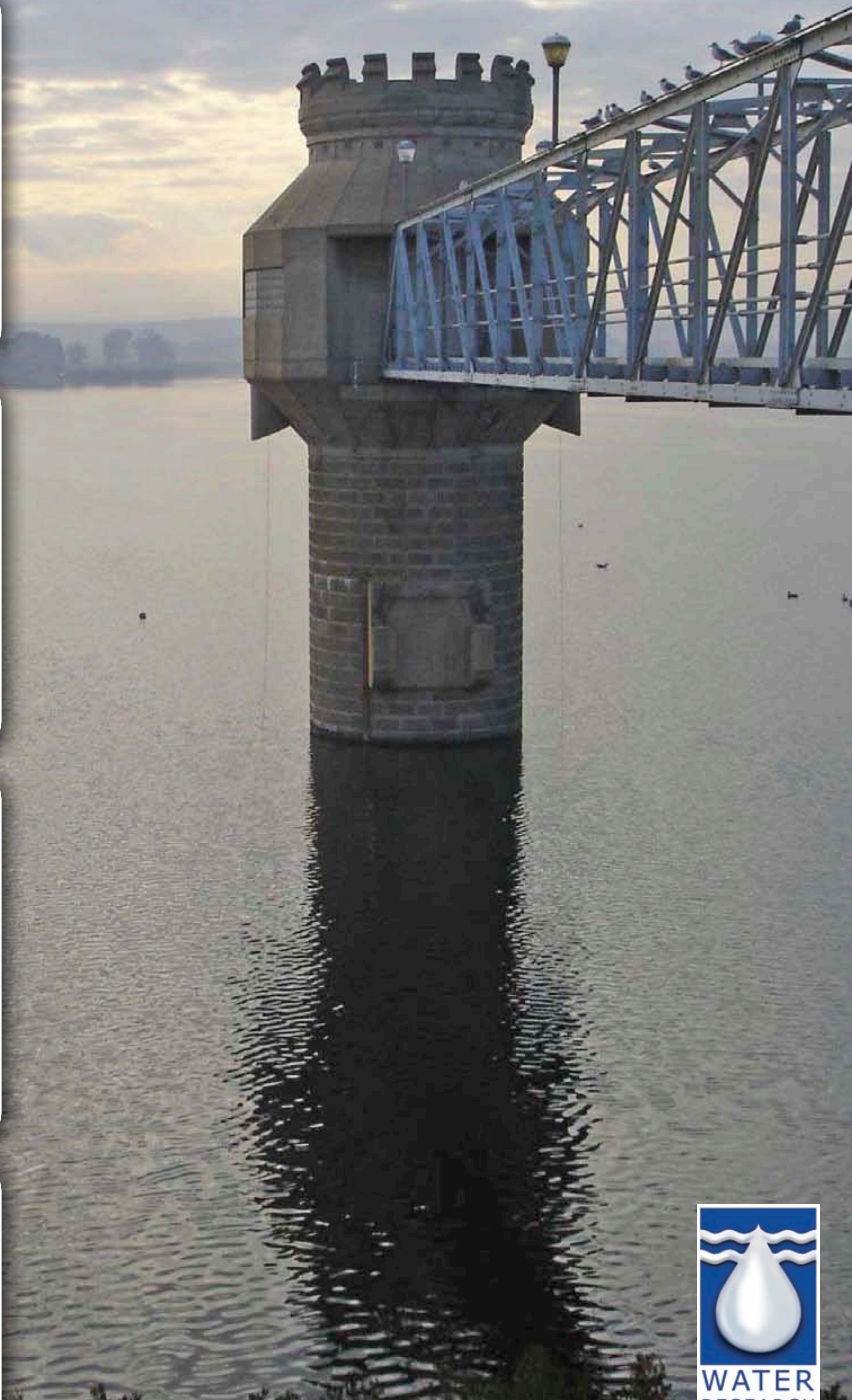
Investigating the Applicability of Ecological Informatics Modelling Techniques for Predicting Harmfull Algal Blooms in Hypertrophic Reservoirs of South Africa



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INVESTIGATING THE APPLICABILITY OF ECOLOGICAL INFORMATICS MODELLING TECHNIQUES FOR PREDICTING HARMFULL ALGAL BLOOMS IN HYPERTROPHIC RESERVOIRS OF SOUTH AFRICA

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EXECUTIVE SUMMARY

1. MOTIVATION

Cyanobacterial blooms and their effects are widespread, frequent and typically seasonal. The increasing number of events of cyanobacterial blooms in South African impoundments and rivers is a cause of concern to the Department of Water Affairs and Forestry (Van Ginkel & Conradie, 2001; Harding & Paxton, 2001; Downing & Van Ginkel, 2002; Van Ginkel, 2003).

Potable drinking water facilities often wait for problems to occur before they initiate interventions to protect users from exposure to potentially toxic events in hypertrophic impoundments. This lack of decision support tools to managers, to be prepared to managing cyanobacteria and algae bloom events, has been a problem throughout South Africa and especially at smaller drinking water facilities. The Ecological Society of America has decided in 2004 that uniformity and training in such tools, namely ecological informatics, is one of the main aims of the society.

Ecological Informatics is defined as interdisciplinary framework promoting the use of advanced computational technology for the elucidation of principles of information processing at and between all levels of complexity of ecosystems – from genes to ecological networks – and aiding transparent decision-making in relation to important issues in ecology such as sustainability, biodiversity and global warming. Biologically-inspired computation techniques such as fuzzy logic, cellular automata, artificial neural networks, evolutionary algorithms and adaptive agents are considered as core concepts of ecological informatics www.waite.adelaide.edu.au/ISEI/.

The use of ecological informatics models is limited in South Africa and a visit of Prof. Recknagel, and the Eutrophication Management Workshop, highlighted the potential for the application of ecological inspired models. The technology of these models is advanced and their applicability to South African ecological systems has not yet been investigated fully.

It is imperative to improve South Africa’s predictive capabilities and the use of these models on South African data will determine the applicability of it to South African ecosystems. This project will address the application of these models in the management of cyanobacterial blooms in South African conditions.

The preliminary testing of the model SALMO and the preliminary results of the pattern analysis by non-supervised artificial neural networks on data from Roodeplaat Dam emphasized the need to investigate the full potential use of these models and that the application of these models may be highly applicable to South African conditions.

The Department of Water affairs and Forestry has data available for a number of impoundments that can be used to test different models for application as management tools in the National Eutrophication Monitoring Programme. The outcome of the project will benefit South Africa nationally and locally because the application of the models will have been tested on South African resource data. Local capacity to use and apply these models will be improved after an Ecological Informatics Workshop and the applicability to other ecosystems have been made known to other researchers in South Africa. A cyanobacterial bloom prediction tool to be used by local water resource managers will be one of the major outcomes of the project. The model application will improve our knowledge regarding the limnological conditions within and the management of eutrophication in South African dams.

Hypothesis

A number of hypotheses were set before the commencement of the study to be included in the investigation and the development of a predictive tool for harmful algal blooms:

1) A holistic approach is required to accommodate different levels of external (climate) and internal (trophic linkages and benthic-pelagic coupling) variability and their interactions. Therefore, the integration of biological and meteorological information is needed to understand and estimate the consequences of climate variations on the development of toxic cyanobacterial blooms.

   A detailed literature survey was done to determine the most important physical, chemical and biological factors in the development of harmful algal blooms. The literature survey also investigated the potential impact of climatic conditions on the development of harmful algal blooms, with special reference to cyanobacteria, which is the largest noxious phytoplankton problem within South African fresh water systems.

This hypothesis also led to the inclusion of a number of climatic variables in the statistical analysis of the collected data, to determine the potential use of climatic variables in predicting harmful algal blooms.

2. A water body is one entity and when a cyanobacterial bloom does occur, there are toxins to be found in the system.

   This hypothesis aimed to investigate the distribution and potential for toxic cyanobacteria that may impact on recreational users, even though the regular sampling site does not indicate any or low cyanobacterial toxicity within the water column.

3. Ecological Modelling methods are available to be tested and used to predict harmful algal blooms.

   This hypothesis was tested and proved to be quite applicable in the hypertrophic reservoirs of South Africa.

2. OBJECTIVES

1. To write a comprehensive literature review on the use of various methods to predict algal blooms and the application of these tools.

2. To collect and collate an extensive dataset of five eutrophic impoundments in South Africa containing climatological data, physical and chemical data.

3. To adapt the deterministic SALMO OO model for application as an algal bloom prediction tool for use by local water resource managers and potable water treatment works.

4. To apply ecological informatics in the field of algal bloom prediction.

5. Organise an Ecological Informatics Workshop to make known the cyanobacterial toxin prediction tool and to expand South African knowledge on the application of artificial neural network modelling and evolutionary algorithim approaches in ecosystem research

3. RESULTS AND DISCUSSION

The hypertrophic reservoirs, Bon Accord, Hartbeespoort, Klipvoor, Rietvlei and Roodeplaat, situated in South Africa are, warm monomictic reservoirs, downstream of the most populated areas of South Africa. These reservoirs are known to experience annual cyanobacterial blooms of especially, the toxin producing cyanobacterium, *Microcystis aeruginosa*. These reservoirs lie within similar climatic conditions, with warm wet summers and dry, fairly cold winters. With this study in mind, five years of monitoring to determine the phytoplankton community trends and the presence of cyanobacterial toxins was initiated. During these five years Hartbeespoort and Roodeplaat were dominated primarily by *Microcystis aeruginosa.* Bon Accord, Klipvoor and Rietvlei reservoirs experienced both *Microcystis aeruginosa* and *Ceratium hirundinella* blooms annually.

Total microcystin (TM) concentrations were found to be orders of a magnitude higher in South Africa (> 10 000 ug/L) than in other countries (between 10 ug/L and 100 ug/L). The presence of TMs in all the reservoirs was primarily associated with the dominance and blooms of *Microcystis aeruginosa*. The depth distribution of the toxins measured in the Hartbeespoort and Roodeplaat Reservoirs indicated that during the periods of excessive *Microcystis aeruginosa* biovolume, toxins are often found all the way through the water column.

Multivariate analyses of the reservoir's data indicated that the five reservoirs are similar in both algal community and physico-chemical variables. The multivariate analyses showed that of the environmental factors, temperature is the most important factor, and can be used as an indicator of climatic conditions, in the development of cyanobacteria biovolume in these systems. Other environmental variables important to the development of algal blooms are dissolved inorganic phosphorous (DIP), dissolved inorganic nitrogen (DIN), the DIN:DIP ratio; total phosphorous (TP), total nitrogen (TN) and Chl *a* concentration.

A number of generic and deterministic ecological models were tested on the data to determine their applicability for predicting harmful algal blooms in hypertrophic reservoirs in the northern central parts of South African. A summary of the key findings are as follows:

1) The relatively simple Vollenweider model is easy to apply and provides a manager with a quick answer. Relatively little information is needed to apply the model. It also provides the manager with the possibility of testing different management scenarios.

2) The simulation library SALMO-OO allows forecasting abundances of cyanobacteria, green algae and diatoms in response to eutrophication control scenarios. It takes the complex limnological characteristics of reservoirs into consideration and it supplies the manager with a tool to test different management scenarios to assist in decision-making. The results were, however, only partly successful with large over and under predictions of nutrients and algal groups, even after the growth equations were adapted.

3) Artificial neural network modelling techniques, both the supervised multilayered feed forward neural network and the non-supervised self-organising map were tested for the applicability to predict algal blooms in South African hypertrophic reservoirs.

   The multi-layered feed forward neural network model tested, provides visual predicted successes, but the strict tolerances set by the model, to determine acceptable prediction as part of the outcome of the model, may be a problem to validate the results and ensure that an acceptable amount of good predictions were found.

   The Self Organising Mapping (SOM) method technique is applicable to investigate before and after impact scenarios. This is more of a knowledge development tool than a predictive tool.

4) Finally, the Hybrid Evolutionary Algorithm (HEA) method was used to develop algorithms for algal bloom prediction. The RULE set discovery by HEA was tested on long-term data in three reservoirs using different scenarios of real time, 7-days forward, 14-days forward, 21-days forward and 28-days forward forecasting respectively of the abundance of the cyanobacterium, *Microcystis aeruginosa*. The developed rule sets are highly applicable to the hypertrophic reservoirs of South Africa. These methods however need, to be tested in other South African reservoirs to determine the applicability under different trophic status and different climatic conditions.

The same method was used to develop a real time algorithm for the dinoflagellate, *Ceratium hirundinella*. The developed RULE set was then tested on the data of two "unseen" reservoirs (Bon Accord and Klipvoor) that both experienced extreme *Ceratium hirundinella* blooms during the study period. This application was found to be highly applicable to these reservoirs. This suggests that the developed RULE set may potentially also be applicable to reservoirs in other climatic areas of South Africa.

Recommendations:

The study showed that eutrophication and the associated problems is a real threat to South African fresh water resources but that modelling methods do exist to assist in managing the problem. The list of recommendations needs to be taken further by a number of stakeholders, e.g. the Department of Water Affairs and Forestry, future CMAs, Universities and other researchers:

a) The project determined the necessary variables and institutions should monitor these variables for future modelling exercises.
b) Include total microcystin monitoring in impacted fresh water resources at least during the summer periods to enable resource managers to issue warnings to all potentially impacted stakeholders.
c) Initiate and test available management options to minimise serious eutrophication levels in South Africa.
d) Manage the risk imposed by the cyanobacterial blooms and the associated toxins produced in the water resources, on drinking water facilities and the health of recreational users.
e) In view of the successes of the modelling results initiate the testing of the developed tool in the short-term forecasting, for the algal blooms of *Microcystis* and *Ceratium,* to develop on-line water quality monitoring for early-warning and real-time forecasting for reservoir managers.
f) The cause and effects of the changing composition of the phytoplankton (increasing Dinoflagellate blooms) for these five reservoirs need to be investigated.
g) Institutions involved in reservoir management or use should monitor at different depths to determine the best depth for abstraction for treatment purposes.

h) Initiate, develop and maintain capacity in South Africa to use the Hybrid Evolutionary Algorithm (HEA) RULE set development in all research spheres, as the method is applicable to any type of numerical data.

4. INFORMATION AND KNOWLEDGE DISSEMINATION

4.1 Workshop

As part of the original contract it was agreed to host a workshop in collaboration with Prof Friedrich Recknagel and other WRC research programs using similar research techniques. The workshop: *Applicability of Modeling techniques and Biomanipulation in the aquatic environment* was held from 28-30 July 2008. The workshop was attended by 50 delegates from different companies and institutions in the water related industry. The well-known Ecological Informatics Specialist, Prof Friedrech Recknagel from Adelaide University, was the key speaker at the workshop. Prof Recknagel has experience in Lake Catchment restoration and management, wetlands management and the predictive modelling of aquatic ecosystems. Various other South African specialists in the field also attend as speakers, namely Mr M Watson; Dr M Graham, Dr W Harding, Dr S Jooste and Mr N Rossow.

4.2 Conferences attended

Bezuidenhoudt, J, Van Ginkel, CE, Du Plessis, S & Van Rensburg, L. Applicability of ANN models as a possible early warning tool for algal bloom prediction. Fourth International Conference on Environmental Science and Technology, 28-31 July 2008, Houston Texas, USA. Paper

4.3 Papers published

VAN GINKEL, CE, SILBERBAUER, M.J., DU PLESSIS, S. AND CARELSEN, CIC (2006). Monitoring microcystin toxin and chlorophyll in five South African impoundments. Verh. Internat. Verein. Limnol. (29): 1611-1616.

During November 2007 Mrs Van Ginkel submitted in her PhD thesis at the North-West University, Potchefstroom. The thesis titled: *Investigating the applicability of ecological* *informatics modelling techniques for predicting harmful algal blooms in hypertrophic reservoirs of South Africa*,

5. PROJECT CAPACITY DEVELOPMENT

Dr CE van Ginkel obtained her PhD during 2008. Her thesis included all of the work discussed in this report. During this research program, Mr Jaco Bezuidenhout significantly expanded his expertise in the fields of statistical analyses and modelling. He also had the opportunity to present the work he had done at an international conference.

After the workshop, Prof Recknagel and his collaborator Prof Chen from Beijing University, Beijing China, agreed to present a short course in Ecosystems modelling at the North West University, Potchefstroom as from 2009. The course will be managed by Dr S du Plessis.

ACKNOWLEDGEMENTS

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Steering Committee:

Dr S Liphadzi – Chairman
Dr S Mitchell – WRC
Prof L van Rensburg – NWU
Dr S Jooste – DWAF
Dr N Griffen – RU
Me L Coetzee – Tshwane Rietvlei
Me A Swanepoel – Rand Water
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LIST OF ABBREVIATIONS

Alk	Total alkalinity as $CaCO_3$
Ana_B	*Anabaena* biovolume
Asl	above sea level
ATMax	Maximum air temperature on day of sampling
ATMin	Minimum air temperature on day o sampling
BA	Bon Accord
Ca	calcium
ChlA	chlorophyll *a*
ChloroBi	Chlorophyte biovolume
ChrysoBi	Chrysophyte biovolume
Cl	chloride
CPV	Cumulative percentage variance
CryptoBi	cryptophyte biovolume
CTMax	Maximum cyanobacterial toxin concentration
CTMean	Mean cyanobacterial toxin concentration
CTMin	Minimum cyanobacterial toxin concentration
CTTot	Total cyanotoxin producing group biovolume
CyanoBio	cyanophyte biovolume
Cyl_B	*Cylindrospermopsis* biovolume
DIN	Dissolved inorganic nitrogen (NO_3 + NO_2 + NH_4 -N)
DIN:DIP	Dissolved inorganic nitrogen to dissolved inorganic phosphorous ratio
DIP	Dissolved inorganic phosphorous (measured as PO_4-P)
EC	Electrical conductivity
EV	Eigenvalue
EuglenoB	Euglenophyte biovolume
z_{eu}:z_{mix}	euphotic depth: mixing depth ratio
fsl	full supply level
HBP	Hartbeespoort
HEA	Hybrid evolutionary algorithm
K	potassium
KV	Klipvoor
MATMax14	Mean maximum air temperature 14 days before sampling
MATMin14	Mean minimum air temperature 14 days before sampling
MIB	2-methylisoborneol
Mg	magnesium
Mic_B	*Microcystis* biovolume
MT	Mean daily temperature
MT5	Mean temperature 0-5m in water column
Na	sodium
NH_3	Ammonia
Osc_B	*Oscillatoria* biovolume
OxyDV	Oxygen depleted volume
PCA	Primary component analysis.
pH	Is the logarithm of the reciprocal of the concentration of free hydrogen ions. It measures the activity of the hydrogen ion.
PhyrrBio	Phyrrophyta biovolume (dinoflagellates)
Pse_B	*Pseudoanabaena* biovolume

Rad	Radiation on day of sampling
Rad14	Mean Radiation 14days before sampling
RDA	Redundancy analysis
RDP	Roodeplaat
RV	Rietvlei
Secchi	Secchi disc reading
SO_4	Sulphate
Spec/Env Corr	Species and environmental variable correlation
TDS	Total dissolved salts
Tin14	Total inflow 14 days before sampling
TM	Total microcystin
TMO	Total monthly outflow
TN	Total nitrogen (KN + NO_2 + NO_3)
TN:TP	Total nitrogen to total phosphorous ratio
TotNONCT	Total non-cyanotoxin producing group biovolume
TotVol	Total volume on day of sampling
TP	Total phosphorous
TR14	Total rainfall 14 days before sampling
TV	Total variance
WST	Water surface temperature

CHAPTER 1

INTRODUCTION

Worldwide and in South Africa, there seem to be an increase in the frequency of cyanobacterial and dinoflagellate blooms recorded (Codd *et al.*, 2005; Guven & Howard, 2006; Harding & Paxton, 2001; Van Ginkel *et al.*, 2001). This may be the result of increased eutrophication and/or increased and more effective monitoring of phytoplankton in the water resources. A number of factors can contribute to the phenomenon, of which the impact of global warning (Burroughs, 2003; Guven & Howard, 2006; IPCC, 1992; Mitchell, 1991 as quoted by Kunz *et al.,* 1995) and the then likely increases in water temperatures (Van Ginkel & Silberbauer, 2007), especially the increases in minimum temperatures (Kunz *et al.,* 1995; Mühlenbruch-Tegen, 1992) is but one.

Cyanobacteria blooms, as a symptom of eutrophication, have a notorious reputation to develop rapidly in biovolume from obscurity to massive blooms in nutrient enriched systems. It can then just as abruptly recede. Some waters exhibit frequent and even sustained aggregations of cyanobacteria, while others experience evanescent, but often extremely noxious growth events. A significant proportion of cyanobacteria genera produce one or more of a range of cyanotoxins (WHO, 1999) and many are associated with taste and odour problems for Water Treatment Works (Swanepoel *et al.*, 2007). If water containing high cyanobacterial toxin concentrations is ingested (in drinking or in recreational waters), they present a risk to human and animal health (Pouria *et al.*, 1998; WHO, 1999).

The hypertrophic reservoirs, Bon Accord, Hartbeespoort, Klipvoor, Rietvlei and Roodeplaat, in South Africa are warm, monomictic reservoirs, known to experience annual cyanobacterial blooms of the toxin producing *Microcystis aeruginosa* (Robarts, 1984; NIWR, 1985; Chutter, 1989; Zohary & Robarts, 1989; Chutter & Rossouw, 1991; Van Ginkel *et al.*, 2000a; Van Ginkel *et* al., 2000b, Harding *et al.*, 2004a). Hartbeespoort, Rietvlei and Roodeplaat reservoirs release water to downstream Water Treatment Works that withdrew water for potable use, and this presents a potential threat to the health of users. The extent of geosmin, MIB and cyanobacterial toxins associated with the cyanobacterial blooms highlighted the need to develop trustworthy short and long-term forecasting for hypertrophic systems so that Water Treatment Works can prepare for these algal bloom events.

These harmful algal/cyanobacterial blooms, often experienced in South African hyper-eutrophic fresh water systems, and its unpredictability, usually catch the water resource manager off-guard. Toxicity of these blooms is equally unexpected as blooms are not necessary toxic according to the literature. The water resource manager needs a modelling tool that can predict harmful bloom formation based on physical and chemical characteristics of the impoundment, including climatic conditions.

The main aim of this project was to investigate the applicability of ecological infomatics modelling techniques to develop a predictive tool for harmful algal blooms in South Africa. This will enable water resources managers, managers of water treatment facilities and managers of recreational water use to be prepared for harmful algal blooms, e.g. 1) In planning management action timeously, 2) in purchasing activated carbon, and 3) To plan recreational activities and warn recreational users.

A number of hypotheses were set before the commencement of the study to be included in the investigation and the development of a predictive tool for harmful algal blooms:

1.1 In ecological studies a holistic approach is required to understand how ecosystems accommodate different levels of external (climate) and internal (trophic linkages and benthic-pelagic coupling) variability and their interactions. The integration of biological and meteorological information is needed to understand and estimate the consequences of climate variations on the development of toxic cyanobacterial blooms.

A detailed literature survey was done to determine the most important physical, chemical and biological factors in the development of harmful algal blooms. The literature survey also investigated the potential impact of climatic conditions on the development of harmful algal blooms, with special reference to cyanobacteria, which is the largest noxious phytoplankton problem within South African fresh water systems.

This hypothesis also led to the inclusion of a number of climatic variables in the statistical analysis of the collected data, to determine the potential use of climatic variables in predicting harmful algal blooms.

1.2 A water body is one entity and when a cyanobacterial bloom does occur, there are toxins to be found in the system.

This hypothesis aimed to investigate the distribution and potential for toxic cyanobacteria that may impact on recreational users, even though the regular sampling site does not indicate any or low cyanobacterial toxicity within the water column.

1.3 Various Deterministic and Ecological Modelling methods are available to be tested for the applicability to predict harmful algal blooms.

A number of different types of models were tested and variable successes were achieved. The Hybrid Evolutionary Algorithms proved to be quite useful to develop algorithms that can be used in the prediction of cyanobacterial and algal bloomforming species in the hypertrophic reservoirs of South Africa.

Five years (October 2000-September 2005) of data was collected on the above mentioned five hypertrophic reservoirs to test the hypothesis and to use in the ecological modelling of blooms of harmful algal genera. Climatic variables were included to determine the potential impact of the weather patterns on the development of the problem algae/cyanobacteria. Another fourteen years of additional data was extracted from the Water Management System (WMS) of the Department of Water Affairs and Forestry and was used in the Hybrid Evolutionary Algorithm method to develop predictive capability.

CHAPTER 2

MODELLING METHODS

2.1 VOLLENWEIDER MODEL

The Vollenweider Model is a simple empirical model based on the relationship between the total phosphorus and Chl *a* measured in a system, rather than understanding the biological processes of the system. The Vollenweider model was developed as an eutrophication management tool. It does not provide information on the algal or cyanobacterial species that may pose a problem in a system (Vollenweider, 1976).

$$\mathbf{Chl}\ \boldsymbol{a} = \mathbf{0.28 * TP^{0.98}} \qquad \textbf{(2.1)}$$

Where Chl *a* is the predicted mean Chl *a* concentration in mg/m^3 which is equal to ug/L and TP is the mean total phosphorus concentration in the early summer measured in mg/m^3.

$$\mathbf{TP = (L * t) / z * (1 / (1+ sqrt(z)))} \qquad \textbf{(2.2)}$$

Where:

- L is the specific phosphorus load (mg/m^2/year).
- t is the water residence time determined as volume/flow.
- z is the mean water depth measured in meter and determined as volume/surface area.

Case studies were done for the hypertrophic Hartbeespoort, Klipvoor and Roodeplaat Reservoirs looking at different management scenarios as inflow data that is essential for applying the Vollenweider Model, was available for these three Reservoirs. Bon Accord and Rietvlei Reservoirs were excluded because of a lack of inflow data.

The information needed to do the Vollenweider model is shown in Table 1.

Table 1: Method to determine the constant parameters included for the Vollenweider Model.

Parameter	Definition	Unit	Calculation
TAI	Total Annual Inflow	m^3/year	Sum of 365 consecutive daily flows
MIP	Mean In stream PO^4-P	mg/m^3	Annual Average PO^4-P concentrations
MAPL	Mean Annual PO^4-P load	mg/year	TAI x MIP
SA	Surface Area	m^2	Known surface area at full supply level
PAL	Phosphorus Area Load	mg/m^2/year	MAPL/SA
V	Volume	m^3	Volume at full supply level
RT	Residence Time	year	V/TAI
MD	Mean depth	m	V/SA
TP	Mean Annual Total phosphorus	ug/l	Annual Mean TP concentrations to determine the effectiveness and applicability of the model
Chl *a*	Mean Annual Chl *a*	ug/l	Annual Mean Chl *a* concentrations to determine the effectiveness and applicability of the model

Three management scenarios were investigated, namely a) TP reduction by 50%, b) TP elimination by 90%, and c) Doubling of the residence time.

2.2 SALMO MODEL

The SALMO model developed by Bendorf and Recknagel (1982), is a process-based deterministic model that uses inflow, PO_4-P and NO_3-N concentrations in the inflow, solar radiation and water temperature to determine phytoplankton biovolume, functional algal groups, zooplankton biovolume and oxygen concentrations in the lake. Although only a few input variables are considered the model considers a great number of internal control mechanisms. The model has been tested on a number of lakes with different trophic states by Bendorf and Recknagel (1982).

Constant parameters determinations are shown in Table 2. The number of the first decade of ice cover in South Africa is 1, as no ice cover is found. The first four constant parameters are basically determining the different seasons, while the other constants indicate the start situation in the reservoir regarding biological conditions and nutrient and oxygen concentrations as well as the underwater light conditions.

Table 2: Methods to determine the constant parameters included in SALMO.

Parameter	**Definition**	**Unit**	**Calculation**
STW	Number of first decade with ice cover		
VZF	Number of first decade after ice cover		
STS	Number of first decade with thermocline		
VZH	Number of first decade after thermocline		
X1(0), X2(0), X3(0)	Biovolume of cyanobacteria on day 1 Biovolume of diatoms on day 1 Biovolume of green algae on day 1	cm^3/m^3 cm^3/m^3 cm^3/m^3	(Chl *a* x %Cyanobacteria x 0,75) x 3 (Chl *a* x %diatoms x 0,75) x 3 (Chl *a* x %Chlorophyta x 0,75) x 3
Z1(0)	Biovolume of zooplankton on day 1	cm^3/m^3	Not available
D(0)	concentration of detritus on day 1	mg/l	[Suspended Solids]
P(0)	concentration of PO4-P on day 1	mg/l	[PO4-P]
N(0)	concentration of NO3-N on day 1	mg/l	[NO3-N]
O(0)	concentration of diss. oxygen on day 1	mg/l	Average [DO] for 0-5 m depth
LTMAX	Maximum underwater light transmission		$LTMAX = (\varepsilon_{min} – 0.92)/(-0.46)$ $\varepsilon_{min} = 4.6 / (1.7*z_{secchi})$

SALMO-OO data input start with the winter period and the data for Roodeplaat, Hartbeespoort and Klipvoor dams for the period July 2003 to June 2004 was prepared as 36decade periods as required by SALMO-OO. All the input variables required by SALMO-OO, the units and the method of calculation are shown in Table 3. The daily inflows of the Hartbeespoort, Klipvoor and Roodeplaat dams were available and it is essential in the model. It was decided to exclude Bon Accord and Rietvlei from this section as no flow data, which is essential for the SALMO-OO Model, was available.

Table 3. Methods to determine the input variables included in SALMO.

Variable	Definition	Unit	Calculation
V	Total water volume of the whole lake	million m^3	Calculate V for total water depth of day 1 of each decade by means of the depth to volume relationship
VE	Epilimnion water volume	million m^3	Calculate difference of V-VH
VH	Hypolimnion water volume	million m^3	Calculate VH for hypolimnion depth of day 1 of each decade in summer by means of the depth to volume relationship
ZMIXREAL	Maximum water depth of lake during spring, autumn and winter or Depth of thermocline during summer	m	To be determined by depth at which maximum temperature difference per meter occurs
ZMIX	Mean mixing depth of total volume or epilimnion	m	Ratio of total volume V to total area during spring, autumn and winter or Ratio of epilimnion volume VE to total area during summer
ZHM	Mean mixing depth of hypolimnion	m	Ratio of hypolimnion volume VH to hypolimnion area during summer
QIN	Mean daily flow of streams entering the lake surface	m^3/day	
QHIN	Portion of the mean flow of streams entering the hypolimnion	m^3/day	
QOUT	Mean daily outflow from the lake surface	m3/day	QOUT = $(\Sigma QIN - (V_{i+1} - V_i))/10$
QHOUT	Mean daily outflow from the hypolimnion	m3/day	
SRF	Factor reflecting strong rain events with implications for limiting underwater light	-	Absolute maximum ratio of flow measurements of consecutive days for each decade: abs(max (Q_i/Q_{i-1}))
I	Mean global solar radiation	J/cm^2 /day	
T	Mean water temperature over the lake depth or the epilimnion depth	°C	
TH	Mean water temperature over the hypolimnion depth	°C	
PIN	Weighted mean PO4-P concentration of streams entering the lake	mg/m^3	
NIN	Weighted mean NO3-N concentration of streams entering the lake	g/m^3	
POMIN	Weighted mean detritus concentration of streams entering the lake	g/m^3	In-lake suspended solids concentration

A study by Cetin *et al.* (2005) investigated more process models for algal growth and grazing to be implemented in SALMO-OO to determine the applicability of such libraries of different growth and grazing equations on the modelling of lake ecosystems of different trophic status and climate. The original SALMO-OO model was used in this study. The growth and grazing equations of Arhonditsis and Brett (2005), a model developed for the eutrophic Lake Washington (USA), was used additionally to improve the results. The main differences in the two models are the maximum photosynthesis rate per day, the half-saturation constant for P uptake by algae, phytoplankton settling velocity, optimum temperature for phytoplankton growth and the preference factor for each algal functional group.

