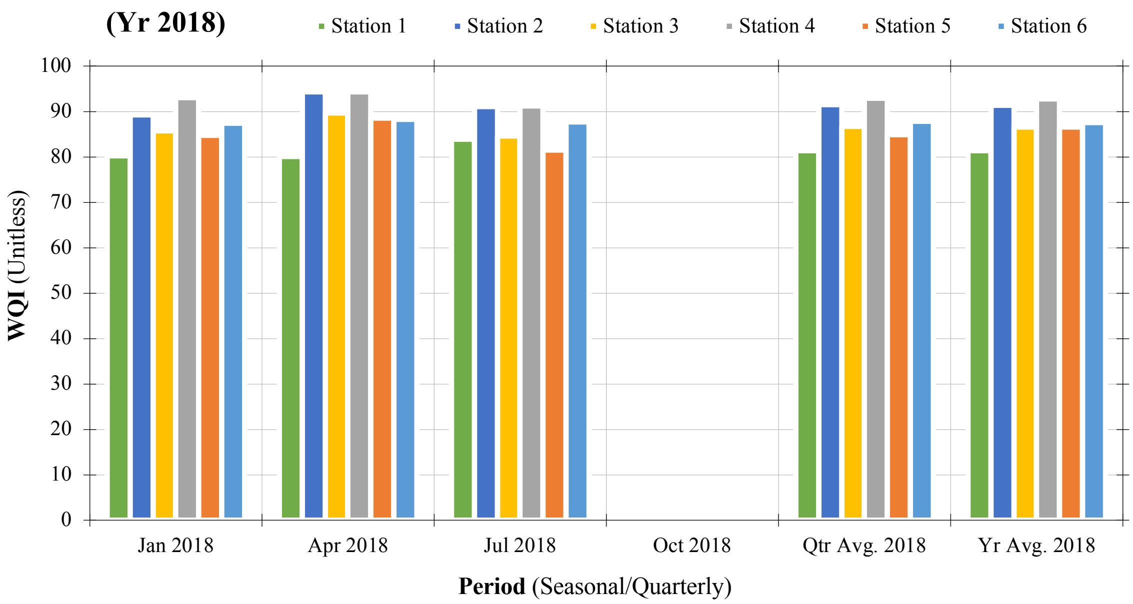

Figure 5.14: Seasonal water quality variability for Umgeni water quality data gathered monthly for over four years starting from 2014 until 2018

Source: ANN results from TIBCO Statistica Automated Neural Networks Software, TIBCO Software Inc. (2020).

Notes: Quarter average is denoted by "Qtr Avg." The yearly average is represented as "Yr Avg." Quartly average figures are seasonal mean index scores considering WQI scores for January, April, July and October only. The yearly average figures are mean index values considering the WQI ratings for the entire year.

Using the index scores generated by the newly developed artificial neural network model, the results suggest that water quality with the four river catchments can be classified as class 2 – acceptable water quality. The region has the lowest index score of 77.713 (class 2) recorded at sampling station 5 for Umzinto Dam within Umzinto/Umuziwezinto River catchment area. The lowest index score resulted from the high concentration level of NH_3, Chl-a, Mn and turbidity with observed values of 0.99 µg/ℓ 8.29 mg/ℓ, 0.53 mg/ℓ and 7.10 NTU, respectively. Station 4 located at Midmar Dam with Umgeni River catchment have the highest WQI rating of 94.337 (class 2) during April 2018 (Figure 5.13 and 5.14).

Two stations situated upstream of the drainage region recorded the minimal variations in WQI values, with station 1 having WQI range of 77.798 – 88.109, and station 4 ranging from 83.616 to 94.337. sampling stations 2, 3, 5 and 6 are located downstream of the catchment towards the Indian Ocean. From the assessment, WQI ratings highlighted that river systems are affected more with the increase in socio-economic activities along the river's watercourse. The situation is more evident on areas surrounding the Durban-Pietermaritzburg with stations 2 and 3 having significant water quality variations ranging from 78.452 – 94.316 and 79.637 – 93.830, respectively. Chl-a, NO_3 and turbidity are the main polluting agents influencing water quality scores for Umgeni

Water Board with maximum concentrations corresponding to 92.22 µg/ℓ, 9.58 mg/ℓ and 367.00 NTU, respectively.

Excessive levels of NO_3 are recorded during the summer seasons, with anthropogenic activities being the possible source of contamination, especially considering the socio-economic developments around the sampling stations. As common and naturally forming ion, NO_3 is regarded as the most notable pollutant in river systems. When viewed in isolation, nitrate is as a low-toxic compound, but when transformed to nitrite (NO_2), it becomes increasingly toxic to both human health and aqua life. Hence, the need for routine water quality monitoring, thereby evaluating water quality trends over time and space. Similar to NO_3, high levels of turbidity are also evident during the summer seasons owing to a diverse range of sources. These indicate algal blooms, wastewater and industrial effluent, decomposition of organic matter, soil erosion, reservoir drawdown flashing, among others combined with NO_3, turbidity contributes heavily towards the deterioration of water quality within the six sampling stations. Chl-a concentrations are influenced by eutrophication resulting from soluble nutrients emanating from phosphorus and nitrogen compounds. These enriching nutrients usually originate from human-based operations which includes, but not limited to wastewater discharge and fertiliser runoff.

Evaluating water quality trends for various drainage basins supports the objective of establishing water quality monitoring tools with broad application. Of significant importance, the artificial neural network model could simulate WQI scores generated using the universal water quality index model (Figure 5.11). The correlation between the UWQI values and ANN model scores is exceptional with similar prediction patterns. Such accuracy upholds the preparedness of the neural network to evaluate water quality and identify water quality trends within the South African river basins.

5.5 Surrogate water quality index model (Proxy WQI)

Often, water quality index (WQI) models are heavily parameterised, requiring an extensive amount of data, thereby limiting their application due to input parameter demand. To govern such tendencies, a surrogate WQI is proposed. A surrogate model is an abridged version of an outright WQI, thereto function with limited input data. It represents a quick and easy method of translating complex water quality data into simple, but yet testable measure. Though less-detailed, proxy models are equally competent and fundamentally identical to the original unbridged models, but with reduced computational precision (Razavi et al., 2012). Although having less accurate arithmetic aptitude, the advantages of surrogate models outbalance such unfavourable attributes and compensate the numerical divergence.

The proposed proxy WQI has been established to be rationally implemented in lieu of the high-fidelity model, referred here as the universal water quality index (UWQI). The primary objective of developing and applying the suggested surrogate WQI is to make better use of typically restricted water resource monitoring budgets (Razavi et al., 2012). Therefore, the proposed surrogate WQI aims to provide a more straightforward and cost-effective model that simulates the output of a complex high-fidelity model (Asher et al., 2015).

Undoubtedly, the success of the surrogate WQI and its advantages will ultimately intensify regular water resource monitoring in South Africa. In the same context, thirteen variables applicable to UWQI have been subjected to multivariate statistical analysis to select the most meaningful proxy variables for the surrogate WQI. Subsequently, chlorophyll-a, electrical conductivity and pondus Hydrogenium and turbidity are the final four proxy parameters. Minimising the input parameters can significantly reduce time, effort and cost required to evaluate water resources, thereby making the process more feasible and economically viable (Bhosekar and Ierapetritou, 2018, Tripathi and Singal, 2019b, Jahin et al., 2020).

In this study, the terms "surrogate model," "proxy model" and "low-fidelity model" bear the same meaning and are used interchangeably.

5.5.1 A rationale for developing the proxy model (multiple linear regression model)

Consider a range of data comprising of n statistical units (observations) of the response variable y (dependent variable) and p-*vector* of regressors x (independent explanatory variable). Then, their mathematical relationship is designated as a linear regression model in the form (Jurečková, 2011, Vatanpour et al., 2020, Banda and Kumarasamy, 2020b):

$$y = b_0 + b_1x_1 + b_2x_2 + ... + b_px_p + \varepsilon \qquad \text{Eq. 5.30}$$

The observations are assumed to be the result of random deviations from an underlying relationship between the dependent variable (y) and the independent variable (x). With regards to observed data, the linear function is defined as (Jurečková, 2011, Vatanpour et al., 2020, Banda and Kumarasamy, 2020b):

$$y_i = b_0 + b_1x_{i1} + b_2x_{i2} + ... + b_px_{ip} + \varepsilon_i \qquad \text{Eq. 5.31}$$

Where $i = 1, 2, \ldots, n$ and variables ε_i symbolise unobservable regression model errors. Which are presumed to be independent and identically distributed random variables; with a distribution function F and density f. Of which, the density is unknown and expected to be symmetric at zero

(0). The corresponding coefficients b_1 to b_p and intercept term b_0, are unknown values calculated based on the dependent variable $y = (y_1, y_2, \ldots, y_n)$ and independent variable $x = (x_{i1}, x_{i2}, \ldots, x_{ip})$. Besides the conventional least-squares method, various statistical estimators of model coefficient (b) exist and they are documented in the existing literature. Some of the methods are distributionally robust (less sensitive to deviations from the assumed distribution factors), whilst others are resistant to the leverage points in the design matrix and have a high breakdown point (Jurečková, 2011, Banda and Kumarasamy, 2020b).

Following the above rationale, linear regression was considered in the development of the proxy water quality index model, and the results are documented in the following subsections.

5.5.2 Parameter selection for the surrogate WQI

A combination of two methods has been adopted in the selection of the most suitable explanatory variables for the suggested proxy model. The methods include, (1) the Rand Corporation's Delphi Technique (Delphi method) and, (2) multivariate statistical analysis. Figure 5.15 illustrates the two-stage screening process established to select significant water quality parameters.

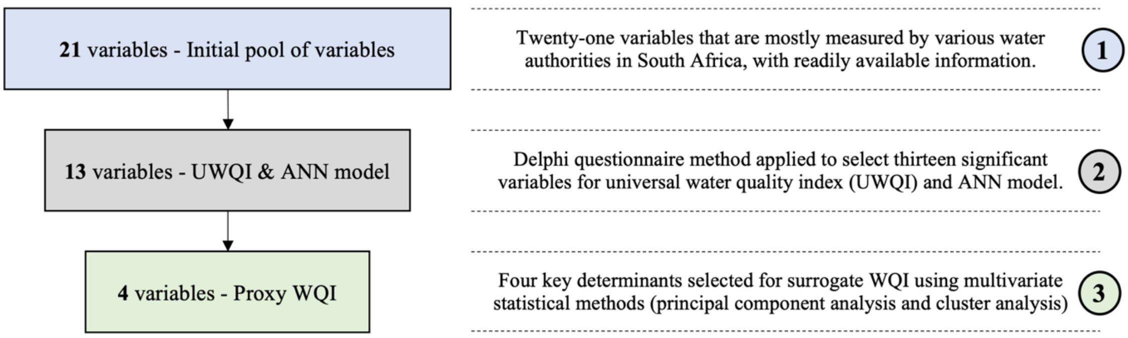

Figure 5.15: Flow diagram illustrating the two-stage screening process employed for selecting the significant water quality parameters

Source: Authors diagram (Banda and Kumarasamy, 2020b)

Notes: Statistical analysis was performed using water quality dataset from Umgeni Water Board (UWB) monitored monthly from 2014 to 2018.

The Delphi method has been employed to abridge the list of parameters from twenty-one to thirteen variables which apply to the universal water quality index (UWQI). Furthermore, statistical analysis assisted in reducing the parameters to four proxy variables applicable to the surrogate water quality index (WQI). Principal component analysis (PCA) have been performed for pattern recognition and outlining the framework of the project data. At the same time, hierarchical cluster analysis (HCA) helped to establish the degree of similarity among water quality parameters. Accordingly, chlorophyll-a (Chl-a), electrical conductivity (EC), turbidity

(Turb) and pondus Hydrogenium (pH) are the final four proxy parameters considered for the surrogate WQI. Additional information relating to the selection of these input variables is discussed and presented in the succeeding sections.

5.5.3 Multivariate statistical analysis

5.5.3.1 Principal component analysis (PCA)

Considering that water quality is generally described using multiple physicochemical and biological variables; principal component analysis (PCA) can ideally transform complex multivariate datasets to a minimal and manageable number of factors without loss of information (Jolliffe, 2011, Awomeso et al., 2020). More importantly, PCA preserves the structure and pattern of the original dataset to the maximum extent possible (Tripathi and Singal, 2019b, Jahin et al., 2020). PCA is an accurate and extensive method for parameter reduction; which is significant and can drastically lower assessment cost, time and effort, thereby promoting routine monitoring. The rationale behind PCA is centred on decreasing dimensions of a multivariate dataset through summarising information dispersed in several dimensions into a reduced number of dimensions that are not correlated (Kim et al., 2019a, Nnorom et al., 2019, Tripathi and Singal, 2019b). The technique eliminates collinearity amongst explanatory variables, discard redundant or significantly correlated variables and develop new uncorrelated variables known as principal components (PCs) (Paca et al., 2019, Njuguna et al., 2020). The application of statistical techniques in the development of water quality indices (WQIs) lessens biasness and makes them more objective in nature (Tripathi and Singal, 2019b).

The first step in performing PCA involves delineating the number of PCs that can adequately explain the structure and pattern of a given dataset. This process is accomplished by the use of (a) scree-plot, (b) real data eigenvalues, and (c) randomly generated eigenvalues. It should be noted that, although it is common practice to disregard low-variance PCs, sometimes they can be useful in their own right; for instance, they can assist in identifying outliers and enhance quality control (Jolliffe, 2011). Ideally for PCA to draw purposeful and reliable conclusions, the standard advice is to retain factors characterised by the following (Tripathi and Singal, 2019a):

(i) Associated eigenvalues that are greater than one (> 1.000);
(ii) Initial eigenvalues percentage of variance of greater than ten percent (> 10.0 %); and
(iii) Cumulative percentage of variance of greater than sixty percent (> 60.0 %).

However, these are just suggestive figures and should be regarded as indicative of the ideal situation. Notably, different opinions exist in the existing literature, especially on the cumulative percentage of variance contribution. Tripathi and Singal (2019a) suggest a minimum of 60.0 %, whereas Jolliffe (2011), and Gradilla-Hernández et al. (2020) propose a range between 70.0 % and 90.0 % with an acknowledgement that the value can be higher or lower depending on the context of the dataset.

A scree-plot developed using real data eigenvalues assisted in identifying the number of principal components to be extracted. Corresponding to the scree-plot sagging point; principal components with eigenvalues greater than one (latent-root-one) were considered significant to explain the underlying structure of the dataset (Horn, 1965, Mitra et al., 2018, Rezaei et al., 2019, Tripathi and Singal, 2019a, Jahin et al., 2020, Patil et al., 2020). Complementary, Parallels Analysis Engine (PAE) aided in confirming the number of factors retained. Using research data, PAE computed eigenvalues from randomly generated correlation matrices, which were used to intercept the cut-off point on the scree-plot diagram. Both PCA and PAE eigenvalues were presented graphically as two different plots, and their intercept point established the number of factors retained during multivariate statistical analysis (Horn, 1965, Patil et al., 2007). All the principal components above the PAE graph were considered; in this case, the first five factors were deemed statistically important. The results of this procedure are graphically displayed in Figure 5.16.

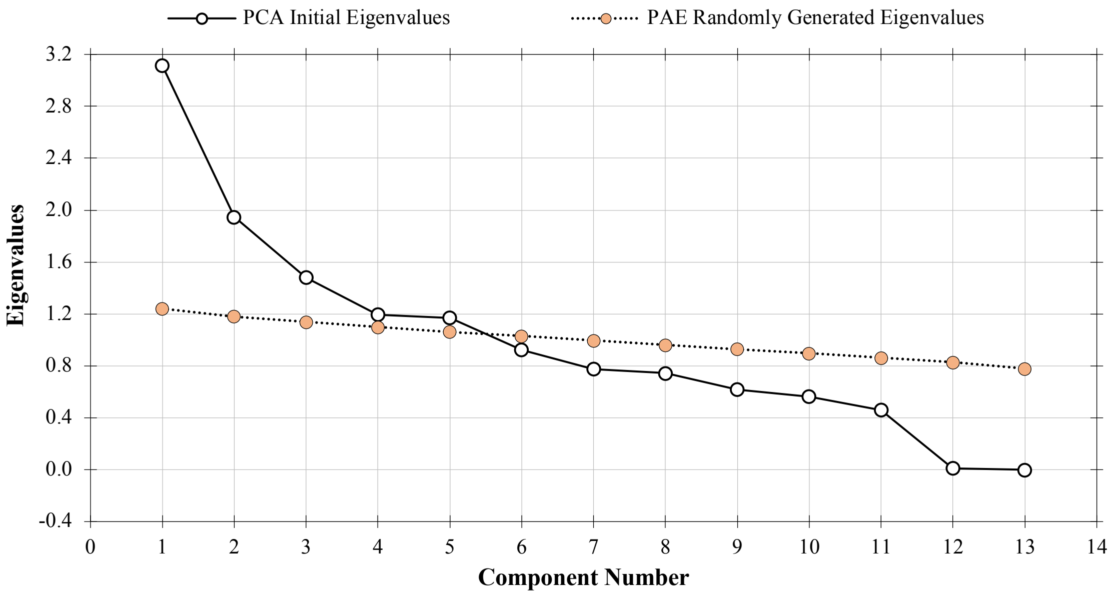

Figure 5.16: Determination of the number of Principal Components (PCs) to be extracted using eigenvalues from Principal Component Analysis (PCA) and randomly generated eigenvalues from Parallel Analysis Engine (PAE)

Source: Authors' diagram illustrating PCA results from IBM SPSS Statistics (SPSS Inc., 2016) and Parallel Analysis Engine (Patil et al., 2007).

Notes: Randomly generated correlation matrix was established using PEA and PCA correlation matrix was set using research dataset from Umgeni Water Board (UWB).

In order to obtain meaningful and more accurate results, the dataset subjected to Principal Component Analysis (PCA) should have a minimum of 150 - 300 test cases (Sutadian et al., 2017, Tripathi and Singal, 2019a, 2019b, Jahin et al., 2020). Accordingly, the current study used 416 test cases monitored from six sampling stations observed monthly for four years (refer to Table 5.1). The case study surpasses the recommended threshold, thus satisfying the stated criterion. The study performed Kaiser-Meyer-Olkin (KMO) and Bartlett's test of sphericity to authenticate the suitability of the dataset to effectively handle principal component analysis (PCA) and factor analysis (FA). KMO is the measure of sampling adequacy that signifies the degree of variance caused by underlying principal components (PCs) (Mitra et al., 2018). Generally, KMO values below 0.500 are undesirable, whereas values ranging from 0.500 to 0.700 are considered sufficient, and higher values (above 0.700) are outstanding (Nnorom et al., 2019, Tripathi and Singal, 2019b, Ustaoğlu et al., 2019, Patil et al., 2020). The current study achieved KMO value of 0.510, which is satisfactory.

Bartlett's test examines the possibility of the correlation matrix being an identity matrix. If such a case exists; Bartlett's test of sphericity assumes that all variables are unrelated and dimensionality reduction is not feasible, thus making PCA and FA inapplicable. Bartlett's test scores less than 0.050 are favourable and suggest that significant relationships exist among variables (Tripathi and Singal, 2019b). In the current case, Bartlett's significance level is 0.000, thus confirming the appropriateness to perform principal component analysis and factor analysis. Table 5.14 presents the correlation matrix, KMO and Bartlett's test results.

Table 5.14: Correlation matrix, KMO and Bartlett's test results for the thirteen physicochemical variables shortlisted for multivariate statistical analysis

	NH_3	Ca	Cl	Chl-a	EC	F	$CaCO_3$	Mg	Mn	NO_3	pH	SO_4	Turb
NH_3	1.000												
Ca	0.077	1.000											
Cl	0.092	-0.012	1.000										
Chl-a	-0.090	-0.061	-0.178	1.000									
EC	**0.359**	0.186	0.153	-0.078	1.000								
F	0.021	-0.019	-0.006	-0.042	0.057	1.000							
$CaCO_3$	0.066	**0.998**	-0.005	-0.071	0.170	-0.028	1.000						
Mg	0.050	**0.987**	0.003	-0.086	0.149	-0.041	**0.995**	1.000					
Mn	0.196	-0.054	0.031	0.024	0.201	-0.022	-0.046	-0.033	1.000				
NO_3	**0.399**	-0.020	0.223	-0.125	0.256	0.012	-0.023	-0.028	-0.066	1.000			
pH	0.006	0.032	-0.194	-0.018	0.070	0.034	0.024	0.014	-0.170	0.012	1.000		
SO_4	0.115	0.138	0.091	-0.078	0.126	0.028	0.128	0.115	-0.226	0.215	0.066	1.000	
Turb	0.173	0.113	0.191	-0.090	0.183	0.272	0.109	0.101	0.125	-0.006	-0.070	-0.134	1.000
Kaiser-Meyer-Olkin (KMO) measure of sampling adequacy							0.510						
Bartlett's Test of Sphericity significance							0.000						

Source: UWB (2014 to 2018), statistical analysis results from IBM SPSS Statistics (SPSS Inc., 2016).

Notes: Kaiser-Meyer-Olkin (KMO) measure of sampling adequacy is 0.510, which is satisfactory, and Bartlett's Test of Sphericity is 0.000, thus confirming the appropriateness of the dataset. Parameters are abbreviated as follows: ammonia (NH_3), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), electrical conductivity (EC), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), pondus Hydrogenium (pH), sulphate (SO_4) and turbidity (Turb).

Correlation matrix assisted in evaluating inter-relationships between the thirteen water quality variables shortlisted for statistical analysis. Similar to Wang (2018), Nnorom et al. (2019), Ustaoğlu et al. (2019), and Patil et al. (2020), the classification adopted is defined as follows: (a) $r < 0.300$, considered of no relevance; (b) $0.300 \leq r < 0.500$, less relevance; (c) $0.500 \leq r < 0.800$, median relevance; and (d) $r \geq 0.800$, high relevance. Considering such groupings, the analysis indicates that Mg is highly related to Ca and $CaCO_3$. Though with less relevance, the results suggest that NH_3 is correlated with EC and NO_3.

As a common practice, rotation (Oblimin with Kaiser Normalisation) was executed to ensure that variables with higher loading values are not considered on the same factor. Rotation transforms the factorial axes into a structure where each of the retained factors is preferably loaded with only one variable. Furthermore, primarily where few principal components (PCs) exist, rotation restricts variables to overlay factor loadings on more than one principal component (PC) (Tripathi and Singal, 2019a). Post rotation, the leading parameters with the highest loadings are grouped as intermediate composites and assigned weights. The weights are then aggregated, and their compound effect is proportional to the percentage of variance explained by a particular component (Tripathi and Singal, 2019a).

Considering that water quality parameters have different units, standardisation (z-scores) harmonised the dataset to a common scale with zero mean and unit standard deviation (Jolliffe, 2011, Paca et al., 2019, Jahin et al., 2020, Liew et al., 2020, Njuguna et al., 2020, Tripathi and Singal, 2019b). Principal component analysis (PCA) helped in reducing the dimensionality of the dataset and summarised the variables to five important components. The first five principal components (PCs) retained accounted for 68.5 % of the total variance with eigenvalues greater than one (> 1.000). For ease reference and factor interpretation, factor loadings are classified as "weak," "moderate," and "strong" corresponding to absolute loading values of 0.300 to 0.500, 0.500 to 0.800 and > 0.800 respectively (Nnorom et al., 2019, Rezaei et al., 2019, Ustaoğlu et al., 2019).

Having strong positive loadings of 0.979, 0.972 and 0.979 for Ca, Mg and $CaCO_3$ respectively, the first component (PC 1) accounts for 23.9 % of the total variance with eigenvalue of 3.118. The second PC features moderate loadings of -0.681, 0.624 and 0.522 corresponding to NH_3, NO_3 and EC with eigenvalue of 1.948 and variance of approximately 15.0 %. Moderate factor loadings of SO_4 (-0.654), Mn (0.624), and Turb (0.522) dominate the third component (PC 3) which represents 11.4 % of the original variability with eigenvalue of 1.482. Signifying 9.2 % variance and eigenvalue of 1.195, the fourth factor (PC 4) contains fluoride as the most significant variable with a strong positive factor loading of 0.763. Lastly, the fifth component (PC 5) accounts for 9.0 % of the total variance with eigenvalue of 1.171. Two parameters dominate this component, thus Cl and pH, with moderate factor loadings of -0.629 and 0.610 respectively. The five extracted principal components (PCs) are presented in Table 5.15.