2.3 ARTIFICIAL NEURAL NETWORKS (ANN)

Neural networks are simple computational tools for examining data and developing models that help to identify interesting patterns or structures in the data. The data used to develop these models is known as training data. Once a neural network has been exposed to the training data, and has learnt the patterns that exist in the data, it can be applied to new data (the testing data) thereby achieving a variety of outcomes (Smith, 2002).

The method of ANN has been inspired by the biological nervous system, hence the name of the modelling technique. One of the most significant advantages of ANN is their ability to learn from a limited set of data. A well-trained and verified ANN for the specific problem at hand recognises the data and makes predictions with often desirable accuracy (Karul and Soyupak, 2006). However, one has to be wary of the pitfalls of neural networks, e.g. overtraining of a limited data set. Where too much training occurs, the network only memorizes the training set and loses its ability to generalize to new data (Mendelsohn, 1993).

Two known types of ANN, a) the multilayered feed forward neural network (MFNN) and b) the self-organising map (SOM) were tested and are discussed as part of the study.

2.3.1 Multilayered Feed Forward Neural Network (MFNN)

The multilayered feed forward neural network (MFNN), is an example of a neural network trained with supervised learning (Rumelhart & McClelland, 1986). With the models that have supervised learning, the data used for training contains the complete information about the characteristics of the data and the observable outcome. The study aims at developing a model that can learn the relationship between the inputs (the environmental variables) and the outputs (the algal groups). The MFNN is trained repeatedly with numerical data of the inputs and the outputs in order to develop a model by learning to represent the relationships correctly (Figure 1). The method includes a three layer feed forward neural network.

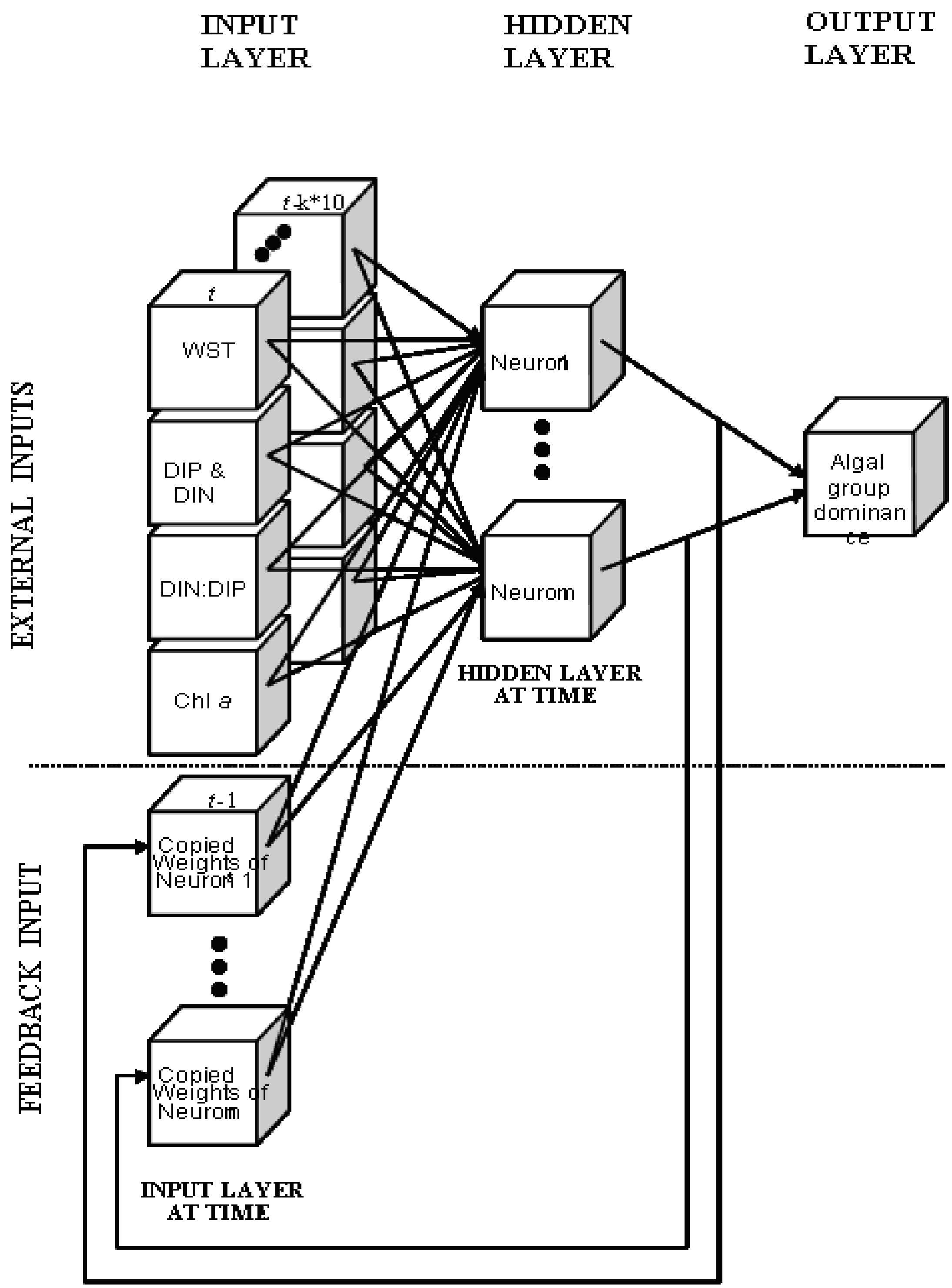


Figure 1 The structure of the supervised MFNN as used in this study (redrawn from Recknagel *et al.*, 2006).

The input layer in this study, includes the variables WST, DIP, DIN, DIN:DIP and Chl *a*. This then feeds into the hidden layer (Neuron 1-n), which is fed into the feedback inputs. The final layer is the output, in this case the algae group as determined by the input data.

The software package initially selected for the study was NeuroSolutions 5.04, by NeuroDimensions Inc. Due to certain limitations encountered during the study, the package Forecaster XL, was subsequently selected. Both NeuroSolutions 5.04 and Forecaster XL are subsequently discussed.

2.3.1.1 NeuroSolutions 5.04

The multivariate analysis the final set of environmental variables used for the training of the artificial neural networks (ANN) included the following measured parameters: water surface temperature (WST), dissolved inorganic phosphorous (DIP), dissolved inorganic nitrogen (DIN), the DIN:DIP ratio; and Chl *a* concentration. Furthermore, the community data was grouped into cyanotoxin (CT) producers and non-cyanotoxin producers (Non-CT) to simplify the modelling process.

2.3.1.2 Forecaster XL

The same data used with NeuroSolutions 5.04 was re-analysed with the Forecaster XL package, another MFNN. Firstly, the single dam (Hartbeespoort Dam) data was analysed (Experiment 1-4). Secondly, the analysis was done on the five reservoirs data (Experiment 5-12). In both these investigations, three approaches were followed to attempt the best fit and to determine the usefulness of the modelling techniques to South African Reservoirs and the importance of the main variables on the outcome of the model.

a) Firstly, prediction of the algae blooms with only the environmental variables included and without the measured algae dominance, and
b) Secondly, including the environmental variables as well as the algae dominance data.
c) Thirdly, including the environmental variables, algal dominance and Chl *a*.

The cyanobacteria were divided into two different groups, namely the Non-cyanotoxin group (Non-CT) and the Cyanotoxin producing group (CT). The Non-CT group included species like

Pseudoanabaena and *Merismopedia.* The CT group included all the known cyanobacterial toxin producers, e.g. *Microcystis*, *Anabaena*, *Oscillatoria* and *Cylindrospermopsis*.

2.3.2 Self-Organising Map (SOM)

The second type of neural network investigated is the self-organizing map (SOM). SOM is the most common example of a neural network, trained with un-supervised learning, and was developed by Kohonen (1982; 1988). The SOM requires that the data contain inputs that describe the characteristics of the variables or fields. The SOM then learns to ordinate and cluster or segment the data based on the similarities and differences of the input variables only (Smith, 2002, Recknagel *et al*., 2006).

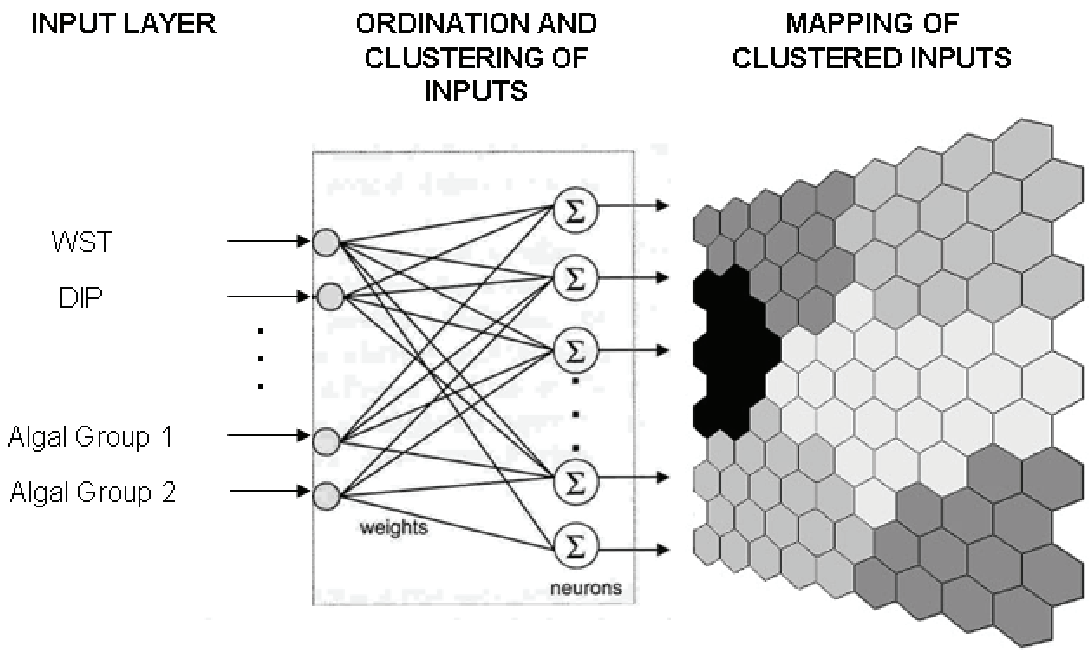


Figure 2 The structure of the non-supervised SOM for ordination and clustering of inputs (redrawn from Recknagel *et al.*, 2006)

The SOM also has an input layer with the known variables and a hidden layer where the ordination and clustering are created with the mapping of the clustered output as the output layer (Figure 2).

The learning process, in the hidden layer, is roughly as follows:

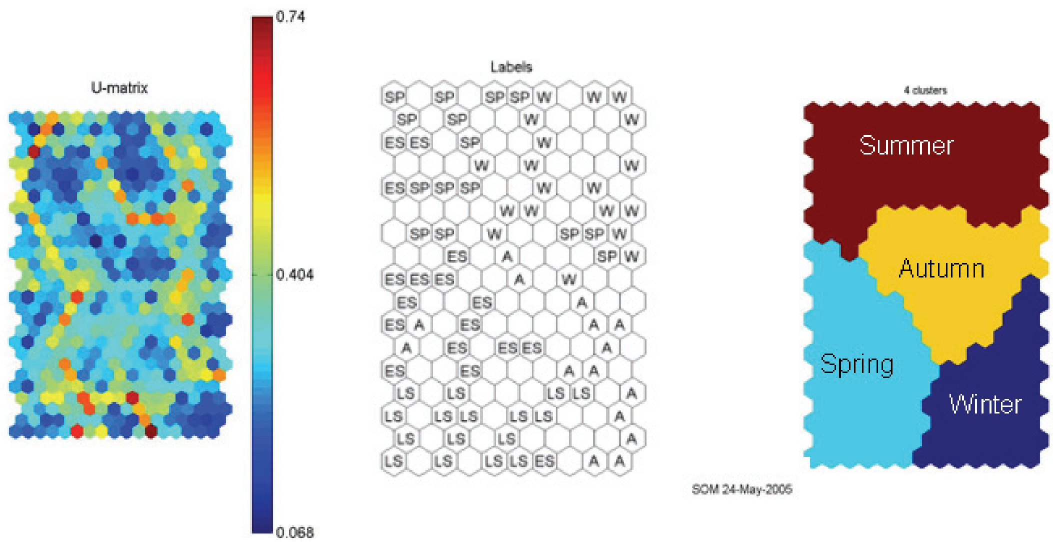
a) It initialises the weights for each output unit;

b) It cycles until weight changes are negligible for each input pattern (by presenting the input pattern, finding the winning output unit, finding all units in the neighbourhood of the winner and update the weight vectors for all those units; and

c) It reduces the size of neighbourhoods if required (Kohonen, 2007).

The non-supervised SOM as introduced by Kohonen (1982, 1988) was applied to the before and after impact data sets to ordinate, cluster and map the nutrients, Chl *a* and algal groups with respect to seasons to determine if significant changes took place since the establishment of the Zeekoegat WCW that discharge directly into the Roodeplaat Reservoir.

The result of the training of the non-supervised SOM, by means of the normalised input data the Euclidean distance between the inputs, is calculated and then visualised as a distance matrix (the U matrix – Fig. 3a) and a partition map (K-means) (See Fig. 3b).



a) Distance matrix map (U-matrix) b) Partitioned map (K-means)

Figure 3 The non-supervised SOMs ordination and clustering maps shown as a) a distance matrix map and b) a partitioned map (Redrawn from Recknagel *et al.*, 2006)

The criteria for the ordination of the seasons are shown in Table 4 and were selected using the air temperatures.

Table 4 The classification of seasons for the SOM modelling

Classification Criteria	Period
Summer	November-March
Autumn	April-May
Winter	June-July
Spring	August-October

2.4 Rule development by Hybrid Evolutionary Algorithms (HEA)

The bi-weekly data from three reservoirs, the Hartbeespoort, Rietvlei and Roodeplaat reservoirs for the period 1991 to 2004 were used. Simple linear interpolations were done with each data variable from each reservoir to create daily data sets. These interpolated data sets for the Hartbeespoort, Rietvlei and Roodeplaat Reservoirs were merged because of the similarity in hypertrophic and climatic conditions and because the CANOCO analysis showed that, there was no distinct difference between the studied hypertrophic systems. For this study the data training were done with data from 1991 to 2003, and 1993 and 2004 were used for testing the rule sets, giving a total of 36 years for training and 6 years for testing. These two years were chosen because the extent of *Microcystis* dominance was low in 1993 and high in 2004 in the Hartbeespoort Reservoir. This enables the modeller to determine if the extent of high values and low values can be correctly forecasted (Recknagel, 2006, *Pers. Comm.*).

A number of experiments were done to determine the potential to use the developed rule set for prediction of real time forecasting of *Microcystis*, 7-days, 14-days, 21-days and 28-days ahead forecasting including Chl *a* as one of the environmental variables. One experiment was done to determine the rule set when Chl *a*, was not included as environmental variable. Similarly, the method was also used to develop a rule set for the real time forecasting of the dinoflagellate, *Ceratium*, a species that is becoming increasingly a nuisance within the studied reservoirs.

The evolutionary algorithm (EA) methods mimics processes of biological evolution, natural selection and genetic variation. The method uses genetic operators and the 'survival of the fittest' principle to search for suitable representations of a problem solution (Cao *et al.*, 2006). The ability of the method to apply self-organization, self-learning, intrinsic parallelism and generality, enables EAs to be applied to recognize patterns, predict outcomes, optimize control and do parallel processing (Goldberg, 1989; Bäck *et al.*, 1997).

The basic framework of the rule discovery for *Microcystis* biovolume in hypertrophic South African reservoirs is represented in Fig 4. The detailed algorithm for the rule discovery and parameter optimization by HEA is the same as used by Cao *et al*. (2006) (Fig 5).

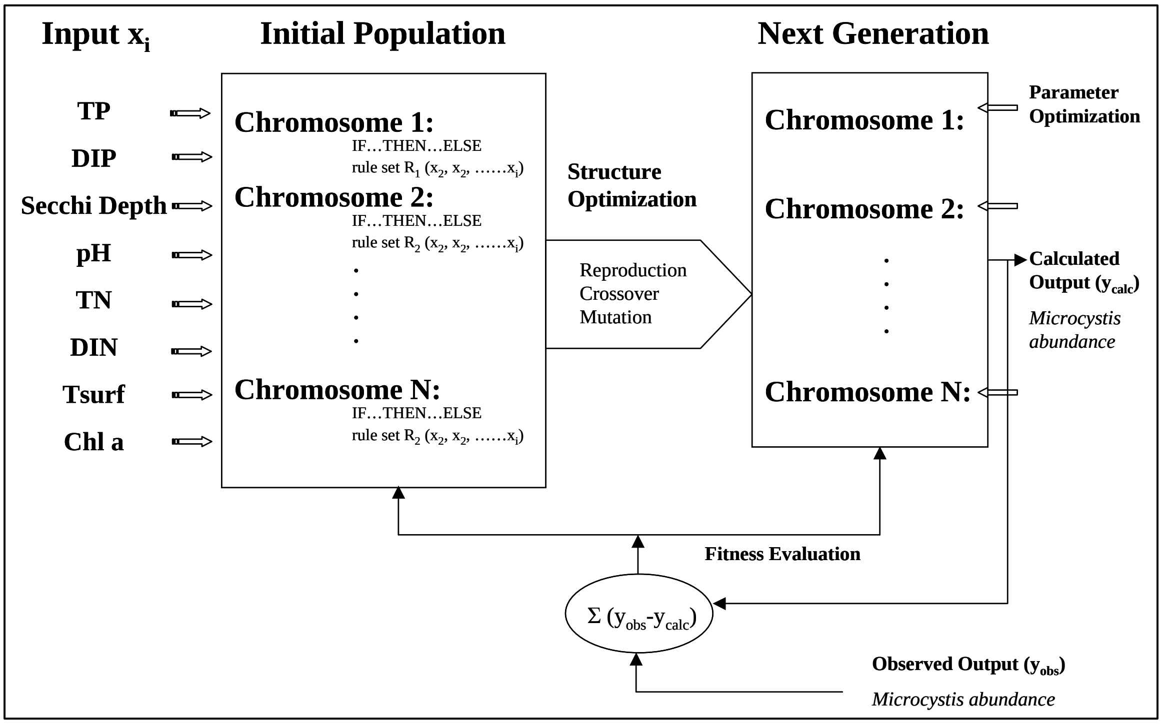


Figure 4 Conceptual diagram of HEA for the discovery of a predictive rule set for *Microcystis* biovolume in three hypertrophic South African reservoirs. The same model was used for the real time prediction of the dinoflagellate biovolume predictive rule set.

Genetic programming (GP) is used in the HEA to generate and optimize the structure of rule sets. The genetic algorithm (GA) is used to optimize the parameters of the rule set. GP computer programs are represented as parse trees, where a branch node represents an element from the functions set (this can be arithmetic operators, logic operators and elementary functions of at least one argument). A leaf node can be an element from a terminal set (this can be variables, constants and functions of no arguments) (Muttil and Lee, 2005; Cao *et al.*, 2006). With each run of the program the results are evaluated by means of 'fitness cases'. Fitter results are selected for recombination to create the next generation by using the genetic operators, e.g. crossover and mutation. These steps are repeated for consecutive generations until the criteria for termination of the program are met. A general genetic algorithm is then used to optimize the random parameters in the rule set.

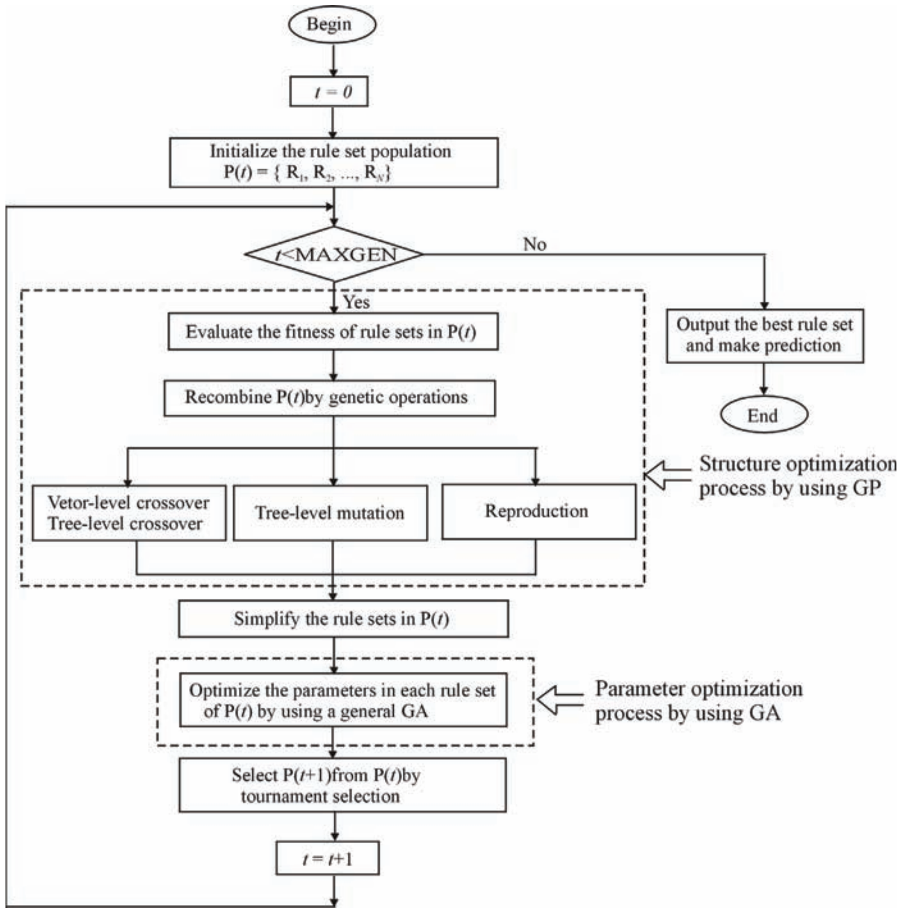


Figure 5 Flow chart showing the process of the HEA (redrawn from Cao *et al.*, 2006).

The rule sets are expressed in an IF THEN/ELSE tree format and are simplified as discussed in Cao *et al.*, 2006. This allows for the development of the rule set to consider and make provision for different conditions within the data set. The model output includes a list of the variables used within each run, as well as the list of outcomes and the effectiveness of each run (Appendix A).

For the experimental programming using HEA, the Hartbeespoort, Rietvlei and Roodeplaat reservoirs data was used to do real time prediction for *Microcystis* and the dinoflagellate, *Ceratium*. These two species were selected because they formed the major blooms in the five reservoirs. Experiments 1, 3, 4, 5, 6 were run to model real-time, 7-days forward, 14-days forward, 21-days forward and 28-days forward for the prediction of the seasonal succession of *Microcystis*. The daily input data of the following variables: TP, DIP, Secchi depth, pH, TN, DIN, Tsurf, Chl *a* and *Microcystis* biovolume were used.

The data preparation for the forwards experiments were done by shifting the daily algae biovolume data backwards the number of days that are shown in the forward prediction. Training was then done on this data set.

In Experiment 2 Chl *a* was omitted as an environmental variable to see if a reliable rule set could be developed without the Chl *a* as indicator of biovolume. In Experiment 7 a rule-set was developed for the dinoflagellate, *Ceratium*. The daily input data of the following variables: TP, DIP, Secchi depth, pH, SO4, TN, DIN, Tsurf, Chl *a*, and dinoflagellate biovolume were used. For the application of HEA during this study an initial population of 200, a maximum of 100 generations and 20 runs were done on the data set. The experiment was performed on a Hydra supercomputer (IBM eServer 1350 Linux) with a peak speed of 1.2 TFlops using C++ programming language. The parameter settings are listed in Table 5.

Table 5 Parameter settings of the hybrid evolutionary algorithm rule set discovery for the Hartbeespoort, Rietvlei and Roodeplaat reservoirs

Structure Optimization	N = 15341 F_L = {AND, OR} F_C = {>,<, ¡Ã, ¡Â} F_A ={+,-,*,/,sin,cos, exp,ln} MAXK = 4 $D_{IF} = D_{THEN/ELSE}$ = 4 MAXGEN = 100
Parameter Optimization (GA)	Popsize = 200 a = -0.5 b = 1.5 M = 8 MAX = 500

To validate the results of the rule sets the correlation coefficient of the measured and fitted data and the Root Mean Square Error (RMSE) of the training error, and the testing error are provided as outcomes of the model. The RMSE are calculated as follows:

$$\sqrt{\frac{1}{m}\sum_{i=1}^{m}(\hat{y}_i - y_i)^2} \qquad \textbf{(2.3)}$$

Where m is the number, of testing data points, y_i and $\hat{y}_i$ are the *i*th observation and the *i*th predicted value of the output variable *Microcystis/*dinoflagellate biovolume.

More validation was done on the best rule set for every Experiment by determining the Average Actual Error (A AE) and the Mean Square Error (MSE) by conventional methods.

To consider the impurities between the actual measurements and the predicted values in the model outcome the Relative Tolerance was set at 10% for the training data and 30% for the testing set, to determine the percentage good and bad predictions within each best rule set for the training and the testing data sets of each experiment. The formula, used to determine the Relative Tolerance, is shown in formula 5.5 and 5.6 (Greenberg, 2003).

$$\mathbf{|v\text{-}V| \leq \tau_r |V| + \tau_a} \qquad \textbf{(2.5)}$$

Where V is the measured value, v the predicted value, τ_r is the Relative Tolerance and τ_a is the Absolute Tolerance.

However, when the measured value V = 0, then

$$\mathbf{|v| \leq \tau_0,} \qquad \textbf{(5.6)}$$

Where τ_0 = 3. This Tolerance is pre-determined to be an acceptable outcome of the model.

Sensitivity analysis for each environmental variable, used in the RULE set, was done by determining the biovolume outcome if an environmental variable changes stepwise within the range of the data for the specific variable. This was done for each variable used in a rule set. The median of the other variables used in a rule set, was used to determine the impact of a specific environmental variable. The impact on the biovolume outcome of the environmental variables used within each rule set was plotted together to verify the most important variable regarding the effect and greatest impact on the algal biovolume changes. The greater the slope, the greater is the impact on the outcome of the model.

CHAPTER 3

MODELLING RESULTS

3.1 VOLLENWEIDER MODEL

The Vollenweider model is an easy to apply empirical model but does not take all the biological processes, into consideration. The model assumes that the system is in a steady state when Thornton and Walmsley (1981) tested the Vollenweider (1976) and Dillen and Rigler (1974) models on South African conditions, it was found that there is a certain degree of potential for predicting the steady state of a system.

This model was developed for eutrophication management purposes and can be used to determine the trophic conditions within a system, and allows the modeller to apply quick management scenarios.

Table 6 shows that for the Hartbeespoort Dam, the model over-predicts the TP concentrations by 28.0% and under-predicts the Chl *a* concentration with 68.1%. In the Klipvoor and Roodeplaat dams, the model under estimated the TP concentration with 78.8% and 29.8% respectively. The Chl *a* concentrations was under-estimated in the Klipvoor Dam by only 5.8% and in the Roodeplaat Dam, an over estimation of Chl *a* of 26.5% was found. There is therefore no uniformity in the predictions between these three Reservoirs. However, IETC (2000) maintains that this model can have uncertainties from as low as 30% up to 300%. This may be quite acceptable because of the differences that may exist between these reservoirs. The acceptable discrepancies that are allowed are much higher than the 10% to 30% that are acceptable for the Forecaster XL ANN model that was tested with the data from the hypertrophic South African reservoirs.

The scenarios were randomly selected to test different scenarios and to show what the potential outcome of management actions can be. The 50% P elimination (Table 6) showed that there will be a significant reduction in the predicted TP, Chl *a*, and PO_4-P concentrations. This may be enough to improve the hypertrophic status to eutrophic in all three the reservoirs. The 90% elimination of P may change the reservoirs water quality into an oligotrophic state. This may not be achievable due to potential costs involved and it must be kept in mind that there may be uncertainties between 30% and 300%, especially if the under prediction in the case of the Klipvoor Dam is considered.

The Vollenweider Model is, therefore, still quite a usable tool for managers, but the potential discrepancies must be kept in mind when this model is used. It is a useful tool when a system is fairly unknown and little data is available to assist the manager in making decisions regarding such a system.

Table 6 Input variables for the Vollenweider Model with the results found by applying three different management scenarios in the hypertrophic Hartbeespoort, Klipvoor and Roodeplaat dams.

Input Variable/Scenarios	**Hartbeespoort**	**Klipvoor**	**Roodeplaat**
TAI (m^3/year)	985270000	113426870	63850000
MIP (mg/m^3)	373	742	369
MAPL (mg/year)	367505710000	84162737540	23554999558
SA (m^2)	20624100	7580000	3970000
PAL (mg/ m^2/year)	17819	11103	5933
V (m^3)	194637710	43800000	41900000
RT (year)	0.20	0.39	0.66
MD (m)	9	6	11
TP (ug/L)	101	751	205
Chl *a* (ug/L)	123	142	33.2
PO_4-P (ug/L)	52.1	50	112
Predicted Reference concentrations	TP: 130 Chl *a*: 39.2 PO_4-P: 43.5	TP: 159 Chl *a*: 47.1 PO_4-P: 52.9	TP: 144 Chl *a*: 42.0 PO_4-P: 48.1
Scenario P Elimination 50%	TP: 65 Chl *a*: 20.9 PO_4-P:21.7	TP: 79 Chl *a*: 24.9 PO_4-P: 26.5	TP: 72 Chl *a*: 22.9 PO_4-P: 24.0
Scenario P Elimination 90%	TP: 13 Chl *a*: 6.3 PO_4-P: 4.3	TP: 16 Chl *a*: 7.1 PO_4-P: 5.3	TP: 15 Chl *a*: 6.7 PO_4-P: 4.8
Scenario Doubling the residence time	TP: 264 Chl *a*: 76.6 PO_4-P: 88.0	TP: 164 Chl *a*: 48.7 PO_4-P: 54.8	TP: 88 Chl *a*: 27.3 PO_4-P: 29.3

3.2 Lake simulation library SALMO-OO

The results discussed here will focus on the outputs from the SALMO-OO model and the improvements made by replacing the original SALMO-OO growth model by the growth model of Arhonditsis and Brett (2005) for Lake Washington. The simulation library SALMO-OO developed by the object-oriented implementation of the lake ecosystem model SALMO-OO (Recknagel and Benndorf, 1982; Benndorf and Recknagel, 1982; Recknagel *et al.*, 1995) is the core of a lake simulation library, implemented within JAVA. It provides optional access to alternative causal representations of ecological processes in lakes such as photosynthesis and respiration of diatoms, green and blue-green algae; grazing of diatoms, green and blue-green algae by zooplankton; growth of herbivorous zooplankton, and predation of zooplankton by planktivorous fish. Alternative process representations were adopted from published lake ecosystem models different to SALMO such as Park et al. (1974), Hongping and Jianyi (2002), and Arhonditsis and Brett (2005).

The original SALMO-OO over-estimated the phosphorus and total algal population in Hartbeespoort and Roodeplaat Reservoirs (Fig 6 & 8). The actual and forecasted results for the Klipvoor Reservoir were much closer, although a certain period during 2003 in Klipvoor was over-estimated (Fig 7). The correlation coefficients of all three of the reservoirs between the measured and predicted variables was low and does not seem to reflect the conditions in the reservoirs, with the original SALMO-OO (Fig 6-Fig 8).

The application of the Arhonditsis and Brett (2005) growth equation in SALMO-OO did reduce the errors. In the Hartbeespoort Reservoir the fitted PO_4-P concentrations were much closer to the actual measured data, and the RMSE was improved from 79.67 to 37.67 (Fig. 6), however, the measured and predicted peaks did not correspond well. With SALMO-OO the total algal biovolume of the Hartbeespoort were slightly over-estimated and there was an improvement of the RMSE from 24.18 to 19.87, after the application of the Arhonditsis and Brett (2005) equation.

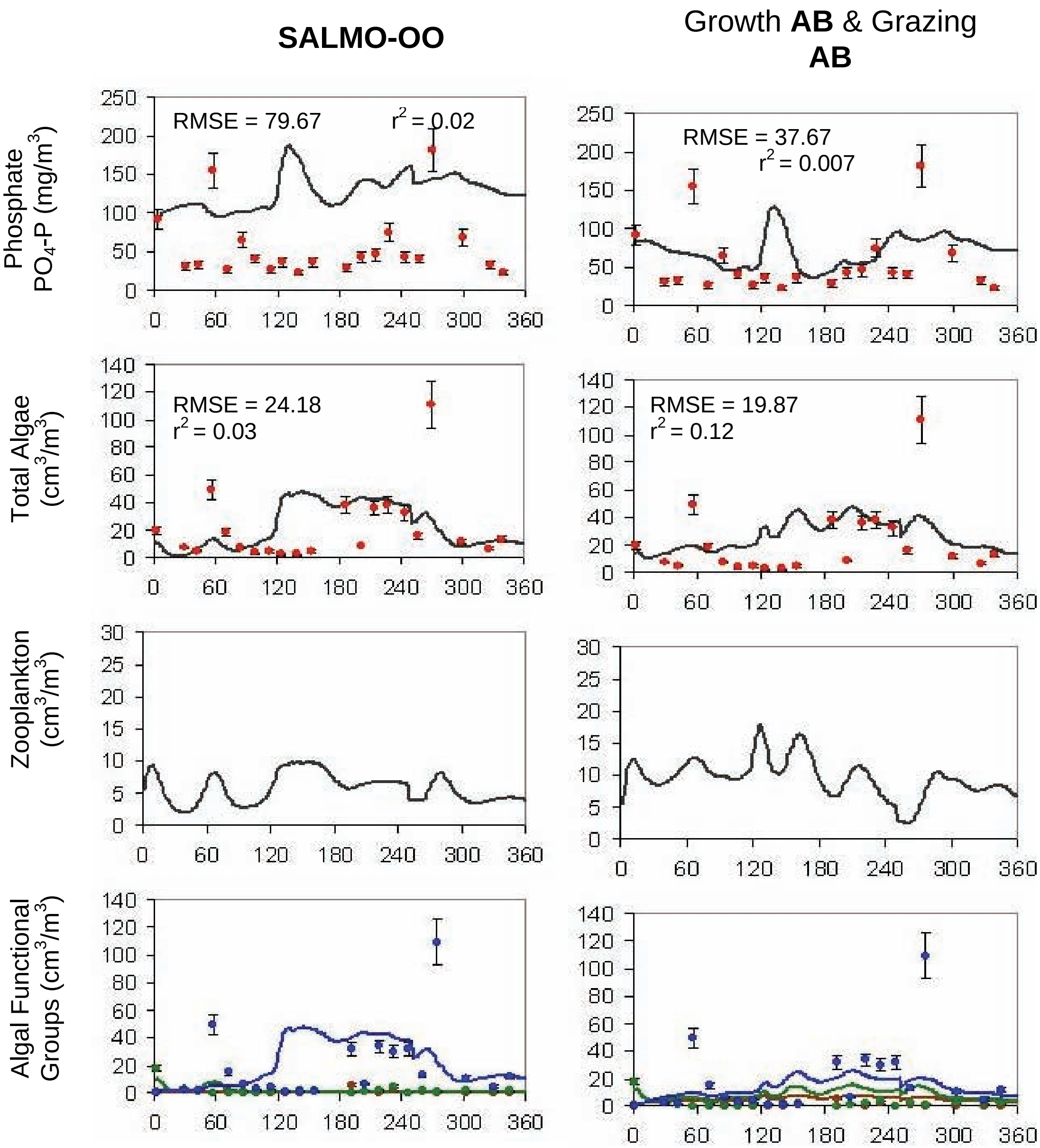


Figure 6 Comparison of output results (line) with real measured data (markers) for the Hartbeespoort Reservoir with the original SALMO-OO growth and grazing equations; and with the adaptation of the growth and grazing equations from Arhonditsis and Brett (AB) (2005). Zooplankton is part of the model output and is thus included in the graph, although no zooplankton data was available.

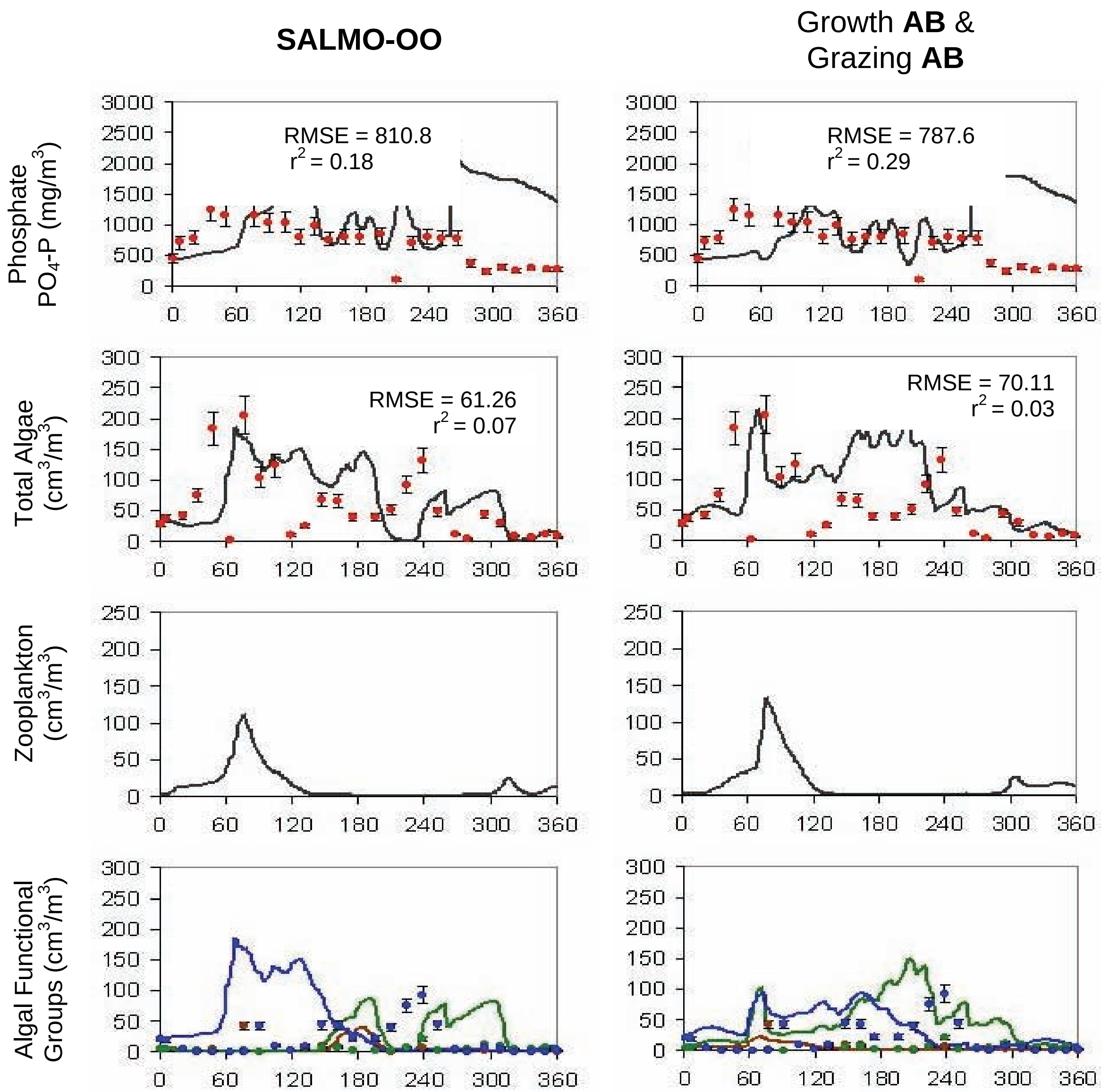


Figure 7 Comparison of output results (line) with real measured data (markers) for the Klipvoor Reservoir with the original SALMO-OO growth and grazing equations; and with the adaptation of the growth and grazing equations from Arhonditsis and Brett (AB) (2005). Zooplankton is part of the model output and is thus included in the graph, although no zooplankton data was available.

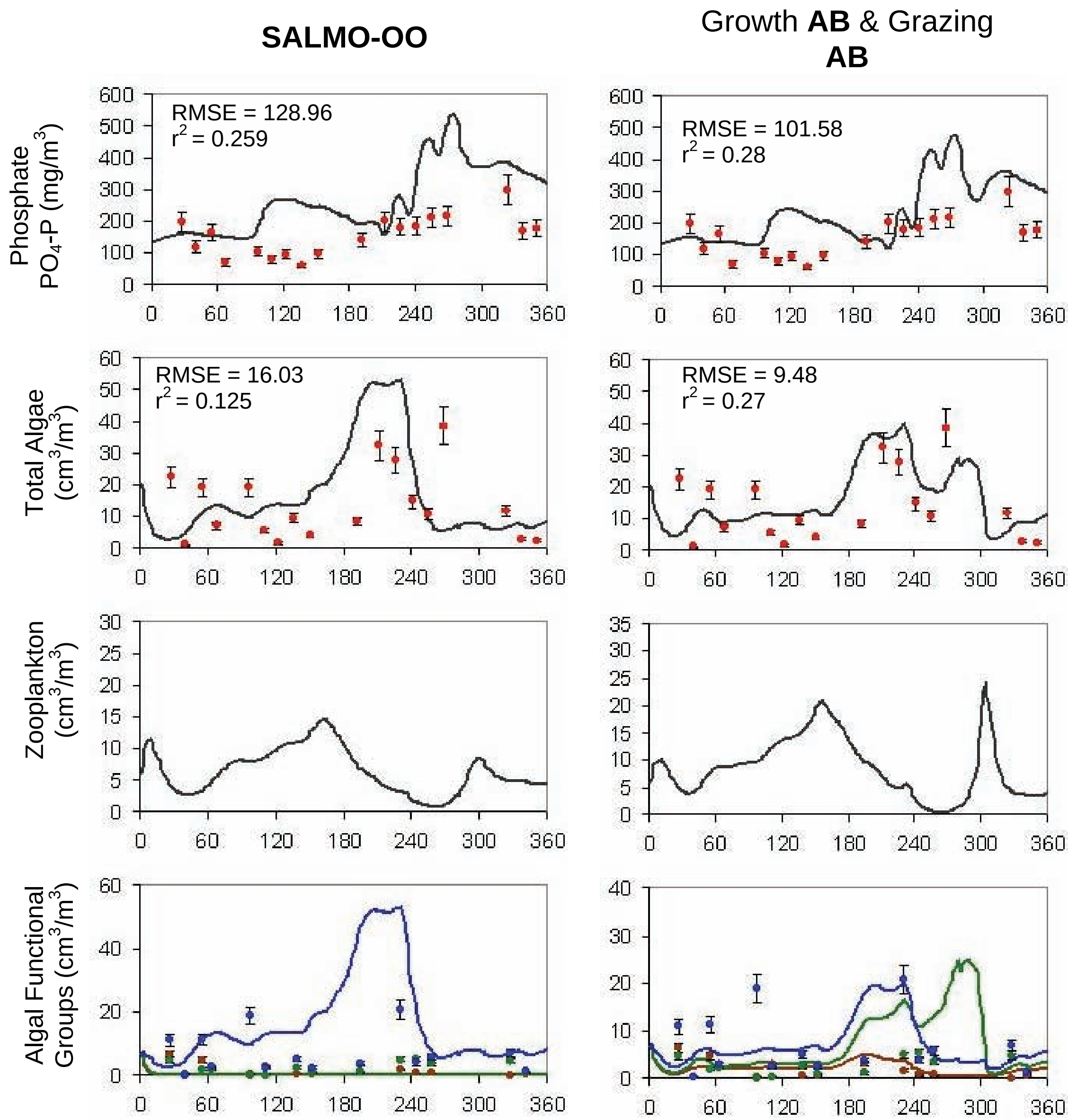


Figure 8 Comparison of output results (line) with real measured data (markers) for the Roodeplaat Reservoir with the original SALMO-OO growth and grazing equations; and with the adaptation of the growth and grazing equations from Arhonditsis and Brett (AB) (2005). Zooplankton is part of the model output and is thus included in the graph, although no zooplankton data was available.

3.3 Artificial Neural Networks

The artificial neural networks (ANN) are a black box approach where the modeller does not know what is happening within the hidden layer of the model. The modeller does not need to know the complex characteristics within a water system to apply the model. However, the results can be quite accurate regarding the prediction of the outcomes. The outcomes of the model, despite the black box approach, can add insight as weights are allocated to the environmental variables in predictions. This supplies the modeller with the most important environmental variables in predicting algal biomass and blooms.

3.3.1 Results with Multilayered Feed forward Neural Network

3.3.1.1 NeuroSolutions 5.04

Originally, data from Roodeplaat Dam was modelled with the ANN (NeuroSolutions 5.04). This modelling package achieved very good results. The results using this model are summarized in Table 7. The package was able to achieve 93.75% accuracy with the cyanotoxin producing group (CTTot exp) and 90 % accuracy with the non-cyanotoxin (TotNONCT) producing group. A graphical representation of the results is presented in Figure 9 and Figure 10.

The normalised mean square error (NMSE) and the mean square error (MSE) are the performance measurements used to determine the accuracy of the model. The NeuroSolutions gives both the MSE and the NMSE as well as the mean actual error (MAE). The smaller these values the more accurate the prediction results. According to Velickov (2004), the NMSE is dimensionless and provides a better indicator for the error measurement since it is normalised by the error of the observed data. The r-value as indicated in Table 7 shows that there was a very good correlation between the predicted and the measured data. However, the minimum and maximum absolute errors do show that there are potentially, large uncertainties in the outcomes.

Attempts were made to construct the solution equation, using NeuroSolutions 5.04 and other packages. However, the main disadvantage of ANN modelling is that it is a black box approach, and the developed algorithm, that provides the output of the model, could not be determined. However, it must be kept in mind that the aim of the study was to test the applicability of the models for harmful algal bloom prediction, and not to develop improved knowledge of the models as such.

The final step was to include the data from all the reservoirs in the training data set and leave one reservoir out for testing the model.

Table 7: Summary of the initial neural network results using NeuroSolutions for prediction of the cyanotoxin producing group (CTTot exp) and the non-cyanotoxin producing group (TotNONCT).

Performance	***CTTot exp***	***TotNONCT***
MSE	225.9431157	1088.47948
NMSE	0.024515995	0.011171232
MAE	12.91183814	21.47676731
Min Abs Error	0.597656353	0.136831959
Max Abs Error	33.21688555	142.0277588
r	0.987846519	0.994490043
Percent Correct	93.75	90

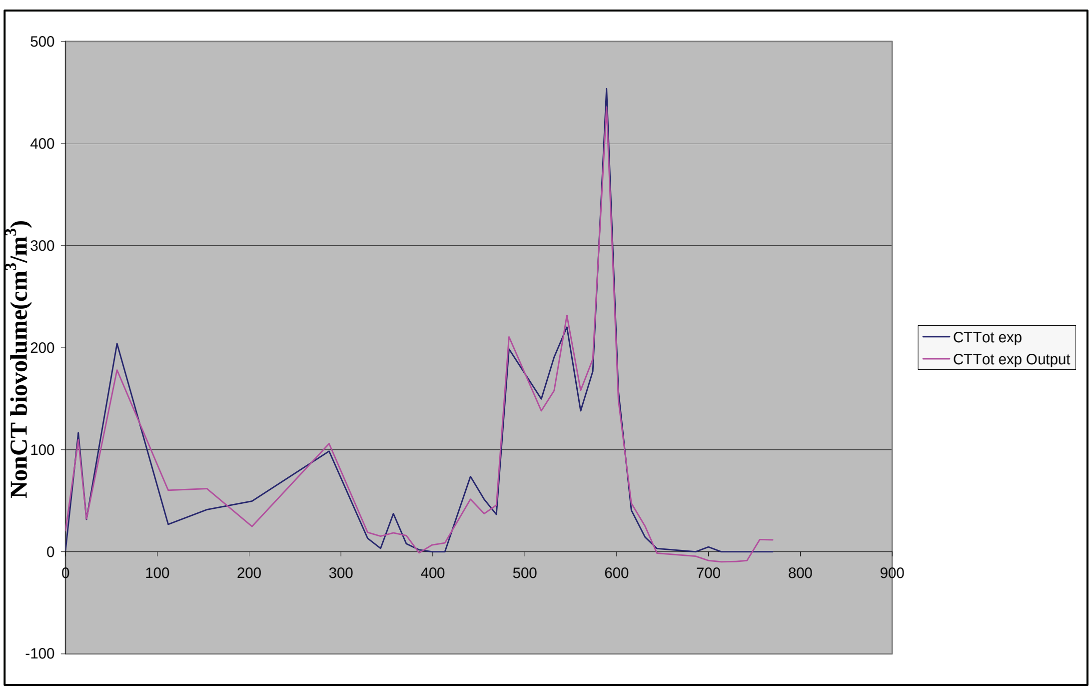


Figure 9 Results from the NeuroSolutions 5.04 ANN for the cyanotoxin producing group (CTTot exp), showing real time forecasting on the Roodeplaat Dam data.

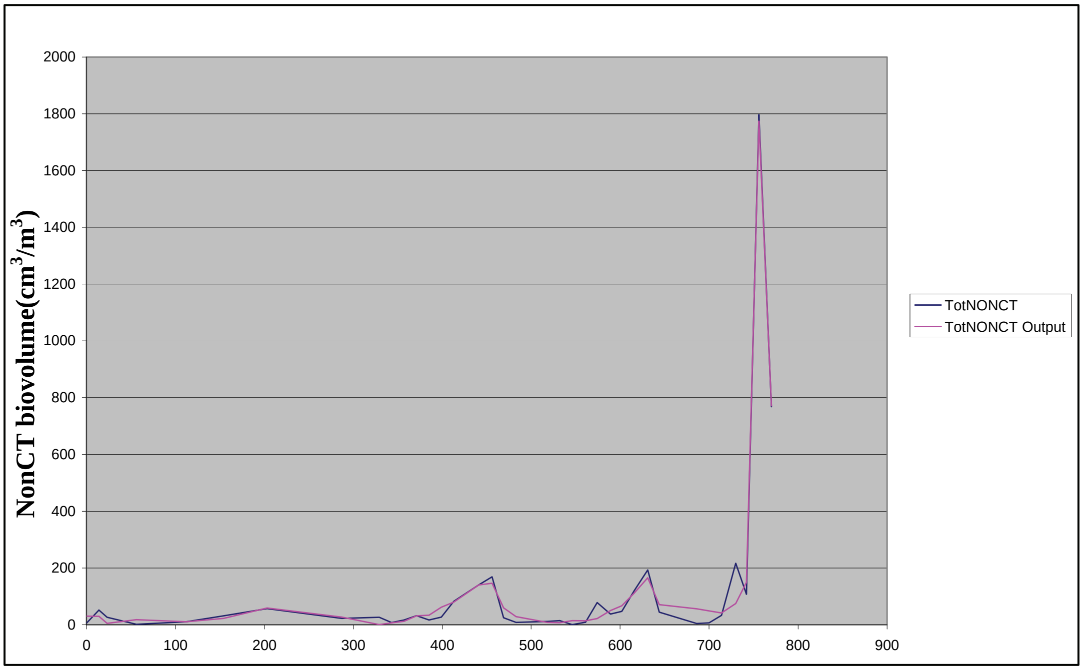


Figure 10 Results from the NeuroSolutions 5.04 ANN for the Non-CT producing group (TotNONCT), showing real time forecasting (pink line) versus the actual data (blue line).

3.3.1.2 Forecaster XL

At first only the data from Hartbeespoort Dam was modelled with the ANN (Forecaster XL). This modelling package achieved very good results and gave a better understanding of the results because of the build in verification. For each experiment, the results from this model are summarized in two graphs and a table, showing the errors and the relative tolerances of the training and testing data set. The percentage relative tolerance of the prediction versus actual data in the modelling package for the training set is 10%, and with the testing data set 30%. The model is, therefore, quite strict with itself in accepting the efficiency of the model.

At the end of this section a summary of the results are shown. This is done to compare the outcome of the experiments and to compare the important variables to be included in modelling the forecasts for the cyanotoxin producing cyanobacteria (CT) and the non-cyanotoxin producing cyanobacteria (Non-CT) groups.

Modelling using data from a single dam

Experiment 1: Non-cyanotoxin producer (Non-CT) group with only selected environment variables as input (single dam)

Using only the measured environmental variables for the period 2000 to 2005 for the modelling exercise, the following results were obtained. The r^2 value was 0.9595 and the correlation was 0.9807. Figure 11 shows the actual measurements against the forecasted results for the Non-CT producing group. The results show that the forecasted results do occasionally over, or under predict, yet have very good correlations as mentioned. According to the results in Table 8, the number of good results is 0, which means that more than a 30% error was found within predicting and comparing all the test results.

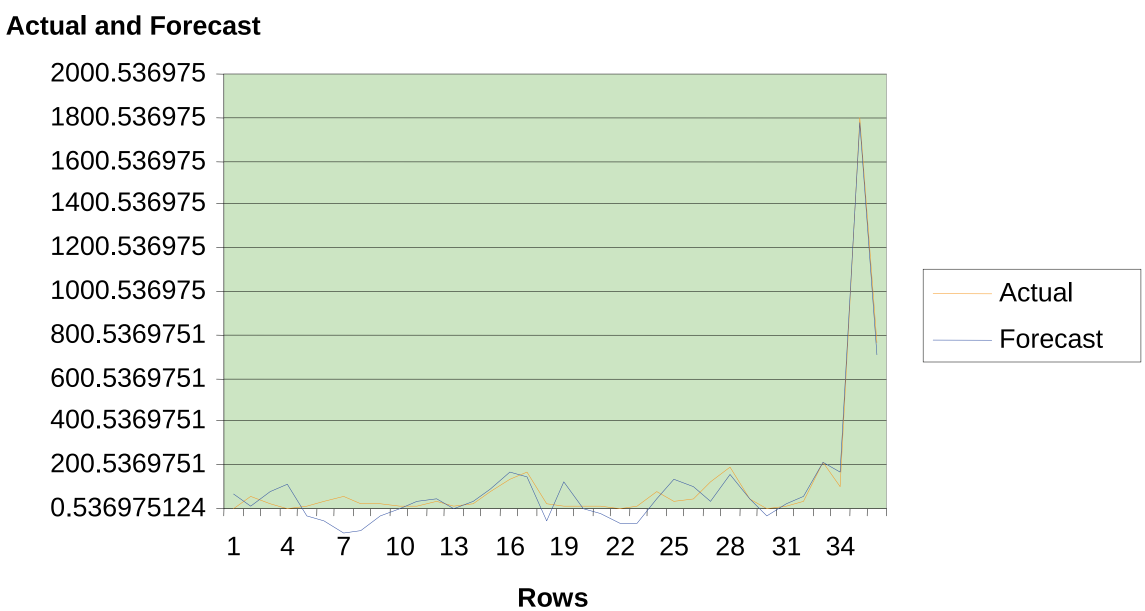


Figure 11 Actual (orange line) versus forecast (blue line) results for Non-CT producing group biovolume using only environmental variables and Chl *a* concentration as input with the Forecaster XL ANN software package.

Table 8 A summary of the modelling result output with the Forecaster XL ANN software package for the Non-CT producing group using only environmental variables and Chl *a* concentration as inputs.

	Training set	**Test set**
# of rows:	30	6
CCR:	n/a	n/a
Average AE:	46.791955	62.012307
Average MSE:	3862.6524	4339.2413
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	5 (17%)	0 (0%)
# of Bad forecasts:	25 (83%)	6 (100%)

One of the excellent features of this model is the graph that shows the percentage of importance of each variable that are used in forecasting the outcomes. Fig. 12 shows that with this first modelling attempt Chl *a*, was by far the most important variable in determining the outcomes of the modelling results.

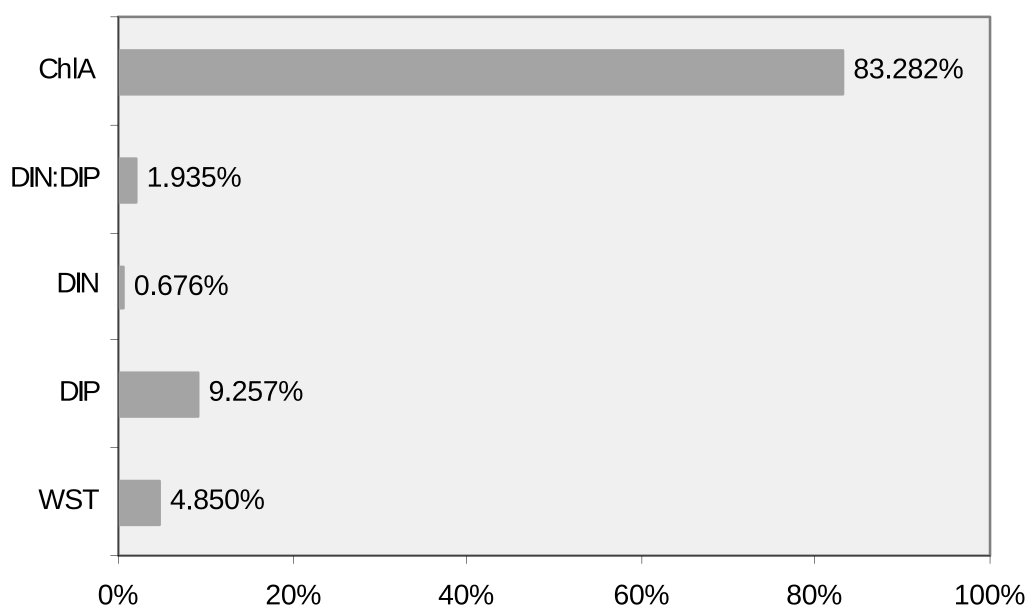


Figure 12 Percentage contributions of measured environmental parameters and Chl *a* concentration to ANN prediction for the Non-CT group in the Hartbeespoort Dam.

Secondly, the DIP concentration, and thirdly, the WST contributed to the outcome of the model. These results, therefore, indicate that the initial biomass is the most important determinant for future bloom development. Next are the nutrients, specifically in the form of DIP, and thirdly, the WST as a climate indicator in determining the forecasting of cyanobacterial biovolume.

<u>Experiment 2:</u> Cyanotoxin producer (CT) group with only selected environment variables as input (single dam)

In this second experiment with Forecaster XL only the selected environmental variables (See Section 4.2.5) were used to achieve results with predictive capacity for the CT group of the phytoplankton community. The correlation coefficient (r^2) value was 0.2746 and the correlation was 0.5620. The periods of dominance by the CT group was forecasted quite well although there are a number of over and under predictions (Fig. 13).

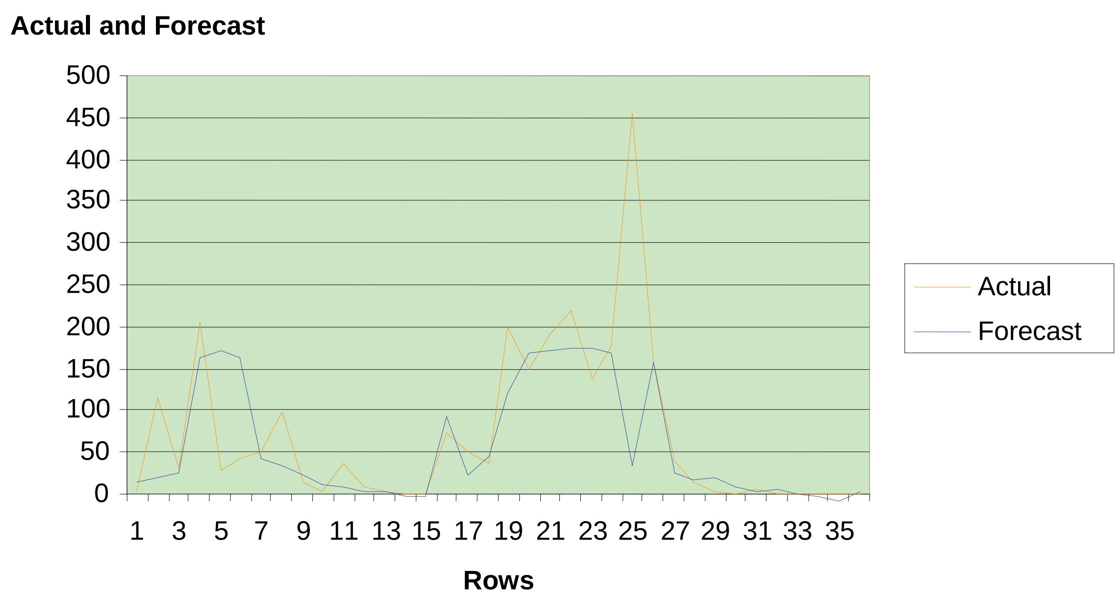


Figure 13 Actual (orange line) versus forecasted (blue line) results for CT`producing group using only environmental variables and Chl *a* concentration as inputs for the Forecaster XL ANN Software package on the Hartbeespoort Dam data.

In this case, the percentage of accurate forecasts with the training set was only 7%. With the testing set, the number of good predictions with a tolerance of 30% was 50% (Table 9).

This is still not accurate enough for the model as the average MSE and the average actual error (AE) for the testing set was much higher than with the training set.

In this instance the results show that in predicting the CT group the most important environmental variable is WST with a 60.91% contribution to the modelling success and secondly the DIP with a contribution of 18.17% (Fig. 14). DIN:DIP and DIN is also showing more importance (8.303% and 7.028% respectively) in the contribution to the outcome of the modelling results than the initial biomass, as indicated by the Chl *a* concentration. Multivariate analyses has shown that WST, as the climatic indicator, (See Section 4.2.5) is the most important environmental variable. The importance of phosphorous and the DIN:DIP ratio is in accordance with existing literature (Vollenweider, 1990; Rossouw, 2000; Rossouw and Görgens, 2005).

Table 9 A summary of the modelling result output with the Forecaster XL ANN software package for the cyanotoxin (CT) producing group using only environmental variables and Chl *a* concentration as input.

	Training set	**Test set**
# of rows:	30	6
CCR:	n/a	n/a
Average AE:	23.211721	102.33326
Average MSE:	1731.8002	31450.745
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	2 (7%)	3 (50%)
# of Bad forecasts:	28 (93%)	3 (50%)

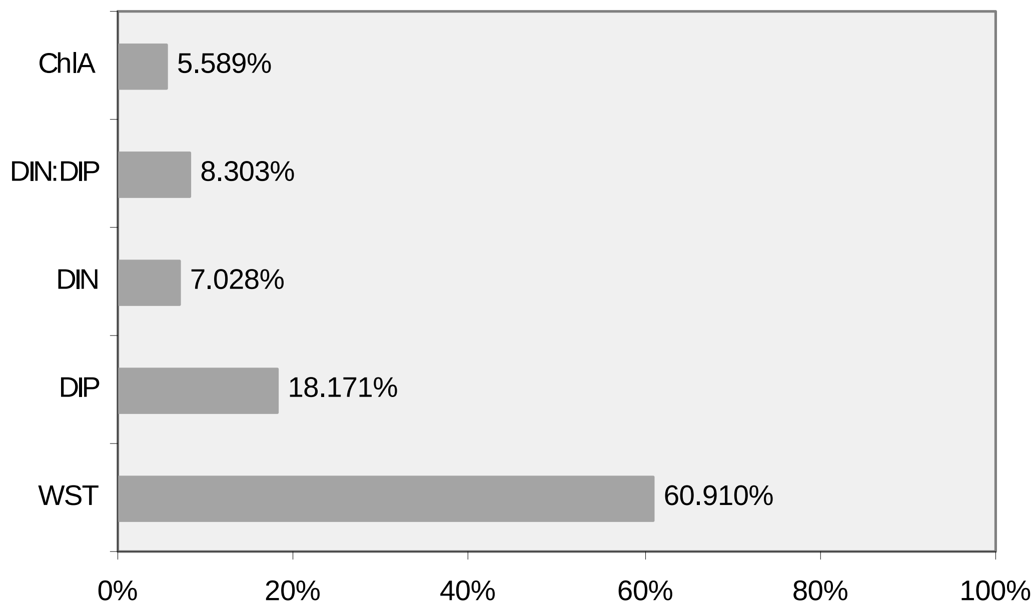


Figure 14 Percentage contributions of measured environmental parameters and Chl *a* concentration to ANN prediction of the CT group.