Table 5.15: Principal component analysis vectors of coefficients for the first five Principal Components (PCs) with eigenvalues greater than one (> 1.000) for Umgeni water quality data (2014 to 2018)

Variable symbol and name		**Principal components (PCs)[a]**					**Communalities**
		PC 1	PC 2	PC 3	PC 4	PC 5	
Ca	Calcium	**0.979**	-0.175	0.035	-0.019	-0.003	0.991
$CaCO_3$	Hardness	**0.979**	-0.184	0.043	-0.027	-0.020	0.995
Mg	Magnesium	**0.972**	-0.194	0.053	-0.035	-0.043	0.987
NH_3	Ammonia	0.191	**0.681**	-0.042	-0.223	0.308	0.647
NO_3	Nitrate	0.080	**0.636**	-0.428	-0.124	-0.012	0.609
EC	Electrical Conductivity	0.313	**0.593**	0.029	-0.120	0.321	0.569
SO_4	Sulphate	0.215	0.182	**-0.654**	0.069	-0.105	0.523
Mn	Manganese	-0.033	0.277	**0.624**	-0.408	0.195	0.671
Turb	Turbidity	0.188	0.372	**0.522**	0.472	0.008	0.669
F	Fluoride	0.001	0.188	0.171	**0.763**	0.188	0.682
Cl	Chloride	0.067	0.492	0.039	0.042	**-0.629**	0.646
pH	pondus Hydrogenium	0.042	-0.110	-0.395	0.261	**0.610**	0.610
Chl-a	Chlorophyll-a	-0.148	-0.296	0.118	-0.260	0.345	0.310
Eigenvalues (> 1.0)		3.118	1.948	1.482	1.195	1.171	
Percentage of variance (%)		23.949	14.986	11.397	9.192	9.008	
Cumulative variance (%)		23.949	38.935	50.332	59.525	68.533	

Source: PCA results from IBM SPSS Statistics (SPSS Inc., 2016)

Notes: [a] five components extracted using Principal Component Analysis (PCA) as the extraction method. Rotation method: Oblimin with Kaiser Normalization and rotation converged in seven iterations. The statistical analysis was performed using Umgeni water quality data for four years, from 2014 to 2018.

Principal component analysis (PCA) is the most used tool in exploratory data analysis. It provides an accurate interpretation of multi-constituent measurements which enables a better understanding of water quality composition (Jolliffe, 2011, Rezaei et al., 2019, Gradilla-Hernández et al., 2020, Tripathi and Singal, 2019b). PCA is a standard primary method used for pattern recognition, and the technique is regarded as the simplest of the true eigenvector-based multivariate analyses. One of the most influential and informative graphical illustrations of multivariate analysis is through the use of biplots. They optimally represent relationships between variables and principal components. Biplots suggests groups of highly correlated variables using an approximation of the original multidimensional space (Gradilla-Hernández et al., 2020, Patil et al., 2020). Biplots are illustrated in either two or three-dimensional subspace. On that basis, the statistical results of the current study are further explained using 2D and 3D biplots in Figure 5.18 and 5.17 respectively.

Figure 5.17: 2D biplot of the first five retained principal components

Source: Authors' diagram showing PCA results from IBM SPSS Statistics (SPSS Inc., 2016).

Notes: The five principal components are denoted as PC 1, PC 2, PC 3, PC 4 and PC 5. Parameters are abbreviated as follows: ammonia (NH_3), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), electrical conductivity (EC), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), pondus Hydrogenium (pH), sulphate (SO_4) and turbidity (Turb).

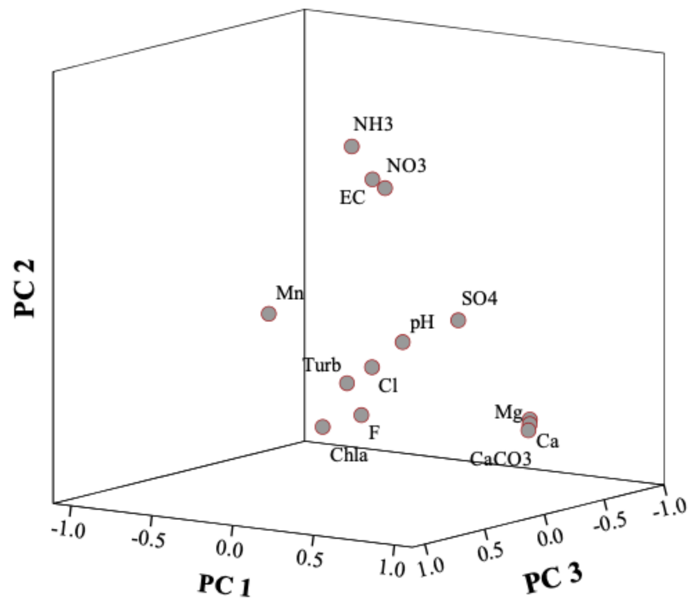

Figure 5.18: 3D biplot illustrating the relationship between highly correlated variables and the first three principal components

Source: Authors' diagram representing PCA results from IBM SPSS Statistics (SPSS Inc., 2016).

Notes: PC 1, PC 2, and PC 3 are principal components one, two and three, respectively. Parameters are abbreviated as follows: ammonia (NH_3), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), electrical conductivity (EC), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), pondus Hydrogenium (pH), sulphate (SO_4) and turbidity (Turb).

5.5.3.2 Hierarchical cluster analysis (HCA)

Hierarchical cluster analysis (HCA) essentially outlined the hierarchical relationships between variables and assisted in arranging thirteen variables into corresponding clusters. Various hierarchical clustering methods exist, but in this doctoral study, centroid based clustering algorithms and Ward's hierarchical clustering methods were examined. Eventually, Ward's technique was preferred amongst the two approaches. Ward's procedure generates approximately identical grouped clusters, unlike the other techniques were groupings are not equally proportional (Gradilla-Hernández et al., 2020).

Cluster analysis uses a distance matrix, and the model intervals were calculated using squared Euclidean distance technique (Gradilla-Hernández et al., 2020, Grzywna and Bronowicka-Mielniczuk, 2020). The method is regarded as the best option and most appropriate measure of distance in the physical world. Since variables are measured in different units, standardisation was performed to transform the observed measurements into a common scale. The tree diagram in Figure 5.19 represents the hierarchical clustering dendrogram for the thirteen explanatory variables considered in the analysis.

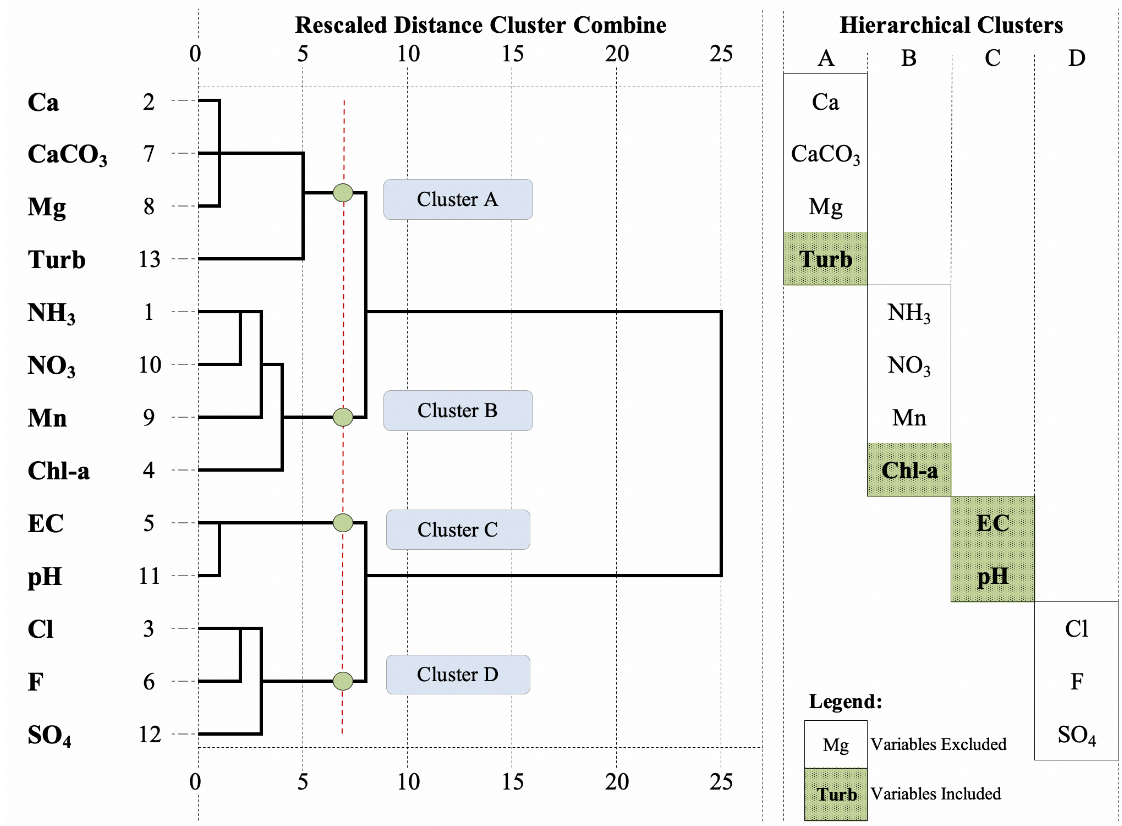

Figure 5.19: Hierarchical clustering dendrogram model for water quality variables using Ward's Linkage and Euclidean Distance method (Hierarchical Cluster Analysis)

Source: Authors' diagram showing HCA results from IBM SPSS Statistics (SPSS Inc., 2016).

Notes: Parameters are abbreviated as follows: ammonia (NH_3), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), electrical conductivity (EC), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), pondus Hydrogenium (pH), sulphate (SO_4) and turbidity (Turb).

As expected, extremely correlated variables are clustered together. For example, variables from principal component one are all clustered together under 'Hierarchical Cluster A.' Likewise, variables in principal component two are included in the second group of the hierarchical cluster dendrogram. The four clusters assisted in selecting the final four proxy variables incorporated in the surrogate index. At this stage, two sets of variables were considered as input parameters for the surrogate water quality index (WQI). The sets are grouped as (Banda and Kumarasamy, 2020b):

(i) Turb, Chl-a, EC and SO4 – referred to as proxy WQI(a); and
(ii) Turb, Chl-a, EC and pH – documented as proxy WQI(b).

Multivariate statistical analyses are highly objective, and their application in WQI development makes the process unbiased (Rezaei et al., 2019, Tripathi and Singal, 2019a, 2019b, Jahin et al., 2020). However, the process does not incorporate local conditions and or expert opinion.

Nevertheless, this study integrated professional judgement through the decision to include pH as input parameter, even though the variable is extremely correlated to EC. The individual importance of pH could not be neglected, hence the need to evaluate the performance of proxy WQI(b).

5.5.3.3 Multiple linear regression (MLR)

As previously stated, multiple linear regression (MLR) analysis was performed to establish regression coefficients of the two preliminary surrogate index models. Multiple regression is a statistical procedure that predicts the values of the dependent (response) variable from a multiple independent (exploratory) variables. More precisely, multiple regression analysis enables the estimation of y-value for specified values of $x_1, x_2, \ldots, x_k$ (Liew et al., 2020, Vatanpour et al., 2020). Durbin-Watson (DW) method was employed considering that water quality data is time-series; each case or test is time-based. DW technique uses the "line of best fit" technique to establish the linear regression equation. All the significant proxy variables were subjected to MLR to determine optimal linear fitting and generate the best regression coefficients used to establish an empirical mathematical equation applicable in evaluating the cleanness of surface water.

Following the results of the multiple linear regression (MLR), the subsequent mathematical coefficients in Table 5.16 have been suggested for the two preliminary proxy models.

Table 5.16: Multiple linear regression (MLR) coefficients for two preliminary surrogate index models, proxy WQI(a) and proxy WQI(b)

Multiple Linear Regression Coefficients[a]

Model	Var.	Unstd. Coeff.		Std. Coeff.	t	Sig.	95 % Confidence Interval for B		Correlations			Collinearity Statistics	
		B	Std. Error	Beta			Lower Bound	Upper Bound	Zero order	Partial	Part	Tol.	VIF
Proxy WQI(a)	Const.	87.047	0.474		183.490	0.000	86.116	87.979					
	Turb	-0.088	0.007	-0.452	-12.644	0.000	-0.101	-0.074	-0.424	-0.449	-0.433	0.918	1.090
	EC	-0.196	0.028	-0.336	-7.049	0.000	-0.251	-0.141	-0.173	-0.270	-0.241	0.516	1.940
	SO4	0.108	0.046	0.113	2.346	0.019	0.018	0.198	-0.028	0.093	0.080	0.510	1.961
	Chl-a	-0.042	0.021	-0.069	-1.978	0.048	-0.084	0.000	-0.152	-0.078	-0.068	0.963	1.038
Proxy WQI(b)	Const.	85.273	2.969		28.726	0.000	79.444	91.102					
	Chl-a	-0.042	0.022	-0.068	-1.921	0.055	-0.084	0.001	-0.152	-0.076	-0.066	0.946	1.057
	EC	-0.151	0.020	-0.259	-7.375	0.000	-0.191	-0.111	-0.173	-0.281	-0.254	0.959	1.043
	pH	0.224	0.378	0.021	0.593	0.553	-0.518	0.966	0.003	0.024	0.020	0.977	1.024
	Turb	-0.090	0.007	-0.462	-12.964	0.000	-0.103	-0.076	-0.424	-0.458	-0.446	0.930	1.075

Source: MLR results from IBM SPSS Statistics (SPSS Inc., 2016).

Notes: [a]Dependent variable: UWQI (universal water quality index value). Abbreviations are defined as follows: chlorophyll-a (Chl-a), electrical conductivity (EC), pondus Hydrogenium (pH), sulphate (SO_4), turbidity (Turb), constant (Const.), unstandardised (Unstd.), standardised (Std.), coefficient (Coeff.), significance (Sig.), tolerance (Tol.) and variance inflation factor (VIF).

Once the multiple regression equation is developed, the appropriateness and predictive ability of the model can be examined using values of known scenarios. Therefore, to validate the selection of four key proxy variables, the two preliminary surrogate water quality indices were subjected to a scenario-based analysis. The outcome of the procedure is documented in the following subsection.

5.5.4 Scenario-based analysis to determine the most appropriate surrogate WQI

Following the same procedure performed for UWQI; the two proxy WQIs have been examined to delineate their proficiency and ability to analyse water quality data. The eleven scenarios and parameter values used herein, are identical to those applied for UWQI, and the scenario-based analysis results for the surrogate WQIs are included as Table 5.17 and Figure 5.20. Both proxy WQIs have similar predictive patterns, which are consistent with the ideal graph. Furthermore, both models have corresponding water quality scores for base-case and best-case scenarios. Except for the worst-case scenario, the two indices have different results, with proxy WQI(b) being much closer to the ideal graph than proxy WQI(a). Ultimately, the analysis proved that; surrogate WQI(a) struggles to evaluate water quality samples with higher parameter concentrations. Against this background, proxy WQI(b) is then considered as the most appropriate surrogate index developed for this study.

Table 5.17: Comparison of the proxy water quality indices (a) and (b) using the scenario-based analysis to establish the functionality and predictive capacity of the models

Sample identity	Water quality index results from the scenario-based analysis					
	Ideal WQI results		Proxy WQI(a) results		Proxy WQI(b) results	
	Index score	WQI class	Index score	WQI class	Index score	WQI class
Max.	99.506	1.0	77.033	1	76.229	1
Avg.	37.571	4.0	46.743	4	43.515	4
1	0.000	5.0	23.088	5	6.389	5
2	0.177	5.0	24.698	5	11.499	5
3	0.827	5.0	26.287	4	16.479	5
4	6.250	5.0	26.152	4	26.458	4
5	20.254	5.0	39.387	4	39.895	4
6	25.027	4.0	42.694	4	43.252	4
7	30.269	4.0	46.001	4	46.609	4
8	56.250	3.0	59.286	3	60.097	3
9	80.976	2.0	77.033	2	75.837	2
10	93.749	2.0	76.261	2	75.917	2
11	99.506	1.0	73.285	3	76.229	2

Source: Ideal WQI values are generated using sub-index key points, and the other WQI results are extracts from the surrogate WQI(a) and WQI(b) suggested for the study (Banda and Kumarasamy, 2020b, 2020c).

Notes: Samples used for scenario analysis are predictive values ideal for establishing a specific set of results as demonstrated with the ideal WQI results columns. With increments of five scores, eleven probable scenarios have been considered to illustrate the model's ability to predict scores of all ranges, from class one (excellent) to class five (worse).

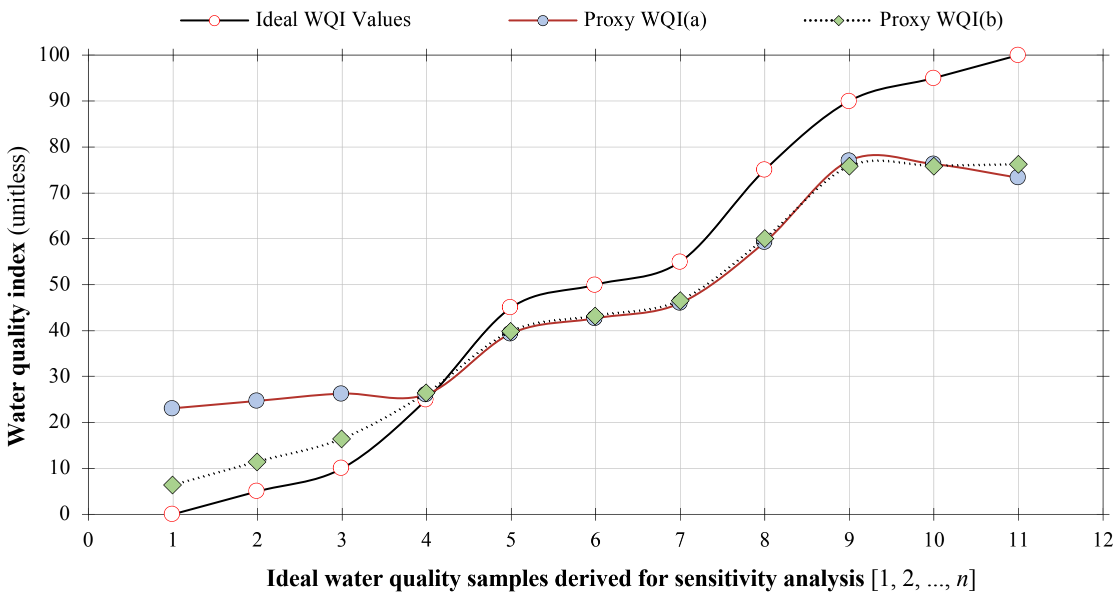

Figure 5.20: Plot diagram showing the results of the scenario-based analysis of the developed proxy water quality indices (a) and (b) against ideal water quality values derived from eleven probable scenarios

Source: Ideal WQI values are generated using sub-index key points, and the other WQI results are extracts from the surrogate WQI(a) and WQI(b) suggested for the study (Banda and Kumarasamy, 2020b, 2020c).

Notes: The eleven cases presented herein are similar to those applied for UWQI, and they are represented as samples 1, 2, …, n, which corresponds respectively to water quality (WQI) values of 0, 5, 10, 25 (worst-cases); 45, 50, 55 (base cases); and 75, 90, 95, 100 (best cases).

The model, as represented by Equation 5.32; functions with four input variables, namely, turbidity (Turb), chlorophyll-a (Chl-a), electrical conductivity (EC) and pondus Hydrogenium (pH). This aligns with objective five, which involves establishing four proxy determinants for the surrogate WQI and assign relative coefficients for the model (Banda and Kumarasamy, 2020b).

$$\mathrm{WQI} = 85.273 - 0.042\mathrm{Chl{-}a} + 0.224\mathrm{pH} - 0.090\mathrm{Turb} - 0.151\mathrm{EC} \qquad \text{Eq. 5.32}$$

where: WQI is the calculated index value ranging from zero to hundred, with zero representing water of poor quality and hundred denoting water of the highest quality;

Chl−a is the observed chlorophyll-a concentration in micrograms per litre (μg/ℓ);

pH is the observed pondus Hydrogenium levels which are unitless;

Turb is the observed turbidity concentration measured in Nephelometric Turbidity Units (NTU); and

EC is the electrical conductivity concentration in micro Siemens per meter (μS/m).

Umgeni water quality data have been examined further to demonstrate the applicability of the proposed surrogate index, and the results are presented in the following plot diagram (Figure 5.21).

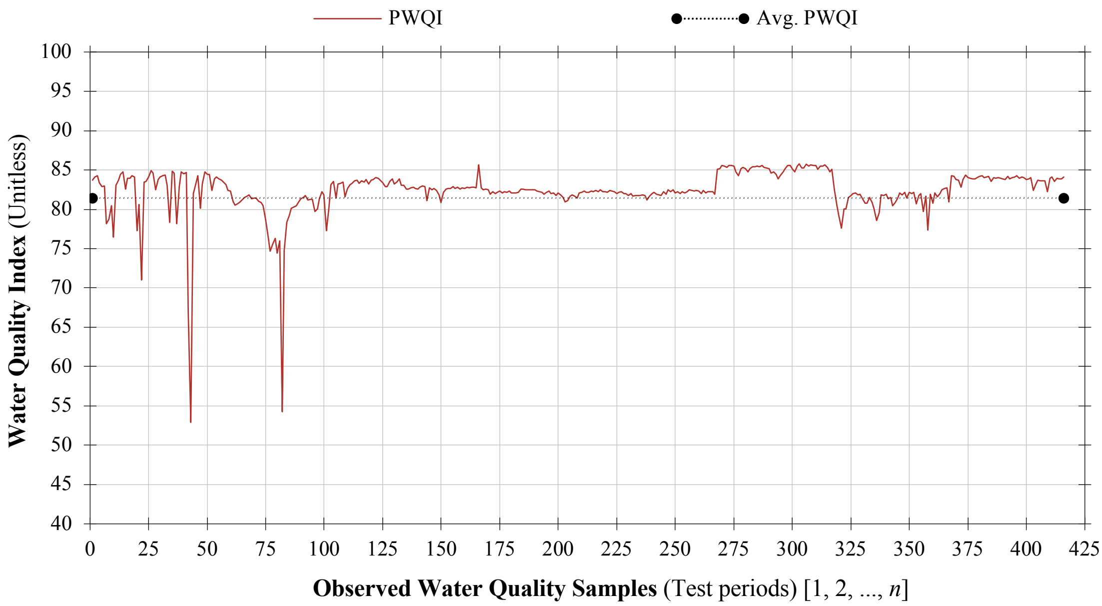

Figure 5.21: Water quality index results calculated using the proposed surrogate water quality index (Proxy WQI) for Umgeni water quality data gathered monthly for over four years starting from 2014 until 2018

Source: WQI results are extracts from the WQVM (Banda and Kumarasamy, 2020b).

Notes: The Umgeni water quality data is from eight sampling stations which fall under four different catchment areas. The catchments include Umgeni River catchment (Henley, Inanda and Midmar Dams); Umdloti River catchment (Hazelmere Dam); Nungwane River catchment (Nungwane Dam); and lastly Umzinto/Umuziwezinto River catchment (Umzinto Dam).

A scientifically balanced surrogate water quality index (WQI) have been suggested. The multivariate statistical approach has been virtually adopted and employed for selecting four proxy parameters and establishing their relative coefficients. Two models were developed, each with four indicators; in fact, the first three variables are similar except the forth parameter of each model. The identical variables are turbidity (Turb), chlorophyll-a (Chl-a), and electrical conductivity (EC). Proxy WQI(a) has sulphate (SO_4) as the fourth parameter, whereas proxy WQI(b) uses pondus Hydrogenium (pH) instead. Both models are technically sensible, with the latter model being considered as the most applicable proxy index. The four parameters retained in the proposed proxy model can be easily measured, even using remote sensors; which would drastically reduce time, effort and cost of evaluating water quality across South African river catchments.

The development of the Surrogate WQI is an attempt to provide an alternative index, better functional with minimum variables, especially in the absence of a full-dataset applicable to the proposed universal water quality index (UWQI). Though with a slight prediction disparity, the proxy WQI can systematically replicate the prediction capabilities of the suggested UWQI. This being that, the Surrogate WQI developed under this study is regarded as an achievement and considered successful enough to fulfil objective three of the research. The objective is defined as developing a surrogate water quality index model that can operate with four key determinants as a proxy to the unbridged UWQI.

Index scores from the universal water quality index (UWQI), artificial neural network (ANN) model and surrogate WQI are all classified using a common index categorisation schema. The focus is on maintaining a standardised unit and compare results of the same group. The index categorisation schema developed for the study is described in the following section.

5.6 Index categorisation schema

Water quality index (WQI) classification approach integrates WQI results into a much simpler, but yet decisive expression that can describe the spatial and temporal changes in water quality. Water categorisation has brought more clarity and understanding in the interpretation of water quality index scores, making it more favourable to non-technical individuals and water management officials. Accordingly, an increasing scale index with values ranging from zero to hundred (0 to 100) with categorisation classes ranging from class 1 to class 5 has been adopted for the classification of the universal water quality index scores. Class 1 water quality with a possible maximum index score of hundred (100) represents water quality of the highest degree. In contrast, Class 5 water quality with an index score close or equal to zero (0) denotes water quality of the lowest degree.

Table 5.18 indicates the index score classification for the universal water quality index (UWQI) for South African river catchments. The indexing schema satisfies the requirements of objective six of the study, which involves the production of water classification grading and water categorisation schema suitable for the proposed water quality index and water quality variability model. Similar to the methods used by Abrahão et al. (2007), Rabee et al. (2011), Rubio-Arias et al. (2012), and Sutadian et al. (2018), appropriate mathematical functions with logical linguistic descriptors such as less than, equal to and greater than have been assigned to each categorisation class. By so doing, the categorisation schema can accommodate all possible index scores regardless of the decimal value.