<u>Experiment 3:</u> Non-Cyanotoxin producer (Non-CT) group algae dominance, Chl *a* concentration and environment variables as input to the Forexter XL model (single dam)

With this experiment, the algal dominance was included in the modelling together with the measured environmental variables and the Chl *a* concentration to determine the predictive capacity for the Non-CT group. The actual data is the measured data, while the forecasted data is the predicted outcome of the model. The r^2 value was 0.9963 and the correlation was 0.9982. The results are shown in Fig. 15.

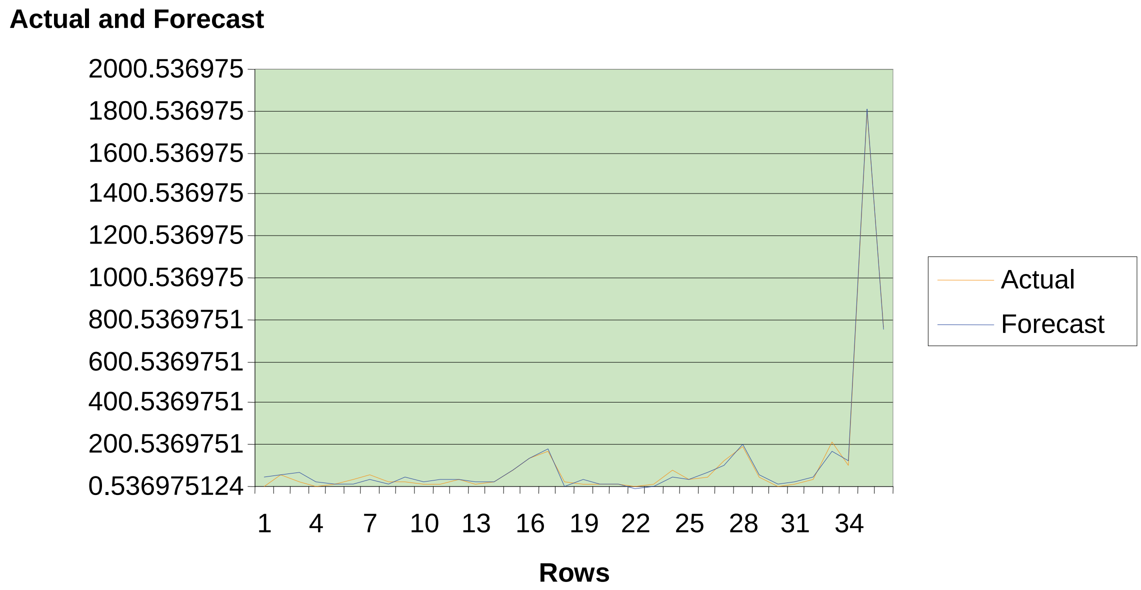


Figure 15 Actual (orange line) versus forecasted (blue line) results for the Non-CT producing group using algal dominance, environmental variables and Chl *a* concentration as inputs for the Forecaster XL ANN Software package.

Table 10 A summary of the modelling result output with the Forecaster XL ANN software package for the Non-CT producing group using algal dominance, environmental variables and Chl *a* concentration as inputs.

	Training set	**Test set**
# of rows:	30	6
CCR:	n/a	n/a
Average AE:	13.922402	23.618138
Average MSE:	293.51034	692.71795
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	7 (23%)	2 (33%)
# of Bad forecasts:	23 (77%)	4 (67%)

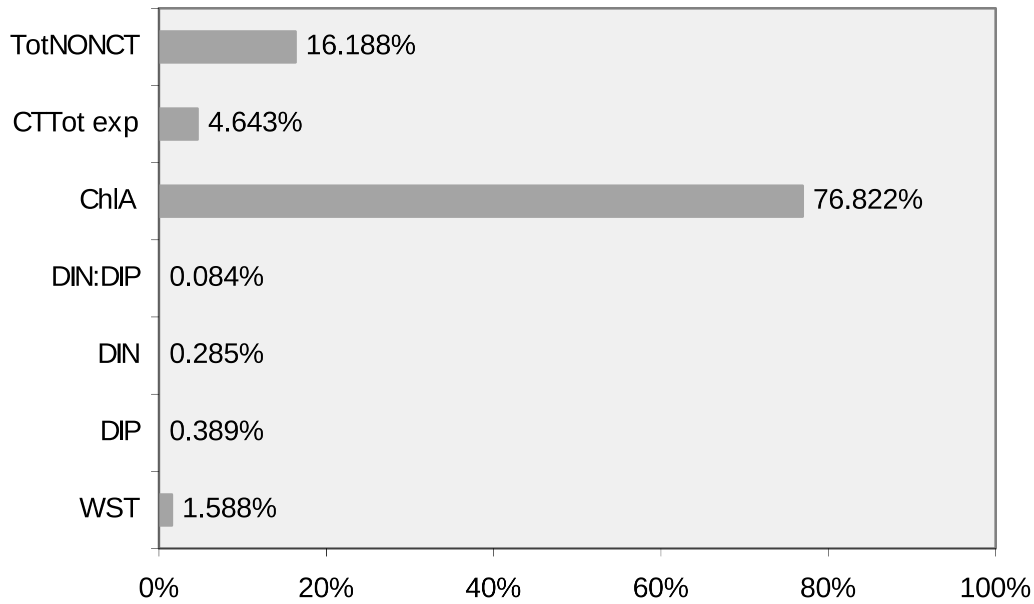


Figure 16 Percentage contributions of algal dominance, selected environmental parameters and Chl *a* concentration to ANN prediction for the Non-CT group.

The results with experiment 3 indicate that with the inclusion of the algal group dominance the average actual error (Average AE) is much smaller than with the previous results (Table 10). The number of good predictions with the training set is only 23%, but the 10% tolerance might be too strict. With the testing dataset the percentage good predictions for the Non-CT group is 33%. This is much higher than what was found with Experiment 1.

The most important variables in the prediction of the Non-CT group are again Chl *a*, with an importance of 76.822% (Fig. 16). Secondly, the dominance determination of the total Non-CT groups that was added in this experiment was used and the importance of the input was 16.188%. Thirdly, the CT group dominance values were used and had an importance of 4.643%. Fourthly, the WST had an importance of only 1.588%.

With experiment 3, the nutrient components did not feature as important factors in determining the algal group contribution in the phytoplankton community. There are two ways of looking at the results. Firstly, it may indicate that including the Chl *a* concentration as a variable in the Forecaster XL model, minimises the effect of the selected environmental variables for forecasting purposes. Secondly, it may indicate that the Chl *a* concentration as an indicator of the biomass/biovolume is closely related to the specific species dominant in the system.

<u>Experiment 4:</u> Cyanotoxin producer (CT) group algae counts and environment variables as input (single dam)

Using the measured environmental variables together with the algal group dominance in the reservoir the results shown in Fig. 17 were obtained. The r^2 value was 0.9843 and the correlation was 0.9932. The correlations show, therefore, good results.

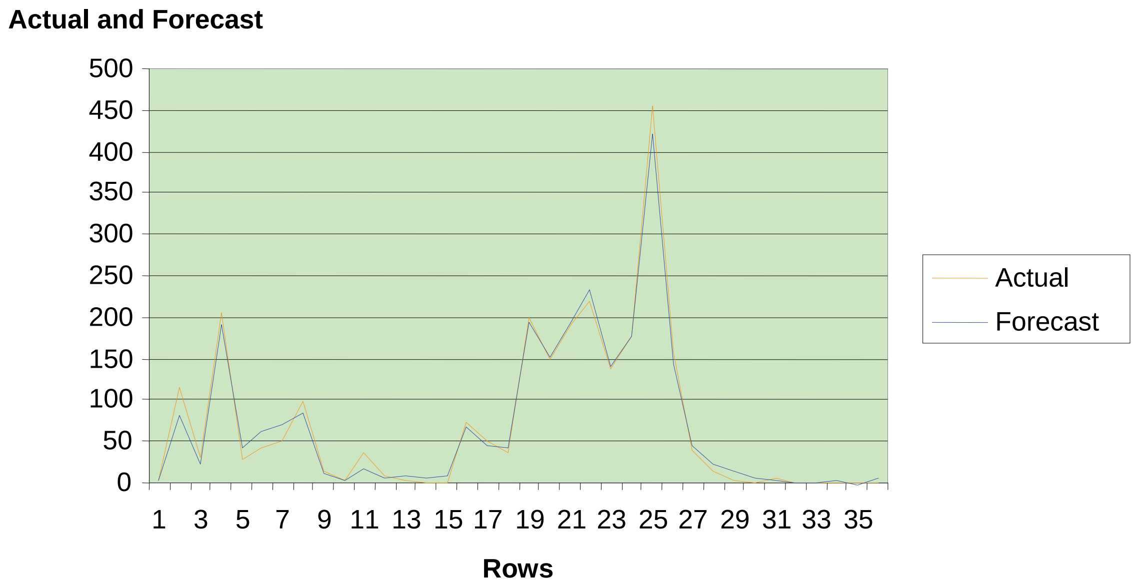


Figure 17 Actual (orange line) versus forecasted (blue line) results for the CT producing group using algal dominance, selected environmental variables and Chl *a* concentration as inputs for the Forecaster XL ANN Software package.

The summary of the modelling results is shown in Table 11. The results show that the average actual error (Average AE) is much lower than any of the previous results (Experiments 1-3). This indicates that the results are significant. However, the tolerance values for the training set are again not within the acceptable tolerance of the model of 10%. Only 37% of the results fall within the 10% tolerance limit. With the training data set, only 17% good forecasts are within the tolerance limit of 30%.

Table 11 A summary of the modelling result output with the Forecaster XL ANN software package for the CT producing group using algal dominance, environmental variables and Chl *a* concentration as inputs.

	Training set	**Test set**
# of rows:	30	6
CCR:	n/a	n/a
Average AE:	6.5620637	17.712396
Average MSE:	88.862874	421.084
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	11 (37%)	1 (17%)
# of Bad forecasts:	19 (63%)	5 (83%)

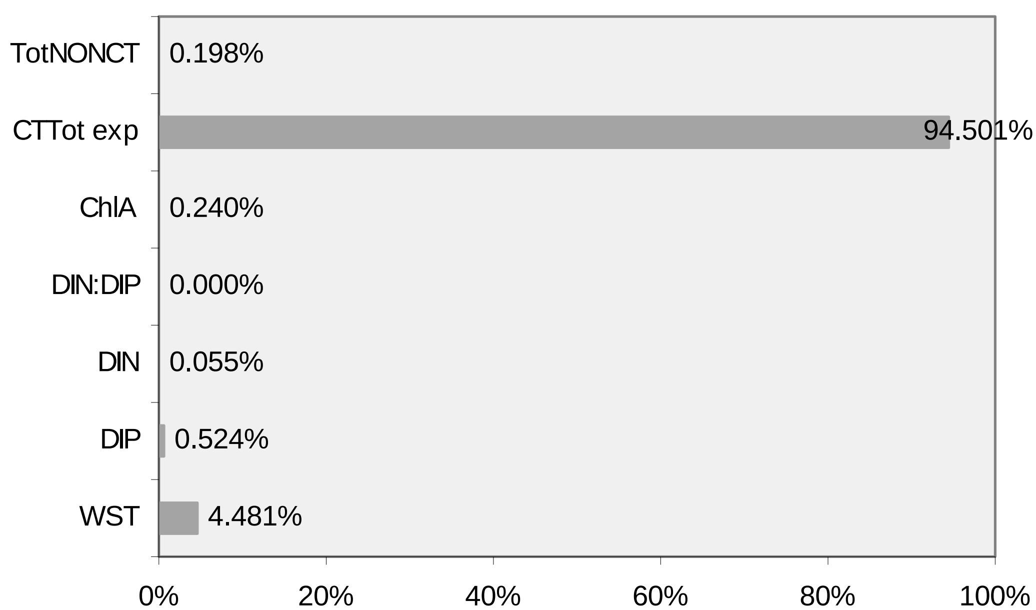


Figure 18 Percentage contributions of algal dominance, selected environmental parameters and Chl *a* concentration to ANN prediction for the CT group.

The percentage contribution of the selected environmental and biological components that were used as input for experiment 4 to predict the CT group, are shown in Fig. 18. In this experiment the total CT dominance contributed 94.501% to the outcomes of the results. This is basically using the forecasted variable to predict itself. WST was the second most important contributor to the outcomes with only 4.481% contribution and the DIP contributes only 0.524%. In this instance the DIN:DIP ratio did not contribute at all to the outcome of the model.

Modelling using data from all the dams

With the combining of all the dams' data, the experiments were again repeated as with the single dam data to determine if the outcomes are consistent with the first four experiments.

Experiment 5: Non-cyanotoxin producer (Non-CT) group with selected environment variables as input (all dams)

With Experiment 5, only the measured environmental variables were used as input into the model and the results obtained are shown in Fig. 19. The r^2 value was 0.9331 and the correlation was 0.9684. The correlation values indicate very good results and there is a linear relationship between the actual data and the forecasted data.

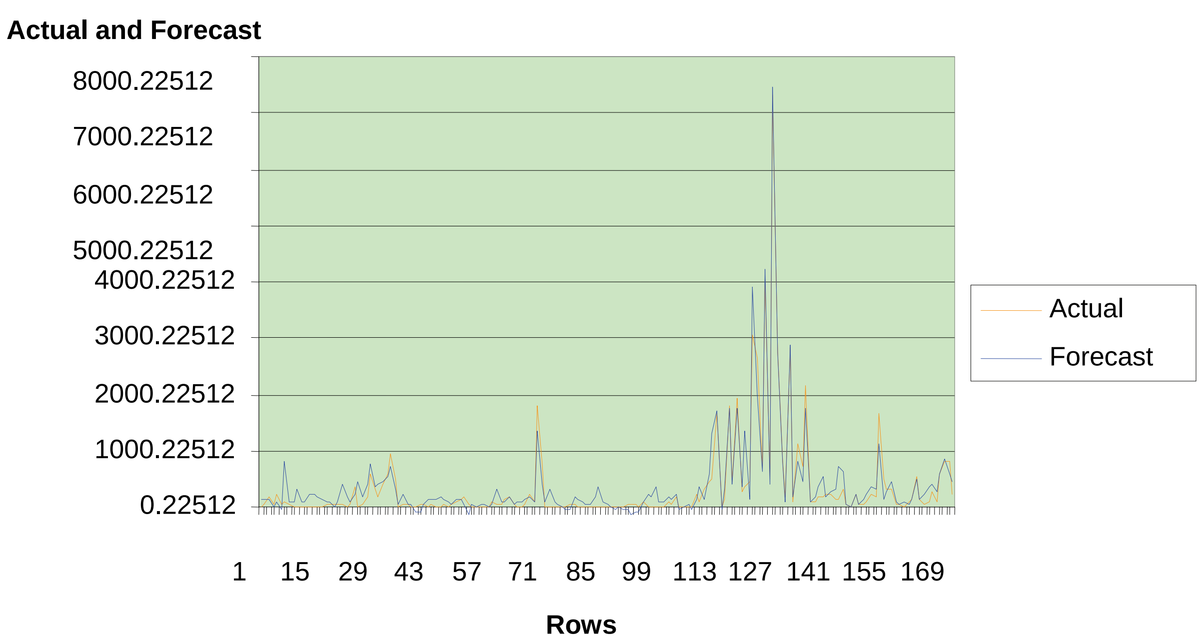


Figure 19 Actual (orange line) versus forecasted (blue line) results for the Non-CT producing group using environmental variables and Chl *a* concentration as inputs for the Forecaster XL ANN Software package.

The Average AE (Table 12) is low and indicates that the results indicate good results. However, the number of good results with both the training dataset (13%) and with the testing dataset (17%) is not acceptable.

Table 12 A summary of the modelling result output with the Forecaster XL ANN software package for the Non-CT producing group using selected environmental variables d Chl *a* as inputs.

	Training set	**Test set**
# of rows:	142	29
CCR:	n/a	n/a
Average AE:	136.34151	140.71186
Average MSE:	42747.538	54454.783
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	18 (13%)	5 (17%)
# of Bad forecasts:	124 (87%)	24 (83%)

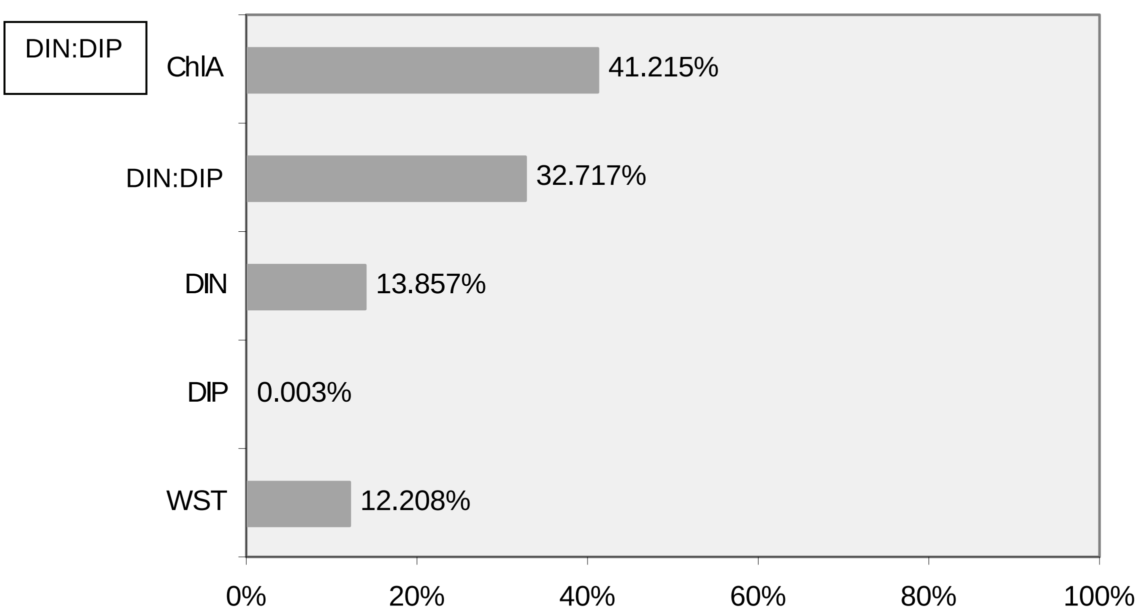


Figure 20 Percentage contributions of selected environmental parameters and Chl *a* concentration to ANN prediction for the Non-CT group.

Fig. 20 shows the percentage contribution of the measured and input variables to determine the Non-CT group's forecasts. As indicated, the main contribution to the outcome is the Chl *a* concentration. Secondly, the DIN:DIP ratio contributed 32.717%. Thirdly, the DIN concentrations contributed 13.857% to the outcomes of the model. Fourthly, the WST contributed 12.208%. These results show that nitrogen may be more important than phosphorus in the forecasting of the Non-CT group of the phytoplankton community.

Experiment 5 (all dams) can be compared to Experiment 1 (single dam). For both experiments, the Chl *a* concentration is the dominant variable that determines the outcome. Secondly, the nutrients are important. However, for the single dam the DIP concentration is more important, while the combination of the data from the different dams shows that DIN is the more important of the two nutrients. For modelling the combined dams, the DIN:DIP ratio is more pronounced than with the single dam.

<u>Experiment 6:</u> Cyanotoxin producer (CT) group with only selected environment variables and Chl *a* concentration as input (all dams)

In Experiment 6 the environmental variables and the Chl *a* concentration were used as input into the model. The actual and forecasted results are shown in Fig. 21. The r^2 value was 0.6866 and the correlation was 0.8311, which indicate good correlation between the actual and forecasted data.

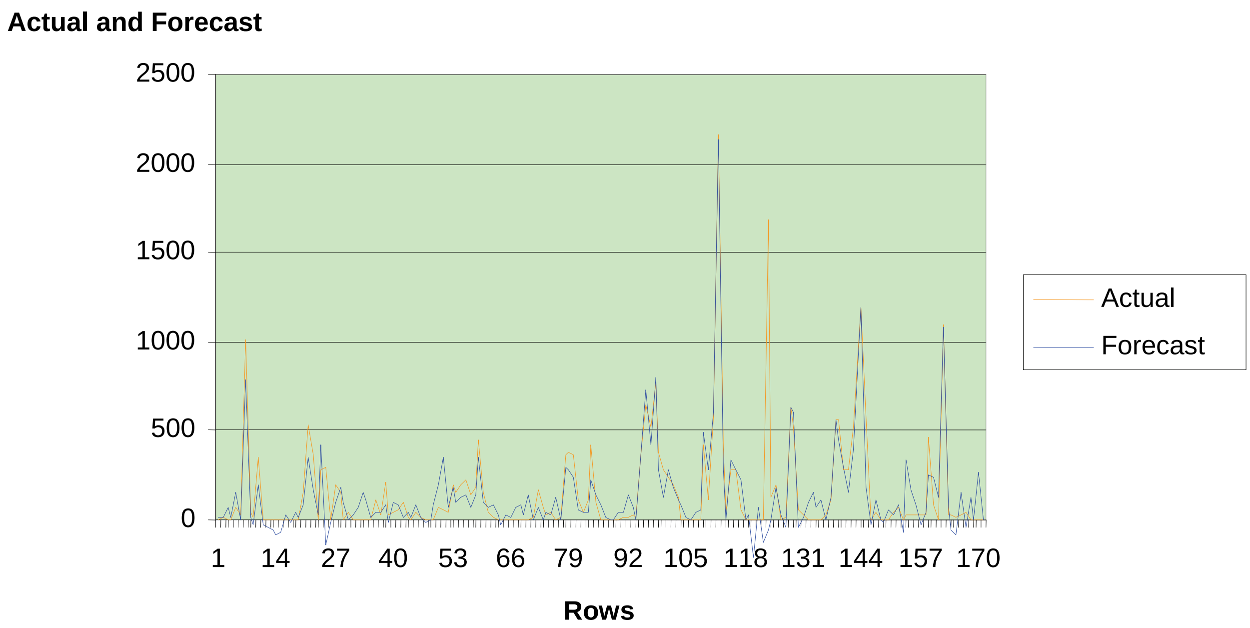


Figure 21 Actual (orange line) versus forecasted (blue line) results for the CT producing group using only environmental variables as inputs for the Forecaster XL ANN Software package.

The results shown in Table 13, show that here are larger errors than before, and this makes the model outcome not acceptable. The number of good forecasts for the training dataset is 11% and for the testing dataset was only 17%. Again, one needs to look at the tolerance level and determine whether the model is not too strict regarding the percentage tolerance allowed. It may also indicate that increasing the dataset do not necessarily improve the results.

Table 13 A summary of the modelling result output with the Forecaster XL ANN software package for the CT producing group using selected environmental variables and Chl *a* as inputs.

	Training set	**Test set**
# of rows:	142	29
CCR:	n/a	n/a
Average AE:	66.752897	142.20048
Average MSE:	8735.5117	118584.66
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	15 (11%)	5 (17%)
# of Bad forecasts:	127 (89%)	24 (83%)

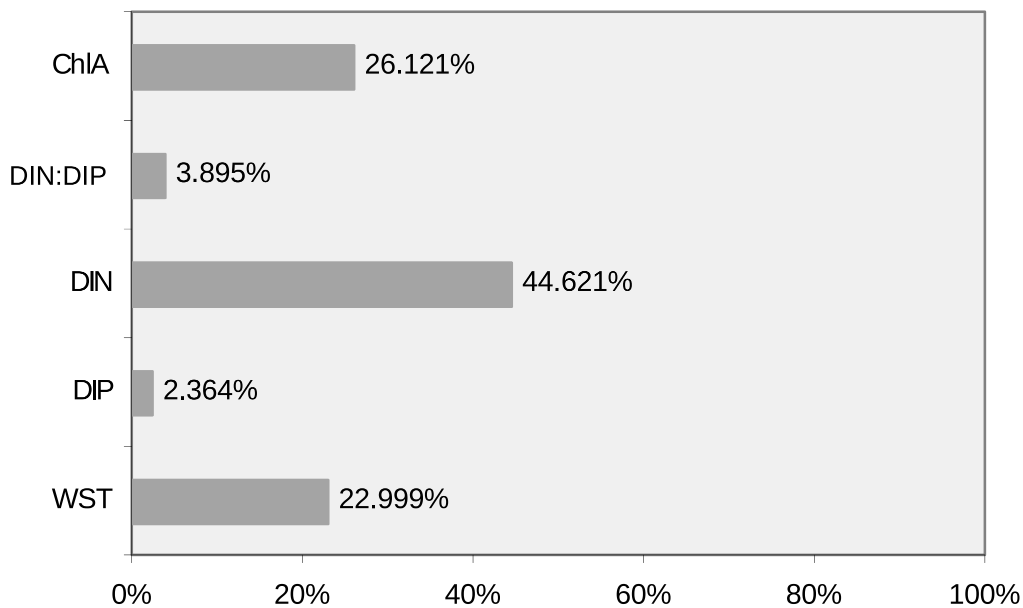


Figure 22 Percentage contributions of selected environmental parameters and Chl *a* concentration to ANN prediction for the CT group.

In the outcome of this modelling experiment the most important contributing variables (Fig. 22) are the DIN concentrations (44.621%), then the Chl *a* concentration (26.121% and lastly the WST values (22.999%). However, all the input variables were used to determine the result.

When the results of single dam experiment (Experiment 2) are compared to Experiment 6 (all dams), there is no trend in the important variables that determine the outcome of the forecast. For the single dam, the most important variable is temperature that contributes over 60% towards the outcome of the results. The DIP concentration is the second most important variable for the single dam scenario. In Experiment 6 the DIN concentration is the most important environmental variable, contributing more than 40% towards the outcome of the results. The Chl *a* concentration and the DIN concentration is almost equally important, contributing over 20% towards the outcome of the results.

<u>Experiment 7:</u> Non-Cyanotoxin producer (Non-CT) group using algae dominance, selected environment variables and Chl *a* concentration as input (all dams)

In Experiment 7, to forecast the Non-CT group the selected environmental variables, the algal dominance and the Chl *a* concentration were used as the input to the model. The results obtained are shown in Fig. 23. The r^2 value was 0.9863 and the correlation was 0.9932. This indicates an extremely good correlation between the actual and the forecasted datasets.

In Table 14, there is a summary of the modelling results regarding the extent of the errors, the tolerance type and the number of good and bad forecasts according to the model. Results show that the average actual error is 65 for the training dataset and 86 for the testing dataset. The number of good forecasts in the training set is 18% and for the testing data set 28%. Within the tolerance levels of 10% and 30%, respectively this is quite acceptable.

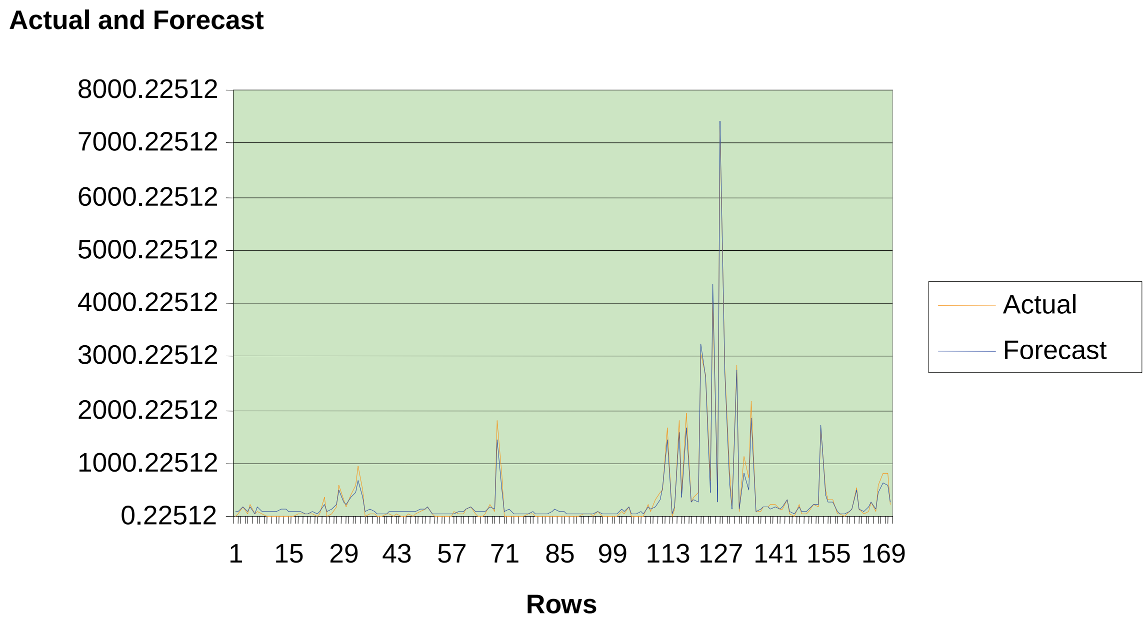


Figure 23 Actual (orange line) versus forecasted (blue line) results for the Non-CT producing group using only environmental variables as inputs for the Forecaster XL ANN Software package.

Table 14 A summary of the modelling results for the Non-CT producing group using algal dominance, selected environmental variables and Chl *a* concentration as inputs.

	Training set	**Test set**
# of rows:	142	29
CCR:	n/a	n/a
Average AE:	64.584469	85.779019
Average MSE:	8357.8507	13143.261
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	25 (18%)	8 (28%)
# of Bad forecasts:	117 (82%)	21 (72%)

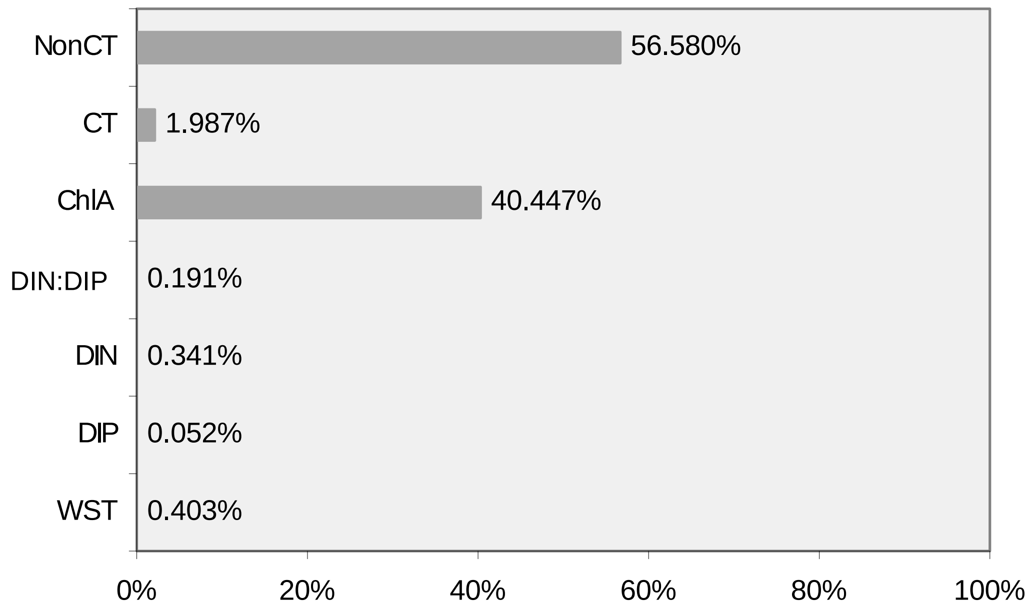


Figure 24 Percentage contributions of algal dominance, selected environmental parameters and Chl *a* concentration to ANN prediction for the Non-CT producing group in all the dams.

Results (Fig. 24) show that the environmental parameters that contribute most to the outcomes of the model are the Non-CT counts (56.58% and the Chl *a* concentration (40.447%). The CT algal counts contribute only 1.987% to the outcome. All the other input variables contribute very little to the outcomes of the model and the suggestion is that these variables are not important in establishing the Non-CT group contribution to the phytoplankton community.

Experiment 7 (for all dams) when compared to Experiment 3 (for the single dam) indicates that the Chl *a* concentration and the Non-CT dominance are important in forecasting real time outcomes of both the experiments. This indicates that the use of both these variables may not be applicable for future use.

Experiment 8: Cyanotoxin producer (CT) group algae counts and environment variables as input (all dams)

In Experiment 8 to forecast the CT Group, algae dominance, the selected environmental variables together with the Chl *a* concentration were used as input into the model. The results obtained are shown in Fig. 25. The r^2 value was 0.9911 and the correlation was 0.9962. This correlation is extremely good and statistically highly significant.

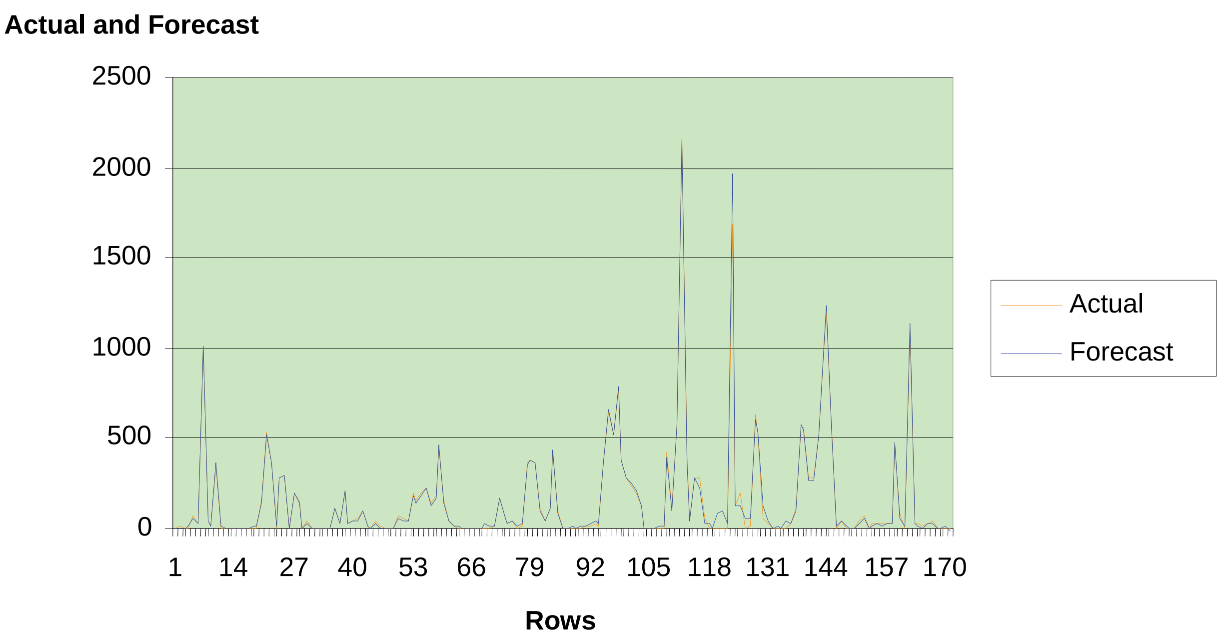


Figure 25 Actual (orange line) versus forecasted (blue line) results for the CT producing algae group using environmental variables and algae counts as inputs for the Forecaster XL ANN Software package.

The results of the model as shown in Table 15 also show that the model predicts the outcomes very well as the average actual error is very small and the average mean square error (MSE) is lower than any of the experiments before. The number of good forecasts has increased to 38% for the training dataset and to 52% with the testing dataset.

Table 15 A summary of the modelling results for CT producing group using algal dominance, selected environmental variables and Chl *a* concentration as inputs.

	Training set	**Test set**
# of rows:	142	29
CCR:	n/a	n/a
Average AE:	12.951232	8.2859074
Average MSE:	889.96353	239.1688
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	54 (38%)	15 (52%)
# of Bad forecasts:	88 (62%)	14 (48%)

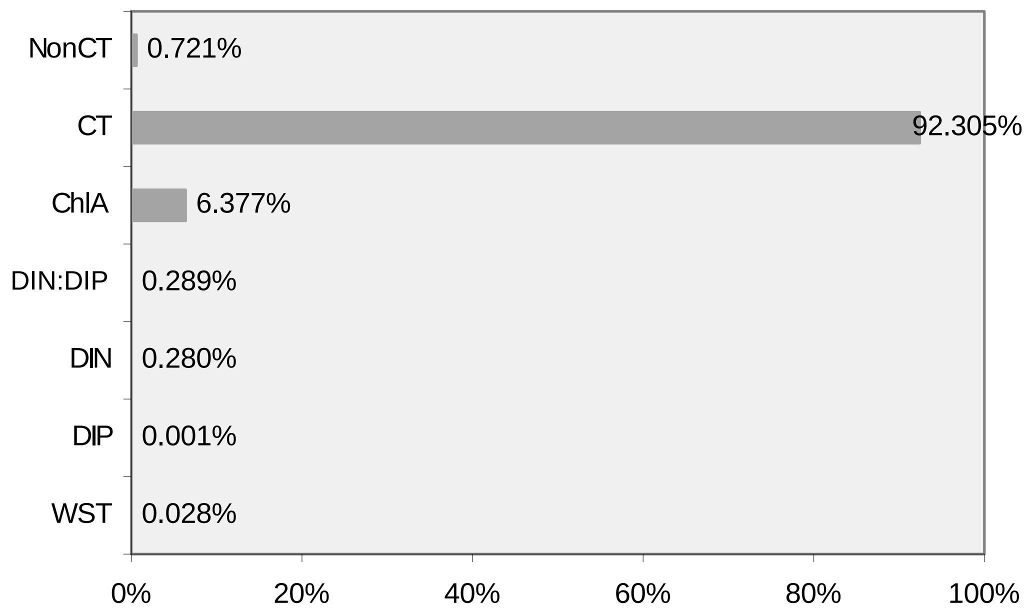


Figure 26 Percentage contributions of algal dominance data, selected environmental parameters and Chl *a* concentration as result of the Forecaster XL forecasting of the CT producing group.

In Fig. 26 it is shown that the CT group counts contributed 92.305% to the outcomes of the model. The Chl *a* concentrations contributed 6.377% and the non-CT group counts 0.721% to the outcomes.

This shows that it is basically the CT counts itself that are used to predict the CT biovolume and this is not quite what one would want from a prediction model. Other factors, e.g. the environmental variables, need to contribute towards the successful forecasts of the outcome variable.

When Experiment 8 (all dams) is compared to Experiment 4 (single dam), the CT biovolume contribute in both instances over 90% to the outcome of the forecast. In the case of Experiment 4 the WST is an important environmental variable contributing to the results, while in the case of Experiment 8 the Chl *a* concentration is more important.

Experiment 9: Non-Cyanotoxin producer (Non-CT) group environment variables, chlorophyll omitted, as input (all dams)

In Experiment 9 the input variables used were only the measured environmental variables. Both the algae counts, and the Chl *a* concentrations, were omitted from the input variables. The results obtained are shown in Fig. 27. The r^2 value was 0.3973 and the correlation was 0.7233. This is not such a good correlation, however, the fact that the Chl *a*, and the algal counts have been left out as input variables makes it more usable as forecasting tool.

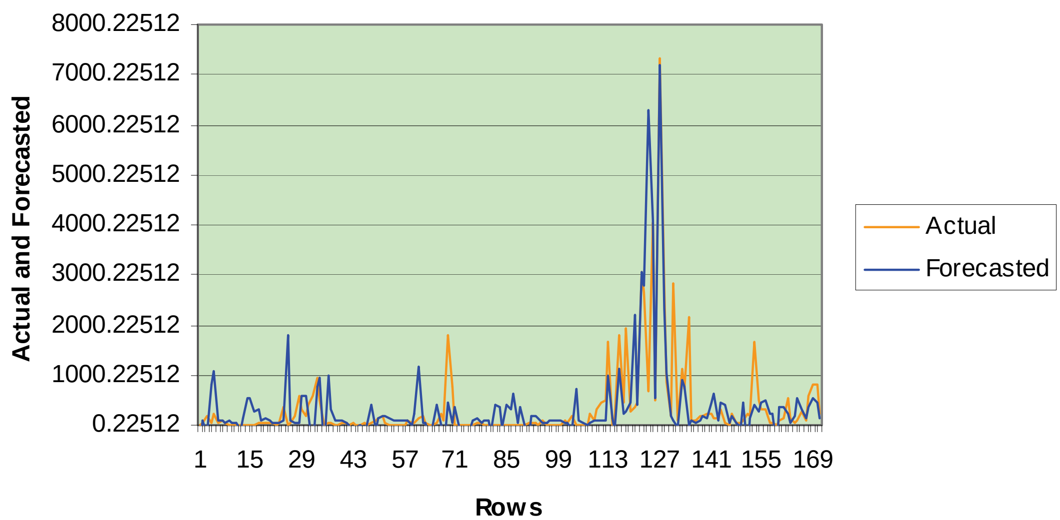


Figure 27 Actual (orange line) versus forecasted (blue line) results for the Non-CT producing group using only selected environmental variables as inputs for the Forecaster XL ANN Software package.

The errors and tolerances used in the model are shown in Table 16. The training dataset and the testing dataset errors were not as good as with experiment 8, but are still acceptable within the variability of the results. However, the number of good forecasts in the training set is only 6% and for the testing data set only 17%.

Table 16 A summary of the modelling results for the Non-CT producing group using only environmental variables as inputs.

	Training set	**Test set**
# of rows:	142	29
CCR:	n/a	n/a
Average AE:	266.95715	484.59321
Average MSE:	238219.96	1281396.3
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	9 (6%)	5 (17%)
# of Bad forecasts:	133 (94%)	24 (83%)

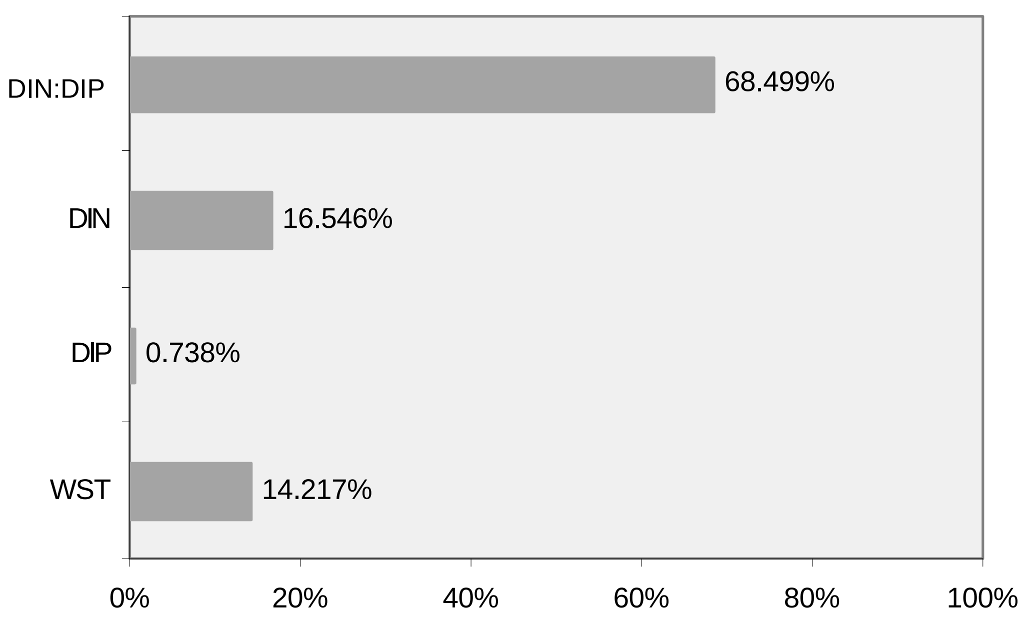


Figure 28 Percentage contributions of the selected environmental parameters to Forecaster XL forecasts for the Non-CT group.

In this case, where only the environmental variables were used as input to the model, the DIN:DIP ratio contributes 68.499% to the outcome(non-CT group) of the model (Fig. 28). This is contradictory to Chutter & Rossouw (1991) that suggests that the N:P ratio is a driving force for the presence of the CT group. The other environmental variables that contribute to the outcome are the DIN concentrations with a contribution of 16.546% and the WST with a contribution of 14.217%. The DIP concentrations indicate that only 0.738% of the outcome is caused by the contribution of DIP. Therefore, these results show that the driving forces behind the forecasts of the non-CT group are the N:P ration, DIN concentrations and the WST at a given time.

<u>Experiment 10:</u> Cyanotoxin producer (CT) group environment variables, Chl *a* omitted, as input (all dams)

In Experiment 10, the algae counts and the Chl *a*, concentrations are not included as input variables. Only the measured environmental variables are used as input into the model and the results obtained are shown in Figure 29. The r^2 value was 0.4681 and the correlation was 0.7018.

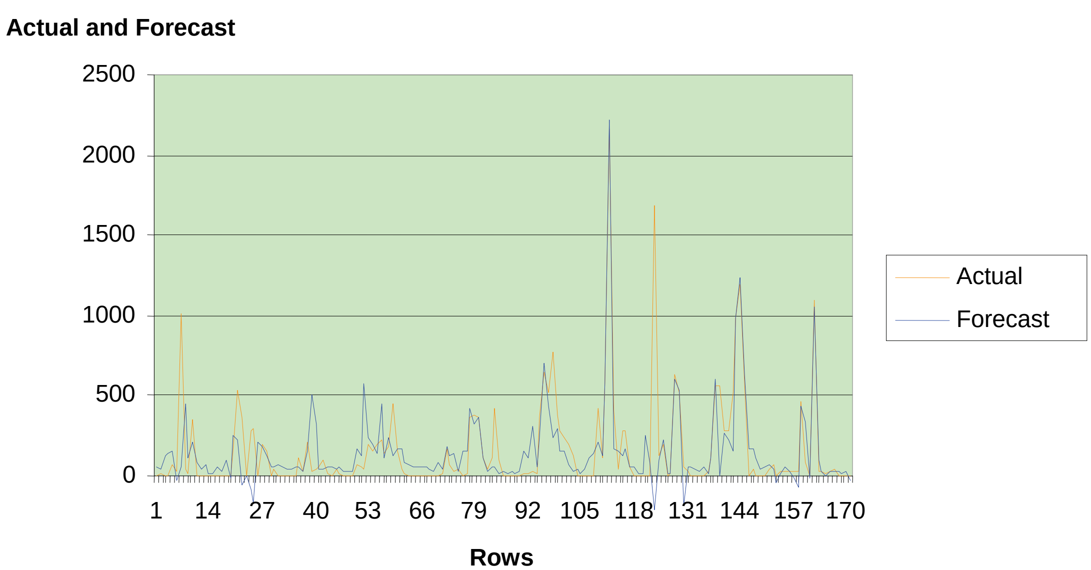


Figure 29 Actual (orange line) versus forecasted (blue line) results for the CT producing group using only environmental variables as inputs for the Forecaster XL ANN Software package.

The errors and the tolerances of the results of the model for Experiment 10 are shown in Table 17. The average actual errors (AE) may be within acceptable limits but the average MSE are quite high. The number of good forecasts according to the model is only 12% in the training dataset and 10% for the testing dataset.

Table 17 A summary of the modelling results for the CT producing group using only the selected environmental variables as inputs.

	Training set	**Test set**
# of rows:	142	29
CCR:	n/a	n/a
Average AE:	90.393001	171.97215
Average MSE:	41676.174	69798.824
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	17 (12%)	3 (10%)
# of Bad forecasts:	125 (88%)	26 (90%)

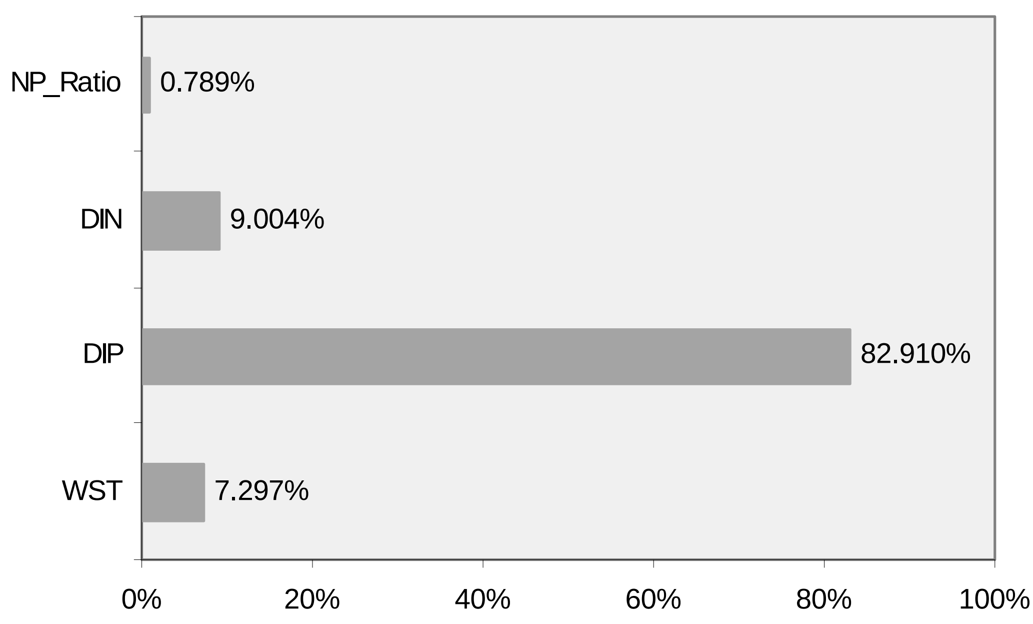


Figure 30 Percentage contributions of selected environmental parameters to Forecaster XL forecast for the CT producing group.

In the forecast of the CT group, using only the selected environmental variables as input it is shown in Fig. 30 that the DIP concentrations contributed most to the model's outcome. The second most important environmental variable was the DIN concentrations with a contribution of 9.004%. This indicates the importance of the nutrients in forecasting the composition of the algal community. It seems that the DIP is the most important environmental variable in determining the presence of the CT group. The WST is also important in the outcome of the model by predicting the CT Group. With this experiment the N:P ratio was the least important variable in predicting the CT Group.

Experiment 11: Prediction of the Non-cyanotoxin producer (Non-CT) group including environment variables and algae dominance; chlorophyll omitted, as input (all dams)

In Experiment 11 the Chl *a* concentrations are not included as input variables. Only the measured environmental variables and the algae dominance are used as input into the model and the results obtained are shown in Fig. 31. The r^2 value was 0.9799 and the correlation was 0.9904.

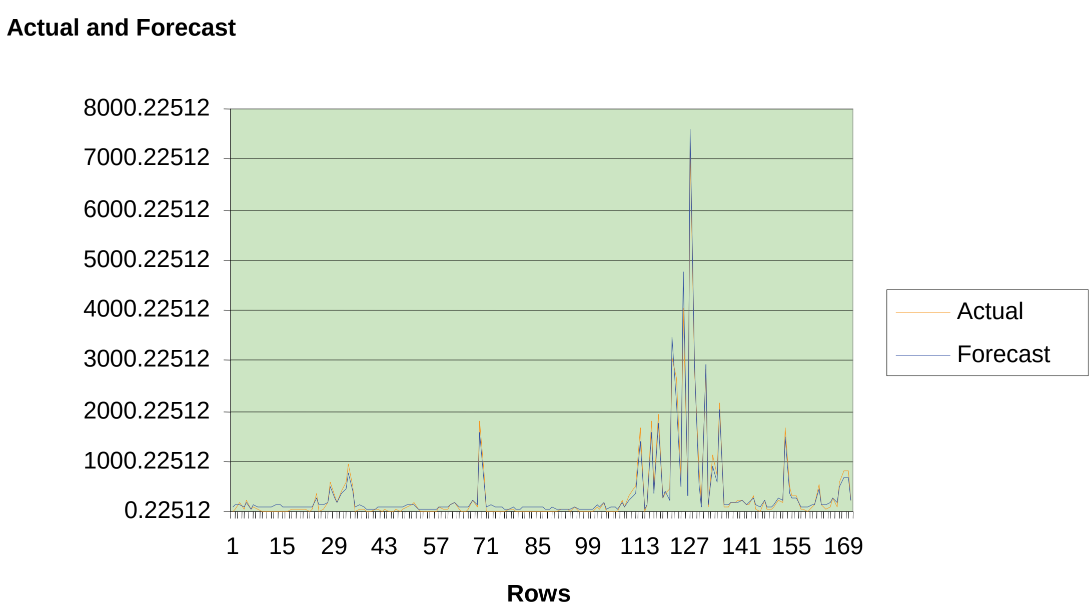


Figure 31 Actual (orange line) versus forecasted (blue line) results for the Non-CT producing group using only environmental variables and algal counts as inputs for the Forecaster XL ANN Software package.

The errors and the tolerances of the results of the model for Experiment 11 are shown in Table 18. The average actual errors (AE) may be within acceptable limits but the average MSE are quite high. The number of good forecasts according to the model is only 17% in the training dataset and 24% for the testing dataset.

Table 18 A summary of the modelling results of the Non-CT producing group using the selected environmental variables, algal dominance and Chl *a* concentration as inputs.

	Training set	**Test set**
# of rows:	142	29
CCR:	n/a	n/a
Average AE:	79.179105	73.15253
Average MSE:	14788.918	6900.0463
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	24 (17%)	7 (24%)
# of Bad forecasts:	118 (83%)	22 (76%)

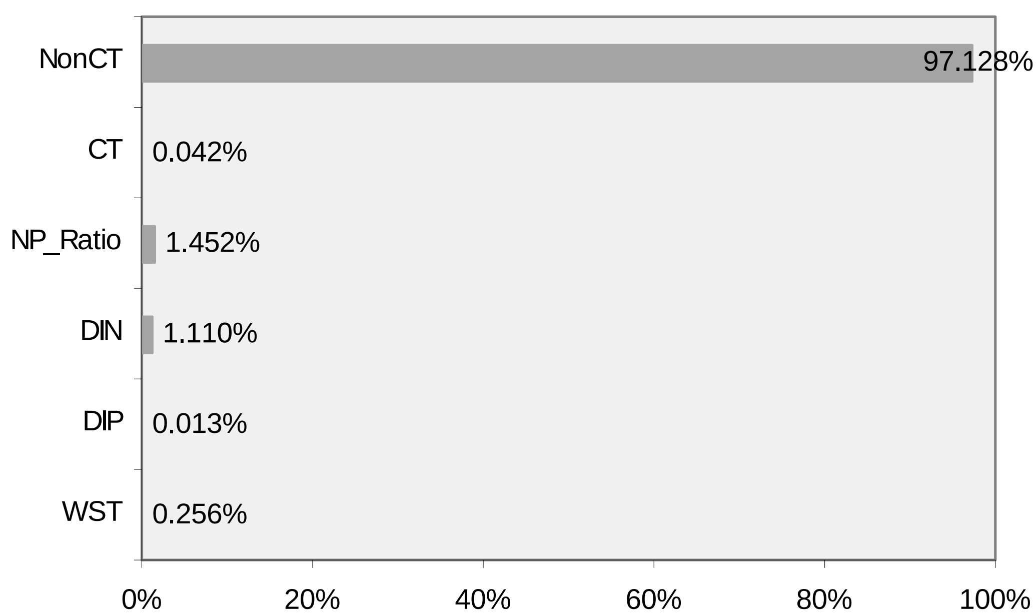


Figure 32 Percentage contributions of algal dominance, selected environmental parameters and Chl *a* concentration to ANN prediction for the Non-CT group.

In the forecast of the Non-CT group using only the environmental variables and algal dominance as inputs, it is shown in Fig. 32 that the algal dominance contributed most (97.128%) to the model outcome. The second most important environmental variable was the N:P ratio (1.452%) and thirdly, the DIN concentrations contribute 1.110%. The WST is used in determining the outcome of the model by predicting the Non-CT Group, however the contribution is very small. This indicates that the DIN concentrations may be more important in the development and forecasting of the Non-CT group.

Experiment 12: Prediction of the Cyanotoxin producer (CT) group including the environment variables and algae dominance; chlorophyll omitted, as input (all dams)

In Experiment 12 the Chl *a* concentrations are not included as input variables. Only the measured environmental variables and the algae counts are used as input into the model and the results obtained are shown in Figure 33. There is very little distinction between the actual and predicted values. The r^2 value was 0.9811 and the correlation was 0.9911. This is a very good correlation.

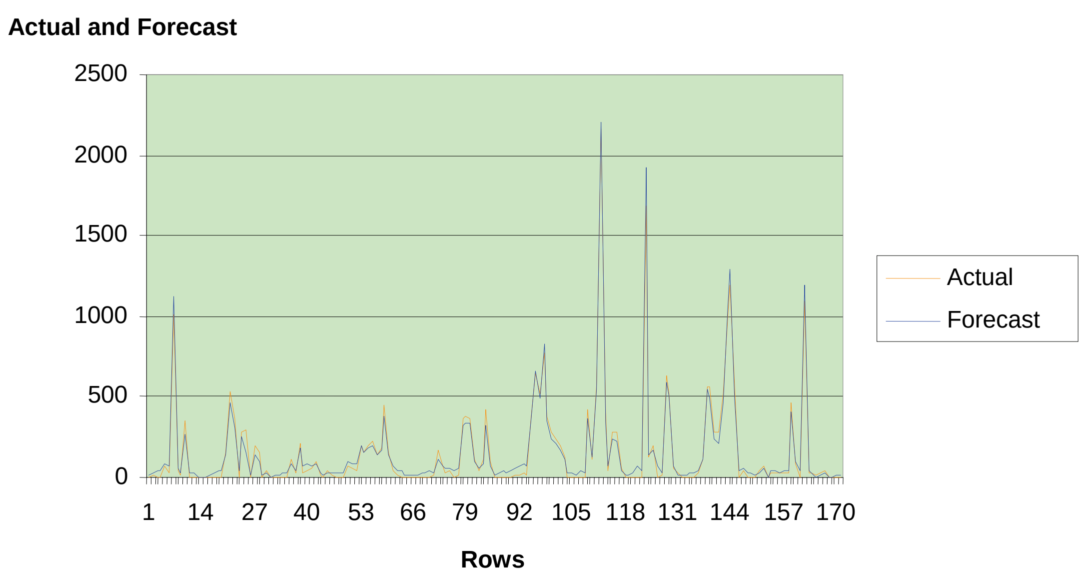


Figure 33 Actual (orange line) versus forecasted (blue line) results for the CT producing group using only environmental variables and algal counts as inputs for the Forecaster XL ANN Software package.

The errors and the tolerances of the results of the model for Experiment 12 are shown in Table 19. The average actual errors (AE) may and the average MSE are quite high. The number of good forecasts according to the model is 20% in the training dataset and 31% for the testing dataset. The acceptance of a 30% tolerance is quite strict and does not give very acceptable results.

Table 19 A summary of the modelling results for the CT producing group using algal dominance and selected environmental variables as inputs.

	Training set	**Test set**
# of rows:	142	29
CCR:	n/a	n/a
Average AE:	30.124946	32.220362
Average MSE:	1597.2205	1915.5839
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
# of Good forecasts:	28 (20%)	9 (31%)
# of Bad forecasts:	114 (80%)	20 (69%)

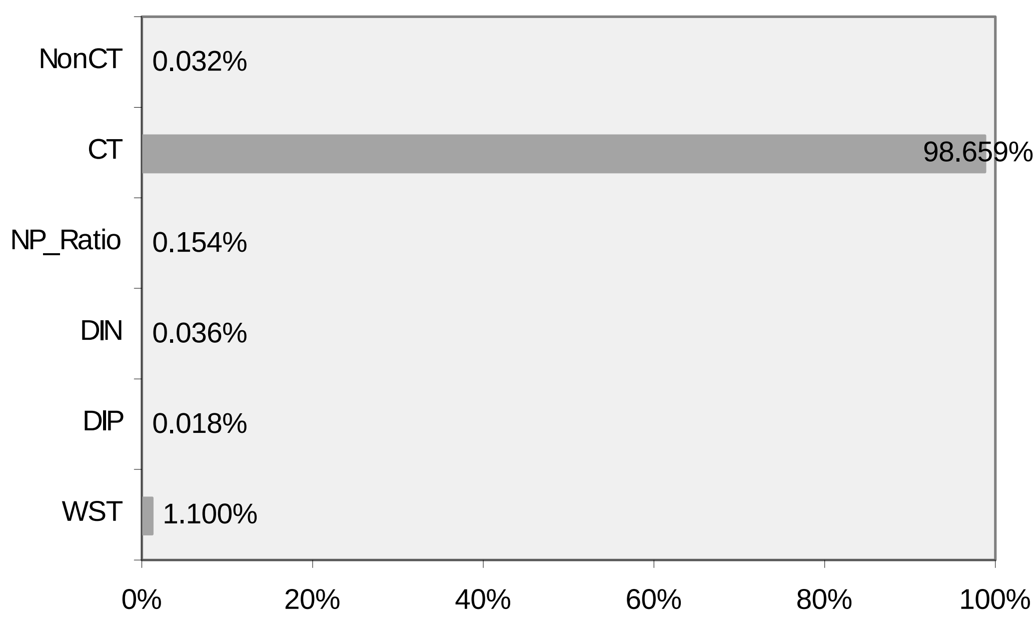


Figure 34 Percentage contributions of the algal dominance and the selected environmental parameters to ANN prediction for the CT group.

In the forecast of the Cyanotoxin group using the environmental variables and algal dominance as inputs it is shown in Fig. 34 that the algal dominance contributed most (98.659%) to the model outcome. The second most important environmental variable is the WST (1.100%) and thirdly the N:P ratio contributed 0.154%. The DIN and DIP concentrations do not contribute significantly to the outcome of this experiment.

The results achieved with the MFNN (Forecaster XL) look promising, and give an output that shows the successes and failures of the results. The percentage tolerance of the modelling package with the training set is 10% and with the testing set is 30%. The presentation of the most important factors in determining the output of the model, does give a researcher insight into the driving environmental variables that were fed into the model.

The modelling results did not show very high successes, however, the user friendliness of the program and the ease with which it can be used within the Microsoft background make it a good choice for further use and testing. The one main problem of the program is that it does not supply the user with the developed algorithms used within the model.

3.3.1.3 Comparison of the Forecaster XL experiments

A comparison of the 12 experiments with Forecaster XL is shown in Table 20. In forecasting the CT group, the experiments show that whenever either the algal dominance and/or the Chl *a* concentration is omitted as input variable to Forecaster XL, WST, DIP and DIN is the most important variables in determining the outcome of the model. Only in one experiment (Exp 9) did the DIN:DIP ratio show up as an important variable in determining the CT biovolume.