Table 5.18: Index score classification for the universal water quality index (UWQI) for South African river catchments

ID	Water quality classification Description of rank and classification	Index score
1	**Class 1 – Good water quality** Water quality is protected with a virtual absence of threat or impairment; conditions very close to natural or pristine levels	95 < Index ≤ 100
2	**Class 2 – Acceptable water quality** Water quality is usually protected with only a minor degree of threat or impairment; conditions rarely depart from natural or desirable levels	75 < Index ≤ 95
3	**Class 3 – Regular water quality** Water quality is usually protected but occasionally threatened or impaired; conditions sometimes depart from natural or desirable levels	50 < Index ≤ 75
4	**Class 4 – Bad water quality** Water quality is frequently threatened or impaired; conditions often depart from natural or desirable levels	25 < Index ≤ 50
5	**Class 5 – Very bad water quality** Water quality is almost always threatened or impaired; conditions usually depart from natural or desirable levels	0 < Index ≤ 25

Source: Banda and Kumarasamy (2020c, 2020b); a modified version of the water quality index (WQI) categorisation schema suggested by Banda (2015).

Notes: Class 1 index values (excellent) can only be obtained if all measurements are within objectives virtually all the time.

This method ultimately assists in developing more flexible and precise water quality variability models (WQVMs). More importantly, the established categorisation schema aids in closing gaps identified in the existing literature and present a progressive approach that will contribute significantly towards water quality indices development. Such an academic contribution reflects on the efficiency of the model and attributes to the success of the current study.

5.7 Water quality variability model (WQVM)

In practice, most water quality indices (WQIs) are presented as mathematical expressions that are somewhat difficult to apply in the real world (Banda, 2015). Such research tendencies contributed to the absence of a holistic water monitoring tool that is appropriate for most, if not all the South African river catchments. The lack of such an algorithmic model substantiates the attempt to apply even the most fundamental logical functions and establish a practically-oriented monitoring tool. Henceforth, Microsoft Excel functions are employed to combine three WQI models into a virtual toolkit.

WQVM, a software-based toolkit earmarked for analysing water quality data through the application of three distinctive WQIs, which are founded on different indexing methods. All the three WQIs are developed under this study, and they are: (a) universal water quality index, (b) artificial neural network model, and (c) surrogate water quality index. The WQVM enables the definition of multiple water quality parameters, thereby solving practical problems in the field of water science. Following study objectives seven and eight, the proposed WQVM is aimed at promoting and improving water quality monitoring programs, by providing a simple, convenient and user-friendly monitoring tool. Undoubtedly, the suggested toolkit has an effect on increasing productivity in water resources assessment and optimising decision making, amongst water scientists and professionals.

There are no definite modelling functions generated for water quality analysis; basically, there are no prescribed functions built for any particular modelling environment. Instead, the choice and effectiveness of procedures applicable to any modelling project depend on our modelling skills-sets, competence and acquaintance with available best practices. To an extent, the options are influenced and governed by the resources at our disposal, more than our knowledge and expertise.

5.7.1 The rationale for using Microsoft Excel

At present, Microsoft Excel remains as one of the most popular and pervasive computer programs. Its widespread have transformed the application to become commonplace, with an estimated users' nearing 750 million, and figures are ever-rising (Avdic, 2018). The software arranges data in cells containing rows and columns used to perform simple arithmetic to complex computational analysis. It enables us to skillfully administer cumbersome formulas and provides a platform to handle complex mathematical expressions that are problematic and otherwise unsolvable using ordinary arithmetic operators.

Excel strikes a balance between usability and functionality; hence the program is regarded as the most useful and ubiquitous computing tools, surpassing most computer-assisted audit tools (CAATs) (Varma and Khan, 2014). In simple terms, Excel is straightforward, convenient and user-friendly. All these merits consequently influenced the choice of using Microsoft Excel to build the water quality variability model (WQVM). Using the Excel platform reduces application barriers and presents end-users with a more familiar interface. The level of acceptance is then expected to be higher than suggesting utterly new software.

5.7.2 Microsoft Excel-based WQVM

Taking account of the merits as mentioned earlier, computational tools contained in Excel were used to integrate three water quality indices (WQIs) and form an ultimate monitoring tool. The WQVM consist of user interface page and various hidden calculation spreadsheets. The user interface page is subdivided into input and output segments. The input section is designed to accommodate one thousand samples with a maximum of thirteen predefined water quality variables. The stated data input limitations are due to the conditions under which the model was developed, other than the computational capacity of the software. Nonetheless, one thousand samples are considerably more than enough, that is nearly twenty years of weekly observed data.

Regardless of the model preference, inputting of water quality parameters is done once for all the three WQIs. Maximum of thirteen variables are required to perform a more precise and dependable water quality evaluation; otherwise, the model is designed to function with four proxy variables. Both UWQI and ANN models can accommodate the maximum thirteen variables, whereas the surrogate WQI is capacitated to handle only four variables. The preferred degree of accuracy and end-user preferences defines the amount of input data. The parameter input arrangement is governed by the input requirements of the underlying WQIs, which are the basis at which the WQVM is developed (Banda, 2015).

The output section presents the model results in numeric, graphical and descriptive order. The model results include, (i) digital WQI score displayed as ratio equivalent to percentage, (ii) visual presentation showing the rises and the falls of the index values, and (iii) descriptive analysis that is based on a categorisation schema consisting of five classes related to the degree of purity. The five levels are; Class 1 (good quality), Class 2 (acceptable quality), Class 3 (regular quality), Class 4 (bad quality), and lastly Class 5 (very bad quality). A block diagram of the WQVM is shown in Figure 5.22.

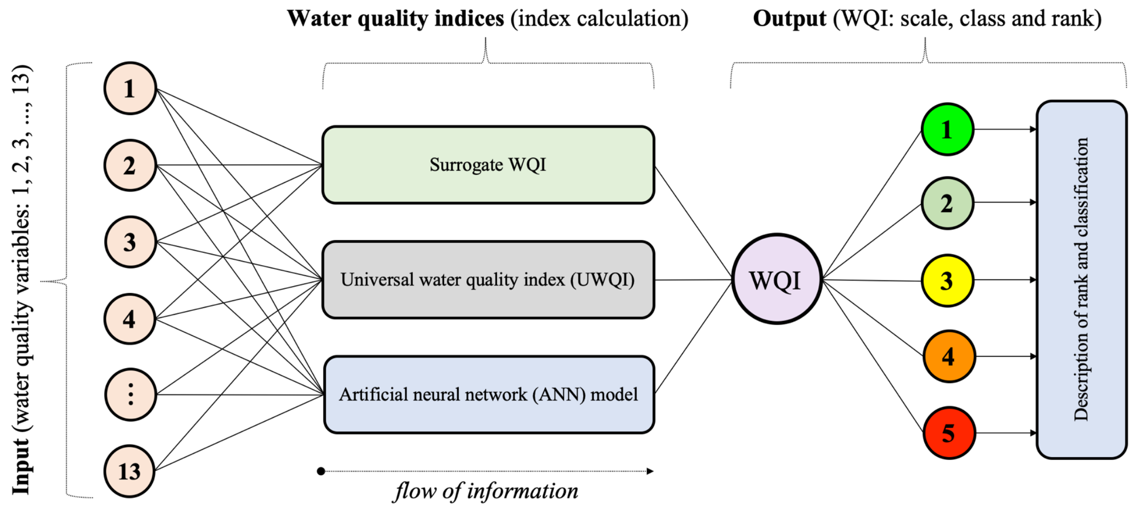

Figure 5.22: Block diagram showing the structure of the water quality variability model (WQVM) developed using Microsoft Excel

Source: Authors' diagram which combines Figure 3.2 (UWQI), Figure 3.3 (ANN), Figure 3.4 (surrogate WQI) and Figure 3.5 (categorisation schema).

Notes: The thirteen explanatory variables are as follows: ammonia (NH_3), calcium (Ca), chloride (Cl), chlorophyll-a (Chl-a), electrical conductivity (EC), fluoride (F), hardness ($CaCO_3$), magnesium (Mg), manganese (Mn), nitrate (NO_3), pondus Hydrogenium (pH), sulphate (SO_4) and turbidity (Turb). The model uses three different water quality indices defined as, (i) universal water quality index (UWQI) model $(2/3)(\sum f(x_i)w_i)^{1.0880563}$ with unequal weights, (ii) artificial neural network (ANN) model that uses nineteen neuro-nodes, seventy predetermined channel weight coefficients and six bias constants, and (iii) surrogate or proxy WQI model in the form of $f(x) = b_0 + b_1x_1 + b_2x_2 + ... + b_4x_4 + \varepsilon$. The water quality categories assume the "green-yellow-red" colour gradient, corresponding to the relevant water quality classes from excellent (class 1) to worse (class 5).

With an attempt to protect information oversights and overrides, data validation schemes were created using Excel built-in functions together with customised IF statements. Such blueprints are necessary to identify potential calculations errors and impending functional problems. In so doing, model formulas are adequately protected, and it reduces the risk of program failure and system crash.

Tables and figures are drawn from the WQVM form part of the research results presented herein Chapter Five and Annexure E of this thesis, which signifies Excels capabilities in analysing water quality data. More so, the results validate the usefulness of the techniques employed; whilst demonstrating the ability of Excel to process high volumes of data. Needless to mention that, techniques presented in this study, provide fast and accurate ways to evaluate water resources. More importantly, the proposed WQVM show much promise and potential. If accorded adequate exposure, the model could afford water professional with a robust and steady tool that can interpret and transform water quality information, from one form to another.

Furthermore, the proposed WQVM gives rise to a well-balanced monitoring structure that assumes a standardised mechanism. Which, in turn, encourages justice and impartiality in resource allocation and national prioritisation programs. Above all, the model promotes water resource monitoring and easy the capturing of spatial and temporal changes in surface water. All these collectively address significant gaps that exist in the South African water sector, which is an important milestone, not only for the study but the country at large.

CHAPTER 6

6. CONCLUSION AND RECOMMENDATIONS

6.1 Introduction

Water quality monitoring is an essential environmental management task and the most demanding activity of the twenty-first century. Practical monitoring tools are then necessary to minimise the burden and promote regular water quality assessment programs. Water quality indices (WQIs) are useful tools which utilise a pollution-based method to perform a holistic analysis of any given water body. WQIs provides more straightforward and scientifically justifiable index scores, usually ranging from zero (worst quality) to hundred (excellent quality). The index ratings are non-dimensional and can be interpreted easily, even by non-technical individuals.

Various indexing models exist; however, most of them are region-specific and oriented to a particular source. The approach governs the index application boundaries and limits its horizon. Such an academic gap prompted the need to consider universally acceptable water quality indices. Henceforth, the current study attempts to put forward flexible water resource monitoring tools that are broadly acknowledged. With immediate attention being given to nationally applicable index model which works for most, if not all the river catchments in South Africa. The research outcomes have the potential to intensify water resource monitoring and facilitate a unified of assessing spatio-temporal trends in river systems.

Therefore, the study presents five distinctive water quality indicators for appraising water status of South African river catchments. The proposed tools are:

(a) Universal water quality index (UWQI) developed using conventional methods involving parameter weights, sub-index functions and an aggregation formula;

(b) Artificial neural networks (ANN) model based on an artificial intelligence algorithm that simulates the functionality of human brains;

(c) Surrogate water quality index (proxy WQI) established through the application of multivariate statistical techniques. The proxy WQI functions as an abridged version of the outright UWQI and operates with limited input parameters;

(d) Water quality variability model (WQVM) that combine the UWQI, ANN model and proxy WQI to become a software-based and practically-oriented monitoring tool; and

(e) An index classification system aimed at interpreting WQI scores resulting from the newly developed water quality monitoring tools.

The research framework is aligned towards satisfying the seven objectives of the study, and the targeted goals were successfully achieved. Subsequently, Chapter Six presents the conclusions and recommendations drawn from the results of this study.

6.2 Conclusion

A unified index model for assessing water contamination levels and facilitate river control functions have been established using expert opinion gathered through participatory based Delphi method and extracts from previously published studies. The universal water quality index (UWQI) is an increasing scale index operating with thirteen fixed variables, parameter weight coefficients, sixty-two sub-index functions, and weighted arithmetic aggregation model. The index scores follow the common percentage hierarchy ranging from zero to hundred, which corresponds to bad and good water quality, respectively. The WQI values are further ranked using a standardised classification system founded on five categories.

The UWQI demonstrated its predictive supremacy through evaluation of spatial and temporal trends of four different drainage basins in KwaZulu-Natal, a coastal province located east of South Africa. Based on the study results, the model is technically stable with a traceable predictive pattern. Such success advocates the readiness of the UWQI to appropriately appraise water quality trends and thus satisfying the requirements of objective one and four of the study.

Similar to statistically derived models, artificial neural network (ANN) models are developed using dependent (target) variable henceforth their level of reliability in prediction depends upon the accuracy of the base-model or source of the dependent variable. Subsequently, their level of reliability in forecast relies on the accuracy of the base-model generating the dependent variable. Without paying enough attention, problems emanating from the parent model might be rolled-forward and influence the descending model. The computational power of artificial intelligence (AI) towards evaluating water quality trends has been verified. The study established as a three-layered parallel-distributed feed-forward neural network model for assessing long-term spatial and temporal water quality variations within South African river systems.

Index scores from the universal water quality index (UWQI) together with water quality data from Umgeni were utilised to formulate a fully-connected neural network model. The dataset consists of 416 samples having thirteen water quality variables measured monthly on six different sampling sites for a period exceeding four years. The ANN model expressed a significantly high degree of accuracy by registering an overall correlation coefficient (R) and coefficient of determination (R^2) corresponding to 0.985 and 0.970, respectively. Accordingly, the R-values achieved are satisfactory, suggesting an increased predictive performance and well-defined neural network.

Findings from the study insinuate that artificial neural networks (ANNs) are powerful and efficient analytical tools for evaluating surface water quality. The results further substantiate the usefulness of modelling ANNs as an effective alternative to traditional and statistical methods modelling methods, thereby satisfying objective two and the study hypothesis. Consequently, the study should encourage water scientists and water resources professionals to considered neural networks as a comprehensive and highly effective technique for assessing water quality trends. Therefore, artificial neural networks are recommended for routine monitoring of environmental resources. Hopefully, the study provides a useful platform beneficial for the application of artificial neural networks.

Further to the two above stated models; a scientifically balanced surrogate water quality index (WQI) has been suggested. The multivariate statistical method has been virtually adopted and employed for selecting four proxy parameters and establishing their relative coefficients. Two models were developed, each with four indicators; in fact, the first three variables are similar except the forth parameter of each model. The identical variables are chlorophyll-a (Chl-a), electrical conductivity (EC) and turbidity (Turb). Proxy WQI(a) has sulphate (SO_4) as the fourth parameter, whereas proxy WQI(b) uses pondus Hydrogenium (pH) instead. Both models are technically sensible, with the latter model being considered as the most applicable proxy index. The four parameters retained in the proposed proxy model can be easily measured, even using remote sensors; which would drastically reduce time, effort and cost of evaluating water quality across South African river catchments.

The proxy WQI is not intended at substituting comprehensive water quality evaluations; instead, it is designed to deliver a quick guide of water resources status. The proxy model which should assist water quality experts, policymakers and the public by communicating water quality data in a more consistent and on-going manner. Developing the surrogate WQI is an attempt to provide an alternative index, better functional with minimum variables, especially in the absence of a full-dataset applicable to high-fidelity model referred to as universal water quality index (UWQI). Though with a slight prediction disparity, the proxy WQI can systematically replicate the prediction capabilities of the UWQI. The surrogate WQI developed under this study is regarded as an achievement and considered successful enough to fulfil objectives three and five of the research. The objective is defined as developing a surrogate water quality index model that can operate with four key determinants as a proxy to the unbridged UWQI.

Classification of index scores is regarded as useful, and the approach offers advantages over the typical index range. Water quality rankings associated with descriptive statements are easily comprehended instead of a single-digit score. Therefore, the current study proposes an index categorisation schema with five-classes distinguished as class 1, 2, 3, 4, and 5. The upper rank (class 1) denotes "good water quality," whereas the lowly-ranked class 5 represents "very bad water quality." The classification system was perfectly aligned with the three WQIs and the water quality variability model developed for the study, which is an accomplishment of objective six of the research work.

Typically water quality index models are presented as mathematical codes that's are somewhat difficult to comprehend and inappropriate for practical use. In an attempt to break such barriers; the study developed a practical-based water quality variability model (WQVM). The WQVM integrates the functionality of the three WQIs (UWQI, ANN model and proxy WQI) and provides a hybrid Microsoft Excel-based application. Thirteen water quality variables are defined as the input parameters (NH_3, Ca, Cl, Chl-a, EC, F, $CaCO_3$, Mg, Mn, NO_3, pH, SO_4 and turbidity). The model is capable of producing a single-digit unitless index score together with a descriptive index rank. Microsft Excel was adopted since it's commonplace and to maximise on the computational abilities of such a familiar software. The WQVM is readily available upon request and through the University of KwaZulu-Natal structures. Providing such a useful tool fulfils objective seven and promote the application of the proposed three water quality indices (WQIs).

Over four hundred water quality samples from six sampling stations located in four different river catchments are evaluated using UWQI, ANN model and the surrogate WQI. Chapter Five of the thesis provide details of the trend analysis. The spatial and temporal changes in water quality for Umgeni Water Board are evident over four years, with a varying sequence comprising of index scores as high as 95.154 (class one), an average of 87.780 (class two) and the lowest score of 75.985 (borderline of class two) across the six sites. The best surface water quality was recorded at station 2 during the summer period of 2017, whereas the lowest water quality was recorded at station 5 during August 2014. The main pollution contributors are NO_3 (station 2, 3, 4 and 6), turbidity (station 1, 2, 5 and 6), Chl-a (station 2 and 3) and lastly, Mn on station 5.

The sources of pollution may be associated with anthropogenic activities considering the socio-economic developments surrounding the affected sampling stations. Otherwise, the rest of the water quality parameters are virtually within permissible levels. There is a need for regular water quality appraisal to monitor concentration levels against pollution control regulations and record the variability trends, especially for sampling stations located within the Durban-Pietermaritzburg business corridor. The application of the proposed water quality monitoring tools can well serve and perform sustainable water resource functions for river basin management.

6.3 Recommendations

The research data suffered a considerable amount of missing values, and this might have impacted on the accuracy of the results obtained. It is therefore recommended that Water Boards (WBs) and Water Service Authorities (WSAs) improve on water quality sampling activities. Such improvements will bear a positive impact on future studies and ultimately promote the production of efficient water management and monitoring tools.

Considering the lack of well-defined water quality objectives and targeted water quality ranges for South Africa, it is highly necessary to initiate a research study focusing on refining the existing water quality limits and guidelines for South African authorities. It would be more practical if the objectives are not generalised, instead be established for every distinctive water use.

In an attempt to improve the developed surrogate WQI and water quality variability model (WQVM), further refinement of the regression coefficients should be considered. Such an improvement would be advantageous in modifying the suggested proxy model into a more robust and compact application tool. Nevertheless, both current models are virtually useful and can be vigilantly employed to assess surface water quality.

The study opens a path for unified WQIs to be considered in South Africa, as the first attempt to demonstrate the use of nationally applicable indices. It is highly expected that the study impacts on methods of developing future water quality indices, contribute to our understanding of index models and supplement our knowledge in water quality science. It is needful to research into unified WQIs formed based on multivariate statistical approaches. Further research is required to understand better the performance of objective methods on nationally applicable indices and address the effects of subjectivity on traditional methods of establishing WQIs.

As an on-going study, additional data from other river catchments should be considered and evaluated using the suggested UWQI. The assessment will further demonstrate the universality of the model and perhaps, guide on necessary modification requirements. Nevertheless, the initial step towards the ultimate goal has been achieved, which is, the development of a universal water quality index (UWQI).

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ANNEXURES

Annexure A: Details of reviewed water quality indices (WQIs)

In Chapter Two, fifteen significant water quality indices (WQIs) were discussed, essentially to establish the existing knowledge and provide background information to the current study. Consequently, this works as guidance towards the selection of the most appropriate research methods and ensure that objectives set in Chapter One are attained, which becomes a logical basis (rationale) for evaluating more existing WQIs. Hence the purpose of this Annexure (Section) is to provide further information on existing WQIs and enables the researcher to anticipate the most appropriate methods. It also provides a theoretical framework to justify the outcome of the study and substantiate the choices made.

There are numerous water quality indices developed since the 19th century, and it is extensive work and beyond reach to attempt discussing all of them under this study; therefore, only forty WQIs are mentioned in Table A.1 below.

Table A.1: Specific details of the reviewed WQIs

Identity		Specific details of the reviewed water quality indices (WQIs) **(a)** Name and associated authors, **(b)** Region of application and purpose, **(c)** Selected water quality parameters, **(d)** Sub-indices and weights, and **(e)** Aggregation method (mathematical composition)
1	(a)	Horton Water Quality Index (Horton's WQI). Horton (1965), Debels et al. (2005), Lumb et al. (2011a), and Lumb et al. (2011b)
	(b)	Developed for United States of America for general assessment of water quality, through the Ohio River Valley Water Sanitation Commission in USA
	(c)	**8 parameters:** Alkalinity, carbon chloroform extract, chlorides, coliform density, dissolved oxygen, pondus Hydrogenium [pH], sewage treatment and specific conductance. Note that, temperature and pollution are included as factors rather than parameters
	(d)	Horton's rating scales and unequal weights were used with the weights ranging from 1 to 4
	(e)	The WQI utilities an Arithmetic weighted mean function
2	(a)	National Sanitation Foundation Water Quality Index (NSF WQI). Brown et al. (1970), Brown et al. (1973), Deininger (1980), dos Santos Simões et al. (2008), Bonanno and Giudice (2010), and Lumb et al. (2011b)
	(b)	Developed for United States of America and further applied in Brazil, India and Iran. Created for general assessment of water quality
	(c)	**11 parameters:** dissolved oxygen, faecal coliform, pondus Hydrogenium [pH], five-day biochemical oxygen demand, phosphates, nitrates, temperature, turbidity, total solids, pesticides and toxic elements
	(d)	Associated rating curves and unequal weights were developed through Delphi Method of involving expert's opinions. Sum of weights equals to 1. Pesticides and toxic elements were handled differently without weights
	(e)	Additive aggregation function was used for the first version in 1970, whereas, multiplicative was adopted for the second version in 1973

Identity		Specific details of the reviewed water quality indices (WQIs) **(a)** Name and associated authors, **(b)** Region of application and purpose, **(c)** Selected water quality parameters, **(d)** Sub-indices and weights, and **(e)** Aggregation method (mathematical composition)
3	(a)	Water Pollution Index (WPI). **Nemerow (1971), Xu et al. (2010)**
	(b)	Index instituted by United States of America specifically for direct and indirect human contact uses as well as remote contact uses
	(c)	**15 parameters:** alkalinity, chloride, colour, dissolved oxygen, faecal coliform, hardness, temperature, total dissolved solids, total nitrogen, turbidity, manganese, pH, suspended solids, sulphates and Iron
	(d)	Sub-indices are generated based on the mean and highest ratio between the particular parameter value over the standard allowable limits. The index is developed using equal weightage
	(e)	WPI utilises the root mean square model to aggregate the equally weighted sub-indices and obtain one final index value
4	(a)	Prati Single Index of Pollution (Prati's Pollution Index). **Prati et al. (1971)**
	(b)	Italy index of pollution instituted to describe the extent of surface water pollution
	(c)	**13 parameters:** alkyl benzene sulfonates, ammonia, carbon chloroform extract, chemical oxygen demand (based on permanganate), chlorine, dissolved oxygen, five-day biochemical oxygen demand, Iron, manganese, nitrates, pH and suspended solids
	(d)	All parameters are considered as indices of pollution with unequal weights adding to a total sum of 1
	(e)	Additive method is used to combine the indices of pollution to provide the pollution index value
5	(a)	Harkin Water Quality Index (Harkin's WQI). Harkins (1974), Landwehr et al. (1974)
	(b)	A scientific tool initiated for collective evaluation of water quality within the United State of America
	(c)	**No parameter guidelines:** any number of parameters may be used to compute the water quality index (WQI) value depending upon the intended ultimate use and or objective of the evaluation
	(d)	In cognisance of the permissible limits (target values), standardisation of the variables is performed to achieve one dimensional scale of the water quality parameters. Unequal weights are assigned with total sum of one whole number
	(e)	A non-parametric classification statistical procedure is used to establish the WQI value, through Multivariate Kendall's Static technique
6	(a)	Walski and Parker Water Quality Index (Walski WQI). **Walski and Parker (1974)**
	(b)	Index for analysing the suitability of water resources earmarked for recreational uses in the United States of America (USA)
	(c)	**10 parameters:** coliform count, colour, grease, nutrients, odour, pH, suspended solids, temperature, toxicity and turbidity
	(d)	All parameters are considered as sub-indices with unequal weights adding to a total sum of 1
	(e)	Additive aggregation equation is utilised to describe the water quality index (WQI)
7	(a)	Scottish Research Development Department Water Quality Index (SRDD Index) SRDD (1976), Bordalo et al. (2001), Bordalo et al. (2006), Carvalho et al. (2011), and Dadolahi-Sohrab et al. (2012)
	(b)	Water quality index developed by the Scottish Government for general water quality assessment in Scotland. Though SRDD Index was applied in several studies for Spain, Portugal, Thailand and Iran
	(c)	**10 parameters**: dissolved oxygen, pH, free and saline ammonia, five-day biochemical oxygen demand, total oxidised nitrogen, suspended solids, phosphorus, E. coli, conductivity and temperature