Whenever Chl *a* concentration is included as an input variable and the algal dominance is omitted in the model, it usually came up as the most important variable in predicting the outcome of the Non-CT group. This indicates that the extent of the Chl *a* is important in forecasting new biomass, specifically, for the Non-CT producing group. Chl *a* seem to be not so important in the forecasting of the CT group. There is no consistency regarding this group (Table 20).

If algal dominance is used as input variable, it dominates the contribution of the input variables. This is using the forecasted variable to predict the biovolume, and it should not be used in this type of modelling exercise.

Table 20 Comparison of the experiments done with the MFF ANN modelling results of ForecasterXL showing the average actual errors, the good and bad forecasts and the contribution of the environmental, biomass and Chl *a* towards the output of each experiment.

Experiment	**Average Actual Error**	**Good Forecasts (%)**	**Bad Forecasts (%)**	**Contribution of Environmental Variables to modelling Results (%)**						
				Non-CT	**CT**	**Chl *a***	**DIN:DIP**	**DIN**	**DIP**	**WST**
Single Dam										
Experiment 1: Non-CT, Chl *a* & Environmental Variables				-	-	83.28	1.935	0.676	9.257	4.850
- Testing Data Set	46.792	17	83							
- Training Data Set	62.012	0	100							
Experiment 2: CT, Chl *a* & Environmental Variables				-	-	5.589	8.303	7.028	18.171	60.910
- Testing Data Set	23.212	7	93							
- Training Data Set	102.333	50	50							
Experiment 3: Non-CT, Environmental Variables, Algal dominance & Chl *a*				16.188	4.643	76.822	0.084	0.285	0.389	1.588
- Testing Data Set	13.922	23	77							
- Training Data Set	23.618	33	67							
Experiment 4: CT, Environmental Variables, Algal dominance & Chl *a*				0.198	94.501	0.240	0.000	0.055	0.524	4.481
- Testing Data Set	6.562	37	17							
- Training Data Set	17.712	63	83							

Experiment	Average Actual Error	Good Forecasts (%)	Bad Forecasts (%)	Contribution of Environmental Variables to modelling Results (%)						
				Non-CT	CT	Chl *a*	DIN:DIP	DIN	DIP	WST
All dams										
Experiment 5: Non-CT, Environmental Variables & Chl *a*				-	-	41.215	32.717	13.857	0.003	12.208
- Testing Data Set	136.342	13	87							
- Training Data Set	140.712	17	83							
Experiment 6: CT, Environmental Variables & Chl *a*				-	-	26.121	3.895	44.621	2.364	22.999
- Testing Data Set	66.753	11	89							
- Training Data Set	142.200	17	83							
Experiment 7: Non-CT, Environmental Variables, Algal dominance & Chl *a*				56.58	1.987	40.447	0.191	0.341	0.052	0.403
- Testing Data Set	64.584	18	82							
- Training Data Set	85.779	28	72							
Experiment 8: CT, Environmental Variables, Algal dominance & Chl *a*				0.721	92.305	6.377	0.289	0.280	0.001	0.028
- Testing Data Set	12.952	38	62							
- Training Data Set	8.286	52	48							
Experiment 9: Non-CT & Environmental Variables				-	-	-	68.499	16.549	0.738	14.217
- Testing Data Set	266.957	6	94							
- Training Data Set	484.593	17	83							

Experiment	Average Actual Error	Good Forecasts (%)	Bad Forecasts (%)	Contribution of Environmental Variables to modelling Results (%)						
				Non-CT	**CT**	**Chl *a***	**DIN:DIP**	**DIN**	**DIP**	**WST**
All Dams										
Experiment 10: CT & Environmental Variables				-	-	-	0.789	9.004	82.910	7.297
- Testing Data Set	90.393	12	88							
- Training Data Set	171.97	10	90							
Experiment 11: Non-CT & Environmental Variables & Algal Dominance				97.128	0.024	-	1.452	1.110	0.013	0.256
- Testing Data Set	79.179	17	83							
- Training Data Set	73.153	24	76							
Experiment 12: CT & Environmental Variables & Algal dominance				0.032	98.659	-	0.154	0.036	0.018	1.100
- Testing Data Set	30.125	20	80							
- Training Data Set	32.220	31	69							

3.3.2 Self-Organising Map (SOM)

The primary application for the SOM is clustering and data segmentation. Non-supervised neural networks learn to ordinate, cluster or group the data patterns only by inspecting the similarities between the inputs (Smith, 2002; Recknagel *et al*., 2006). Clustering involves classifying or ordinating the data into groups based upon the natural structure of the data, rather than known pre-defined classifications. The data from the Roodeplaat Dam was divided into two groups (before 1991 and after 1991) to represent the before and after Zeekoegat Waste Water Treatment Works (WCW) conditions. The WCW discharge directly into the Roodeplaat Dam since 1991 and the impact of the establishment of a WCW on a reservoir can be expressed in the ordination and clustering mapping of the unsupervised SOM.

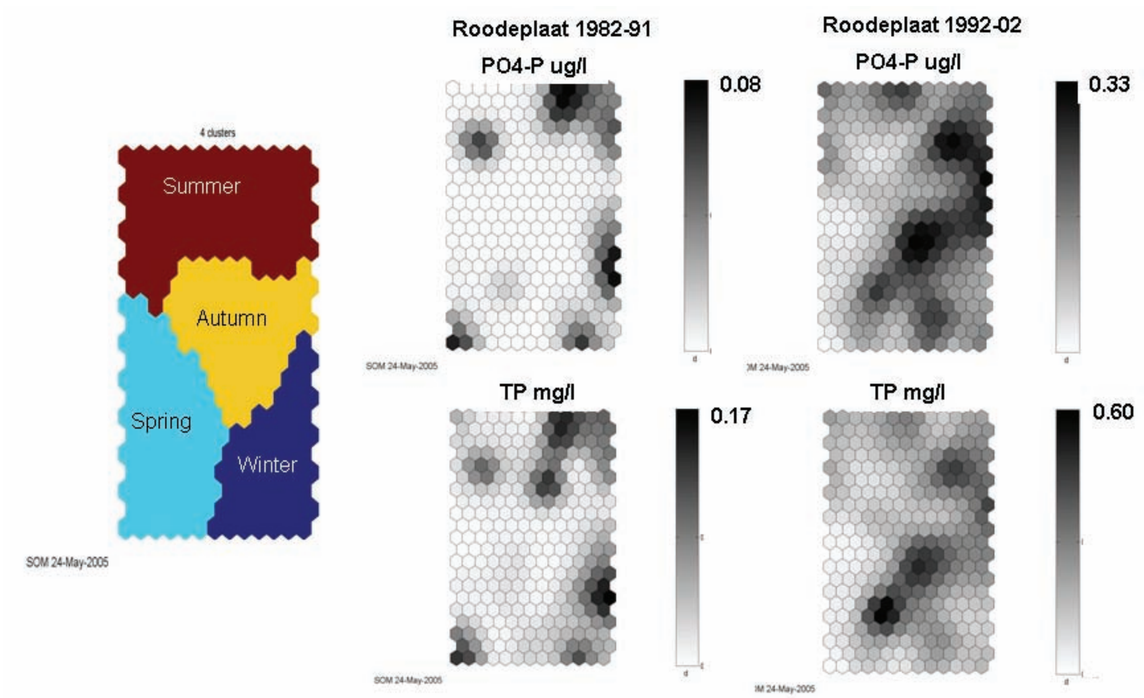


Figure 35 The ordination and clustering map of the PO_4-P (DIP) and TP concentrations in the Roodeplaat Reservoir for the before and after construction of Zeekoegat WCW that show the changes in the water quality.

In Fig 35, it is shown that there was a large increase in the maximum concentrations of both the PO_4-P and TP in the Roodeplaat Reservoir in response to the impact of the Zeekoegat WCW. The maximum PO_4-P concentration increased from 0.08mg/L to 0.33mg/L. The maximum TP concentration increased from 0.17mg/L to 0.60mg/L. The seasonal occurrence of the higher

PO_4-P concentrations shifted from small peaks in all seasons, but primarily in summer to extreme high concentrations throughout the year. The changes in TP concentration showed similar patterns. The impact of the WCW was severe and the Roodeplaat Dam has since been shifted into hypertrophic conditions, as can be seen from this data as well.

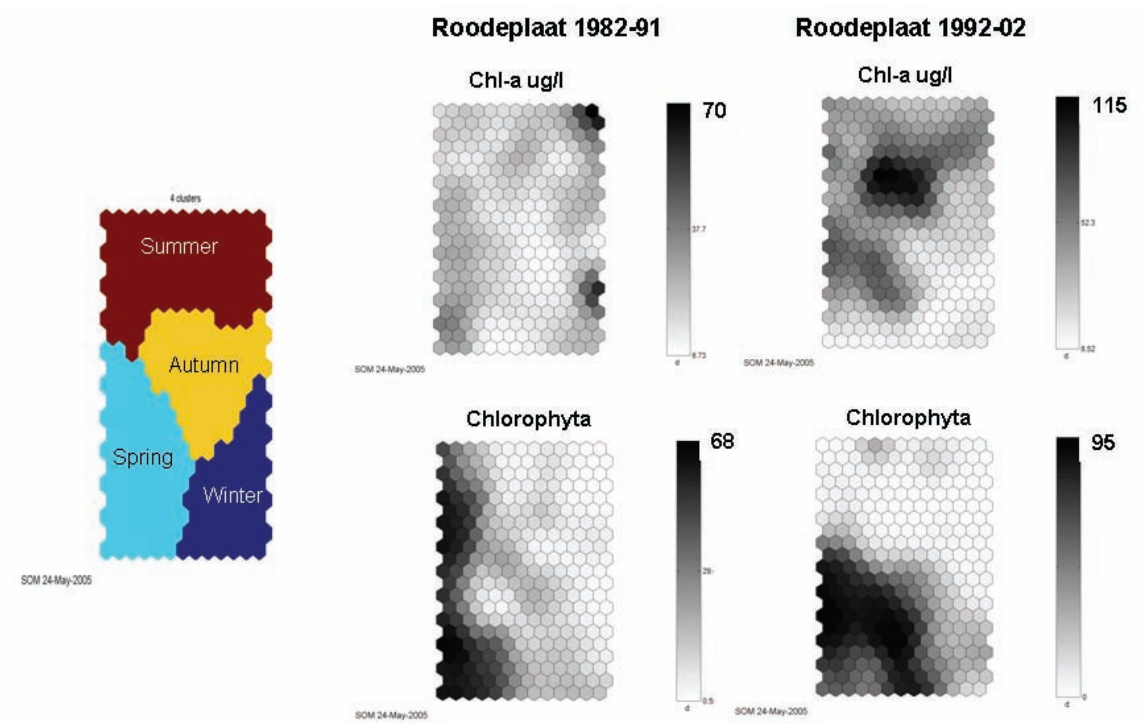


Figure 36 The ordination and clustering map of the Chl *a* compared to the Chlorophyta dominance in the Roodeplaat Reservoir for the before and after construction of Zeekoegat WCW that show the changes in the water quality.

The modelling results also show an increase in the Chl *a* concentration between the before and after Zeekoegat WCW establishment. Chl *a* concentrations, increased from a maximum of 70 ug/L to a maximum of 115 ug/l (Fig. 36). The occurrence of maximum Chl *a*, concentrations shifted from small peaks in the summer and the winter to large peaks during summer and smaller peaks throughout the year. The dominance of the Chlorophyta (green algae) shifted from being dominant during spring and summer before the establishment of the WCW to being dominant primarily during spring. The dominance of the Chlorophyta during spring was replaced by dominance of cyanobacteria (Cyanophyta) (Fig. 37). Before the WCW was established, cyanobacteria were prominent throughout the year but the dominant period shifted to primarily summer through autumn with much higher biovolume overall as shown by the Chl *a* concentrations.

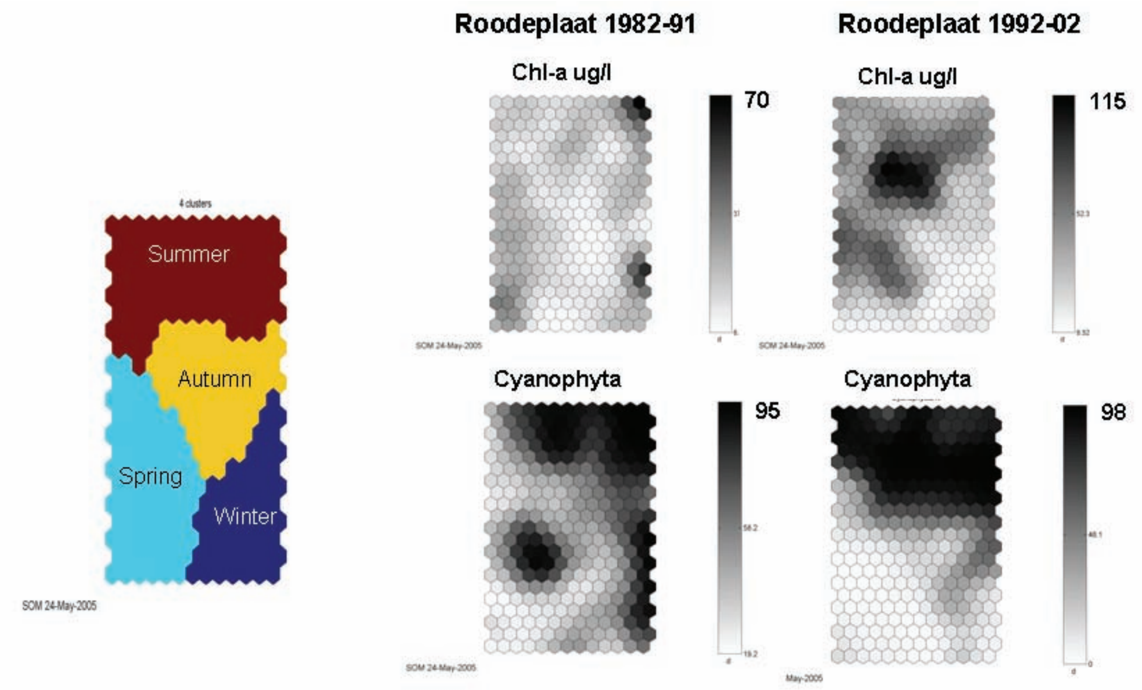


Figure 37 The ordination and clustering map of the Chl *a* compared to the Cyanophyta dominance in the Roodeplaat Reservoir for the before and after construction of Zeekoegat WCW that show the changes in the water quality.

The ordination and clustering map as output of the SOM method showed an increase in the maximum dominance of the diatoms from 41% to 52%. The diatoms have been and still are limited to be dominant primarily in the winter periods when biovolume is low (Fig. 38). The impact of the WCW on the diatoms was therefore not so severe.

The SOM modelling method showed potential for further use in South Africa as it can be used to potentially:

- Investigate, before and after situations,
- To determine the potential effects of management actions,
- Or changes in the environmental conditions.

This method is not a prediction model but can assist in the search for answers in cause and effect investigations.

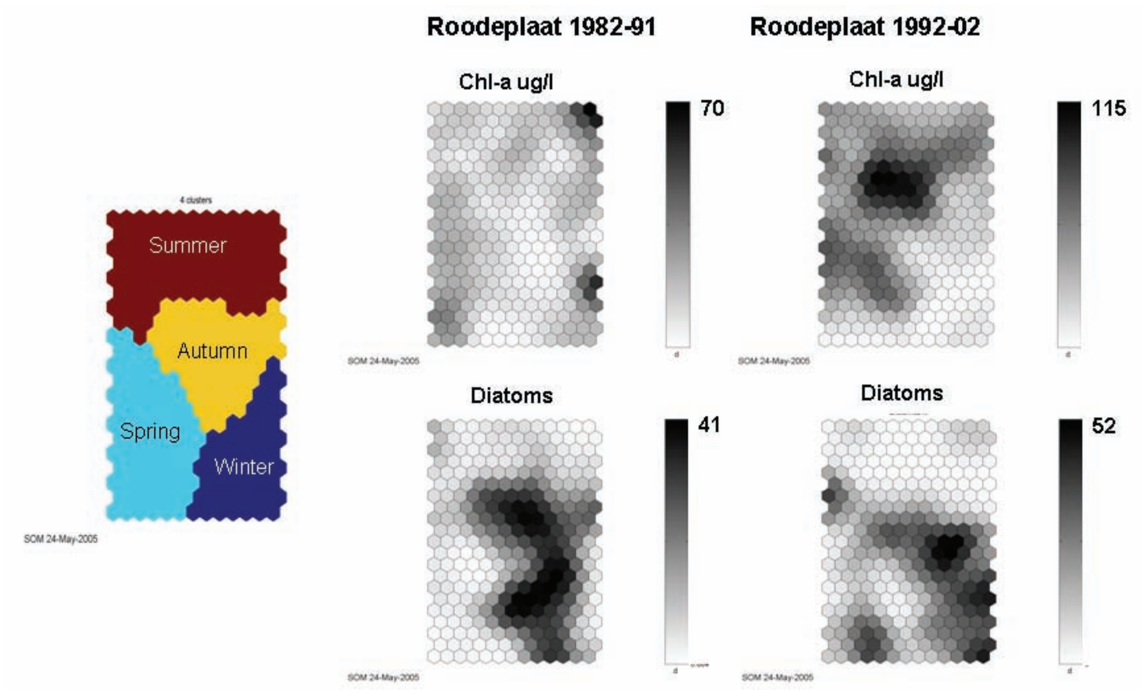


Figure 38 The ordination and clustering map of the Chl *a* compared to the diatom dominance in the Roodeplaat Reservoir for the before and after construction of Zeekoegat WCW that show the changes in the water quality.

3.4 Rule Set Development by Hybrid Evolutionary Algorithms

Previous studies on algal communities have demonstrated that highly complex ecological time series can be successfully probed to develop rule sets as prediction tools, by using hybrid evolutionary algorithms (HEA) (Cao *et al.,* 2005). The HEA is an adaptive method that mimics ecological evolutionary processes, natural selection and genetic variations. A number of experiments were done to determine the most applicable and usable rule set in the prediction of *Microcystis* and the dinoflagellate, *Ceratium*.

Each experiment will be discussed separately, showing the best-developed rule set for each experiment. Selected outcomes of each experiment are shown in Appendix A. All the results from the HEA experiments are available on the CD attached.

3.4.1 **HEA Experiment 1**: Real-time prediction simulation and rule-set discovery for *Microcystis* including Chl *a*, as an environmental factor.

The 36 years of real-time daily data (See Section 5.1.4) of the Hartbeespoort, Rietvlei and Roodeplaat reservoirs was used as training data to develop a rule set for the prediction of *Microcystis* biovolume as shown in Fig. 39.

The correlation coefficient ($r^2 = 0.88$) and the root mean square error (RMSE = 9.3357) for the training data and the correlation coefficient ($r^2 = 0.73$) and the root mean square error (RMSE = 7.4620) for the tested data indicate that the predictions are quite good. The model manages to predict the peaks and lows as well, as shown in Fig. 35 and Fig. 36. The predictions for the Hartbeespoort and the Roodeplaat Dam were much better than for the Rietvlei Reservoir.

More validation was done by determining the Average Actual Error (A AE) and the mean square error (MSE) as shown in Table 21. To further test the results of the experiment and to determine the impurities between the actual data and the test data set (Greenberg, 2003), the relative tolerance of the training set and of the testing data set was determined and is shown in Table 21.

The results show that with a set relative tolerance of 10% in the training set and with a relative tolerance of 30% for the testing data set, there are respectively 38.5% and 44.8% good predictions 61.5% and 55.2% bad predictions. This is a very strict relative tolerance when compared to the up to 300% that is allowed in the Vollenweider Model (IETC, 2000).

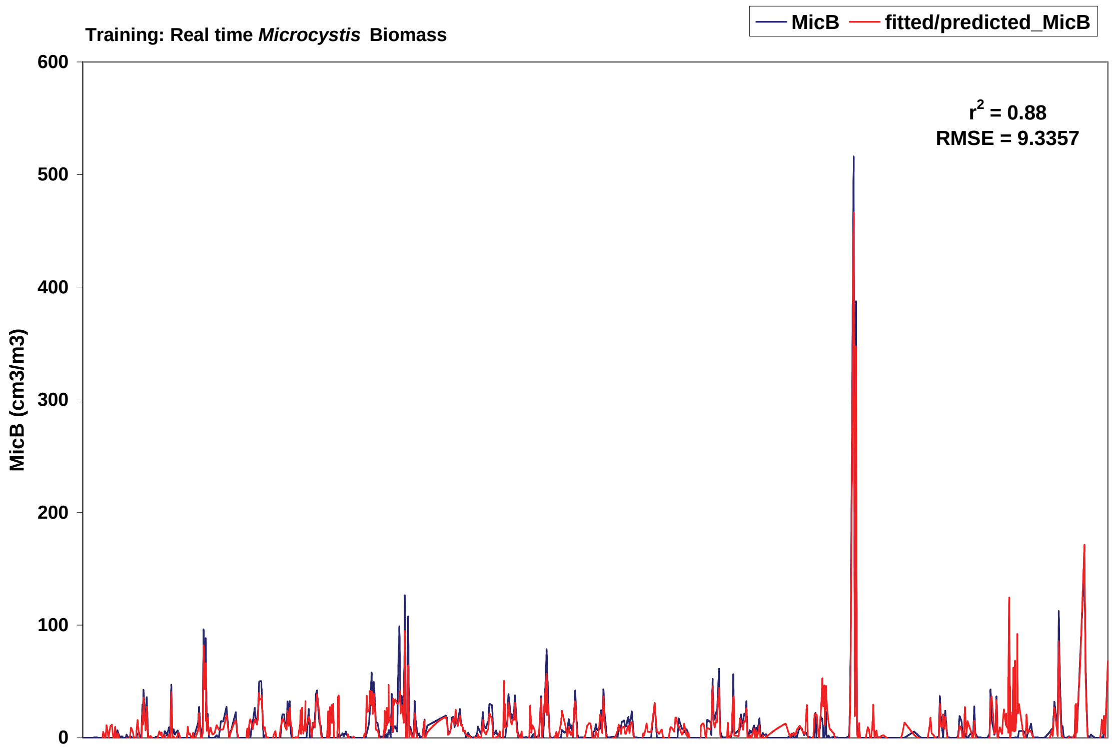


Figure 39 Training results of the real-time forecasting of *Microcystis* biovolume including Chl *a*, as an environmental variable in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs during the development of the rule set for HEA Experiment 1.

Fig. 40 shows the results of the tested data and it is clear that the rule set fits the Hartbeespoort and Roodeplaat reservoirs data better than the Rietvlei data, where under and over predictions are found. This may be due to the fact that Rietvlei also experienced dinoflagellate blooms during the study period. However, the magnitudes of the maximum *Microcystis* biovolume peaks are predicted quite well in all three of the reservoirs.

Table 21 Summary of the average actual error (AE), the mean square error (MSE) and the relative tolerance of the training and testing data sets of the *Microcystis* biovolume including Chl *a* as an environmental variable in real time rule set development.

	Training set	**Test set**
# of rows:	13148	2193
Average AE:	0.10422	0.974735
MSE:	8.414296	7.063562
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
Good predictions:	38.5%	44.8%
Bad predictions:	61.5%	55.2%

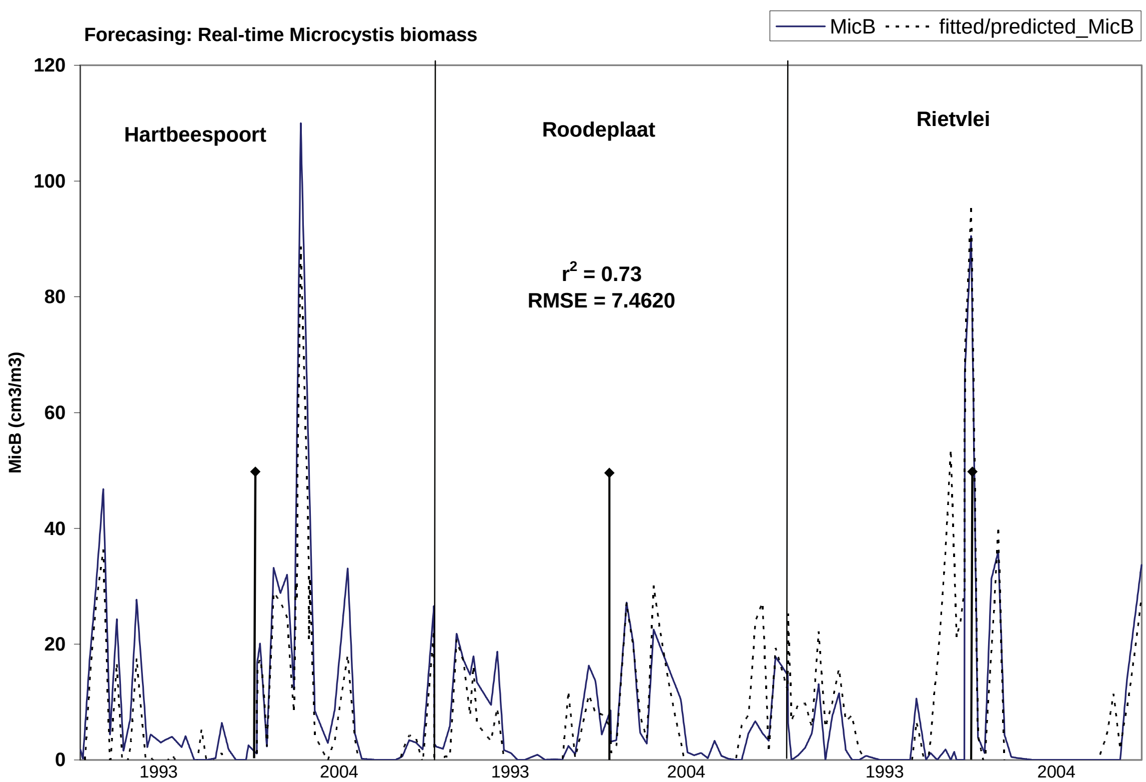


Figure 40 Testing results of the real-time forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs using the rule set as shown in Figure 41.

The conditions for the developed rule set (Fig. 41) include TP and Chl *a* concentrations that are used to determine if the THEN branch or the ELSE branch of the rule set is to be used for forecasting *Microcystis* biovolume. The sensitivity analysis that was done on the real-time testing data for the three reservoirs to determine the *Microcystis* biovolume show that with the THEN branch of the rule set surface temperature and total nitrogen are the variables to which the determination of the *Microcystis* biovolume is most sensitive to. Low TN concentrations and high surface temperatures are associated with high *Microcystis* biovolume. This suggests that the *Microcystis* biovolume decreases with an increase in the TN concentrations. The Tsurf has the expected opposite reaction. The higher the temperature rise, the larger the *Microcystis* biovolume grow.

The ELSE branch of the rule set is used when Chl *a* concentrations are below 120.519 ug/L and total phosphorous concentrations are higher than 227.982 ug/L. In the ELSE branch of the rule set Chl *a*, is the variable that the *Microcystis* biovolume is most sensitive to. Both pH and Tsurf are also used in the developed RULE set to predict the *Microcystis* biovolume but is not so important in determining changes in the *Microcystis* biovolume under these high total phosphorous conditions.

These results indicate that under phosphorus concentrations smaller than 431.729 ug/L (expressed as TP) the increases in *Microcystis* biovolume are driven negatively by high nitrogen concentrations and positively by the surface temperature (Tsurf).

Under the ELSE rule set, where TP concentrations exceed 431.729 ug/L the *Microcystis* biovolume that develops is primarily driven by the initial biomass (as indicated by the Chl *a* concentration). Temperature is still also impacting on the developing *Microcystis* biovolume, but is not as important as the Chl *a*.

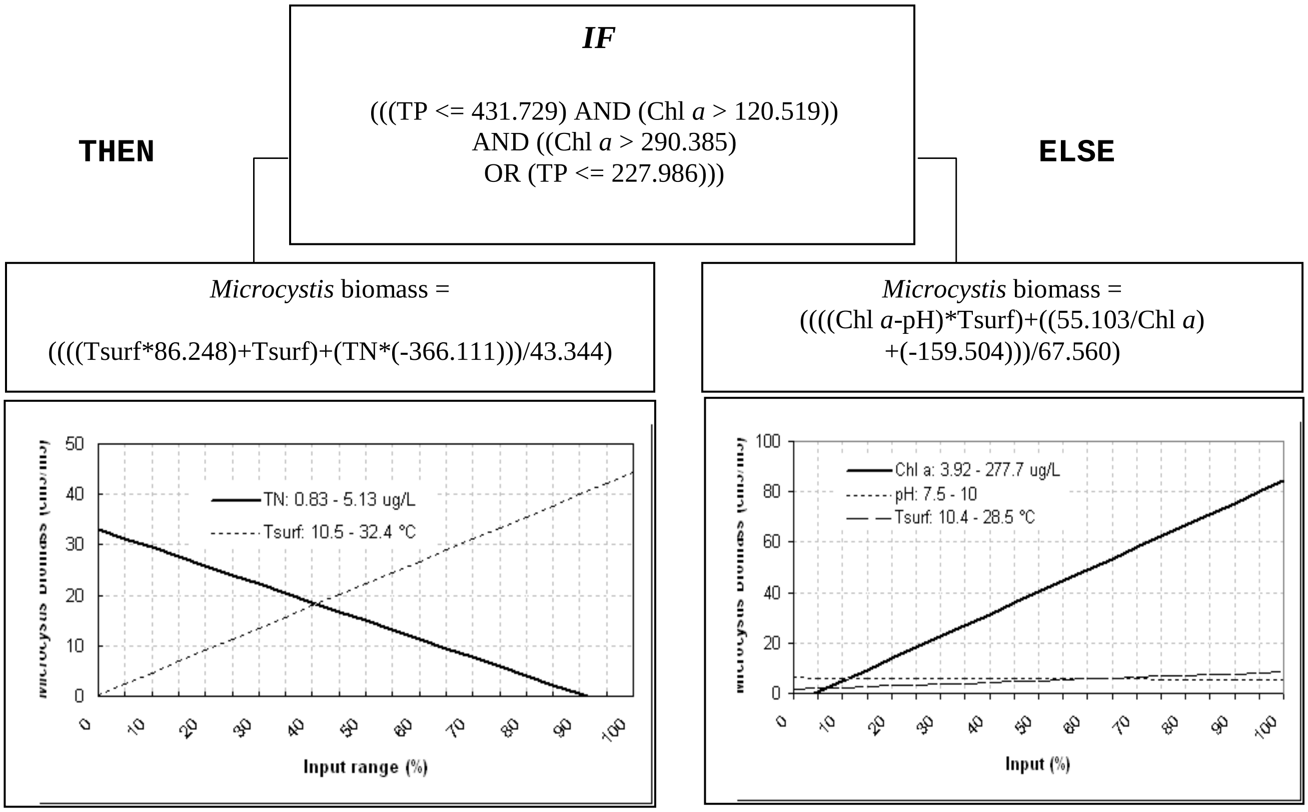


Figure 41 Sensitivity analysis of the input data for the THEN-branch (left) and the ELSE-branch (right) of the best developed rule set for real-time forecasting of *Microcystis* biovolume using the median concentrations of the most important environmental variables to determine the sensitivity of the *Microcystis* biovolume prediction to each variable.

3.4.2 **<u>HEA Experiment 2</u>**: Real-time prediction simulation and rule-set discovery for *Microcystis* excluding Chl *a*, as an environmental variable.

In the set-up of this experiment, no Chl *a* values, were included as an environmental variable. In Fig. 42 it is shown that, the predicted results are not as good as the previous experiment (HEA Experiment 1), therefore, for all subsequent experiments Chl *a* was included. A number of the peaks were not predicted correctly. However, the correlation coefficient (r^2 = 0.81) and the root mean square error (RMSE = 11.7002) for the training data and the correlation coefficient (r^2 = 0.46) and the root mean square error (RMSE = 10.3676) for the tested data indicate that the predictions are still quite good. The model does manage to predict the peaks and lows quite accurately as shown in Fig. 42 and Fig. 43. Again, the predictions for the Hartbeespoort and the Roodeplaat Dam were better than for the Rietvlei Reservoir.