Identity		Specific details of the reviewed water quality indices (WQIs) — **(a)** Name and associated authors, **(b)** Region of application and purpose, **(c)** Selected water quality parameters, **(d)** Sub-indices and weights, and **(e)** Aggregation method (mathematical composition)
	(d)	Conceptually similar to NSF WQI, the parameter rating curves and unequal weights were developed through Rand Corporation's Delphi Technique with the sum of all weights adding to 1
	(e)	Final index value was established based on the additive aggregation function
8	(a)	Ross Water Quality Index (Ross WQI). **Ross (1977)**
	(b)	Established for the United Kingdom territory for general water quality assessment
	(c)	**4 parameters:** ammoniac nitrogen, dissolved oxygen, five-day biochemical oxygen demand and suspended solids
	(d)	Sub-indices with rating curves developed through Rand Corporation's Delphi Technique with unequal weights and the sum of all weights adding to 10
	(e)	Additive aggregation method is used by Ross WQI
9	(a)	STORET Water Quality Index (STORET Index). **Canter (1977)**, Ministry of the Environment of Indonesia (2003)
	(b)	Index for general water quality evaluation for the North America
	(c)	**No specified list of parameters**. Rather variables are categorised into 3 groups (biological, chemical and physical)
	(d)	Unequally weighted 3 group sub-indices derived from an analysis of monitored parameter values against the permissible limits
	(e)	The additive function is used to combine the group sub-indices into a single index value
10	(a)	Stoner Water Quality Index (Stoner' Index). **Stoner (1978)**
	(b)	WQI specifically modelled for assessing the suitability of irrigation water within the United States of America
	(c)	**16 parameters (irrigation):** aluminium, arsenic, beryllium, boron, cadmium, chromium, cobalt, copper, faecal coliform, fluoride, manganese, nickel, sodium absorption ratio [SAR], specific conductance, vanadium and zinc **13 parameters (water supply):** ammonia-nitrogen, chloride, colour, copper, faecal coliform, fluoride, Iron, methylene active blue substance [MBAS], nitrate-nitrogen, pH, phenols, sulphate and zinc
	(d)	All water quality parameters are taken as a sub-index with unequal weights adding to a total sum of 1
	(e)	Additive aggregation function is used to provide the final index number
11	(a)	Oregon water quality index (OWQI) Dunnette (1979), Cude (2001), and Sarkar and Abbasi (2006)
	(b)	Utilised by Oregon (pacific northwest, west coast) and Idaho (north-western region), United States of America. Both indices were developed for general water quality assessment of Oregon and Idaho States
	(c)	**6 parameters (first version):** dissolved oxygen, faecal coliform, pH, five-day biochemical oxygen demand, nitrates, ammonia and total solids **8 parameters (second version):** temperature and total phosphorus, adding to the parameters of the first version of the water quality index (WQI)
	(d)	Both indices used logarithmic transforms to convert water quality variables into sub-indices values. The first version used unequally weights with total sum of weight adding to 1, while, the second version used equal weights
	(e)	Additive formula and un-weighted harmonic mean of squares of the sub-indices were used to aggregated the final WQI value for both the first version and second version of the index respectively
12	(a)	Martínez de Bascarón Water Quality Index (Bascarón Index). Martínez de Bascarón (1979), Pesce and Wunderlin (2000), Debels et al. (2005), Abrahão et al. (2007), Sánchez et al. (2007), Kannel et al. (2007), and Koçer and Sevgili (2014)

Identity		Specific details of the reviewed water quality indices (WQIs) **(a)** Name and associated authors, **(b)** Region of application and purpose, **(c)** Selected water quality parameters, **(d)** Sub-indices and weights, and **(e)** Aggregation method (mathematical composition)
	(b)	Formulated for use in Spain and later modified by various researchers for application in Argentina, Brazil, Korea and India. Original index was for general water quality assessment, but the evolution of the index, was targeting specific uses
	(c)	**26 parameters:** pH, five-days biochemical oxygen demand, dissolved oxygen, temperature, total coliform, colour, turbidity, permanganate reduction, detergents, hardness, pesticides, oil and grease, sulphates, nitrates, cyanides, sodium, free carbon dioxide, ammonia nitrogen, chloride, conductivity, magnesium, phosphorus, nitrites, calcium and apparent aspect
	(d)	Sub-indices generated from segmented (piecewise) linear transformation. Unequal weights were assigned with a total sum of 54
	(e)	The final index value was obtained through the application of a modified additive function
13	(a)	Bhargava's Water Quality Index (Bhargava's Index). Bhargava (1985), Al-Ani et al. (1987), and Avvannavar and Shrihari (2008)
	(b)	Established to evaluate water quality of River Yamuna, Delhi, India
	(c)	**Identified 4 parameter groups:** (i) coliform organisms to represent bacterial variables, (ii) toxicants, heavy metals, etc., (iii) physical parameters and (iv) organic and inorganic nontoxic substances
	(d)	Water quality parameters clustered in the same group were aggregated to obtain 4 different group sub-indices. Unequal weights with a total summing up to 1
	(e)	Bhargava's index used a modified multiplicative model
14	(a)	House's Water Quality Index (House's Index). House (1986, 1989, 1990), Tyson and House (1989), and Carvalho et al. (2011)
	(b)	Water quality index for the United Kingdom, which was further modified for application in Spain. Its purposes included general assessment of water quality, appraisal of portable water supply and evaluating suitability of aquaculture
	(c)	**9 parameters:** dissolved oxygen, ammonia nitrogen, pH, five-day biochemical oxygen demand, chlorides, total coliform, total phosphorus, nitrates and temperature
	(d)	Conceptually similar to NSF WQI, the parameter rating curves and unequal weights were developed through Rand Corporation's Delphi Technique with the sum of all weights adding to 1
	(e)	Final index value was established based on the additive aggregation function
15	(a)	Dinius Water Quality Index (Dinius WQI). Dinius (1987), Sarkar and Abbasi (2006)
	(b)	Dinius WQI established in United Kingdom for general water quality evaluation, which included public water supply, recreation, fisheries, shellfish, agriculture and industrial waters
	(c)	**12 parameters:** alkalinity, chlorides, coliform count, colour, dissolved oxygen, E-coli count, five-day biochemical oxygen demand, hardness, nitrates, pH, specific conductance and temperature
	(d)	Parameter sub-indices with unequal weightage assigned based on the evaluation of importance by the Delphi panel members
	(e)	Multiplicative aggregation function is utilised to combine all the sub-index functions into one overall index value
16	(a)	Smith Water Quality Index (Smith's WQI). **Smith (1987, 1990)**
	(b)	River and stream water quality index for New Zealand. Used to assess suitability of water resources for various uses such as bathing, water supply and fish spawning

Identity		Specific details of the reviewed water quality indices (WQIs) **(a)** Name and associated authors, **(b)** Region of application and purpose, **(c)** Selected water quality parameters, **(d)** Sub-indices and weights, and **(e)** Aggregation method (mathematical composition)
	(c)	**7 parameters (water supply):** ammonia, dissolved oxygen, faecal coliform, five-day biochemical oxygen demand (unfiltered), temperature, turbidity and suspended solids **6 parameters (general and bathing):** dissolved oxygen, faecal coliform, five-day biochemical oxygen demand (unfiltered), temperature, turbidity and suspended solids **4 parameters (fish spawning):** five-day biochemical oxygen demand (unfiltered), temperature, turbidity and suspended solids
	(d)	Sub-indices and rating curves developed through a panel of experts (Delphi's Method) with sum of unequal weights adding to 1
	(e)	The lowest value of all the sub-indices is retained as the final index value, thus the minimum operator technique
17	(a)	Ved Prakashi Water Quality Index (Ved Prakashi's Index). **1990**
	(b)	Index for India attempting to evaluate the general water quality status of Indian water resources
	(c)	**4 parameters:** biochemical oxygen demand, dissolved oxygen, faecal coliforms and pH
	(d)	Each water quality variable was considered as a sub-index with unequal weights adding to a total sum of 1
	(e)	Parameter sub-indices were combined using the additive aggregation function
18	(a)	Diljido Water Quality Index (Diljido's Index). **Dojlido et al. (1994)**
	(b)	Mathematical tool developed in Serbia for analysing the water quality status of various water sources
	(c)	**7 basic parameters:** ammonia, chemical oxygen demand (Mg), chlorides, dissolved oxygen, dissolved solids, five-day biochemical oxygen demand, suspended solids, phosphates **19 additional parameters:** cadmium, chemical oxygen demand (Cr), chlorides, chromium, copper, free cyanides, hardness, lead, iron, manganese, mercury, nickel, nitrate, organic nitrogen, phenols, total chromium, sulphates and zinc
	(d)	Sub-indices with equal weights
	(e)	Combination of parameter sub-indices was achieved through the application of a mathematical function simply known as the harmonic mean square root formula (harmonic model)
19	(a)	British Columbia water quality index (BCWQI). Zandbergen and Hall (1998), CCME (2001a), Bharti and Katyal (2011)
	(b)	Though adaptive to various applications, the BCWQI was designed for general water quality assessment for the British Columbia Province in Canada
	(c)	**No prescribed list of parameters**, instead, a minimum of 4 parameters are required and there is no defined maximum number of parameters
	(d)	The index does not use neither sub-indices nor weights, rather the deviation of the monitored parameter value form the standards is used to describe water quality
	(e)	No aggregation function, in fact, 3 factors are employed to express the extent of water quality noncompliance and divergence from water quality standards
20	(a)	Status and Sustainability Index (SS Index). Oudin et al. (1999), Fulazzaky (2010)
	(b)	Developed for France mainly for general water quality assessment
	(c)	**15 parameter clusters:** based on their similar nature and their impact on environment. Acidification, colour, metals in bryophytes, microorganisms, mineralisation, mineral micro pollutants, nitrates, non-pesticides, organic micro-pollutants, pesticides, phosphorus matter, phytoplankton, suspended particles and temperature

Identity		Specific details of the reviewed water quality indices (WQIs) **(a)** Name and associated authors, **(b)** Region of application and purpose, **(c)** Selected water quality parameters, **(d)** Sub-indices and weights, and **(e)** Aggregation method (mathematical composition)
	(d)	Colour, nitrates and temperature alteration classes are considered directly as sub-indices, whereas, with the other classes, only one variable with the worst monitored value is considered as sub-index of that particular alteration class, obeying the minimum operator method. All parameters have equal weights
	(e)	Minimum operator function is used to aggregate the final index value
21	(a)	Contact Recreation Index (NZ Recreation Index). **Nagels et al. (2001)**
	(b)	Established in New Zealand for assessing recreational water resources
	(c)	**8 parameters:** Escherichia coli (or faecal coliform), colour, dissolved inorganic nitrogen, dissolved reactive phosphorus, five-day biochemical oxygen demand, pH, turbidity and visual clarity
	(d)	Parameter sub-indices with equal weights
	(e)	The final index value is obtained through the application of the minimum operator function
22	(a)	Canadian Council of Ministers of the Environment Water Quality Index (CCME WQI). CCME (2002), Khan et al. (2003), Khan et al. (2004), Davies (2006), Lumb et al. (2006), Tobin et al. (2007), de Rosemond et al. (2009), Boyacioğlu (2010), Terrado et al. (2010), Nikoo et al. (2011), Sharma and Kansal (2011), Espejo et al. (2012), Hurley et al. (2012), Damo and Icka (2013), and Mostafaei (2014)
	(b)	Originally for Canada and adopted for India, Albania, Chile, Egypt, Iran, Spain, Turkey and Poland. The original WQI was designed for general water quality assessment, whereas the modified indices are for specific uses
	(c)	**No prescribed list of parameters**, instead, a minimum of 4 parameters are required and there is no defined maximum number of parameters
	(d)	The index does not use neither sub-indices nor weights, rather the deviation of the monitored parameter value form the standards is used to describe water quality
	(e)	No aggregation function, in fact, 3 factors (scope, frequency and amplitude) are employed to express the extent of water quality noncompliance and amplitude from the standards
23	(a)	Hallock Water Quality Index (Hallock's Index). **Hallock (2002)**
	(b)	Developed for United States of America for routine stream monitoring exercise
	(c)	**8 parameters**: dissolved oxygen, faecal coliform bacteria, pH, temperature, total nitrogen, total phosphorus, total suspended sediments and turbidity
	(d)	Total suspended sediments and turbidity are combined to become one sub-index using average mean value. Whereas faecal coliform bacteria, pH, and temperature are considered as parameter sub-indices generated from permissible limits. The rest of the parameters are directly considered as sub-indices developed using historical data. All the sub-indices are weighted equally
	(e)	Hallock's Index is based on an additive function
24	(a)	Dalmatian Water Quality Index (Dalmatian Index). **Štambuk-Giljanović (1999, 2003)**
	(b)	Used in Serbia as a tool for general water quality evaluation
	(c)	**9 parameters:** five-day biochemical oxygen demand, dissolved oxygen, corrosion coefficient, mineralisation, protein N, temperature, total coliforms, total nitrate and total phosphorus
	(d)	Parameter sub-indices with unequal weights adding to a total sum of 1
	(e)	Additive or multiplicative functions can be utilised to aggregate the final index rating
25	(a)	Overall Index of Pollution (Indian OIP). **Sargaonkar and Deshpande (2003)**

Identity		Specific details of the reviewed water quality indices (WQIs) **(a)** Name and associated authors, **(b)** Region of application and purpose, **(c)** Selected water quality parameters, **(d)** Sub-indices and weights, and **(e)** Aggregation method (mathematical composition)
	(b)	OIP is designed as an indicator of surface water pollution in India
	(c)	13 parameters: arsenic, biochemical oxygen demand, chloride, colour, dissolved oxygen, fluoride, hardness, nitrate, pH, turbidity, sulphate, total coliform and total dissolved solids
	(d)	Individual water quality parameter sub-indices with equal weights
	(e)	The final OIP value is obtained through the application of additive aggregation function
26	(a)	Liou's Water Quality Index (Liou's WQI). **Liou et al. (2004)**
	(b)	Taiwan WQI developed for general water quality assessment
	(c)	**At least 9 parameters:** ammonia nitrogen, dissolved oxygen, faecal coliform, five-day biochemical oxygen demand, pH, suspend solids, temperature, toxicity and turbidity
	(d)	All parameters have sub-indices, which are further grouped into 3 cluster sub-indices, which are [a] microorganism sub-index (total coliform), [b] organics sub-index (ammonia nitrogen, chemical oxygen demand, dissolved oxygen and five-day biochemical oxygen demand) and finally [c] particulates sub-index (suspended solids and turbidity)
	(e)	Both additive and multiplicative functions are used. Additive formula combines water quality parameters of the same characteristic into group sub-indices (that is, organic and nutrients as well as particulates). Whereas the multiplicative function aggregates all the 3 group sub-indices
27	(a)	Said Water Quality Index (Said's WQI). **Said et al. (2004)**
	(b)	WQI produced for general water quality evaluation of surface water resources in the United States of America
	(c)	**5 parameters:** dissolved oxygen, faecal coliform, total phosphates, turbidity and specific conductivity
	(d)	Utilises equally weighted parameter sub-indices
	(e)	Index value generated through the application of a specific linear function
28	(a)	Fuzzy-based Water Quality Index (Fuzzy Index). Ocampo-Duque et al. (2006), Lermontov et al. (2009), Nikoo et al. (2011), Mahapatra et al. (2012), and Ocampo-Duque et al. (2013)
	(b)	WQI for Spain and introduced in Iran, India, Brazil and Columbia. Fuzzy Index was developed for general water quality evaluation
	(c)	**No guidelines provided**
	(d)	Using fuzzy logic and unequal weights
	(e)	Using fuzzy logic
29	(a)	Universal Water Quality Index - Boyacioğlu Index (UWQI). **Boyacioğlu (2007)**
	(b)	WQI developed to evaluate the suitability of drinking water supplied in Turkey
	(c)	**12 parameters:** arsenic, cadmium, cyanide, dissolved oxygen, five-day biochemical oxygen demand, fluoride, mercury, nitrate-nitrogen, pH, selenium, total coliform and total phosphates
	(d)	Sub-indices are generated in cognisance of the permissible limits governed by Turkey water standards. The WQI utilises unequal weights adding up to a total sum of 1
	(e)	Aggregation of the sub-indices is achieved through the utilisation of an additive formula
30	(a)	Malaysian Water Quality (Malaysian Index). **Shuhaimi-Othman et al. (2007)**
	(b)	Applied in Malaysia for general water quality valuation
	(c)	**6 parameters:** sulphates, phosphate, pH, chemical oxygen demand, nitrates and ammonia nitrogen

Identity		Specific details of the reviewed water quality indices (WQIs) **(a)** Name and associated authors, **(b)** Region of application and purpose, **(c)** Selected water quality parameters, **(d)** Sub-indices and weights, and **(e)** Aggregation method (mathematical composition)
	(d)	Variable directly considered as sub-indices using unequal weights adding up to a total sum of 1
	(e)	Additive aggregation method applied to aggregate the final water quality index value
31	(a)	Hanh Water Quality Index (Hanh's WQI). **Thi Minh Hanh et al. (2011)**
	(b)	WQI formulated to evaluate surface water resources in Vietnam
	(c)	**Minimum of 11 parameters:** ammonium nitrogen, chemical oxygen demand, dissolved oxygen, five-day biochemical oxygen demand, orthophosphate, total coliform, suspended solids, temperature, turbidity and toxicity
	(d)	All parameters have sub-indices, which are further clustered into 3 group sub-indices, thus [a] bacteria sub-index (total coliform), [b] organic and nutrients sub-index (ammonia nitrogen, chemical oxygen demand, dissolved oxygen, five-day biochemical oxygen demand, and orthophosphate) and lastly [c] particulates sub-index (suspended solids and turbidity
	(e)	Both additive and multiplicative functions are used. Additive formula aggregates water quality variables of the same characteristic into clustered parameter sub-indices (that is, organic and nutrients together with particulates). Whilst the multiplicative model combines all the 3 group sub-indices
32	(a)	Almeida Water Quality Index (Almeida's Index). **Almeida et al. (2012)**
	(b)	Research initiative for Argentina, created mainly for water quality assessment of recreational water resources
	(c)	**9 parameters:** chemical oxygen demand, detergents, Escherichia coli, enterococci, faecal coliforms, nitrates, phosphate, pH, and total coliforms
	(d)	Parameter sub-indices with unequal weights adding to a total sum of 1
	(e)	Almeida's Index uses multiplicative function to combine the sub-indices into a single index grading
33	(a)	Vaal Water Quality Index (Vaal WQI). **Banda (2015)**
	(b)	Specifically developed for the Vaal Basin in South African to evaluate the status of surface raw water intended for purification to portable standards
	(c)	**15 parameters:** ammonia/ammonium, calcium, chlorophyll 665, chloride, electrical conductivity, fluoride, hardness, magnesium, manganese, nitrate/nitrite, orthophosphate, pondus Hydrogenium [pH], sulphate, total alkalinity and turbidity
	(d)	Variable directly considered as sub-indices using unequal weights adding up to a total sum of 1
	(e)	Vaal WQI utilises additive aggregation model to combine the unequally weighted sub-indices
34	(a)	Wanda Water Quality Index (Wanda's Index). **Wanda et al. (2016)**
	(b)	Suggested for evaluating water resources for Mpumalanga and North-West Provinces in South Africa
	(c)	**7 parameters:** pondus Hydrogenium [pH], electrical conductivity, five-day biochemical oxygen demand, Escherichia coli [E-coli], temperature, turbidity and nutrients [nitrogen and phosphates)
	(d)	Parameter sub-indices with unequal weights adding to a total sum of 1
	(e)	The final index value is obtained through the application of the modified additive function
35	(a)	Medeiros Water Quality Index (Medeiros WQI). **Medeiros et al. (2017)**
	(b)	Developed for evaluating water quality for Murucupi River Basin, Barcarena City in the Pará State, Brazil
	(c)	**11 parameters:** temperature, pH, total dissolved solids, total suspended solids, dissolved oxygen, five-day biochemical oxygen demand, thermotolerant, coliforms, total nitrogen, total phosphorus, and turbidity

Identity		Specific details of the reviewed water quality indices (WQIs) **(a)** Name and associated authors, **(b)** Region of application and purpose, **(c)** Selected water quality parameters, **(d)** Sub-indices and weights, and **(e)** Aggregation method (mathematical composition)
	(d)	All parameters are considered as sub-indices with unequal weights adding to a total sum of 1
	(e)	Multiplicative aggregation equation is utilised to describe the water quality index (WQI)
36	(a)	García-Ávila Water Quality Index (García-Ávila Index). **García-Ávila et al. (2018)**
	(b)	Developed to analyse drinking water for Azogues City in Ecuador
	(c)	**13 parameters**: turbidity, temperature, electrical conductivity, pondus Hydrogenium [pH], total dissolved solids, total hardness, calcium, magnesium, alkalinity, chlorides, nitrates, sulphates and phosphates
	(d)	Variable directly considered as sub-indices using unequal weights adding up to a total sum of 1
	(e)	García-Ávila Index is based on additive aggregation function that combine unequally weighted sub-indices
37	(a)	Drinking Water Quality Index (DWQI). **Ponsadailakshmi et al. (2018)**
	(b)	Index established to assess the drinking water in Nagapattinam, Tamil Nadu in Southern India
	(c)	**17 parameters:** pondus Hydrogenium [pH], electrical conductivity, sodium, chloride, sulphate, alkalinity, total hardness, calcium, magnesium, iron, fluoride, nitrate, manganese, zinc, chromium, lead and copper
	(d)	Parameter sub-indices with unequal weights adding to a total sum of 1
	(e)	Both arithmetic and geometric methods were applied to aggregate the final water quality index value
38	(a)	Fuzzy-based Water Quality Index (FWQI). **Tiri et al. (2018)**
	(b)	WQI for El Hai Basin in Algeria
	(c)	**10 parameters for both FWQI and the traditional WQI:** pondus Hydrogenium [pH], total dissolved solids, calcium, magnesium, Sodium, potassium, chloride, sulphate, bicarbonate and nitrate
	(d)	Using fuzzy logic and unequal weights the traditional WQI uses parameter sub-indices and unequal weights
	(e)	Using fuzzy logic and the traditional WQI uses additive method to aggregate sub-indices into WQI
39	(a)	West Java Water Quality Index (WJWQI). **Sutadian et al. (2018)**
	(b)	Tool developed to assess water quality in rivers of the West Java Province in Indonesia
	(c)	**17 parameters:** temperature, suspended solids, chemical oxygen demand, dissolved oxygen, nitrite, total phosphate, detergent, phenol, chloride, zinc, lead, mercury, and faecal coliform
	(d)	Parameters directly considered as sub-indices with unequal weights adding up to a total sum of 1
	(e)	WJWQI utilises geometric aggregation model to combine the unequally weighted sub-indices
40	(a)	Mhlongo's Water Quality Index (Mhlongo's Index). **Mhlongo et al. (2018)**
	(b)	Index suggested for evaluating mining water along the Upper Olifants River, Witbank Dam, South Africa
	(c)	**5 parameters:** pondus Hydrogenium [pH], turbidity, total dissolved solids, sulphates and manganese
	(d)	The index does not use neither sub-indices nor weights, rather the deviation of the monitored parameter value form the standards is used to describe water quality
	(e)	No aggregation function, in fact, allowable upper and lower limits are used to express the extent of water quality noncompliance from the national standards

Source: As indicated with each WQI (also see Lumb et al., 2011a, Poonam et al., 2015, Sutadian et al., 2016)

Notes: The listing of the water quality indices (WQIs) in Table A.1 above is based on the year at which the WQI was developed and or published, rather than preference.

Annexure B: Aggregation formulation of the reviewed WQIs

The aggregation functions applicable to the fifteen water quality indices (WQIs) discussed under Chapter Two, Section 2.4.8 are summarised herein Annexure B: Aggregation formulation of the reviewed WQIs, under Table B.1 below. The summary only focuses on the aggregation method used in the calculation of the index value. The fifteen WQIs are widely used and perceived as the most fundamental water quality indices. The original National Sanitation Foundation water quality index (NSF WQI) and the modified NSF WQI are recorded as one in Table B.1, unlike in Section 2.4.8 where they are discussed separately. Therefore, the numbering of the WQIs in the following table, reduces to fourteen.

Although several aggregation techniques have been established, with various modifications being suggested, additive (arithmetic mean) and multiplicative (geometric mean) functions remain as the commonly applied methods. Selection of the most appropriate aggregation technique is an ongoing challenge, considering that each method has its advantages and disadvantages. It is therefore, upon the water quality index (WQI) developer to apply their expertise and knowledge, to select the most suitable method, preferably with minimal disadvantages. The selection process is usually guided by the degree of accuracy required, available data and whether the water quality variables have equal or unequal weights.

Table B.1: Aggregation formulation of the reviewed WQIs

WQI name and symbol description	Aggregation formulation	
1: Horton Water Quality Index (Horton's WQI). Horton (1965), Debels et al. (2005), Lumb et al. (2011a), and Lumb et al. (2011b). **Additive (arithmetic weighted mean)**, where: WQI is the index value, n is the number of variables, s_i is the i^{th} sub-index value which represents the rating number assigned to each variable (0-100), w_i is the i^{th} weight factor (1-4), m_1 is the temperature correction factor (0.5 or 1), and m_2 is the pollution correction factor (0.5 or 1).	$\mathrm{WQI} = \left[\sum_{i=1}^{n} w_i s_i \Big/ \sum_{i=1}^{n} w_i \right] m_1 m_2$	B1.1
2: National Sanitation Foundation Water Quality Index (NSF WQI). Brown et al. (1970), Brown et al. (1973), Deininger (1980), dos Santos Simões et al. (2008), Bonanno and Giudice (2010), and Lumb et al. (2011b). **Additive (1970) and multiplicative (1973)**, where: WQI is the aggregated index value, ρ_i is the measured value of the i^{th} parameter, T_i is the quality rating transformation curve of the i^{th} parameter, q_i is the individual parameter quality rating ($T_i \rho_i = q_i$), n is the total number of weighted parameters, and w_i is the i^{th} weight value such that $w_1 + w_2 + w_3 + \ldots + w_n = 1$ for both Equation B1.2 and Equation B1.3	The first version, 1970 $\mathrm{WQI} = \sum_{i=1}^{n} w_i T_i(\rho_i) = \sum_{i=1}^{n} w_i q_i$	B1.2
	The second version, 1973 $\mathrm{WQI} = \prod_{i=1}^{n} s_i^{wi}$	B1.3
	$w_1 + w_2 + w_3 + \ldots + w_n = 1$	B1.4

WQI name and symbol description	Aggregation formulation	
3: Scottish Research Development Department Water Quality Index (Scottish WQI) SRDD (1976), Bordalo et al. (2001), Bordalo et al. (2006), Carvalho et al. (2011), and Dadolahi-Sohrab et al. (2012). **Additive**, where: WQI is the aggregated index value, n is the number of variables, q_i is the i^{th} sub-index value, and w_i is the i^{th} weight factor such that $w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equation B1.5.	$\text{WQI} = \frac{1}{100}\left(\sum_{i=1}^{n} q_i w_i\right)^2$ $w_1 + w_2 + w_3 + \ldots + w_n = 1$	B1.5 B1.6
4: Oregon Water Quality Index (OWQI) Dunnette (1979), Cude (2001), and Sarkar and Abbasi (2006) **Additive (1979) and unweighted harmonic mean of squares (2001)**, where: WQI is the aggregated index value, n is the number of variables, SI_i is the i^{th} sub-index value, and w_i is the i^{th} weight factor such that $w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equation B1.7.	The first version, 1979 $\text{WQI} = \sum_{i=1}^{n} \text{SI}_i w_i$ $w_1 + w_2 + w_3 + \ldots + w_n = 1$ The second version, 2001 $\text{WQI} = \sqrt{\frac{n}{\sum_{i=1}^{n} \frac{1}{\text{SI}_i^2}}}$	B1.7 B1.8 B1.9
5: Martínez de Bascarón Water Quality Index (Bascarón Index). Martínez de Bascarón (1979), Pesce and Wunderlin (2000), Debels et al. (2005), Abrahão et al. (2007), Sánchez et al. (2007), Kannel et al. (2007), and Koçer and Sevgili (2014). **Modified additive**, where: WQI_{sub} is the subjective water quality index value, WQI_{obj} is the objective water quality index value, WQI_{min} is the minimum water quality index value, n is the number of sub-indices, k is the subjective constant representing the visual impression of river contamination, C_i is the value assigned to parameter i^{th} after normalisation, and P_i is the relative weight assigned to the i^{th} parameter and ranges from 1 to 4 as highest.	Model for the subjective index $\text{WQI}_{sub} = k\frac{\sum_{i=1}^{n} C_i P_i}{\sum_{i=1}^{n} P_i}$ Model for the objective index $\text{WQI}_{obj} = \frac{\sum_{i=1}^{n} C_i P_i}{\sum_{i=1}^{n} P_i}$ Model for the minimum index $\text{WQI}_{\text{min}} = \frac{\sum_{i=1}^{n} C_i P_i}{n}$	B1.10 B1.11 B1.12
6: Bhargava's Water Quality Index (Bhargava's Index). Bhargava (1985), Al-Ani et al. (1987), and Avvannavar and Shrihari (2008). **Modified multiplicative**, where: WQI is the water quality index value, n is the number of variables considered more relevant, and $f_i(P_i)$ is the sensitivity function of the i^{th} parameter which includes the effects of a weighting of the i^{th} parameter.	$\text{WQI} = \left[\prod_{i=1}^{n} f_i(P_i)\right]^{\frac{1}{n}}$	B1.13
7: House's Water Quality Index (House's Index). House (1986, 1989, 1990), Tyson and House (1989), and Carvalho et al. (2011). **Additive**, where: WQI is the aggregated index value, n is the number of variables, q_i is the i^{th} sub-index value, and w_i is the i^{th} weight factor such that $w_1 + w_2 + w_3 + \ldots + w_n = 1$ for Equation B1.14.	$\text{WQI} = \frac{1}{100}\left(\sum_{i=1}^{n} q_i w_i\right)^2$ $w_1 + w_2 + w_3 + \ldots + w_n = 1$	B1.14 B1.15

WQI name and symbol description	Aggregation formulation	
8: Smith Water Quality Index (Smith's WQI). **Smith (1987, 1990)**. **Minimum operator**, where: I_{min} is the lowest sub-index value, I_{sub1} is the sub-index value of the first parameter (1, 2, …, n), and I_{subn} is the sub-index value of the last parameter (1, 2, …, n).	$\mathrm{I}_{min} = \sum \min\left(\mathrm{I}_{sub1}, \mathrm{I}_{sub2}, \ldots, \mathrm{I}_{subn}\right)$	B1.16
9: British Columbia Water Quality Index (BCWQI). Zandbergen and Hall (1998), CCME (2001a), and Bharti and Katyal (2011) **Objective-based model**, where: WQI is the overall water quality index value, F_1 is the percentage of water quality guidelines exceeded, F_2 is the frequency with which objectives not met as a percentage of objectives checked, F_3 is the maximum by which any of the guidelines were exceeded, and 1.453 is the factor to normalise the WQI to a maximum value of 100.	$\mathrm{WQI} = \left(\frac{\sqrt{F_1^2 + F_2^2 + \left(F3/3\right)^2}}{1.453}\right)$	B1.17
10: Canadian Council of Ministers of the Environment Water Quality Index (CCME WQI). CCME (2002), Khan et al. (2003), Khan et al. (2004), Davies (2006), Lumb et al. (2006), Tobin et al. (2007), de Rosemond et al. (2009), Boyacioğlu (2010), Terrado et al. (2010), Nikoo et al. (2011), Sharma and Kansal (2011), Espejo et al. (2012), Hurley et al. (2012), Damo and Icka (2013), and Mostafaei (2014) Objective-based model, where: WQI is the final index value, nse is the normalised sum of excursions, n is the total number of the excursions, F_1 is the scope ("failed variables"), F_2 is the frequency ("failed tests"), F_3 is the amplitude (magnitude of failed tests"), and 1.732 is a factor to normalise the WQI to a maximum value of 1.	$F_1 = \frac{\text{number of failed variables}}{\text{total number of variables}} \times 100$	B1.18
	$F_2 = \frac{\text{number of failed tests}}{\text{total number of tests}} \times 100$	B1.19
	$nse = \frac{\sum_{i=1}^{n} \text{excursion}_i}{\text{total number of tests}}$	B1.20
	$F_3 = \left(\frac{nse}{0.01nse + 0.01}\right)$	B1.21
	$\mathrm{WQI} = 100 - \left(\frac{\sqrt{F_1^2 + F_2^2 + F_3^2}}{1.732}\right)$	B1.22
11: Liou's Water Quality Index (Liou's WQI). **Liou et al. (2004)**. **Combination of additive and multiplicative**, where: RSI is the aggregated river status index value, is the number of sub-indices, w_i is the i^{th} weight value for organic parameters, w_j is the j^{th} weight value for particulate parameters, w_k is the k^{th} weight value for microorganisms, I_i is the i^{th} sub-index value for organic parameters, I_j is the j^{th} sub-index value for particulate parameters, I_k is the sub-index value for microorganisms, and c_{temp}, c_{pH} and c_{tox} are temperature, pondus Hydrogenium (pH) and toxic substance coefficients respectively.	$\mathrm{RSI} = c_{temp} c_{pH} c_{tox} \left[\left(\sum_{i=1}^{3} \mathrm{I}_i w_i\right)\left(\sum_{j=1}^{2} \mathrm{I}_j w_j\right)\left(\sum_{k=1}^{1} \mathrm{I}_k w_k\right)\right]^{\frac{1}{3}}$	B1.23
	$\sum_{i=1}^{n} w_i = 1; \sum_{j=1}^{n} w_j = 1; \text{and} \sum_{k=1}^{n} w_k = 1$	B1.24
12: Fuzzy-based Water Quality Index (Fuzzy Index). Ocampo-Duque et al. (2006), Lermontov et al. (2009), Nikoo et al. (2011), Mahapatra et al. (2012), and Ocampo-Duque et al. (2013). **Fuzzy logic**, where: FWQI is the fuzzy-based water quality index value (between 0 and 100), z is the independent variable of the fuzzy output set in each rule, and a, b, c, and d are membership function parameters.	$\mu(x;a,b,c,d) = \max\left(\min\left(\frac{x-a}{b-a}, 1, \frac{d-x}{d-c}\right), 0\right)$	B1.25
	$\mathrm{FWQI} = \frac{\int \mu(z) \cdot z\mathrm{d}z}{\int \mu(z) z\mathrm{d}z}$	B1.26

WQI name and symbol description	Aggregation formulation	
13: Universal Water Quality Index - Boyacioğlu Index (UWQI). **Boyacioğlu (2007)**. **Additive**, where: UWQI is the universal water quality index value, w_i is the weighted coefficient for the i^{th} parameter presented as decimal, I_i is the sub-index for the i^{th} parameter and n is the total number of the ranked water parameters.	$\mathrm{UWQI} = \sum_{i=1}^{n} w_i \mathrm{I}_i$ $w_1 + w_2 + w_3 + \ldots + w_n = 1$	B1.27 B1.28
14: Vaal Water Quality Index (Vaal WQI). **Banda (2015)** **Additive**, where: WQI is the index value, w_i is the weighted coefficient for the i^{th} parameter presented as decimal, I_i is the sub-index for the i^{th} parameter and n is the total number of the ranked water parameters.	$\mathrm{WQI} = \sum_{i=1}^{n} w_i \mathrm{I}_i$ $w_1 + w_2 + w_3 + \ldots + w_n = 1$	B1.29 B1.30

Source: As indicated with each WQI (also see Lumb et al., 2011a, Poonam et al., 2015, Sutadian et al., 2016)

Notes: The listing of the water quality indices (WQIs) in Table B.1 above is based on the year at which the WQI was developed and or published, rather than preference.

Annexure C: Rand Corporation's Delphi Technique questionnaire sample

Research Questionnaire

Selection of Water Quality Parameters and Weight Ratings for the Development of a Universal Water Quality Index (UWQI)

Doctoral Studies in Engineering (PhD)

Thank you for participating. Please select the appropriate BOX with an [**X**]

Gender Identity: Female ☐ Male ☐

Date and Time of completing the Questionnaire: dd/mm/yyyy ☐☐☐☐☐☐☐☐

Honorific Title		**Highest Qualification**		**Employment Area**
Ms ☐	Prof ☐	Doctoral ☐	HNDip ☐	Academia ☐
Miss ☐	Dr ☐	Masters ☐	NDip ☐	Private Org ☐
Mx ☐	Eng ☐	Honours ☐	NNDip ☐	SOC Ltd ☐
Hon ☐	Mr ☐	PGDip ☐	NCert ☐	Government ☐
Other ☐	Mrs ☐	Under Grad ☐	None ☐	Other ☐

Please indicate the variables you would prefer to be included or excluded in the universal water quality index (UWQI) for South African river catchments, mark ONLY ONCE for each variable as either "Include" or "Exclude" and assign relative significance rating against each parameter designated as "Include." The parameter significance weight rating indicators range from 1 to 5 with, 1 representing the highest significance and 5 relatively low significance. Your cooperation is much appreciated. Thank you.

Water Quality Variable Alphabetic Rank, Name and Symbol			**Preference**		**Significance Weight Rating**				
Item	Parameter Description	Symbol	Include	Exclude	1	2	3	4	5
1	Ammonia	NH_3	☐	☐	☐	☐	☐	☐	☐
2	Biochemical Oxygen Demand	BOD_5	☐	☐	☐	☐	☐	☐	☐
3	Calcium	Ca	☐	☐	☐	☐	☐	☐	☐
4	Chloride	Cl	☐	☐	☐	☐	☐	☐	☐
5	Chlorophyll-a	Chl-a	☐	☐	☐	☐	☐	☐	☐
6	Dissolved Oxygen	DO	☐	☐	☐	☐	☐	☐	☐
7	Electrical Conductivity	EC	☐	☐	☐	☐	☐	☐	☐
8	Faecal Coliforms	CFU	☐	☐	☐	☐	☐	☐	☐
9	Fluoride	F	☐	☐	☐	☐	☐	☐	☐
10	Hardness	$CaCO_3$	☐	☐	☐	☐	☐	☐	☐
11	Magnesium	Mg	☐	☐	☐	☐	☐	☐	☐
12	Manganese	Mn	☐	☐	☐	☐	☐	☐	☐
13	Nitrate	NO_3	☐	☐	☐	☐	☐	☐	☐
14	Nitrite	NO_2	☐	☐	☐	☐	☐	☐	☐
15	Phosphate	PO_4	☐	☐	☐	☐	☐	☐	☐
16	pondus Hydrogenium	pH	☐	☐	☐	☐	☐	☐	☐
17	Sulphate	SO_4	☐	☐	☐	☐	☐	☐	☐
18	Temperature	Temp	☐	☐	☐	☐	☐	☐	☐
19	Total Alkalinity	TA	☐	☐	☐	☐	☐	☐	☐
20	Total Dissolved Solids	TDS	☐	☐	☐	☐	☐	☐	☐
21	Turbidity	Turb	☐	☐	☐	☐	☐	☐	☐

Please ADD up to a maximum of five, any other parameters that should be considered other than the listed above

22	....	....	☐	☐	☐	☐	☐	☐	☐
23	....	....	☐	☐	☐	☐	☐	☐	☐
24	....	....	☐	☐	☐	☐	☐	☐	☐
25	....	....	☐	☐	☐	☐	☐	☐	☐
26	....	....	☐	☐	☐	☐	☐	☐	☐

Comments/Remarks: ....

For the Researcher Only Date Received: Date Captured:

Please return the completed questionnaire form to the following address: Attention: Talent Diotrefe BANDA (Mr.) | Postal: P. O. Box 3154, POLOKWANE, Limpopo Province, South Africa, 0700 | Hand/Postal: 21 Compensatie Street, CDB, POLOKWANE, Limpopo Province, South Africa, 0699 | Email: diotrefetb@yahoo.co.uk

Annexure D: Aggregated significance weight ratings from selected existing water quality indices (WQIs) ranging from 1965 to 2018

Variables[a]		Statistical Summary[b]			Studies considered for expert opinion from existing literature on water quality indices (WQIs)[c]												
Item	Symbol	Included	Excluded	Rating	1	2	3	4	5	6	7	8	9	10	11	12	13
1	NH_3	20	17	**3.503**							2.553	5.000			5.000	4.902	
2	BOD_5	23	14	**3.211**		3.000					0.331		3.190	2.000			
3	Ca	15	22	**1.996**	3.000		5.000		1.702	2.870		2.000			2.000	0.989	2.000
4	Cl	23	14	**1.925**	5.000		3.000	2.079	1.886	2.870	0.010	3.000		1.000	3.000	1.118	3.000
5	Chl-a	1	36	**1.000**											1.000		
6	DO	27	10	**4.214**		4.090		2.700					4.930	4.000			5.000
7	EC	19	18	**2.314**		3.220			1.886	2.050	0.002	3.000			3.000		5.000
8	CFU	23	14	**3.574**				4.833					4.640	4.000		4.859	
9	F	8	29	**3.462**					3.404					3.000	5.000	2.881	2.000
10	$CaCO_3$	15	22	**1.894**	1.000	1.460	4.000		1.702	2.050		3.000		1.000	3.000	0.903	
11	Mg	14	23	**1.933**	3.000		5.000		1.702	2.050		2.000			2.000	1.075	2.000
12	Mn	6	31	**3.109**					3.404						5.000	2.322	
13	NO_3	31	6	**3.007**	5.000	2.570	2.000	1.755	3.818	4.920	0.176	5.000	2.900	3.000	5.000	2.924	4.000
14	NO_2	12	25	**2.572**		2.000					0.110				5.000	2.924	
15	PO_4	20	17	**2.535**				1.566		2.050	4.963		2.900	2.000	4.000		
16	pH	35	2	**2.595**	3.000	2.540	4.000		1.702	4.100	0.221	3.000	3.190	1.000	5.000	0.430	4.000
17	SO_4	16	21	**2.971**	5.000		5.000		2.070	4.100		3.000		2.000	3.000	0.989	4.000
18	Temp	21	16	**2.053**				0.918		2.050			2.900				
19	TA	9	28	**2.317**					1.702	2.870		2.000			3.000		2.000
20	TDS	27	10	**2.959**	5.000	2.750	5.000	1.188		2.870	0.079	5.000	2.030	3.000		3.225	4.000
21	Turb	14	23	**2.623**		2.430				4.920	0.397		2.320	1.000	3.000	2.279	

a Water quality variables listed according to alphabetic order as follows: 1. Ammonia (NH_3) [mg N/ℓ], 2. Biochemical oxygen demand (BOD_5) [mg BOD/ℓ], 3. Calcium (Ca) [mg Ca/ℓ], 4. Chloride (Cl) [mg Ca/ℓ], 5. Chlorophyll-a (Chl-a) [µg/ℓ], 6. Dissolved oxygen (DO) [mg DO/ℓ], 7. Electrical conductivity (EC) [µS/m], 8. Faecal coliforms (CFU) [cfu/100 mℓ], 9. Fluoride (F) [µg F/ℓ], 10. Hardness ($CaCO_3$) [mg $CaCO_3$/ℓ], 11. Magnesium (Mg) [mg Mg/ℓ], 12. Manganese (Mn) [mg Mn/ℓ], 13. Nitrate (NO_3) [mg N/ℓ], 14. Nitrite (NO_2) [mg N/ℓ], 15. Phosphate (PO_4) [mg PO_4/ℓ], 16. pondus Hydrogenium (pH) [Unitless], 17. Sulphate (SO_4) [mg SO_4/ℓ], 18. Temperature (Temp) [°C], 19. Total alkalinity (TA) [mg TA/ℓ], 20. Total dissolved solids (TDS) [mg TDS/ℓ], and 21. Turbidity (Turb) [NTU].

b Statistical summary of significance ratings from existing literature. " Included," denotes the number of WQIs that uses the relevant parameter as an input variable and " Excluded," symbolises the number of WQIs were the parameter is not considered as an input variable. " Rating," is the average significance achieved by taking the mean values recorded ratings, not for the entire thirty-seven WQIs.

c First seventeen of the thirty-seven studies considered for expert opinion from existing literature on WQIs, the studies are ranging from 1965 to 2018 and are listed according to the year of publication in descending order as follows: 1. Yousefi et al. (2018), 2. Ewaid et al. (2018), 3. Tiri et al. (2018), 4. Sutadian et al. (2018), 5. Ponsadailakshmi et al. (2018), 6. García-Ávila et al. (2018), 7. Trikoilidou et al. (2017), 8. Guettaf et al. (2017), 9. Ewaid (2016), 10. Singh et al. (2015), 11. Banda (2015), 12. Abtahi et al. (2015), 13. Sharma et al. (2014).

Variables[a]		Statistical Summary[b]			Studies considered for expert opinion from existing literature on water quality indices (WQIs)[c]											
Item	Symbol	Included	Excluded	Rating	14	15	16	17	18	19	20	21	22	23	24	25
1	NH_3	20	17	**3.503**	3.000		4.000	3.120	3.750	3.000		3.000	3.510	1.650	3.000	4.000
2	BOD_5	23	14	**3.211**	3.000			3.900	4.350	3.000	2.000	3.000	4.590	1.650	3.000	4.500
3	Ca	15	22	**1.996**	1.000	2.000			3.380			1.000			1.000	
4	Cl	23	14	**1.925**	1.000	3.000	1.000		3.610			1.000			1.000	1.000
5	Chl-a	1	36	**1.000**												
6	DO	27	10	**4.214**	4.000			4.940	4.690	4.000	4.000	4.000	4.860	1.650	4.000	5.000
7	EC	19	18	**2.314**	1.000	2.000	3.000	1.560		2.000		1.000	1.620		3.000	
8	CFU	23	14	**3.574**	3.000			3.120	4.690		4.000			5.000	3.000	2.750
9	F	8	29	**3.462**			5.000		3.410		3.000					
10	$CaCO_3$	15	22	**1.894**		2.000			3.300			1.000			1.000	
11	Mg	14	23	**1.933**	1.000	1.000			3.240			1.000			1.000	
12	Mn	6	31	**3.109**			3.000		3.430							
13	NO_3	31	6	**3.007**	2.000	5.000	5.000		3.940	2.000	3.000	2.000	1.890		2.000	2.250
14	NO_2	12	25	**2.572**	2.000		5.000		3.940	2.000		2.000	1.890		2.000	
15	PO_4	20	17	**2.535**	1.000		3.000		3.990	1.000	2.000	1.000	3.240		1.000	
16	pH	35	2	**2.595**	1.000	4.000	3.000	2.340	4.380	1.000	1.000	1.000	2.700		1.000	2.250
17	SO_4	16	21	**2.971**	2.000	4.000	3.000		3.380			2.000			2.000	
18	Temp	21	16	**2.053**	1.000			1.300	4.110	1.000		1.000	2.700		1.000	0.500
19	TA	9	28	**2.317**		2.000			3.580							
20	TDS	27	10	**2.959**	2.000	4.000			3.910	4.000		2.000		2.500	2.000	2.750
21	Turb	14	23	**2.623**	2.000				3.670						2.000	

a Water quality variables listed according to alphabetic order as follows: 1. Ammonia (NH_3) [mg N/ℓ], 2. Biochemical oxygen demand (BOD_5) [mg BOD/ℓ], 3. Calcium (Ca) [mg Ca/ℓ], 4. Chloride (Cl) [mg Ca/ℓ], 5. Chlorophyll-a (Chl-a) [µg/ℓ], 6. Dissolved oxygen (DO) [mg DO/ℓ], 7. Electrical conductivity (EC) [µS/m], 8. Faecal coliforms (CFU) [cfu/100 mℓ], 9. Fluoride (F) [µg F/ℓ], 10. Hardness ($CaCO_3$) [mg $CaCO_3$/ℓ], 11. Magnesium (Mg) [mg Mg/ℓ], 12. Manganese (Mn) [mg Mn/ℓ], 13. Nitrate (NO_3) [mg N/ℓ], 14. Nitrite (NO_2) [mg N/ℓ], 15. Phosphate (PO_4) [mg PO_4/ℓ], 16. pondus Hydrogenium (pH) [Unitless], 17. Sulphate (SO_4) [mg SO_4/ℓ], 18. Temperature (Temp) [ºC], 19. Total alkalinity (TA) [mg TA/ℓ], 20. Total dissolved solids (TDS) [mg TDS/ℓ], and 21. Turbidity (Turb) [NTU].

b Statistical summary of significance ratings from existing literature. " Included," denotes the number of WQIs that uses the relevant parameter as an input variable and " Excluded," symbolises the number of WQIs were the parameter is not considered as an input variable. " Rating," is the average significance achieved by taking the mean values recorded ratings, not for the entire thirty-seven WQIs.

c Last twenty of the thirty-seven studies considered for expert opinion from existing literature on water quality indices (WQIs), the studies are ranging from 1965 to 2018 and are listed according to the year of publication in descending order as follows: 14. Koçer and Sevgili (2014), 15. Hamid et al. (2013), 16. Dzwairo (2011), 17. Carvalho et al. (2011), 18. Kumar and Alappat (2009), 19. Sánchez et al. (2007), 20. Boyacioğlu (2007), 21. Kannel et al. (2007), 22. Debels et al. (2005), 23. Liou et al. (2004), 24. Pesce and Wunderlin (2000), 25. House (1990).