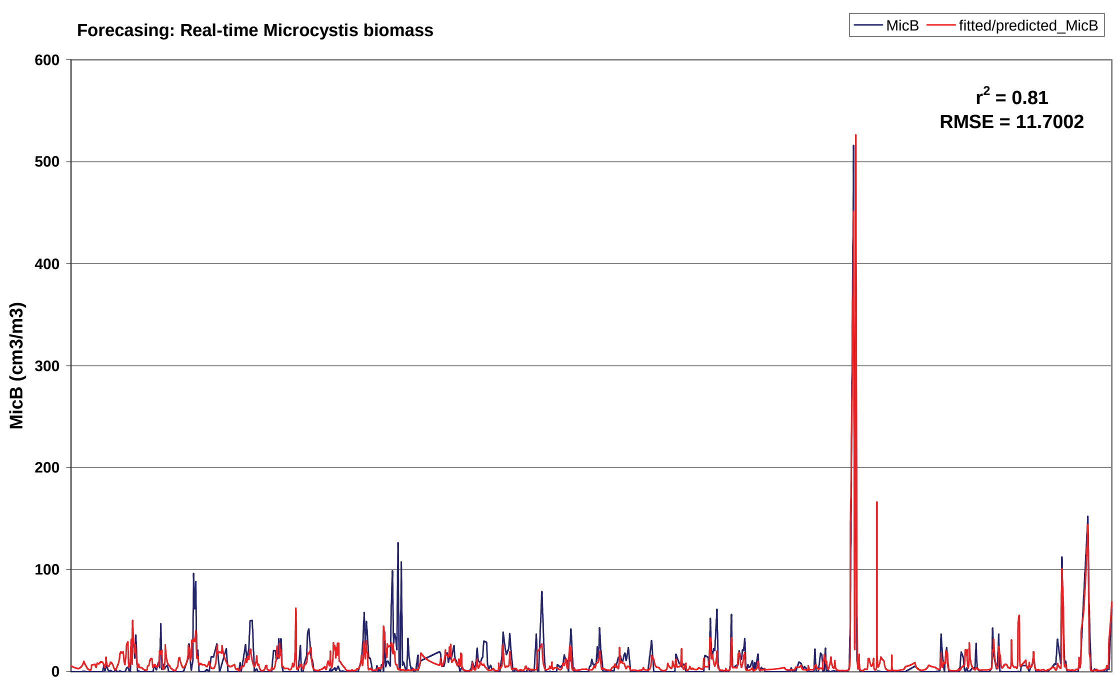


Figure 42 Training results of the real-time forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs during the development of the best rule set for HEA Experiment 2 that excluded Chl *a*, as an environmental factor.

Further validation was done by determining the Average Actual Error (A AE) and the average square error (MSE) as shown in Table 22. The impurities between the actual data and the test data set (Greenberg, 2003) was determined by the relative tolerance of the training set, and of the testing data set, and is shown in Table 22.

The results show that with a set relative tolerance of 10% in the training set and with a relative tolerance of 30% for the testing data set, there are respectively 42.3% and 62.9% good predictions and respectively 57.7% and 37.1% bad predictions. Although this is a very strict relative tolerance, these results are better than the previous experiment, and the number of acceptable predictions is quite good.

Table 22 Summary of the average actual error (AE), the average mean square error (MSE) and the relative tolerance of the training and testing data sets of the *Microcystis* biovolume real time rule set development excluding Chl *a* as an environmental variable.

	Training set	**Test set**
# of rows:	13148	2193
Average AE:	0.342782	1.630976
MSE:	10.52243	7.503751
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
Good predictions:	42.3%	62.9%
Bad predictions:	57.7%	37.1%

A number of times the predictions were under predicting. This was especially the case in the predictions for Rietvlei. The Rietvlei Reservoir is known to lie within a colder area when compared to the Hartbeespoort and the Roodeplaat reservoirs.

The conditions for the developed rule set (Fig. 44) in the absence of Chl *a* concentrations include the TN and Secchi depth as conditional parameters that are used to determine if the THEN branch or the ELSE branch of the rule set is to be used for forecasting *Microcystis* biovolume. For the rule set to use the THEN branch the TN concentration needs to be greater than 0mg/L and smaller than 7.77 mg/L. The Secchi depth to comply with the condition set for the THEN branch should be less than 0.7 m. Otherwise, the ELSE branch applies to determining the *Microcystis* biovolume.

The sensitivity analysis that was done on the real-time testing data for the three reservoirs to determine the *Microcystis* biovolume show that with the THEN branch of the rule set, total phosphorous (TP), total nitrogen (TN), pH and surface temperature (Tsurf) are the variables to which the outcome of the *Microcystis* biovolume is most sensitive to. Within this rule set TP has the highest impact, TN the second highest and Tsurf has a smaller impact on the extent of *Microcystis* biovolume development. The pH, although used in the rule set does not seem to play a significant role in determining the outcome. This phenomenon may be because of the small changes in pH in general. This suggests that the *Microcystis* biovolume increases with increase in the TP, TN and Tsurf.

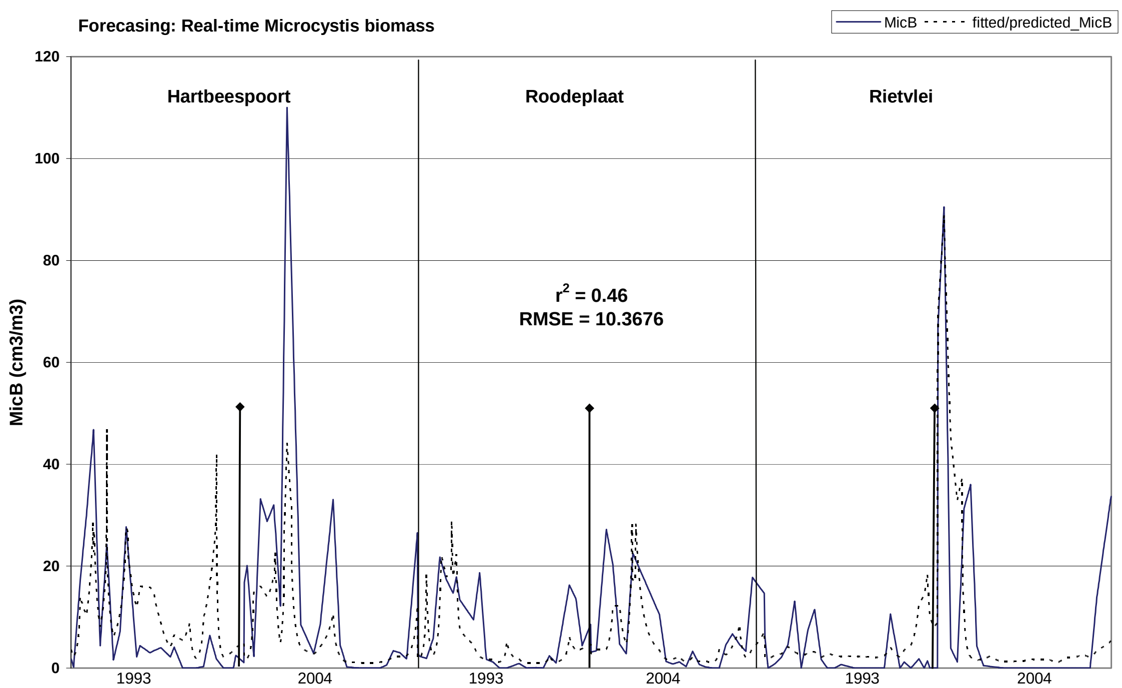


Figure 43 Testing results of the real-time forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs using the best-developed rule set as shown in Figure 5.44, excluding Chl *a*, as an environmental factor.

In the ELSE branch of the rule set, the Secchi depth and the pH are the variables that determine the outcome of the *Microcystis* biovolume. The Secchi depth is the most important variable that negatively impacts on the prediction of the *Microcystis* biovolume. Under low light conditions (shallow Secchi depths), there is a strong decrease in the *Microcystis* biovolume. Again, the pH seems to have no significant impact on the *Microcystis* biovolume outcome when the input ranges increase stepwise.

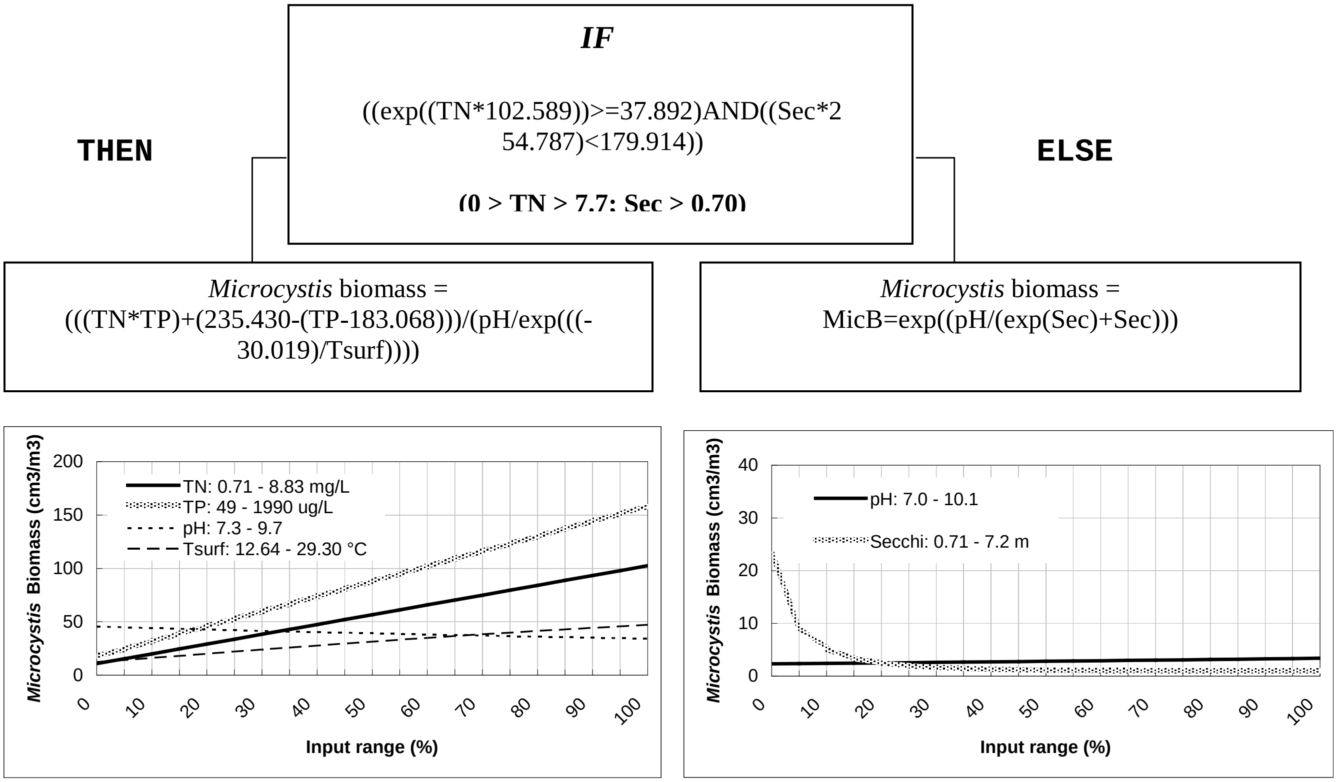


Figure 44 Sensitivity analysis of the input data for the THEN-branch (left) and the ELSE-branch (right) of the best developed rule set for real-time forecasting of *Microcystis* biovolume using the median concentrations of the most important environmental variables (excluding Chl *a*) to determine the sensitivity of the *Microcystis* biovolume prediction to each variable.

3.4.3 **<u>HEA Experiment 3</u>**: 7-Days forward prediction simulation and rule set discovery for *Microcystis*

To develop a rule set for the 7-days forward prediction of *Microcystis* biovolume the daily interpolated data of the 36 years data set was used for training on the Hartbeespoort, Rietvlei and Roodeplaat reservoir. The *Microcystis* biovolume measured data was shifted backwards to create the condition of 7-days forward training. The training results from this experiment are shown in Figure 45.

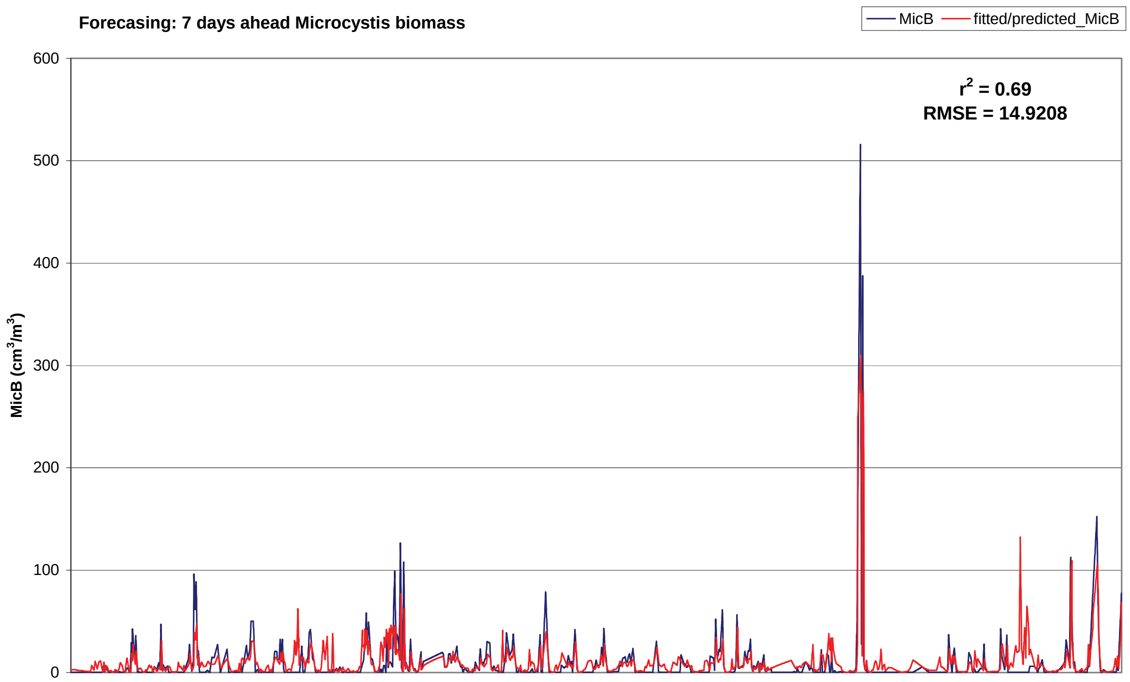


Figure 45 Training results of the 7-days forward forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs using the developed rule set of experiment 3.

The r^2 = 0.69 and the RMSE = 14.9208 for the training data and the r^2 = 0.52 and the RMSE = 9.3582 for the tested data are very good results and show that this 7-days forward prediction can be used on reservoirs with similar trophic status and climatic conditions. Fig. 46 shows the results of the tested data and it is clear that the rule set fits the Hartbeespoort and Roodeplaat reservoirs data better than the Rietvlei data, where under and over predictions are found. However, the magnitudes of the maximum *Microcystis* biovolume peaks are predicted quite well in all three the reservoirs.

Table 23 Summary of the average actual error (AE), the average mean square error (MSE) and the relative tolerance of the training and testing data sets of the 7-days forward forecasting of *Microcystis* biovolume RULE set development.

	Training set	**Test set**
# of rows:	13148	2193
Average AE:	-1.43515	-0.2281
MSE:	12.22073	6.978118
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
Good predictions:	53.9%	70.3%
Bad predictions:	46.1%	29.7%

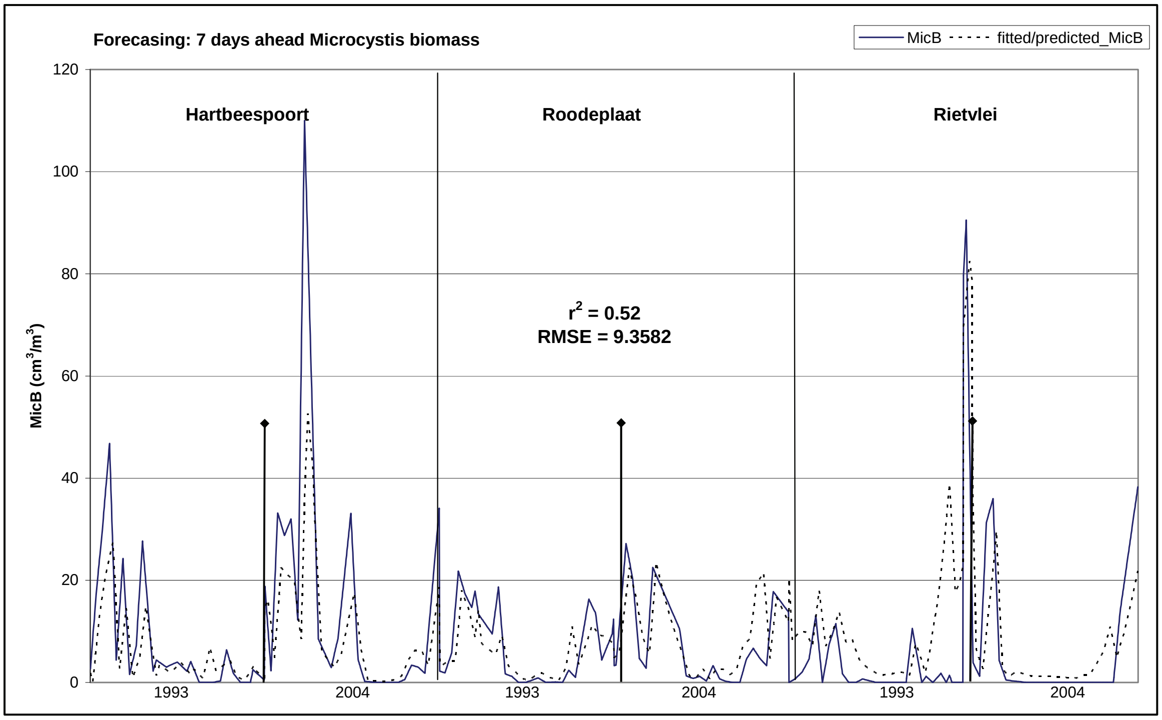


Figure 46 Testing results of the 7-days forward forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs using the best-developed rule set as shown in Figure 43.

The further validation shows that the Relative Tolerance of 10% do give an outcome of 53.9% good predictions for the training data set (Table 23). The Relative Tolerance of 30% for the testing set shows an outcome of 70.3% good predictions.

The smaller MSE found within the The testing data set, when compared to the training data set, show that the predictive capability of the RULE set is better. Fig. 47 illustrates the IF-THEN/ELSE RULE Set and the sensitivity analysis regarding the THEN- and ELSE- branches of the developed RULE Set for the 7-days-ahead prediction of *Microcystis* biovolume in the three reservoirs. Chl *a* concentrations, lower than 175.634 ug/l is the condition to use the RULE Set of the THEN-branch.

In the THEN branch, the Chl *a* concentration and the surface temperature are the variables that are used to predict the *Microcystis* biovolume. The outcome of the *Microcystis* biovolume is sensitive to both these environmental variables. However, Chl *a*, is the most important environmental variable in determining the outcome. The input of Chl *a* ranges between 0.6 and 175.66 ug/l. The surface temperature is the second most important variable regarding the sensitivity of the *Microcystis* biovolume and the surface temperature ranges between 10.4°C and 32.4°C for the study.

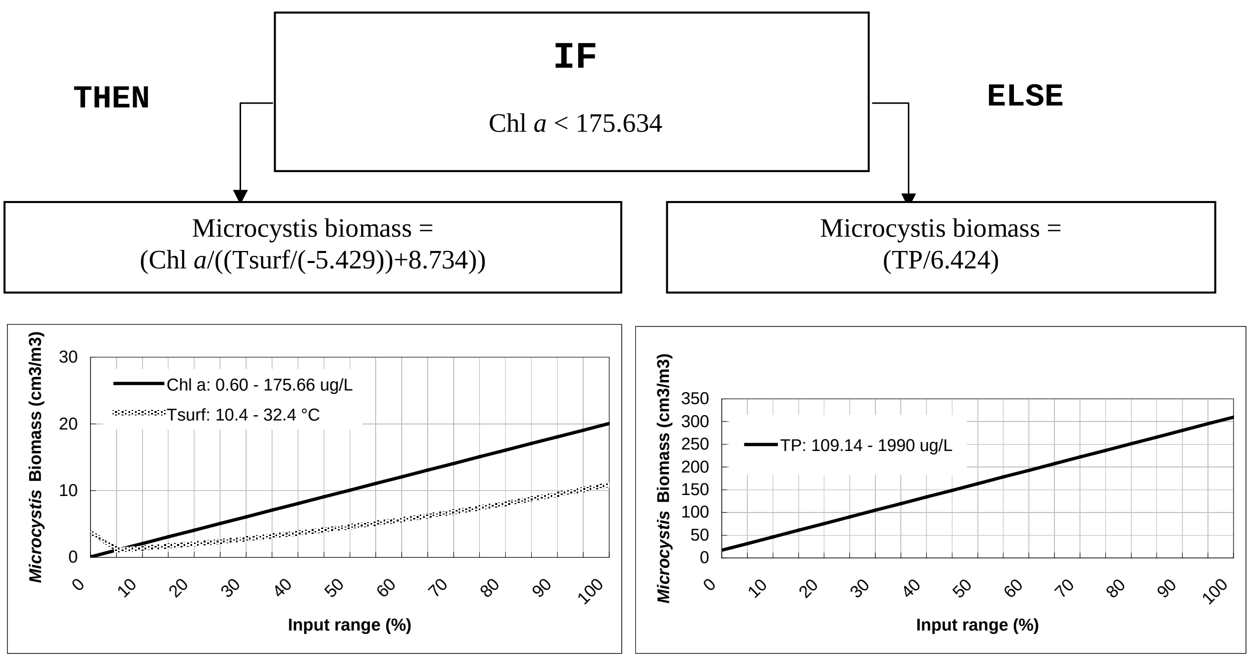


Figure 47 Sensitivity analysis of the input data for the THEN-branch (left) and the ELSE-branch (right) of the best developed rule set for 7-days forward forecasting of *Microcystis* biovolume using the median concentrations of the most important environmental variables to determine the sensitivity of the *Microcystis* biovolume prediction to each variable.

For the ELSE branch, where Chl *a* exceeds 175.634 ug/l, TP is the most important environmental variable that determines the *Microcystis* biovolume (Fig. 43).

These results indicate that the hypertrophic reservoirs have probably such an excess of nutrients available in the system that temperature and the presence of high primary productivity, as indicated by the Chl *a* concentrations, are the main factors that drive the development of further *Microcystis* biovolume. Thus, the initial inoculum of cyanobacteria leads to the extent and further development of *Microcystis* biovolume.

Under high biovolume conditions, it is the TP concentrations present in the system, which drives the ELSE rule set. This is the case during high primary production biovolume conditions and TP is the sole variable used in the ELSE rule set to predict *Microcystis* biovolume. This can be because TP is used at a high rate, which determine the growth rate of the population.

3.4.4 **<u>HEA Experiment 4</u>**: 14-Days forward prediction simulation and rule set discovery for *Microcystis*

To develop a rule set for the 14-days forward prediction of *Microcystis* biovolume the daily interpolated data of the 36 years data set was used for training on the Hartbeespoort, Rietvlei and Roodeplaat reservoir. The *Microcystis* biovolume, measured data, was shifted backwards to create the data set of the 14-days forward training. The training results from this experiment are shown in Figure 48.

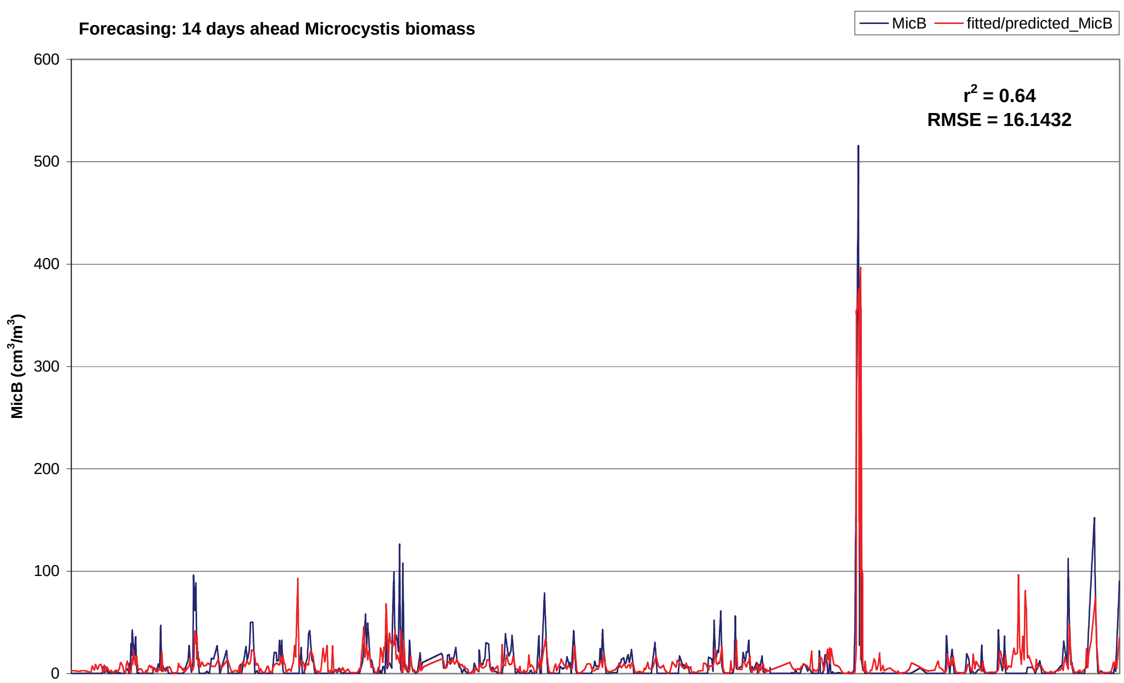


Figure 48 Training results of the 14-days forward forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs during the development of the best rule set for HEA Experiment 4, including Chl *a* as an environmental factor.

The r^2 of 0.64 and the RMSE of 16.1432 for the training data and the r^2 of 0.29 and the RMSE of 11.0926 for the tested data are still good results. However, the results are not as good as with the 7-days forward predictions. The results show that the 14-days forward prediction can be used on reservoirs with similar trophic status and climatic conditions with relative success. Fig. 49 shows the results of the tested data and it is clear that the rule set does predict the peaks, however the extent of the peaks are not predicted accurately.

Table 24 Summary of the average actual error (AE), the mean square error (MSE) and the relative tolerance of the training and testing data sets, of the *Microcystis* biovolume 14-days ahead RULE set development.

	Training set	**Test set**
# of rows:	13148	2193
Mean AE:	-0.34259	1.302998
MSE:	13.85358	5.687873
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
Good predictions:	55.4%	67.5%
Bad predictions:	44.6%	32.5%

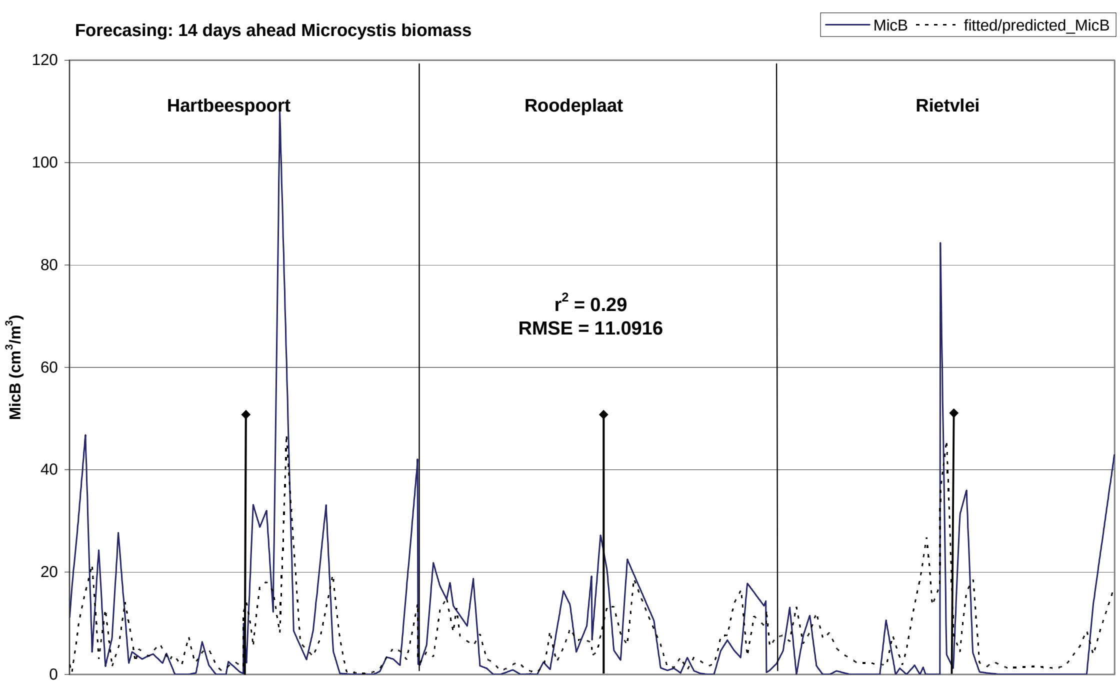


Figure 49 Testing results of the 14-days ahead forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs using the best developed RULE set as shown in Figure 50 including Chl *a* as an environmental variable.

The further validation show that the Relative Tolerance of 10% do give an outcome of 55.4% good predictions for the training data set. The Relative Tolerance of 30% for the testing data set shows an outcome of 67.5% good predictions (Table 24). The decrease in MSE found between the training and the Testing data set show that the predictions capability of the RULE set is still quite good.

Fig. 50 illustrates the IF-THEN/ELSE RULE Set and the sensitivity analysis regarding the THEN- and ELSE- branches of the developed RULE Set for the 14-days forwards prediction of *Microcystis* biovolume in the three reservoirs. Chl *a* concentration lower than, or equal to 194.455 ug/L, or a dissolved inorganic phosphorous concentration of less than 498.225 ug/L, is the condition to use the RULE Set of the THEN-branch.

IF

Chl *a* <= 194.455 OR DIP < 498.225

THEN

Microcystis biomass =
(Chl *a*/ln(|(exp(Sec)*Chl *a*)|))

ELSE

Microcystis biomass =
MicB=((((Chl *a*/pH)+(-18.402))-
((Sec*(-594.824))+62.195))+0.000)

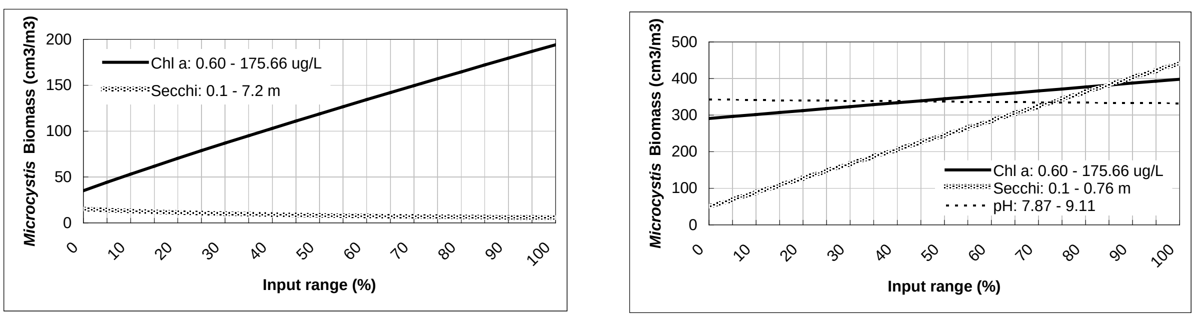


Figure 50 Sensitivity analysis of the input data for the THEN-branch (left) and the ELSE-branch (right) of the best developed rule set for 14-days forward forecasting of *Microcystis* biovolume using the median concentrations of the most important environmental variables to determine the sensitivity of the *Microcystis* biovolume prediction to each variable.