Variables[a]		Statistical Summary[b]			Studies considered for expert opinion from existing literature on water quality indices (WQIs)[c]											
Item	Symbol	Included	Excluded	Rating	26	27	28	29	30	31	32	33	34	35	36	37
1	NH_3	20	17	**3.503**	4.000	3.750		2.590	4.000	3.000			3.240			
2	BOD_5	23	14	**3.211**	4.500	4.100			4.500	3.000	5.000	1.200	4.050	3.000	3.000	
3	Ca	15	22	**1.996**		1.000				1.000						
4	Cl	23	14	**1.925**	1.000	2.700			1.000	1.000						1.000
5	Chl-a	1	36	**1.000**												
6	DO	27	10	**4.214**	5.000	4.670	2.200	2.380	5.000	4.000	5.000	4.800	4.860	5.000	5.000	4.000
7	EC	19	18	**2.314**		3.000				4.000			1.620			2.000
8	CFU	23	14	**3.574**	2.750	3.200	3.180	1.780	2.750	3.000	5.000	2.400	3.240	4.500	4.500	2.000
9	F	8	29	**3.462**												
10	$CaCO_3$	15	22	**1.894**		2.000				1.000						
11	Mg	14	23	**1.933**						1.000						
12	Mn	6	31	**3.109**		1.500										
13	NO_3	31	6	**3.007**	2.250	2.380			2.250	2.000	5.000	1.200		3.000	3.000	
14	NO_2	12	25	**2.572**						2.000						
15	PO_4	20	17	**2.535**		2.830				1.000	5.000		2.160	3.000	3.000	
16	pH	35	2	**2.595**	2.250	3.920	3.130	2.790	2.250	1.000	5.000	1.200	2.430	3.500	3.500	4.000
17	SO_4	16	21	**2.971**						2.000						
18	Temp	21	16	**2.053**	0.500	3.540	3.150	3.590	0.500	1.000	5.000		1.350	3.000	3.000	
19	TA	9	28	**2.317**		2.700										1.000
20	TDS	27	10	**2.959**	2.750	5.000			2.750		5.000	1.200	1.890	2.000	2.000	
21	Turb	14	23	**2.623**		3.700				4.000				2.500	2.500	

a Water quality variables listed according to alphabetic order as follows: 1. Ammonia (NH_3) [mg N/ℓ], 2. Biochemical oxygen demand (BOD_5) [mg BOD/ℓ], 3. Calcium (Ca) [mg Ca/ℓ], 4. Chloride (Cl) [mg Ca/ℓ], 5. Chlorophyll-a (Chl-a) [µg/ℓ], 6. Dissolved oxygen (DO) [mg DO/ℓ], 7. Electrical conductivity (EC) [µS/m], 8. Faecal coliforms (CFU) [cfu/100 mℓ], 9. Fluoride (F) [µg F/ℓ], 10. Hardness ($CaCO_3$) [mg $CaCO_3$/ℓ], 11. Magnesium (Mg) [mg Mg/ℓ], 12. Manganese (Mn) [mg Mn/ℓ], 13. Nitrate (NO_3) [mg N/ℓ], 14. Nitrite (NO_2) [mg N/ℓ], 15. Phosphate (PO_4) [mg PO_4/ℓ], 16. pondus Hydrogenium (pH) [Unitless], 17. Sulphate (SO_4) [mg SO_4/ℓ], 18. Temperature (Temp) [ºC], 19. Total alkalinity (TA) [mg TA/ℓ], 20. Total dissolved solids (TDS) [mg TDS/ℓ], and 21. Turbidity (Turb) [NTU].

b Statistical summary of significance ratings from existing literature. " Included," denotes the number of WQIs that uses the relevant parameter as an input variable and " Excluded," symbolises the number of WQIs were the parameter is not considered as an input variable. " Rating," is the average significance achieved by taking the mean values recorded ratings, not for the entire thirty-seven WQIs.

c Last twenty of the thirty-seven studies considered for expert opinion from existing literature on water quality indices (WQIs), the studies are ranging from 1965 to 2018 and are listed according to the year of publication in descending order as follows: 26. Tyson and House (1989), 27, 28 and 29. Smith (1987), 30. House (1986), 31. Martínez de Bascarón (1979), 32. Cude (2001), 33. Dunnette (1979), 34. SRDD (1976), 35. Brown et al. (1973), 36. Brown et al. (1970), 37. Horton (1965)

Annexure E: Weighted sub-indices and water quality index results

The weighted sub-indices together with the aggregated water quality index values for Umgeni monthly water quality data have been calculated using the universal water quality index (UWQI) and are presented herein as Table E.1. The data set observed by Umgeni Water Board (UWB) at monthly intervals spans for four years from 2014 to 2018. The originally observed parameter concentration levels are summarised in Chapter Five, Section 5.2 in Table 5.1 of this study.

Table E.1: Weighted sub-indices and aggregated water quality index values for Umgeni Water Board in KwaZulu-Natal Province

Weighted sub- indices and aggregated water quality index values for Umgeni Water Board

Identity	NH_3 [mg N/ℓ]	Ca [mg Ca/ℓ]	Cl [mg Cl/ℓ]	Chl-a [µg/ℓ]	EC [µS/m]	F [mg F/ℓ]	$CaCO_3$ [mg $CaCO_3$/ℓ]	Mg [mg Mg/ℓ]	Mn [mg Mn/ℓ]	NO_3 [mg N/ℓ]	pH [Unit-less]	SO_4 [mg SO_4/ℓ]	Turb [NTU]	WQI [Unit-less]
Coeff.[1]	0.1035	0.0726	0.0742	0.0358	0.0692	0.0949	0.0587	0.0710	0.0910	0.0909	0.0911	0.0774	0.0696	1.0000
Max.[2]	9.87	7.19	7.42	3.58	6.92	8.30	5.83	7.09	9.10	8.41	9.11	7.74	6.89	95.154
Min.[3]	4.30	4.89	5.81	0.00	6.92	3.94	4.66	6.93	1.46	0.00	0.00	7.43	0.00	75.985
Avg.[4]	9.48	6.53	7.35	2.84	6.92	8.05	5.54	7.03	8.78	5.54	8.92	7.63	4.08	87.780
1	8.99	6.66	7.42	3.58	6.92	8.30	5.65	7.05	9.10	0.58	9.11	7.72	0.59	80.235
2	9.52	6.53	7.42	2.91	6.92	8.30	5.65	7.06	9.10	0.64	9.11	7.72	1.01	80.454
3	9.87	6.70	7.42	2.81	6.92	8.30	5.65	7.05	8.16	0.84	9.11	7.72	3.36	82.614
4	9.64	6.69	7.42	2.43	6.92	8.30	5.65	7.05	7.97	1.49	9.11	7.71	0.59	79.467
5	9.64	6.61	7.42	1.59	6.92	8.30	5.62	7.04	9.10	3.45	9.11	7.71	0.53	81.703
6	9.87	6.83	7.42	0.00	6.92	8.30	5.70	7.06	9.10	5.91	7.65	7.71	2.53	83.799
7	9.87	6.16	7.42	0.00	6.92	8.30	5.35	7.00	7.94	6.50	9.11	7.74	0.30	81.238
8	9.87	6.85	7.42	0.00	6.92	8.30	5.71	7.06	9.10	1.53	9.11	7.70	0.00	77.989
9	9.87	6.88	7.42	2.53	6.92	8.30	5.72	7.06	9.10	0.00	9.11	7.70	0.00	79.093
10	8.52	6.80	7.42	2.66	6.92	3.94	5.70	7.06	7.43	6.27	9.11	7.73	0.00	77.983
11	9.52	6.81	7.42	3.58	6.92	8.30	5.70	7.06	9.10	4.36	9.11	7.72	0.35	84.820
12	9.52	6.76	7.42	3.20	6.92	8.30	5.68	7.05	9.10	0.53	9.11	7.72	0.53	80.403
13	9.52	6.77	7.42	2.98	6.92	8.30	5.68	7.05	9.10	3.09	9.11	7.72	1.70	84.196
14	9.52	6.67	7.42	3.58	6.92	8.30	5.66	7.05	9.10	0.64	7.65	7.73	5.04	84.089
15	9.52	6.75	7.42	2.75	6.92	8.30	5.67	7.05	9.10	0.53	9.11	7.72	0.32	79.684
16	9.52	6.74	7.42	1.70	6.92	8.30	5.67	7.05	9.10	2.00	9.11	7.71	1.78	81.675
17	7.64	6.57	7.42	3.04	6.92	8.26	5.61	7.04	7.05	6.67	9.11	7.72	1.53	83.340
18	9.52	6.57	7.42	2.98	6.92	8.28	5.61	7.04	9.10	4.64	9.11	7.71	3.20	87.127
19	9.34	6.60	7.42	2.67	6.92	8.29	5.62	7.04	9.10	6.53	8.63	7.71	3.12	88.083
20	9.52	6.63	7.42	2.73	6.92	8.18	5.63	7.04	7.28	5.45	9.11	7.71	0.00	82.332
21	6.82	6.60	7.42	3.15	6.92	8.30	5.63	7.04	6.33	4.91	9.11	7.70	0.00	78.382
22	9.46	6.77	7.42	3.58	6.92	8.30	5.69	7.06	8.16	1.53	9.11	7.71	0.00	80.272
23	9.52	6.74	7.42	3.58	6.92	8.30	5.68	7.06	9.10	1.82	8.63	7.71	0.43	81.542
24	9.52	6.68	7.42	3.01	6.92	8.30	5.66	7.05	9.10	1.91	9.11	7.71	0.49	81.525
25	9.52	6.73	7.42	2.10	6.92	8.30	5.68	7.06	9.10	1.44	9.11	7.73	1.36	81.089
26	9.34	6.68	7.42	3.58	6.92	8.30	5.65	7.05	9.10	1.82	8.63	7.71	4.70	85.833
27	9.52	6.72	7.42	2.53	6.92	8.30	5.67	7.05	9.10	1.91	9.11	7.72	5.57	86.512
28	9.52	6.71	7.42	2.67	6.92	8.30	5.70	7.07	9.10	1.44	9.11	7.73	0.33	80.586
29	9.52	6.71	7.42	2.50	6.92	8.30	5.67	7.05	9.10	1.33	9.11	7.72	0.67	80.594
30	9.52	6.73	7.42	1.44	6.92	8.30	5.67	7.05	9.10	3.64	9.11	7.71	3.62	85.123
31	9.52	6.55	7.42	3.58	6.92	8.30	5.62	7.04	4.28	3.09	9.11	7.71	0.66	78.244
32	9.52	6.82	7.42	3.58	6.92	8.30	5.70	7.06	9.10	0.49	9.11	7.70	0.63	80.961
33	9.52	6.76	7.42	3.58	6.92	8.30	5.69	7.06	9.10	2.18	9.11	7.71	0.38	82.434

Weighted sub- indices and aggregated water quality index values for Umgeni Water Board

Identity	NH_3 [mg N/ℓ]	Ca [mg Ca/ℓ]	Cl [mg Cl/ℓ]	Chl-a [µg/ℓ]	EC [µS/m]	F [mg F/ℓ]	$CaCO_3$ [mg $CaCO_3$/ℓ]	Mg [mg Mg/ℓ]	Mn [mg Mn/ℓ]	NO_3 [mg N/ℓ]	pH [Unit-less]	SO_4 [mg SO_4/ℓ]	Turb [NTU]	WQI [Unit-less]
Coeff.[1]	0.1035	0.0726	0.0742	0.0358	0.0692	0.0949	0.0587	0.0710	0.0910	0.0909	0.0911	0.0774	0.0696	1.0000
Max.[2]	9.87	7.19	7.42	3.58	6.92	8.30	5.83	7.09	9.10	8.41	9.11	7.74	6.89	95.154
Min.[3]	4.30	4.89	5.81	0.00	6.92	3.94	4.66	6.93	1.46	0.00	0.00	7.43	0.00	75.985
Avg.[4]	9.48	6.53	7.35	2.84	6.92	8.05	5.54	7.03	8.78	5.54	8.92	7.63	4.08	87.780
34	9.52	6.93	7.42	2.89	6.92	8.30	5.75	7.07	9.10	0.00	9.11	7.71	0.00	79.210
35	8.99	6.81	7.42	3.00	6.92	8.30	5.70	7.06	9.10	0.33	9.11	7.72	4.45	83.697
36	9.52	6.81	7.42	2.84	6.92	8.30	5.70	7.06	9.10	1.02	9.11	7.72	2.20	82.422
37	9.28	6.86	7.42	3.58	6.92	8.30	5.72	7.06	9.10	0.58	9.11	7.71	0.00	80.203
38	9.52	6.84	7.42	3.10	6.92	8.30	5.71	7.06	9.10	0.15	9.11	7.73	0.34	79.824
39	9.52	6.81	7.42	2.83	6.92	8.30	5.70	7.06	9.10	1.15	9.11	7.73	4.62	85.156
40	9.52	6.61	7.42	3.19	6.92	8.30	5.61	7.03	9.10	0.22	9.11	7.73	2.62	82.063
41	9.52	6.58	7.42	2.72	6.92	8.30	5.62	7.04	9.10	1.36	9.11	7.71	5.83	86.187
42	9.52	6.91	7.42	3.09	6.92	8.30	5.74	7.07	9.10	1.71	9.11	7.70	0.00	81.209
43	9.52	6.79	7.42	3.58	6.92	8.30	5.70	7.06	7.28	1.71	9.11	7.71	0.00	79.614
44	9.52	6.82	7.42	3.03	6.92	8.30	5.71	7.06	9.10	0.91	9.11	7.72	0.13	80.322
45	9.52	6.82	7.42	3.58	6.92	8.30	5.70	7.06	9.10	0.31	9.11	7.72	0.35	80.474
46	9.52	6.73	7.42	2.97	6.92	8.30	5.68	7.05	9.10	1.47	9.11	7.73	0.68	81.311
47	9.52	6.79	7.42	3.58	6.92	8.30	5.67	7.04	9.10	0.07	9.11	7.70	0.00	79.761
48	9.52	6.84	7.42	3.58	6.92	8.30	5.70	7.06	9.10	0.36	9.11	7.72	0.40	80.630
49	9.52	6.79	7.42	3.58	6.92	8.30	5.68	7.05	9.10	0.85	9.11	7.71	1.86	82.625
50	9.52	6.75	7.42	3.58	6.92	8.30	5.67	7.05	9.10	0.00	9.11	7.73	1.11	80.871
51	9.52	6.77	7.42	2.12	6.92	8.30	5.68	7.05	8.16	0.62	8.89	7.72	5.22	83.139
52	9.69	6.90	7.42	3.58	6.92	8.28	5.69	7.05	9.10	6.96	9.11	7.69	0.40	87.873
53	9.69	6.90	7.42	3.58	6.92	8.28	5.69	7.04	9.10	6.95	9.11	7.69	3.01	90.679
54	9.52	6.90	7.42	3.58	6.92	8.29	5.69	7.04	9.10	6.95	9.11	7.69	4.39	91.972
55	9.28	6.90	7.42	3.58	6.92	8.29	5.69	7.04	9.10	6.94	9.11	7.69	2.57	89.750
56	9.34	6.90	7.42	3.58	6.92	8.29	5.69	7.04	9.10	6.94	8.87	7.69	0.82	87.666
57	9.52	6.90	7.42	3.00	6.92	8.29	5.69	7.04	8.16	6.93	9.11	7.69	0.69	86.333
58	9.52	6.90	7.42	3.14	6.92	8.29	5.69	7.04	8.16	6.93	9.11	7.69	0.61	86.390
59	9.52	6.90	7.42	3.06	6.92	8.30	5.69	7.04	8.16	6.92	9.11	7.70	0.48	86.157
60	9.58	6.90	7.42	3.58	6.92	8.30	5.69	7.04	9.10	6.91	9.11	7.70	0.42	87.734
61	9.87	6.90	7.42	3.03	6.92	8.30	5.69	7.04	9.10	6.91	9.11	7.70	0.15	87.160
62	9.87	6.89	7.42	3.12	6.92	8.30	5.69	7.04	9.10	6.77	9.11	7.69	0.05	86.983
63	9.87	6.88	7.42	3.16	6.92	8.30	5.68	7.05	9.10	6.64	9.11	7.68	0.11	86.934
64	9.87	6.87	7.42	2.68	6.92	8.30	5.68	7.05	9.10	6.50	9.11	7.67	0.18	86.334
65	9.87	6.88	7.42	3.58	6.92	8.28	5.69	7.05	9.10	6.52	9.11	7.67	0.23	87.360
66	9.64	6.88	7.42	2.95	6.92	8.26	5.69	7.05	9.10	6.55	9.11	7.68	0.31	86.537
67	9.87	6.89	7.42	3.00	6.92	8.23	5.69	7.05	9.10	6.57	8.87	7.68	0.32	86.592
68	9.87	6.89	7.42	3.20	6.92	8.21	5.70	7.05	9.10	6.59	8.14	7.68	0.33	86.052
69	9.87	6.90	7.42	3.58	6.92	8.19	5.70	7.05	9.10	6.61	9.11	7.69	0.25	87.440
70	9.87	6.90	7.42	3.08	6.92	8.17	5.70	7.05	9.10	6.64	9.11	7.69	0.27	86.942
71	9.87	6.90	7.42	3.19	6.92	8.12	5.70	7.05	9.10	6.53	9.11	7.69	0.29	86.891
72	9.52	6.89	7.42	3.11	6.92	8.07	5.69	7.05	9.10	6.43	7.90	7.69	0.14	84.786
73	9.52	6.90	7.42	3.15	6.92	8.10	5.69	7.05	9.10	5.76	9.11	7.68	0.16	85.480
74	9.52	6.91	7.42	3.06	6.92	8.13	5.70	7.05	9.10	4.97	8.87	7.68	0.05	84.188
75	9.52	6.91	7.42	3.08	6.92	8.16	5.70	7.05	9.10	4.18	9.11	7.68	0.00	83.603
76	9.52	6.92	7.42	3.15	6.92	8.19	5.70	7.05	9.10	3.39	8.87	7.67	0.00	82.618
77	9.52	6.93	7.42	3.19	6.92	8.22	5.70	7.05	9.10	2.61	9.11	7.67	0.00	82.106
78	9.52	6.93	7.42	2.87	6.92	8.22	5.70	7.05	9.10	1.82	9.11	7.66	0.00	80.932
79	9.52	6.92	7.42	2.21	6.92	8.17	5.70	7.05	9.10	4.91	9.11	7.66	0.00	83.467
80	9.52	6.91	7.42	0.00	6.92	8.12	5.70	7.05	9.10	6.98	7.90	7.65	0.00	81.940

Weighted sub- indices and aggregated water quality index values for Umgeni Water Board

Identity	NH_3 [mg N/ℓ]	Ca [mg Ca/ℓ]	Cl [mg Cl/ℓ]	Chl-a [µg/ℓ]	EC [µS/m]	F [mg F/ℓ]	$CaCO_3$ [mg $CaCO_3$/ℓ]	Mg [mg Mg/ℓ]	Mn [mg Mn/ℓ]	NO_3 [mg N/ℓ]	pH [Unit-less]	SO_4 [mg SO_4/ℓ]	Turb [NTU]	WQI [Unit-less]
Coeff.[1]	0.1035	0.0726	0.0742	0.0358	0.0692	0.0949	0.0587	0.0710	0.0910	0.0909	0.0911	0.0774	0.0696	1.0000
Max.[2]	9.87	7.19	7.42	3.58	6.92	8.30	5.83	7.09	9.10	8.41	9.11	7.74	6.89	95.154
Min.[3]	4.30	4.89	5.81	0.00	6.92	3.94	4.66	6.93	1.46	0.00	0.00	7.43	0.00	75.985
Avg.[4]	9.48	6.53	7.35	2.84	6.92	8.05	5.54	7.03	8.78	5.54	8.92	7.63	4.08	87.780
81	9.52	6.90	7.42	0.00	6.92	8.11	5.70	7.05	9.10	7.09	8.14	7.65	0.00	82.295
82	9.52	6.90	7.42	0.00	6.92	8.10	5.69	7.05	9.10	7.20	8.38	7.65	0.00	82.651
83	9.52	6.89	7.42	0.00	6.92	8.09	5.69	7.05	9.10	7.31	7.41	7.65	0.00	81.705
84	9.52	6.89	7.42	1.61	6.92	8.08	5.69	7.05	9.10	7.42	6.44	7.65	0.00	82.485
85	9.52	6.88	7.42	2.22	6.92	8.02	5.69	7.05	9.10	7.35	8.63	7.65	0.00	85.342
86	9.28	6.88	7.42	3.17	6.92	7.96	5.69	7.05	8.16	7.28	7.65	7.65	0.00	83.911
87	9.52	6.87	7.42	2.80	6.92	7.90	5.69	7.05	9.10	7.22	6.68	7.65	0.00	83.595
88	9.52	6.87	7.42	3.58	6.92	7.84	5.69	7.05	9.10	7.15	8.87	7.65	0.03	86.666
89	9.52	6.85	7.42	3.12	6.92	7.94	5.68	7.05	9.10	7.18	8.38	7.65	0.12	85.870
90	9.52	6.83	7.42	3.58	6.92	8.04	5.68	7.05	9.10	7.22	7.41	7.65	0.20	85.526
91	9.52	6.81	7.42	3.58	6.92	8.14	5.67	7.05	9.10	7.25	8.38	7.65	0.25	86.743
92	9.52	6.79	7.42	3.15	6.92	8.24	5.67	7.04	9.10	7.28	7.41	7.65	0.30	85.400
93	9.17	6.80	7.42	3.58	6.92	8.22	5.67	7.04	8.16	7.14	9.11	7.65	0.20	86.028
94	9.52	6.81	7.42	3.58	6.92	8.20	5.67	7.04	8.12	6.99	9.11	7.65	0.23	86.230
95	9.40	6.83	7.42	3.58	6.92	8.18	5.67	7.04	8.12	6.85	8.14	7.66	0.22	84.883
96	9.52	6.84	7.42	3.19	6.92	8.16	5.67	7.04	7.97	6.70	8.14	7.66	0.00	84.039
97	9.52	6.87	7.42	3.15	6.92	8.30	5.67	7.04	9.10	4.64	8.63	7.63	0.00	83.669
98	9.52	6.81	7.42	3.11	6.92	8.30	5.66	7.04	9.10	5.91	7.90	7.64	0.30	84.471
99	9.52	6.80	7.42	3.17	6.92	8.00	5.65	7.04	8.12	6.18	8.87	7.65	0.50	84.697
100	9.52	6.84	7.42	3.11	6.92	7.92	5.67	7.04	9.10	7.73	8.14	7.72	0.41	86.526
101	9.52	6.82	7.42	0.34	6.92	7.97	5.66	7.04	9.10	1.91	9.11	7.64	0.00	77.873
102	9.52	6.84	7.42	0.12	6.92	8.15	5.67	7.04	9.10	7.73	9.11	7.62	0.28	84.365
103	9.52	6.85	7.42	2.40	6.92	8.15	5.67	7.04	9.10	7.73	9.11	7.64	2.37	89.079
104	9.52	6.89	7.42	3.00	6.92	8.16	5.69	7.05	9.10	7.73	7.90	7.63	3.03	89.209
105	9.52	6.88	7.42	1.96	6.92	8.25	5.69	7.05	9.10	7.73	9.11	7.61	0.40	86.613
106	9.46	6.83	7.42	3.01	6.92	8.21	5.67	7.04	7.87	7.73	9.11	7.68	0.86	86.807
107	9.52	6.86	7.42	3.19	6.92	8.25	5.68	7.05	9.10	7.11	9.11	7.70	2.03	89.097
108	9.52	6.84	7.42	3.58	6.92	8.21	5.67	7.04	9.10	7.22	9.11	7.69	3.12	90.727
109	9.52	6.83	7.42	3.03	6.92	8.17	5.67	7.04	9.10	6.87	9.11	7.60	0.37	86.652
110	9.52	6.81	7.42	3.58	6.92	8.17	5.65	7.04	9.10	7.73	9.11	7.57	0.63	88.355
111	9.52	5.80	7.42	2.78	6.92	8.20	5.21	7.00	9.10	7.73	9.11	7.67	4.37	90.072
112	9.52	6.81	7.42	3.58	6.92	8.22	5.66	7.04	9.10	7.62	9.11	7.63	4.12	92.153
113	9.52	6.73	7.42	2.93	6.92	8.21	5.63	7.03	9.10	7.01	8.87	7.59	6.09	92.462
114	9.52	6.77	7.42	3.58	6.92	8.30	5.65	7.04	9.10	7.73	9.11	7.67	6.74	95.154
115	9.52	6.79	7.42	2.26	6.92	8.30	5.65	7.04	9.10	7.73	9.11	7.63	6.68	93.656
116	9.52	6.79	7.42	2.39	6.92	8.27	5.65	7.04	9.10	7.66	9.11	7.64	6.61	93.629
117	9.52	6.82	7.42	1.49	6.92	8.22	5.67	7.04	9.10	7.45	9.11	7.66	6.77	92.628
118	9.52	6.91	7.42	3.17	6.92	8.30	5.70	7.05	9.10	7.39	9.11	7.64	5.13	92.811
119	9.52	6.83	7.42	3.58	6.92	8.21	5.67	7.04	9.10	6.84	9.11	7.64	0.66	87.600
120	9.52	6.73	7.42	3.06	6.92	8.30	5.63	7.03	9.10	7.56	9.11	7.67	4.45	91.868
121	9.52	6.81	7.42	2.45	6.92	8.30	5.71	7.06	9.10	7.15	8.87	7.63	6.69	93.087
122	9.52	6.78	7.42	3.10	6.92	8.30	5.65	7.04	9.10	7.22	9.11	7.64	6.82	94.160
123	9.52	6.66	7.42	3.58	6.92	8.30	5.60	7.02	9.10	7.25	9.11	7.64	6.78	94.462
124	9.52	6.73	7.42	2.99	6.92	8.30	5.63	7.03	9.10	7.73	9.11	7.62	6.75	94.416
125	9.52	6.77	7.42	3.00	6.92	8.30	5.65	7.04	9.10	0.00	8.63	7.65	5.57	84.398
126	9.52	6.77	7.42	2.53	6.92	8.30	5.64	7.03	9.10	7.73	9.11	7.68	0.70	87.497
127	9.52	6.82	7.42	2.21	6.92	8.30	5.66	7.04	9.10	7.73	9.11	7.67	6.66	93.666

Weighted sub- indices and aggregated water quality index values for Umgeni Water Board

Identity	NH_3 [mg N/ℓ]	Ca [mg Ca/ℓ]	Cl [mg Cl/ℓ]	Chl-a [µg/ℓ]	EC [µS/m]	F [mg F/ℓ]	$CaCO_3$ [mg $CaCO_3$/ℓ]	Mg [mg Mg/ℓ]	Mn [mg Mn/ℓ]	NO_3 [mg N/ℓ]	pH [Unit-less]	SO_4 [mg SO_4/ℓ]	Turb [NTU]	WQI [Unit-less]
Coeff.[1]	0.1035	0.0726	0.0742	0.0358	0.0692	0.0949	0.0587	0.0710	0.0910	0.0909	0.0911	0.0774	0.0696	1.0000
Max.[2]	9.87	7.19	7.42	3.58	6.92	8.30	5.83	7.09	9.10	8.41	9.11	7.74	6.89	95.154
Min.[3]	4.30	4.89	5.81	0.00	6.92	3.94	4.66	6.93	1.46	0.00	0.00	7.43	0.00	75.985
Avg.[4]	9.48	6.53	7.35	2.84	6.92	8.05	5.54	7.03	8.78	5.54	8.92	7.63	4.08	87.780
128	9.52	6.75	7.42	1.94	6.92	8.14	5.64	7.03	9.10	7.73	9.11	7.69	6.69	93.136
129	9.52	6.82	7.42	3.22	6.92	8.30	5.66	7.04	9.10	7.52	9.11	7.69	6.81	94.708
130	9.52	6.97	7.42	3.58	6.92	8.26	5.71	7.05	7.87	7.45	8.63	7.68	0.69	86.735
131	9.52	6.84	7.42	3.58	6.92	8.27	5.67	7.04	8.08	6.64	8.87	7.66	2.87	88.489
132	9.52	6.79	7.42	3.18	6.92	8.27	5.66	7.04	9.10	7.01	8.87	7.66	4.62	91.396
133	9.58	5.16	7.42	2.78	6.92	8.11	4.83	6.97	9.10	5.64	9.11	7.54	6.78	89.096
134	9.40	5.14	7.42	2.98	6.92	8.11	4.81	6.97	7.43	7.01	9.11	7.53	6.77	88.749
135	9.87	5.12	7.42	1.63	6.92	8.12	4.80	6.97	9.10	5.91	9.11	7.53	6.79	88.398
136	9.87	5.09	7.42	1.72	6.92	8.12	4.78	6.96	9.10	8.41	9.11	7.53	6.82	91.176
137	9.87	5.07	7.42	2.26	6.92	8.12	4.77	6.96	9.10	7.25	9.11	7.52	6.82	90.471
138	9.87	5.05	7.42	2.48	6.92	8.13	4.76	6.96	9.10	6.50	9.11	7.52	6.84	89.888
139	9.87	5.03	7.42	2.09	6.92	8.13	4.74	6.96	8.01	6.27	9.11	7.52	6.81	87.958
140	9.87	5.00	7.42	2.17	6.92	8.13	4.73	6.96	9.10	8.41	9.11	7.51	6.77	91.440
141	9.87	4.98	7.42	3.03	6.92	8.14	4.71	6.96	9.10	8.41	9.11	7.51	6.84	92.413
142	9.75	4.96	7.42	3.17	6.92	8.14	4.70	6.96	9.10	6.47	9.11	7.51	6.86	90.320
143	9.75	4.94	7.42	3.58	6.92	8.14	4.69	6.95	9.10	6.09	9.11	7.50	6.83	90.282
144	9.87	4.91	7.42	3.58	6.92	8.14	4.67	6.95	9.10	6.40	0.00	7.50	6.85	80.931
145	9.87	4.89	7.42	3.12	6.92	8.15	4.66	6.95	9.10	5.00	9.11	7.50	6.83	88.656
146	9.87	5.13	7.42	3.06	6.92	8.10	5.03	7.02	9.10	7.22	9.11	7.52	6.81	91.673
147	9.87	5.39	7.42	3.00	6.92	8.09	5.13	7.02	9.10	8.14	9.11	7.51	6.81	92.969
148	9.87	5.65	7.42	2.82	6.92	8.08	5.24	7.02	9.10	7.49	9.11	7.51	6.71	92.351
149	9.52	5.91	7.42	2.50	6.92	8.07	5.34	7.02	9.10	7.69	9.11	7.50	3.70	88.955
150	9.52	6.17	7.42	2.64	6.92	8.06	5.44	7.02	9.10	7.62	9.11	7.49	0.51	85.968
151	9.52	6.12	7.42	2.65	6.92	8.01	5.41	7.02	9.10	7.52	9.11	7.51	6.69	92.407
152	9.52	6.13	7.42	2.89	6.92	8.01	5.41	7.02	9.10	7.56	9.11	7.50	6.74	92.755
153	9.52	6.14	7.42	3.04	6.92	8.01	5.42	7.02	9.10	7.32	9.11	7.48	6.78	92.723
154	9.52	6.15	7.42	3.14	6.92	8.01	5.42	7.02	9.10	7.73	9.11	7.47	6.71	93.200
155	9.52	6.17	7.42	3.11	6.92	8.01	5.43	7.02	9.10	7.22	9.11	7.46	6.83	92.746
156	9.52	6.16	7.42	2.98	6.92	7.97	5.42	7.02	9.10	7.49	9.11	7.48	6.84	92.888
157	9.52	6.16	7.42	3.58	6.92	7.92	5.42	7.02	9.10	6.64	9.11	7.50	6.89	92.628
158	9.52	6.16	7.42	3.58	6.92	7.87	5.42	7.02	9.10	4.09	9.11	7.52	6.82	89.771
159	9.52	6.16	7.42	3.22	6.92	8.04	5.41	7.02	9.10	6.18	9.11	7.53	6.85	91.851
160	9.46	6.16	7.42	3.58	6.92	8.07	5.41	7.02	8.06	6.74	9.11	7.54	6.79	91.634
161	9.17	6.15	7.42	3.19	6.92	8.11	5.42	7.02	7.85	6.81	9.11	7.54	6.83	90.828
162	9.52	6.15	7.42	3.58	6.92	8.14	5.42	7.02	7.65	6.09	9.11	7.55	6.82	90.670
163	9.52	6.14	7.42	3.58	6.92	8.13	5.41	7.02	7.43	5.00	9.11	7.60	6.83	89.277
164	9.52	6.15	7.42	3.58	6.92	8.14	5.42	7.02	7.73	4.91	8.87	7.58	6.83	89.258
165	9.52	6.16	7.42	3.00	6.92	8.15	5.43	7.02	8.04	3.45	8.63	7.56	6.81	87.125
166	9.52	6.17	7.42	2.94	6.92	8.17	5.43	7.02	9.10	6.00	8.87	7.54	6.81	91.230
167	9.52	6.13	7.42	3.58	6.92	8.15	5.41	7.02	9.10	6.40	8.63	7.54	6.84	92.041
168	9.52	6.10	7.42	2.71	6.92	8.13	5.39	7.02	9.10	7.52	9.11	7.55	6.84	92.762
169	9.52	6.08	7.42	3.00	6.92	8.02	5.38	7.02	9.10	7.73	9.11	7.54	6.81	93.103
170	9.52	6.07	7.42	3.01	6.92	7.91	5.38	7.02	9.10	6.64	9.11	7.52	6.77	91.752
171	9.52	6.07	7.42	1.47	6.92	7.91	5.38	7.02	9.10	7.73	8.87	7.53	6.68	90.904
172	9.52	6.06	7.42	2.87	6.92	7.91	5.37	7.02	9.10	7.73	9.11	7.54	6.71	92.723
173	9.52	6.06	7.42	1.61	6.92	7.91	5.37	7.02	9.10	6.43	8.87	7.55	6.75	89.738
174	9.52	6.37	7.42	2.28	6.92	7.86	5.58	7.04	9.10	7.08	8.50	7.53	6.73	91.263

Weighted sub- indices and aggregated water quality index values for Umgeni Water Board

Identity	NH_3 [mg N/ℓ]	Ca [mg Ca/ℓ]	Cl [mg Cl/ℓ]	Chl-a [µg/ℓ]	EC [µS/m]	F [mg F/ℓ]	$CaCO_3$ [mg $CaCO_3$/ℓ]	Mg [mg Mg/ℓ]	Mn [mg Mn/ℓ]	NO_3 [mg N/ℓ]	pH [Unit-less]	SO_4 [mg SO_4/ℓ]	Turb [NTU]	WQI [Unit-less]
Coeff.[1]	0.1035	0.0726	0.0742	0.0358	0.0692	0.0949	0.0587	0.0710	0.0910	0.0909	0.0911	0.0774	0.0696	1.0000
Max.[2]	9.87	7.19	7.42	3.58	6.92	8.30	5.83	7.09	9.10	8.41	9.11	7.74	6.89	95.154
Min.[3]	4.30	4.89	5.81	0.00	6.92	3.94	4.66	6.93	1.46	0.00	0.00	7.43	0.00	75.985
Avg.[4]	9.48	6.53	7.35	2.84	6.92	8.05	5.54	7.03	8.78	5.54	8.92	7.63	4.08	87.780
175	9.52	6.69	7.42	2.73	6.92	7.81	5.69	7.07	9.10	7.73	8.14	7.51	6.78	92.522
176	9.52	6.54	7.42	2.62	6.92	7.85	5.64	7.05	9.10	7.73	9.11	7.52	6.77	93.269
177	9.52	6.39	7.42	3.03	6.92	7.90	5.58	7.04	9.10	6.94	9.11	7.53	6.78	92.701
178	9.52	6.25	7.42	2.64	6.92	7.95	5.47	7.03	9.10	7.01	8.87	7.54	6.70	91.768
179	9.52	6.10	7.42	3.58	6.92	8.00	5.36	7.01	9.10	7.73	8.87	7.54	6.66	93.280
180	9.52	6.14	7.42	2.38	6.92	7.96	5.39	7.02	9.10	7.73	8.87	7.54	6.67	92.031
181	9.52	6.15	7.42	2.73	6.92	8.00	5.40	7.02	9.10	7.73	9.11	7.52	6.64	92.700
182	9.52	6.16	7.42	2.47	6.92	8.05	5.40	7.02	9.10	7.52	9.11	7.51	6.69	92.298
183	9.52	6.17	7.42	2.57	6.92	8.10	5.40	7.02	9.10	7.56	9.11	7.50	6.72	92.524
184	9.52	6.18	7.42	3.20	6.92	8.14	5.41	7.02	9.10	7.73	8.87	7.60	6.78	93.366
185	9.46	6.16	7.42	3.12	6.92	8.07	5.41	7.02	9.10	7.73	8.87	7.54	6.82	93.095
186	9.52	6.23	7.42	3.14	6.92	8.00	5.44	7.02	9.10	7.73	9.11	7.49	6.84	93.451
187	9.46	6.23	7.42	3.14	6.92	7.96	5.45	7.02	9.10	7.18	9.11	7.50	6.79	92.713
188	9.46	6.23	7.42	3.09	6.92	8.09	5.46	7.02	9.10	6.57	9.11	7.51	6.84	92.217
189	9.52	6.19	7.42	3.12	6.92	8.08	5.46	7.03	7.95	6.57	9.11	7.53	6.85	91.057
190	9.52	6.15	7.42	3.58	6.92	8.07	5.46	7.03	7.63	6.70	9.11	7.55	6.82	91.297
191	9.52	6.11	7.42	3.04	6.92	8.06	5.37	7.01	7.32	6.94	9.11	7.58	6.84	90.511
192	9.52	6.14	7.42	3.19	6.92	8.01	5.40	7.02	7.54	0.64	9.11	7.59	6.63	83.930
193	9.52	6.34	7.42	3.00	6.92	7.96	5.52	7.03	7.94	1.31	9.11	7.58	6.75	85.292
194	9.52	6.55	7.42	2.84	6.92	7.91	5.61	7.04	9.10	1.71	8.87	7.56	5.39	85.343
195	9.52	6.41	7.42	3.03	6.92	7.94	5.56	7.03	9.10	3.09	9.11	7.56	6.69	88.513
196	9.52	6.26	7.42	3.58	6.92	7.98	5.49	7.03	9.10	1.25	8.87	7.56	6.81	86.784
197	9.52	6.19	7.42	3.17	6.92	7.96	5.44	7.02	9.10	1.02	9.11	7.53	6.26	85.585
198	9.52	6.12	7.42	3.15	6.92	7.95	5.39	7.02	9.10	0.07	9.11	7.51	6.76	84.910
199	9.52	6.05	7.42	2.54	6.92	7.93	5.34	7.01	9.10	7.05	9.11	7.48	6.71	91.533
200	9.52	6.03	7.42	3.58	6.92	7.92	5.32	7.01	9.10	6.40	8.87	7.47	6.74	91.647
201	9.52	6.01	7.42	2.87	6.92	7.91	5.31	7.01	9.10	1.78	9.11	7.45	6.67	86.025
202	9.52	5.92	7.42	1.83	6.92	7.90	5.26	7.01	9.10	1.40	9.11	7.43	6.64	84.288
203	9.52	5.98	7.42	0.45	6.92	7.84	5.20	6.98	9.10	1.25	9.11	7.49	4.20	80.007
204	9.52	6.04	7.42	1.08	6.92	8.01	5.14	6.96	9.10	2.00	9.11	7.54	4.37	81.887
205	9.52	6.04	7.42	2.60	6.92	8.01	5.18	6.97	9.10	1.38	9.11	7.52	5.57	84.171
206	9.52	6.05	7.42	2.69	6.92	8.01	5.23	6.99	9.10	6.87	9.11	7.49	6.43	91.159
207	9.52	6.05	7.42	2.53	6.92	8.01	5.28	7.00	9.10	7.73	9.11	7.47	6.35	91.857
208	9.52	6.05	7.42	2.17	6.92	8.01	5.33	7.01	9.10	0.00	9.11	7.45	6.81	83.685
209	9.52	6.10	7.42	3.13	6.92	7.80	5.36	7.01	9.10	4.82	9.11	7.54	6.83	89.875
210	9.40	6.12	7.42	3.58	6.92	7.77	5.36	7.01	9.10	7.73	9.11	7.53	6.83	93.361
211	9.52	6.14	7.42	3.12	6.92	7.75	5.38	7.01	9.10	2.45	9.11	7.56	6.81	87.345
212	9.52	6.14	7.42	2.86	6.92	7.82	5.39	7.01	9.10	6.27	9.11	7.56	6.71	91.158
213	9.52	6.14	7.42	2.51	6.92	7.89	5.39	7.02	9.10	6.77	9.11	7.56	6.72	91.403
214	9.52	6.14	7.42	3.01	6.92	7.96	5.39	7.02	9.10	6.67	9.11	7.55	6.72	91.914
215	9.52	6.14	7.42	2.67	6.92	8.03	5.39	7.02	9.10	6.91	9.11	7.55	6.74	91.898
216	9.52	6.31	7.42	3.06	6.92	8.01	5.50	7.03	9.10	7.22	9.11	7.57	6.82	93.033
217	9.52	6.24	7.42	2.91	6.92	7.99	5.40	7.01	9.10	0.51	9.11	7.56	6.70	85.281
218	9.52	6.17	7.42	3.06	6.92	7.97	5.29	6.99	9.10	3.18	9.11	7.55	6.74	88.110
219	8.82	6.13	7.42	2.86	6.92	8.00	5.31	7.00	9.10	5.00	8.87	7.53	6.72	88.833
220	9.52	6.09	7.42	2.98	6.92	8.04	5.33	7.01	9.10	4.55	9.11	7.52	6.72	89.501
221	9.52	6.05	7.42	3.10	6.92	8.08	5.35	7.01	9.10	1.51	9.11	7.51	6.66	86.296

Weighted sub- indices and aggregated water quality index values for Umgeni Water Board

Identity	NH_3 [mg N/ℓ]	Ca [mg Ca/ℓ]	Cl [mg Cl/ℓ]	Chl-a [µg/ℓ]	EC [µS/m]	F [mg F/ℓ]	$CaCO_3$ [mg $CaCO_3$/ℓ]	Mg [mg Mg/ℓ]	Mn [mg Mn/ℓ]	NO_3 [mg N/ℓ]	pH [Unit-less]	SO_4 [mg SO_4/ℓ]	Turb [NTU]	WQI [Unit-less]
Coeff.[1]	0.1035	0.0726	0.0742	0.0358	0.0692	0.0949	0.0587	0.0710	0.0910	0.0909	0.0911	0.0774	0.0696	1.0000
Max.[2]	9.87	7.19	7.42	3.58	6.92	8.30	5.83	7.09	9.10	8.41	9.11	7.74	6.89	95.154
Min.[3]	4.30	4.89	5.81	0.00	6.92	3.94	4.66	6.93	1.46	0.00	0.00	7.43	0.00	75.985
Avg.[4]	9.48	6.53	7.35	2.84	6.92	8.05	5.54	7.03	8.78	5.54	8.92	7.63	4.08	87.780
222	9.52	6.07	7.42	3.18	6.92	8.10	5.36	7.01	9.10	2.82	9.11	7.53	6.83	88.062
223	9.52	6.05	7.42	3.09	6.92	8.08	5.34	7.01	9.10	1.42	9.11	7.53	6.79	86.364
224	9.52	6.03	7.42	2.98	6.92	8.06	5.33	7.01	9.10	5.09	9.11	7.53	6.78	90.128
225	9.52	6.00	7.42	2.86	6.92	8.05	5.32	7.01	9.10	3.55	9.11	7.53	6.71	88.208
226	9.52	5.98	7.42	3.15	6.92	8.03	5.31	7.01	9.10	5.82	9.11	7.53	6.75	90.945
227	9.52	6.10	7.42	3.15	6.92	8.03	5.40	7.02	9.10	5.09	9.11	7.53	6.78	90.434
228	9.52	6.22	7.42	3.08	6.92	8.03	5.48	7.03	9.10	2.82	9.11	7.53	6.77	88.124
229	9.52	6.34	7.42	3.03	6.92	8.03	5.57	7.04	9.10	1.27	9.11	7.53	6.82	86.685
230	9.52	6.45	7.42	3.03	6.92	8.03	5.62	7.05	9.10	1.64	7.90	7.53	6.82	85.968
231	9.52	6.34	7.42	2.84	6.92	8.04	5.56	7.04	9.10	4.45	9.11	7.53	6.72	89.824
232	9.52	6.22	7.42	3.01	6.92	8.06	5.47	7.03	9.10	3.45	9.11	7.54	5.13	86.991
233	9.52	6.10	7.42	2.73	6.92	8.07	5.39	7.02	9.10	1.11	9.11	7.54	6.35	85.265
234	8.76	5.98	7.42	2.20	6.92	8.08	5.30	7.01	9.10	4.27	9.11	7.54	6.71	87.450
235	9.52	6.02	7.42	2.63	6.92	8.06	5.32	7.01	9.10	3.73	9.11	7.55	6.52	88.013
236	9.52	6.06	7.42	2.50	6.92	8.05	5.35	7.01	9.10	2.91	9.11	7.56	6.70	87.248
237	9.52	6.10	7.42	1.84	6.92	8.03	5.37	7.02	9.10	3.73	9.11	7.57	6.63	87.413
238	9.52	6.14	7.42	2.68	6.92	8.01	5.40	7.02	9.10	5.73	9.11	7.58	0.66	84.115
239	9.52	6.14	7.42	2.15	6.92	8.00	5.38	7.01	9.10	2.82	9.11	7.57	4.87	84.890
240	9.52	6.14	7.42	2.80	6.92	7.99	5.37	7.01	9.10	2.82	9.11	7.57	5.65	86.388
241	9.52	6.13	7.42	2.92	6.92	7.98	5.35	7.01	9.10	5.18	9.11	7.56	6.17	89.585
242	9.52	6.13	7.42	2.72	6.92	7.97	5.34	7.00	9.10	0.00	8.87	7.55	6.52	83.870
243	9.52	6.12	7.42	2.49	6.92	7.96	5.33	7.00	9.10	4.64	6.93	7.55	6.69	86.647
244	9.52	6.12	7.42	1.12	6.92	7.95	5.31	7.00	9.10	5.09	9.11	7.54	6.69	87.971
245	9.52	6.13	7.42	1.99	6.92	7.94	5.33	7.00	9.10	4.64	7.17	7.54	6.17	85.799
246	9.52	6.14	7.42	2.38	6.92	7.93	5.34	7.00	9.10	6.70	9.11	7.55	6.35	90.748
247	9.52	6.15	7.42	2.80	6.92	7.92	5.36	7.01	9.10	6.36	9.11	7.55	6.79	91.334
248	9.52	6.16	7.42	2.54	6.92	7.90	5.37	7.01	9.10	5.91	9.11	7.55	6.71	90.489
249	9.52	6.17	7.42	2.62	6.92	7.89	5.38	7.01	9.10	6.40	8.87	7.55	6.75	90.907
250	9.52	6.17	7.42	2.22	6.92	7.88	5.40	7.01	9.10	5.73	9.11	7.56	6.62	89.889
251	9.52	6.21	7.42	2.12	6.92	7.85	5.43	7.02	9.10	6.27	9.11	7.55	6.72	90.520
252	9.52	6.25	7.42	2.28	6.92	7.82	5.46	7.02	9.10	0.87	8.38	7.55	6.63	84.038
253	9.52	6.24	7.42	2.16	6.92	7.86	5.45	7.02	9.10	4.18	9.11	7.54	6.63	88.259
254	9.52	6.22	7.42	2.60	6.92	7.90	5.44	7.02	9.10	4.73	8.87	7.54	6.09	88.488
255	9.52	6.21	7.42	2.74	6.92	7.94	5.43	7.02	8.18	1.76	9.11	7.53	6.17	84.827
256	9.52	6.20	7.42	3.15	6.92	7.99	5.42	7.02	8.12	1.69	9.11	7.52	6.62	85.618
257	9.46	6.19	7.42	3.18	6.92	7.99	5.42	7.02	8.11	2.45	9.11	7.53	6.71	86.480
258	9.52	6.18	7.42	2.65	6.92	7.99	5.41	7.02	8.10	2.55	9.11	7.53	6.75	86.089
259	9.40	6.17	7.42	2.90	6.92	7.99	5.40	7.02	8.08	1.71	9.11	7.53	6.82	85.381
260	9.11	6.15	7.42	2.95	6.92	8.00	5.40	7.02	8.07	1.56	9.11	7.53	6.85	84.976
261	8.52	6.14	7.42	2.87	6.92	8.00	5.39	7.02	8.06	1.20	9.11	7.54	6.62	83.585
262	9.52	6.13	7.42	3.58	6.92	8.00	5.38	7.02	8.05	1.24	9.11	7.54	6.85	85.684
263	9.52	6.12	7.42	3.58	6.92	8.03	5.38	7.01	8.12	1.27	9.11	7.54	5.22	84.064
264	9.52	6.11	7.42	3.18	6.92	8.06	5.37	7.01	9.10	0.62	9.11	7.55	6.64	85.533
265	9.52	6.10	7.42	2.77	6.92	8.10	5.37	7.01	9.10	1.25	9.11	7.55	6.71	85.873
266	9.52	6.09	7.42	2.88	6.92	8.13	5.36	7.01	9.10	1.24	9.11	7.55	6.76	86.045
267	9.17	6.09	7.42	2.63	6.92	8.13	5.36	7.01	9.10	0.80	9.11	7.54	6.52	84.653
268	6.53	6.87	7.42	3.13	6.92	8.30	5.73	7.07	9.10	7.01	9.11	7.72	2.29	86.154

Weighted sub- indices and aggregated water quality index values for Umgeni Water Board

Identity	NH_3 [mg N/ℓ]	Ca [mg Ca/ℓ]	Cl [mg Cl/ℓ]	Chl-a [µg/ℓ]	EC [µS/m]	F [mg F/ℓ]	$CaCO_3$ [mg $CaCO_3$/ℓ]	Mg [mg Mg/ℓ]	Mn [mg Mn/ℓ]	NO_3 [mg N/ℓ]	pH [Unit-less]	SO_4 [mg SO_4/ℓ]	Turb [NTU]	WQI [Unit-less]
Coeff.[1]	0.1035	0.0726	0.0742	0.0358	0.0692	0.0949	0.0587	0.0710	0.0910	0.0909	0.0911	0.0774	0.0696	1.0000
Max.[2]	9.87	7.19	7.42	3.58	6.92	8.30	5.83	7.09	9.10	8.41	9.11	7.74	6.89	95.154
Min.[3]	4.30	4.89	5.81	0.00	6.92	3.94	4.66	6.93	1.46	0.00	0.00	7.43	0.00	75.985
Avg.[4]	9.48	6.53	7.35	2.84	6.92	8.05	5.54	7.03	8.78	5.54	8.92	7.63	4.08	87.780
269	9.75	6.86	7.42	2.94	6.92	8.30	5.73	7.07	9.10	7.01	9.11	7.72	3.94	91.205
270	9.87	6.86	7.42	3.12	6.92	8.30	5.73	7.07	9.10	7.05	9.11	7.72	6.74	94.582
271	9.75	6.86	7.42	3.07	6.92	8.30	5.73	7.07	9.10	6.77	9.11	7.72	6.61	93.966
272	7.99	6.86	7.42	3.19	6.92	8.30	5.73	7.07	9.10	0.00	9.11	7.71	5.13	83.299
273	9.87	6.88	7.42	3.01	6.92	8.30	5.73	7.07	9.10	6.77	8.38	7.73	6.43	93.085
274	9.87	7.19	7.42	3.12	6.92	8.30	5.83	7.09	9.10	6.91	9.11	7.72	6.74	94.918
275	9.87	6.86	7.42	2.97	6.92	8.30	5.72	7.07	9.10	7.01	9.11	7.72	6.52	94.129
276	9.52	6.85	7.42	1.05	6.92	8.30	5.73	7.07	9.10	7.42	9.11	7.72	5.04	90.515
277	9.49	6.84	7.42	0.11	6.92	8.30	5.72	7.07	9.10	7.03	9.11	7.72	4.45	88.400
278	9.46	6.84	7.42	2.84	6.92	8.30	5.72	7.07	8.08	6.64	9.11	7.72	5.39	90.794
279	9.28	6.80	7.42	3.17	6.92	8.30	5.71	7.06	9.10	7.45	9.11	7.73	4.03	91.433
280	9.52	6.86	7.42	3.16	6.92	7.78	5.73	7.07	9.10	6.91	9.11	7.72	2.70	89.176
281	9.52	6.86	7.42	2.98	6.92	8.30	5.73	7.07	9.10	6.64	6.68	7.72	3.70	87.718
282	9.52	6.88	7.42	3.58	6.92	8.30	5.73	7.07	9.10	7.15	8.87	7.72	2.37	89.851
283	9.52	6.71	7.42	2.98	6.92	8.30	5.67	7.06	9.10	6.67	9.11	7.71	6.00	92.601
284	9.40	6.86	7.42	2.97	6.92	8.29	5.73	7.07	9.10	7.42	9.11	7.72	6.52	94.053
285	9.52	6.83	7.42	3.04	6.92	8.27	5.72	7.07	9.10	7.37	8.75	7.72	6.39	93.618
286	9.52	6.82	7.42	2.62	6.92	8.30	5.71	7.07	9.10	7.32	8.14	7.72	6.63	92.726
287	9.52	6.82	7.42	3.58	6.92	8.30	5.72	7.07	9.10	7.73	8.38	7.72	6.26	94.079
288	9.52	6.83	7.42	2.56	6.92	8.30	5.72	7.07	9.10	7.73	8.63	7.73	6.26	93.248
289	9.52	6.80	7.42	2.78	6.92	8.30	5.71	7.06	9.10	7.73	9.11	7.72	6.09	93.773
290	9.52	6.79	7.42	3.04	6.92	8.30	5.70	7.06	9.10	7.73	9.11	7.72	4.70	92.544
291	9.52	5.82	7.42	3.01	6.92	8.30	5.24	7.01	9.10	7.45	9.11	7.72	0.65	86.240
292	9.52	6.80	7.42	3.12	6.92	8.30	5.71	7.07	9.10	7.73	8.63	7.72	0.67	87.777
293	9.52	6.83	7.42	2.56	6.92	8.30	5.72	7.07	9.10	7.35	8.63	7.72	0.62	86.759
294	9.52	6.84	7.42	2.56	6.92	7.98	5.72	7.07	9.10	7.28	9.11	7.72	0.51	86.759
295	9.52	6.82	7.42	3.58	6.92	8.30	5.72	7.07	9.10	7.01	9.11	7.72	0.59	87.966
296	9.52	6.84	7.42	2.84	6.92	8.30	5.72	7.07	9.10	6.98	8.87	7.72	0.68	86.995
297	9.52	6.82	7.42	2.83	6.92	8.30	5.71	7.07	9.10	6.09	9.11	7.72	4.12	89.960
298	9.46	6.81	7.42	3.01	6.92	8.30	5.71	7.07	9.10	6.27	8.63	7.73	6.61	92.442
299	9.52	6.66	7.42	3.19	6.92	8.30	5.66	7.05	9.10	7.08	8.63	7.72	6.17	92.857
300	9.52	6.73	7.42	1.73	6.92	8.30	5.69	7.06	9.10	7.45	9.11	7.72	6.66	92.866
301	9.52	6.87	7.42	0.70	6.92	8.30	5.73	7.07	9.10	7.61	9.11	7.72	5.39	90.748
302	9.52	6.86	7.42	3.13	6.92	8.30	5.73	7.07	9.10	7.73	9.11	7.72	6.17	94.349
303	9.52	6.85	7.42	3.15	6.92	8.30	5.72	7.07	9.10	7.71	8.14	7.72	6.72	93.870
304	9.52	6.81	7.42	3.58	6.92	8.30	5.71	7.06	9.10	7.23	9.11	7.71	4.45	92.330
305	9.52	6.84	7.42	2.96	6.92	8.30	5.72	7.07	9.10	7.28	9.11	7.72	3.78	91.048
306	9.52	6.90	7.42	3.10	6.92	8.30	5.74	7.07	9.10	7.25	7.90	7.72	6.62	93.024
307	9.52	6.88	7.42	3.08	6.92	8.30	5.73	7.07	9.10	7.28	9.11	7.72	6.00	93.636
308	9.52	6.81	7.42	3.16	6.92	8.30	5.71	7.06	9.10	6.91	9.11	7.72	6.64	93.905
309	9.52	5.94	7.42	3.12	6.92	8.30	5.27	7.01	9.10	7.45	9.11	7.72	6.72	93.064
310	9.52	6.81	7.42	2.75	6.92	8.30	5.71	7.07	9.10	7.32	8.63	7.72	6.67	93.410
311	9.52	6.80	7.42	1.91	6.92	8.30	5.72	7.07	9.10	7.25	9.11	7.71	6.68	92.964
312	9.52	6.87	7.42	2.56	6.92	8.30	5.74	7.07	9.10	7.45	9.11	7.71	6.69	94.009
313	9.52	6.85	7.42	2.84	6.92	8.30	5.72	7.07	9.10	7.73	9.11	7.71	6.69	94.553
314	9.52	6.83	7.42	2.58	6.92	8.30	5.72	7.07	9.10	7.73	8.80	7.72	6.83	94.061
315	9.52	6.83	7.42	2.38	6.92	8.30	5.72	7.07	9.10	7.73	9.11	7.72	6.66	94.008

Weighted sub- indices and aggregated water quality index values for Umgeni Water Board

Identity	NH_3 [mg N/ℓ]	Ca [mg Ca/ℓ]	Cl [mg Cl/ℓ]	Chl-a [µg/ℓ]	EC [µS/m]	F [mg F/ℓ]	$CaCO_3$ [mg $CaCO_3$/ℓ]	Mg [mg Mg/ℓ]	Mn [mg Mn/ℓ]	NO_3 [mg N/ℓ]	pH [Unit-less]	SO_4 [mg SO_4/ℓ]	Turb [NTU]	WQI [Unit-less]
Coeff.[1]	0.1035	0.0726	0.0742	0.0358	0.0692	0.0949	0.0587	0.0710	0.0910	0.0909	0.0911	0.0774	0.0696	1.0000
Max.[2]	9.87	7.19	7.42	3.58	6.92	8.30	5.83	7.09	9.10	8.41	9.11	7.74	6.89	95.154
Min.[3]	4.30	4.89	5.81	0.00	6.92	3.94	4.66	6.93	1.46	0.00	0.00	7.43	0.00	75.985
Avg.[4]	9.48	6.53	7.35	2.84	6.92	8.05	5.54	7.03	8.78	5.54	8.92	7.63	4.08	87.780
316	9.52	6.87	7.42	2.39	6.92	8.30	5.73	7.07	9.10	7.73	9.11	7.72	1.78	88.804
317	9.52	6.85	7.42	2.24	6.92	8.30	5.72	7.07	9.10	7.73	9.11	7.73	4.37	91.407
318	9.87	6.26	6.66	3.21	6.92	7.69	5.25	6.97	9.10	2.91	8.38	7.62	6.81	86.657
319	9.87	6.24	6.55	3.58	6.92	7.69	5.23	6.97	8.05	6.50	9.11	7.56	5.96	89.422
320	9.58	6.22	6.40	2.64	6.92	7.68	5.22	6.97	2.18	6.60	9.11	7.53	0.63	75.985
321	9.87	6.21	6.25	2.86	6.92	7.67	5.21	6.96	7.61	4.27	9.11	7.58	0.13	79.137
322	9.87	6.19	6.09	2.28	6.92	7.67	5.19	6.96	8.01	8.00	9.11	7.59	4.12	87.035
323	9.69	6.14	6.16	3.58	6.92	4.57	5.12	6.95	7.72	7.52	9.11	7.52	2.87	82.583
324	9.87	6.43	6.47	3.21	6.92	6.99	5.38	6.99	9.10	8.41	9.11	7.58	6.74	92.639
325	9.52	6.10	6.31	3.15	6.92	7.74	5.52	7.05	7.79	5.45	9.11	7.59	5.48	86.730
326	9.52	6.45	6.62	3.08	6.92	7.86	5.44	7.00	7.94	7.73	9.11	7.66	6.67	91.306
327	9.52	6.51	5.81	3.09	6.92	7.79	5.47	7.00	7.97	7.73	9.11	7.68	6.70	90.589
328	9.52	6.47	6.43	2.50	6.92	7.70	5.44	7.00	8.01	7.73	9.11	7.65	6.64	90.379
329	9.52	6.50	7.42	3.01	6.92	7.89	5.47	7.00	8.01	7.73	8.87	7.70	5.91	91.276
330	9.52	6.31	6.58	2.96	6.92	7.80	5.31	6.98	8.12	7.73	9.11	7.62	5.39	89.559
331	9.52	6.17	6.55	2.61	6.92	7.91	5.22	6.97	8.08	1.29	8.14	7.63	2.87	78.318
332	4.30	6.42	6.45	2.35	6.92	8.07	5.40	6.99	4.55	7.05	9.11	7.46	3.12	76.523
333	9.52	6.28	6.44	2.84	6.92	7.94	5.29	6.98	7.72	7.56	8.87	7.48	4.12	86.981
334	9.52	6.21	7.42	3.12	6.92	7.67	5.26	6.98	7.65	6.91	9.11	7.62	6.43	90.043
335	9.52	6.03	6.23	2.98	6.92	5.60	5.11	6.96	7.61	7.73	8.14	7.53	6.67	85.976
336	9.52	5.94	6.25	2.89	6.92	5.51	4.96	6.93	7.47	7.73	9.11	7.63	0.63	80.043
337	9.52	6.05	6.18	3.15	6.92	4.80	5.06	6.94	7.28	7.73	8.38	7.72	6.63	85.265
338	9.52	6.69	6.45	3.11	6.92	7.85	5.65	7.04	8.01	7.73	8.87	7.65	6.68	91.510
339	9.52	6.49	6.26	3.20	6.92	7.73	5.47	7.00	7.87	7.73	8.14	7.60	6.70	89.851
340	9.52	6.42	6.56	3.58	6.92	7.91	5.45	7.01	7.97	7.73	9.11	7.66	6.68	91.893
341	9.52	6.55	6.22	3.03	6.92	8.11	5.52	7.01	8.01	6.64	9.11	7.57	2.95	86.110
342	9.52	6.47	6.37	3.58	6.92	8.09	5.44	7.00	8.08	7.39	9.11	7.58	6.52	91.412
343	8.41	6.45	7.42	2.31	6.92	8.01	5.43	7.00	4.67	7.73	9.11	7.60	1.70	81.372
344	9.52	6.39	6.11	3.22	6.92	6.14	5.59	7.04	8.16	6.67	9.11	7.45	6.17	87.538
345	9.52	7.11	6.64	2.56	6.92	7.84	5.81	7.08	7.50	7.73	9.11	7.55	3.78	88.272
346	9.52	6.61	6.60	3.20	6.92	7.95	5.55	7.01	7.94	7.45	9.11	7.61	4.62	89.275
347	9.52	6.55	6.29	3.21	6.92	6.82	5.50	7.00	8.01	7.32	9.11	7.58	2.53	85.265
348	9.52	6.35	7.42	3.58	6.92	7.78	5.43	7.01	7.79	7.01	9.11	7.67	1.28	85.797
349	9.52	6.51	7.42	3.58	6.92	8.04	5.51	7.01	7.54	7.73	9.11	7.62	0.58	86.034
350	9.52	6.62	7.42	2.66	6.92	7.92	5.59	7.02	7.87	7.73	9.11	7.70	3.03	88.208
351	9.52	6.50	7.42	3.58	6.92	5.82	5.43	6.99	8.05	7.62	9.11	7.65	3.95	87.635
352	9.52	6.60	7.42	3.58	6.92	5.62	5.54	7.01	9.10	7.73	9.11	7.64	6.63	91.792
353	9.52	6.83	7.42	3.58	6.92	7.39	5.65	7.04	9.10	3.55	9.11	7.56	0.36	82.748
354	9.52	6.52	7.42	3.58	6.92	4.80	5.46	7.00	9.10	0.00	9.11	7.57	2.20	77.595
355	9.52	6.50	7.42	3.58	6.92	6.11	5.42	6.99	9.10	7.11	9.11	7.58	6.61	91.310
356	9.52	6.56	7.42	3.21	6.92	7.19	5.51	7.01	1.46	7.05	9.11	7.56	0.24	77.100
357	9.52	6.38	7.42	3.58	6.92	5.74	5.31	6.97	9.10	7.15	9.11	7.61	6.09	90.135
358	9.52	6.86	7.42	3.15	6.92	8.28	5.69	7.05	8.05	6.91	8.87	7.62	0.00	85.208
359	9.52	6.44	7.42	3.21	6.92	5.94	5.35	6.98	9.10	7.73	9.11	7.62	5.91	90.514
360	9.52	6.77	7.42	3.09	6.92	8.17	5.64	7.03	8.08	1.47	9.11	7.61	0.26	79.624
361	9.52	6.64	7.42	2.68	6.92	7.94	5.58	7.02	7.79	7.32	9.11	7.66	0.67	85.161
362	9.52	6.68	7.42	0.00	6.92	8.02	5.60	7.02	8.16	7.73	9.11	7.67	3.87	86.714

Weighted sub- indices and aggregated water quality index values for Umgeni Water Board

Identity	NH_3 [mg N/ℓ]	Ca [mg Ca/ℓ]	Cl [mg Cl/ℓ]	Chl-a [µg/ℓ]	EC [µS/m]	F [mg F/ℓ]	$CaCO_3$ [mg $CaCO_3$/ℓ]	Mg [mg Mg/ℓ]	Mn [mg Mn/ℓ]	NO_3 [mg N/ℓ]	pH [Unit-less]	SO_4 [mg SO_4/ℓ]	Turb [NTU]	WQI [Unit-less]
Coeff.[1]	0.1035	0.0726	0.0742	0.0358	0.0692	0.0949	0.0587	0.0710	0.0910	0.0909	0.0911	0.0774	0.0696	1.0000
Max.[2]	9.87	7.19	7.42	3.58	6.92	8.30	5.83	7.09	9.10	8.41	9.11	7.74	6.89	95.154
Min.[3]	4.30	4.89	5.81	0.00	6.92	3.94	4.66	6.93	1.46	0.00	0.00	7.43	0.00	75.985
Avg.[4]	9.48	6.53	7.35	2.84	6.92	8.05	5.54	7.03	8.78	5.54	8.92	7.63	4.08	87.780
363	9.52	6.68	7.42	1.27	6.92	8.05	5.60	7.02	8.08	6.60	9.11	7.67	0.95	83.679
364	9.52	6.68	7.42	2.48	6.92	8.08	5.60	7.02	8.05	7.73	9.11	7.69	2.62	87.997
365	9.52	6.64	7.42	2.25	6.92	8.04	5.59	7.02	7.76	7.49	8.87	7.68	4.96	89.334
366	8.87	6.64	7.42	2.90	6.92	8.04	5.59	7.02	7.87	7.45	9.11	7.67	6.68	91.530
367	8.82	6.66	7.42	2.76	6.92	7.97	5.59	7.02	7.28	6.60	8.63	7.66	0.51	82.548
368	8.93	7.15	7.42	3.58	6.92	8.30	5.81	7.08	9.10	7.22	9.11	7.73	4.61	92.371
369	9.05	7.16	7.42	3.08	6.92	8.30	5.82	7.08	9.10	6.67	9.11	7.72	3.98	90.709
370	9.28	7.17	7.42	3.02	6.92	8.30	5.82	7.09	9.10	6.50	9.11	7.72	0.68	87.170
371	9.58	7.18	7.42	3.02	6.92	8.30	5.83	7.09	9.10	4.55	9.11	7.71	0.69	85.395
372	9.23	7.19	7.42	2.98	6.92	8.30	5.83	7.09	7.94	6.47	9.11	7.72	0.51	85.620
373	9.05	6.96	7.42	2.94	6.92	8.30	5.71	7.05	9.10	6.60	8.38	7.74	0.68	85.797
374	9.87	6.97	7.42	2.78	6.92	8.30	5.72	7.05	9.10	7.18	7.41	7.70	5.65	91.411
375	9.52	6.97	7.42	2.97	6.92	8.30	5.71	7.05	9.10	7.22	9.11	7.68	3.45	90.699
376	9.52	6.95	7.42	2.20	6.92	8.30	5.71	7.05	9.10	7.73	9.11	7.69	6.67	93.883
377	9.52	6.92	7.42	2.73	6.92	8.30	5.70	7.05	9.10	7.73	9.11	7.70	4.62	92.198
378	9.52	6.92	7.42	2.69	6.92	8.30	5.70	7.05	9.10	7.73	9.11	7.72	4.37	91.919
379	9.28	6.92	7.42	2.80	6.92	8.30	5.70	7.05	9.10	7.56	9.11	7.69	4.79	92.027
380	9.34	6.93	7.42	3.09	6.92	8.30	5.71	7.05	9.10	7.01	8.14	7.70	3.70	89.607
381	9.52	6.98	7.42	3.11	6.92	8.30	5.71	7.05	9.10	7.32	8.63	7.70	5.30	92.474
382	9.52	6.94	7.42	2.89	6.92	8.30	5.70	7.05	9.10	6.91	8.63	7.67	5.22	91.608
383	9.52	6.93	7.42	3.03	6.92	8.30	5.70	7.05	9.10	7.73	9.11	7.70	5.91	93.946
384	9.52	6.90	7.42	3.01	6.92	8.30	5.69	7.04	9.10	7.11	9.11	7.70	5.30	92.554
385	9.52	6.97	7.42	2.48	6.92	8.30	5.73	7.06	9.10	7.45	8.38	7.70	0.69	86.721
386	9.52	6.95	7.42	2.76	6.92	8.30	5.72	7.06	7.83	7.52	8.38	7.69	3.20	88.383
387	9.52	6.92	7.42	2.29	6.92	8.30	5.70	7.05	9.10	7.73	8.38	7.65	5.22	91.550
388	9.52	6.93	7.42	2.79	6.92	8.30	5.71	7.05	9.10	7.73	8.63	7.69	4.37	91.498
389	9.52	6.99	7.42	2.46	6.92	8.30	5.74	7.06	9.10	7.11	9.11	7.71	6.72	93.684
390	9.23	6.87	7.42	2.97	6.92	8.30	5.68	7.04	9.10	7.73	9.11	7.70	4.79	92.244
391	9.52	6.94	7.42	3.58	6.92	8.30	5.70	7.05	9.10	3.09	9.11	7.67	1.78	85.065
392	9.52	6.96	7.42	3.17	6.92	8.30	5.72	7.05	9.10	6.84	9.11	7.72	4.37	91.553
393	9.52	6.97	7.42	3.11	6.92	8.30	5.72	7.05	9.10	4.73	9.11	7.68	2.03	86.652
394	9.52	6.86	7.42	2.98	6.92	8.30	5.68	7.04	9.10	5.18	9.11	7.69	3.45	88.373
395	9.52	6.92	7.42	2.61	6.92	8.30	5.70	7.05	9.10	6.53	8.63	7.70	4.62	90.266
396	9.52	6.96	7.42	2.43	6.92	8.30	5.71	7.05	9.10	6.74	9.11	7.70	6.66	93.087
397	9.52	6.94	7.42	2.99	6.92	8.30	5.70	7.05	9.10	6.09	9.11	7.70	2.11	88.046
398	9.52	6.94	7.42	2.69	6.92	8.30	5.70	7.05	9.10	6.27	9.11	7.70	5.91	92.016
399	6.12	6.65	7.42	2.64	6.92	8.30	5.66	7.05	9.10	7.15	9.11	7.71	4.54	87.418
400	9.52	6.93	7.42	2.63	6.92	8.30	5.70	7.05	9.10	7.21	9.11	7.71	2.20	88.951
401	9.52	7.02	7.42	1.80	6.92	8.30	5.74	7.06	9.10	7.24	9.11	7.70	4.96	91.212
402	9.52	6.98	7.42	2.24	6.92	8.30	5.72	7.05	9.10	7.32	9.11	7.73	5.22	91.996
403	9.52	7.03	7.42	2.85	6.92	8.30	5.74	7.06	9.10	0.98	9.11	7.69	0.35	80.651
404	9.52	6.99	7.42	3.16	6.92	8.30	5.73	7.06	9.10	1.27	9.11	7.70	0.52	81.443
405	9.52	6.99	7.42	3.07	6.92	8.30	5.72	7.05	9.10	1.71	9.11	7.69	0.62	81.898
406	9.52	6.92	7.42	2.98	6.92	8.30	5.72	7.06	9.10	4.55	9.11	7.71	0.61	84.776
407	9.52	6.96	7.42	3.16	6.92	8.30	5.71	7.05	9.10	6.74	7.90	7.71	0.59	86.032
408	9.52	7.01	7.42	2.99	6.92	8.30	5.73	7.05	9.10	0.42	9.11	7.71	0.63	80.482
409	9.52	6.98	7.42	3.07	6.92	8.30	5.71	7.05	9.10	1.91	9.11	7.70	0.31	81.769

Weighted sub- indices and aggregated water quality index values for Umgeni Water Board

Identity	NH_3 [mg N/ℓ]	Ca [mg Ca/ℓ]	Cl [mg Cl/ℓ]	Chl-a [μg/ℓ]	EC [μS/m]	F [mg F/ℓ]	$CaCO_3$ [mg $CaCO_3$/ℓ]	Mg [mg Mg/ℓ]	Mn [mg Mn/ℓ]	NO_3 [mg N/ℓ]	pH [Unit-less]	SO_4 [mg SO_4/ℓ]	Turb [NTU]	WQI [Unit-less]
Coeff.[1]	0.1035	0.0726	0.0742	0.0358	0.0692	0.0949	0.0587	0.0710	0.0910	0.0909	0.0911	0.0774	0.0696	1.0000
Max.[2]	9.87	7.19	7.42	3.58	6.92	8.30	5.83	7.09	9.10	8.41	9.11	7.74	6.89	95.154
Min.[3]	4.30	4.89	5.81	0.00	6.92	3.94	4.66	6.93	1.46	0.00	0.00	7.43	0.00	75.985
Avg.[4]	9.48	6.53	7.35	2.84	6.92	8.05	5.54	7.03	8.78	5.54	8.92	7.63	4.08	87.780
410	9.52	6.99	7.42	2.81	6.92	8.30	5.72	7.05	9.10	6.57	9.11	7.71	1.20	87.465
411	9.52	6.98	7.42	2.82	6.92	8.30	5.71	7.05	9.10	6.36	9.11	7.71	3.37	89.573
412	9.52	6.97	7.42	2.76	6.92	8.30	5.73	7.06	9.10	6.59	9.11	7.72	0.64	86.834
413	9.52	7.00	7.42	2.70	6.92	8.30	5.72	7.05	9.10	6.81	9.11	7.72	1.45	87.905
414	9.52	6.98	7.42	3.04	6.92	8.30	5.72	7.05	9.10	6.57	9.11	7.72	0.68	87.160
415	9.40	6.99	7.42	2.98	6.92	8.30	5.72	7.05	9.10	6.36	9.11	7.72	0.68	86.763
416	9.52	7.00	7.42	3.16	6.92	8.30	5.73	7.06	9.10	5.82	9.11	7.73	1.45	87.348

Source: Universal water quality index model (2020)

Notes: [1] Fixed parameter weight coefficients, [2] Maximum WQI value, [3] Minimum WQI score and [4] Average WQI values. Water quality parameters are listed according to alphabetic, other than the order of importance. The calculated water quality index values are for Umgeni water quality data for four years from 2012 to 2018.