In the THEN branch, the Chl *a* concentration and the Secchi disc depth are the two environmental variables that are used to predict the *Microcystis* biovolume. The outcome of the *Microcystis* biovolume is sensitive to these environmental variables are shown in Fig. 50. Chl *a* is the most important environmental variable in determining the outcome. The input of Chl *a* ranges between 0.6 and 175.66 ug/l. The Secchi disc do have a slight negative impact on the outcome of the *Microcystis* biovolume and the Secchi disc readings ranges between 0.1m and 0.76m for the

THEN RULE set. This indicates that the THEN RULE set is applicable during all turbidity conditions. For the ELSE branch, where exceeds 194.455 ug/L or dissolved, inorganic phosphorous is greater than 498.225 ug/l, the RULE set make use of the Chl *a*, Secchi depth readings and the pH to determine the *Microcystis* biovolume. In this case the Secchi disc reading is the environmental variable that the most important environmental variable in determining the *Microcystis* biovolume (Fig. 50). The ELSE RULE set is applicable to low light conditions as shown by the range of Secchi disc readings in Fig. 50. The Chl *a* concentrations are the second most important variable in the determination of the *Microcystis* biovolume.

As previously shown, these results indicate that these hypertrophic reservoirs have such an excess of nutrients available in the system that the light conditions in the systems (measured as Secchi disc readings) and the presence of high primary productivity (as indicated by the Chl *a* concentrations) is the main environmental variables that is used to determine the predicted development of *Microcystis* biovolume.

3.4.5 <u>HEA Experiment 5</u>: 21-Days forward prediction simulation and rule set discovery for *Microcystis*

To develop a rule set for the 21-days forward prediction of *Microcystis* biovolume the daily interpolated data of the 36 years data set was used for training on the Hartbeespoort, Rietvlei and Roodeplaat reservoir. The *Microcystis* biovolume measured data was shifted backwards to create the condition of 21-days forward training. The training results from this experiment are shown in Figure 51.

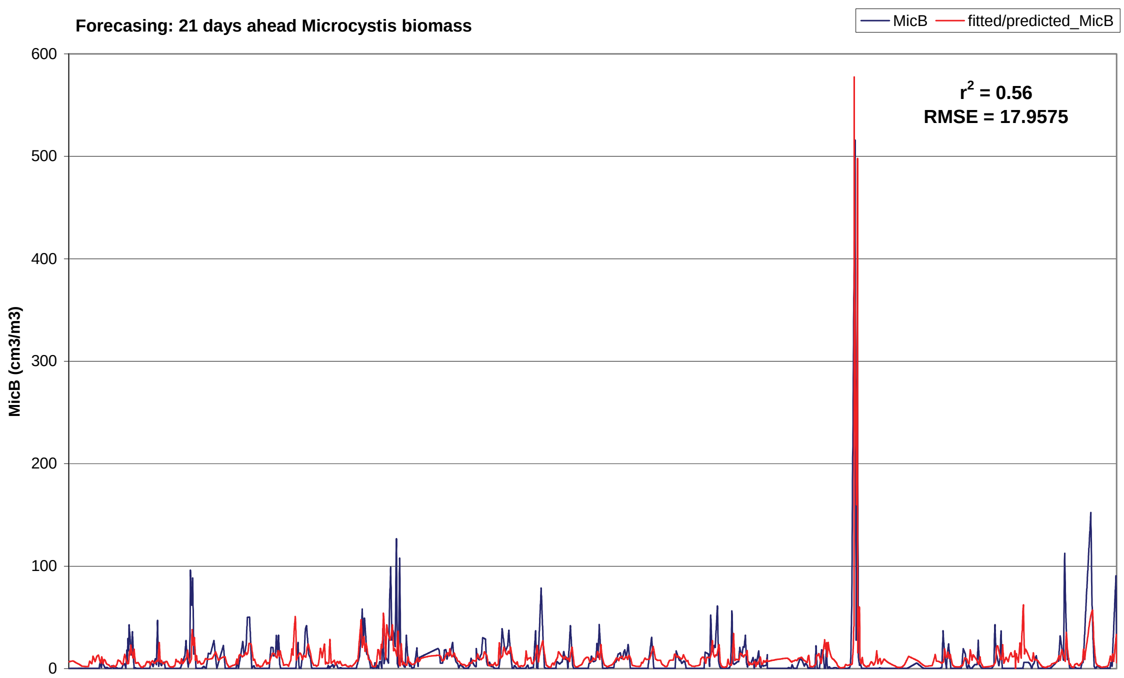


Figure 51 Training results of the 21-days ahead forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs during the development of the best rule set for HEA Experiment 5 including Chl *a* as an environmental factor.

The r^2 of 0.56 and the RMSE of 17.9575 for the training data and the r^2 of 0.15 and the RMSE of 12.0300 for the tested data are still good results. However, the results are not as good as with the previous forward predictions. Despite the lower correlations, the results shown in Fig. 51 and Fig. 52 of the 21-days forward prediction can still be used on reservoirs with similar trophic status and climatic conditions with relative success. Fig. 52 shows the results of the tested data and it is clear that the rule set does predict the peaks, however, the extent of the peaks was not reached and the predictions of this experiment was, therefore, not nearly as good as with the previous experiments.

Table 25 Summary of the average actual error (AE), the average mean square error (MSE) and the relative tolerance of the training and testing data sets of the *Microcystis* biovolume 21-days ahead rule set development.

	Training set	**Test set**
# of rows:	13148	2193
Average AE:	-0.9561	-0.10506
Average MSE:	13.21759	5.892838
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
Good predictions:	55.4%	64.6%
Bad predictions:	44.6%	35.4%

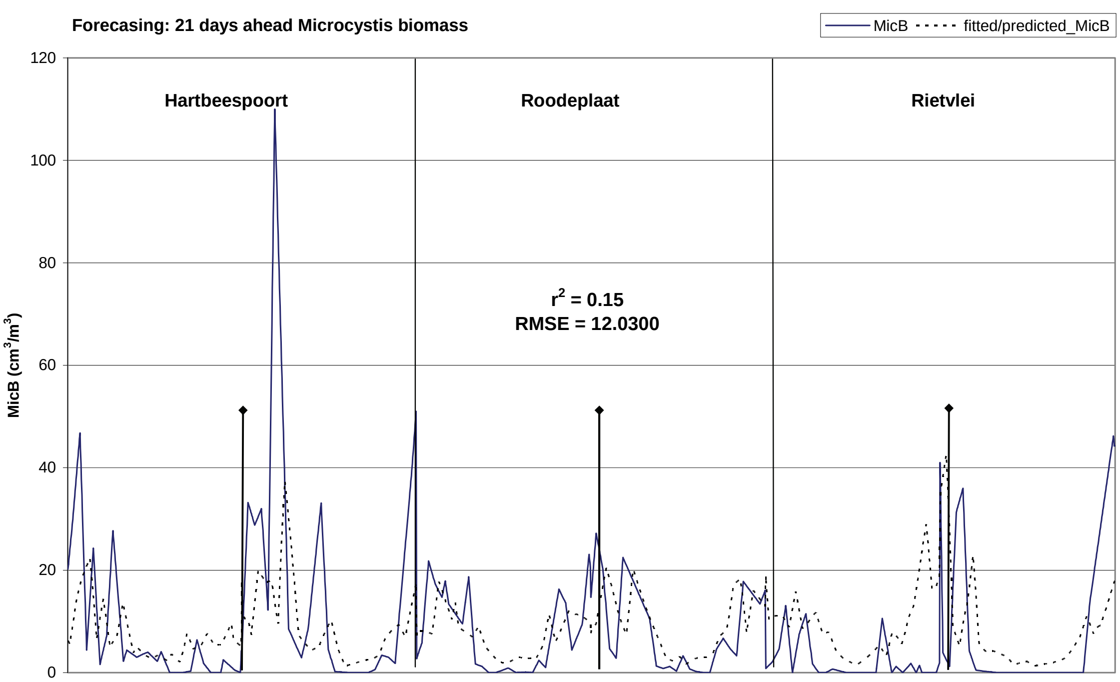


Figure 52 Testing results of the 21-days ahead forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs using the best-developed rule set as shown in Figure 53 including Chl *a* as an environmental variable.

The further validation show that the Relative Tolerance of 10% do give an outcome of 55.4% good predictions for the training data set. The Relative Tolerance of 30% for the testing data set shows an outcome of 64.6% good predictions (Table 25). The decrease in MSE found between the training and the Testing data set show that the predicting capability of the RULE set is still quite good.

Fig. 53 illustrates the IF-THEN/ELSE RULE Set and the sensitivity analysis regarding the THEN- and ELSE- branches of the developed RULE Set for the 21-days forwards prediction of *Microcystis* biovolume in the three reservoirs. There is a number of conditions that are used to determine if the THEN or ELSE branch of the RULE set are used in the prediction. Within the first condition, Chl *a* concentration can range between 0.6 ug/l and 969 ug/l and the TN concentrations vary between 0mg/L and 8.3mg/L. High DIP and TP concentrations are set as potential conditions (Fig. 53). If any of these four conditions as shown in Fig. 53 are met the THEN branch is used to determine the predicted outcome. Only when none of these conditions are met is the ELSE branch used in the predicted outcome.

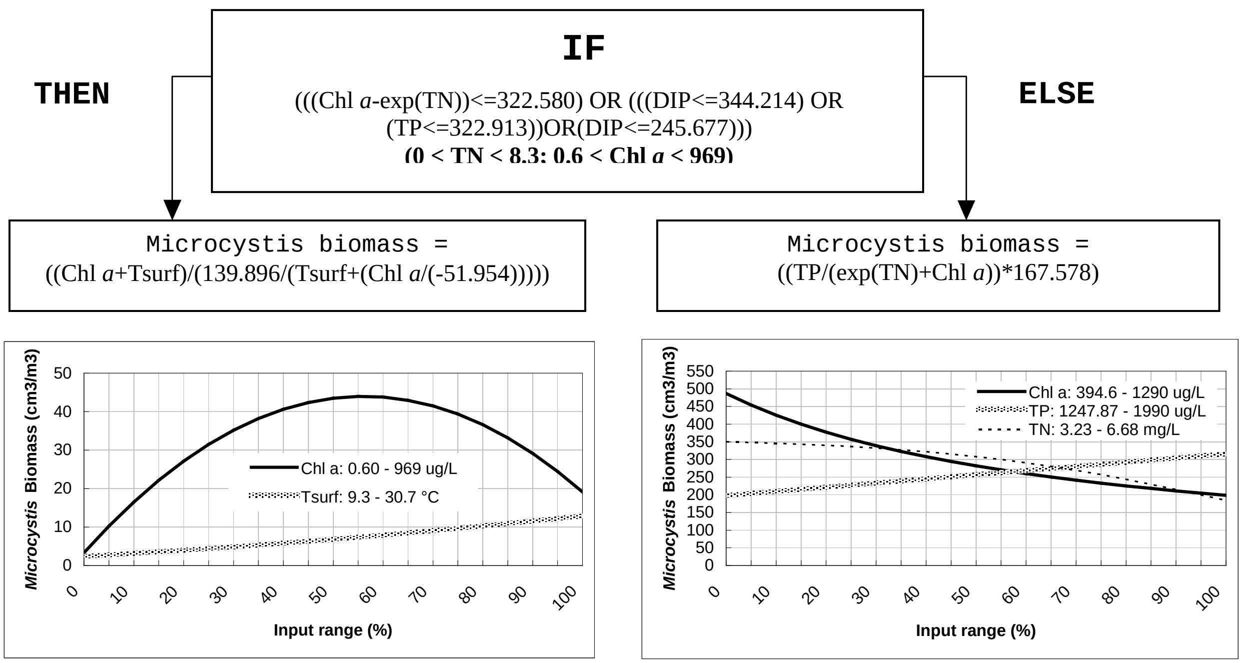


Figure 53 Sensitivity analysis of the input data for the THEN-branch (left) and the ELSE-branch (right) of the best developed rule set for 21-days ahead forecasting of *Microcystis* biovolume using the median concentrations of the most important environmental variables to determine the sensitivity of the *Microcystis* biovolume prediction to each variable.

In the THEN branch, the Chl *a* concentration and the Tsurf measurements are the two environmental variables that are used to predict the *Microcystis* biovolume. The outcome of the *Microcystis* biovolume is sensitive to these environmental variables as shown in Fig. 53. Chl *a* concentration is, once again, the most important environmental variable in determining the outcome. The input of Chl *a* concentration ranges between 0.6 ug/l and 969 ug/l. The Tsurf measurements do have a much smaller impact on the outcome of the *Microcystis* biovolume and the Tsurf measurements ranges between 9.3°C and 30.7°C for the THEN RULE set. It is interesting that at large changes in the Chl *a*, the sensitivity testing for the THEN branch in Fig. 53 indicates that there is much lower *Microcystis* biovolume output, while the Tsurf input changes the development of *Microcystis* biovolume constantly. This may be explained by the shading effect of high biovolume, as indicated by high Chl *a*, on further growth. The THEN RULE set is applied under the lower phosphorus conditions although the set concentrations are still extremely high and typical of the hypertrophic conditions that is found in the set of reservoirs.

For the ELSE branch Chl *a* ranges between 394.6 ug/l and 1290 ug/l, the TP is in excess of 1247.87 ug/l up to 1990 ug/l and TN ranges between 3.23 mg/l and 6.68 mg/L. The nutrients are therefore in very high concentrations present in the systems during the ELSE RULE set determinations. The *Microcystis* biovolume outcome is sensitive to all three these variables under the ELSE RULE set conditions (Fig. 53). The ELSE RULE set is applicable to low light conditions as shown by the range of Secchi disc readings in Fig. 5.53. The Chl *a* concentrations are the second most important variable in the determination of the *Microcystis* biovolume. Both the high Chl *a* and the TN input has a negative impact on the outcome of the ELSE RULE set application, while the TP input has a positive increasing impact on the *Microcystis* biovolume outcome.

3.4.6 **HEA Experiment 6**: 28-Days ahead prediction simulation and rule set discovery for *Microcystis*

To develop a rule set for the 28-days forward prediction of *Microcystis* biovolume the daily interpolated data of the 36 years data set was used for training on the Hartbeespoort, Rietvlei and Roodeplaat reservoir. The *Microcystis* biovolume measured data was shifted backwards to create the condition of 28-days forward training. The training results from this experiment are shown in Fig. 54.

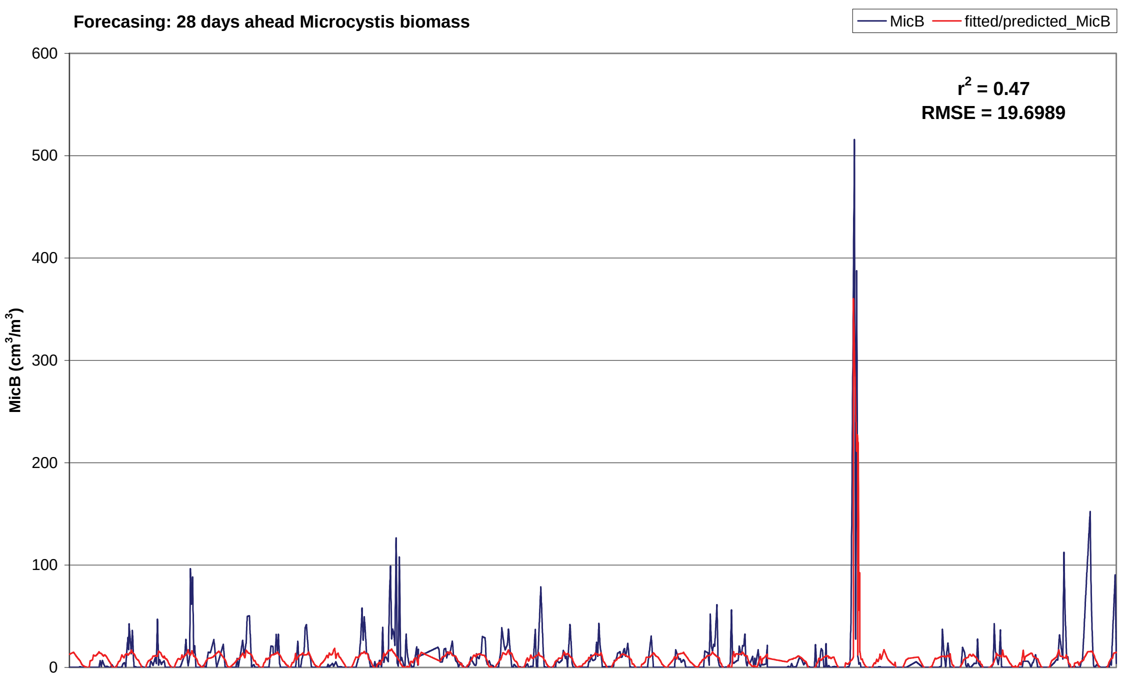


Figure 54 Training results of the 28-days ahead forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs during the development of the best rule set for HEA Experiment 6 including Chl *a* as an environmental factor.

The r^2 of 0.47 and the RMSE of 19.6989 for the training data and the r^2 of 0.20 and the RMSE of 12.0657 for the tested data are still good results. However, the results are not as good as with the previous forward predictions. Despite this results in Fig. 54 and Fig. 55 show that the 28-days forward prediction can still be used on reservoirs with similar trophic status and climatic conditions with relative success. Fig. 55 shows the results of the tested data and it is clear that the rule set does predict the peaks, however, none of the highest peaks were predicted correctly.

Therefore, the 28-days forward predictions were not nearly as good as with the previous experiments, but do predict the cyclic occurrence of *Microcystis* correctly.

Table 26 Summary of the average actual error (AE), the average mean square error (MSE) and the relative tolerance of the training and testing data sets of the *Microcystis* biovolume 28-days ahead rule set development.

	Training set	**Test set**
# of rows:	13148	2193
Average AE:	0.942485	1.805445
Average MSE:	13.55385	4.613223
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
Good predictions:	53.6%	55.5%
Bad predictions:	46.4%	44.5%

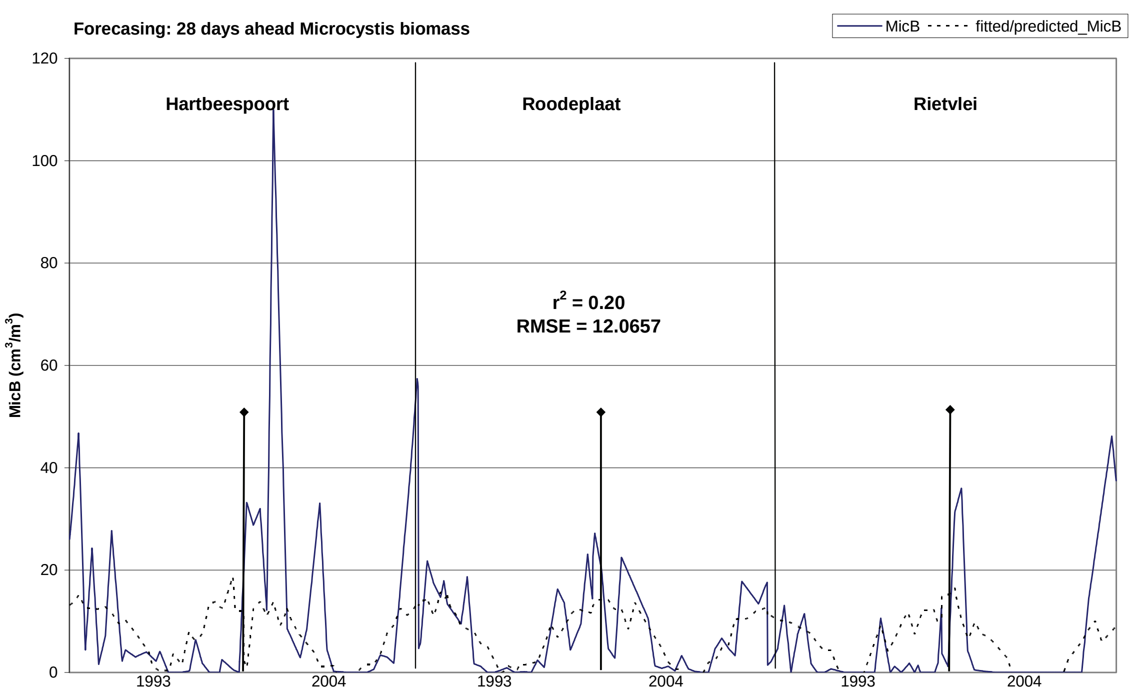


Figure 55 Testing results of the 28-days ahead forecasting of *Microcystis* biovolume (MicB) in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs using the best-developed rule set as shown in Figure 56 including Chl *a* as an environmental variable.

The further validation (Table 26) shows that the Relative Tolerance of 10% do give an outcome of 53.6% good predictions for the training data set. The Relative Tolerance of 30% for the testing data set shows an outcome of 55.5% good predictions. The decrease in MSE found between the training and the Testing data set show that the predicting capability of the RULE set is still quite good.

Fig. 56 illustrates the IF-THEN/ELSE RULE Set and the sensitivity analysis regarding the THEN- and ELSE- branches of the developed RULE Set for the 28-days forwards prediction of *Microcystis* biovolume in the three reservoirs. There is a two conditions that are required for the THEN RULE set to be used, namely DIP concentrations must be higher or equal to 355.453 ug/L and the Chl *a* concentration should be higher or equal to 180.962 ug/L.

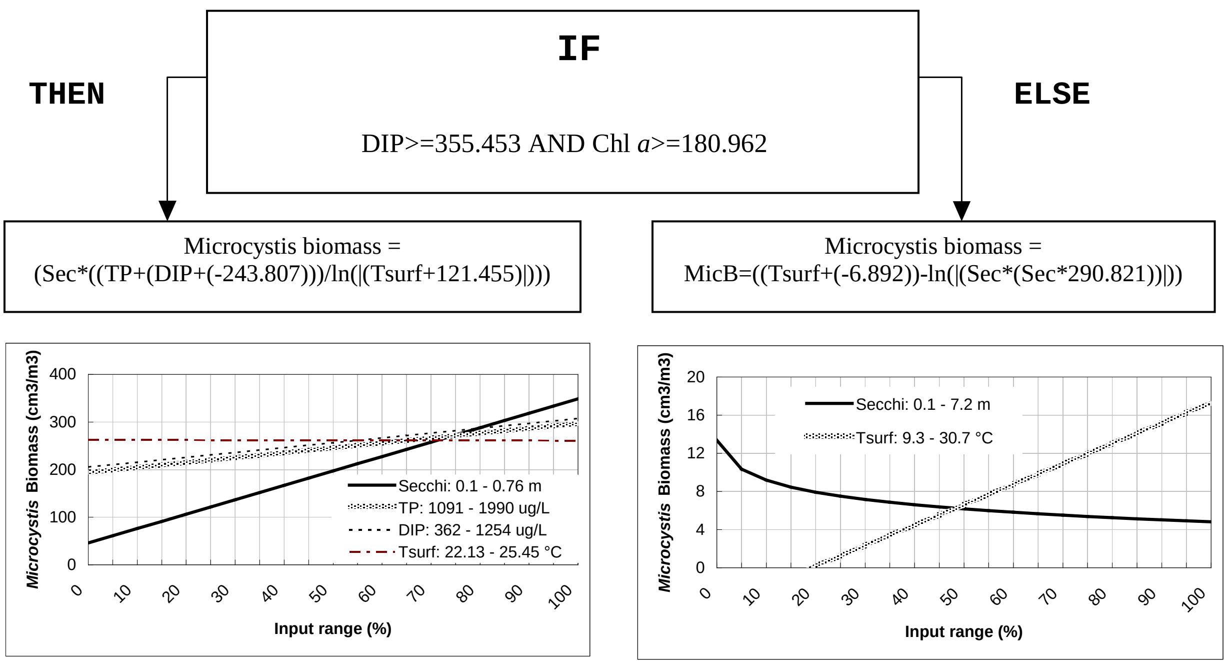


Figure 56 Sensitivity analysis of the input data for the THEN-branch (left) and the ELSE-branch (right) of the best developed rule set for 28-days ahead forecasting of *Microcystis* biovolume using the median concentrations of the most important environmental variables to determine the sensitivity of the *Microcystis* biovolume prediction to each variable.

To use the ELSE RULE set, the DIP and Chl *a* concentrations need to be lower than the mentioned conditions as shown in Fig. 56.

In the THEN branch the Secchi depth reading, the TP and DIP concentrations and the Tsurf measurements are the environmental variables that are used to predict the *Microcystis* biovolume. The outcome of the *Microcystis* biovolume is sensitive to these environmental variables as shown in Fig. 56. In the RULE set for the THEN branch, the changes in Secchi depth readings are the most important variable in determining the outcome of the predicted *Microcystis* biovolume. The second and third environmental variables that cause large changes in the predicted *Microcystis* biovolume outcome is the TP and DIP concentrations. Fourthly, the Tsurf input changes do have a much smaller impact on the outcome of the *Microcystis* biovolume and the Tsurf measurements range between 22.13°C and 25.45°C for the THEN RULE set. It is interesting that the THEN branch is found in this very small temperature range as shown in Fig. 56, indicating optimum temperatures for the development of *Microcystis* biovolume in these reservoirs. The THEN RULE set is applied under extremely high phosphorus (TP and DIP).

For the ELSE branch it is the Tsurf readings and the Secchi disc depth that are the most important environmental variables that affects the large changes in the *Microcystis* biovolume development. The Tsurf ranges between 9.3°C and 30.7°C and has the greatest impact on the model outcome. The Secchi disc readings that range between 0.1m and 7.2m have a negative impact on the *Microcystis* biovolume development.

The ELSE RULE set conditions covers a very wide section of the data and model outcomes, while the THEN RULE set covers only a small section of the data as the Secchi disc reading range and the Tsurf range are very small. The THEN RULE set is applicable to very low light conditions as shown by the range of Secchi disc readings in Fig. 56.

3.4.7 **<u>HEA Experiment 7</u>**: Real-Time Simulation and Rule Set Discovery for the dinoflagellate *Ceratium*

The rule set for the dinoflagellate, *Ceratium*, real time prediction was developed as discussed in the methods and the results were tested on the unseen data of Bon Accord and Klipvoor reservoirs. The method proved effective in the development of a rule set for predicting *Microcystis* biovolume and the method was thus applied to the prediction of dinoflagellate blooms that consists primarily of *Ceratium*. This species seem to be more pronounced since 1999 in the studied reservoir systems (Van Ginkel *et al.,* 2001).

Testing of the Rule Set

The developed rule set was tested for five reservoirs, namely the three reservoirs that it was trained and tested on (Hartbeespoort, Rietvlei and Roodeplaat) (Fig. 57 & Fig. 58) and two unseen reservoirs (Bon Accord and Klipvoor) (Fig. 60 & Fig. 61). Both the latter reservoirs experienced annually large blooms of dinoflagellates (consisting of *Ceratium*) during the period 2000 to 2005. The rule set was applied and tested to 1993 and 2004 on the Hartbeespoort, Rietvlei and Roodeplaat Reservoirs (Fig. 58). The rule set was also tested and applied to the 2000 to 2005 data of the two unseen reservoirs, Bon Accord and Klipvoor (Fig.60 & Fig. 61).

To validate the results of the rule set the correlation coefficient of the measured and fitted data were determined. The Root Mean Square Error (RMSE) of the testing error was also calculated for the different reservoirs to indicate the standard error of the estimate.

Sensitivity Analysis of Developed Rule Set

Sensitivity analyses were done on the tested data for the Hartbeespoort, Rietvlei and Roodeplaat Reservoirs for the period 1993 and 2004. The sensitivity analysis was done for both the THEN and the ELSE rule set (Fig. 59).

The input range changes (as percentage) were determined by applying the rule set to calculate changes in each variable that was used in the rule set, while the other variables median values were used. The starting point of the environmental variable was the minimum and the maximum values measured within the data set. This gives an indication of the importance of each variable in driving the changes (increases or decreases) of the outcome, namely the Dinoflagellate biovolume.

Real-time rule-set discovery for *Ceratium* biovolume in Hartbeespoort, Roodeplaat and Rietvlei Reservoirs

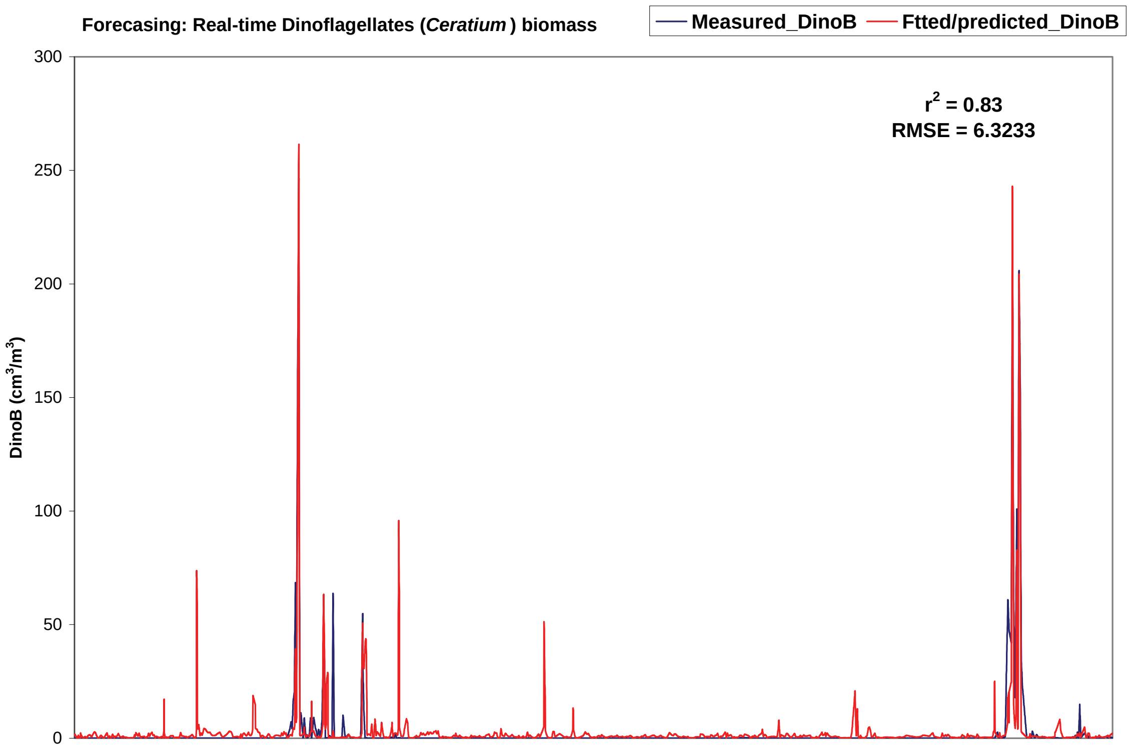


Figure 57 Training results of the real-time forecasting of *Ceratium* biovolume (DinoB), in the Hartbeespoort, Roodeplaat and Rietvlei reservoirs during the development of the best rule set for HEA Experiment 7 including Chl *a* as an environmental factor.

The 36 years of real-time training on the Hartbeespoort, Rietvlei and Roodeplaat reservoir daily data produced a rule set for the prediction of *Ceratium* biovolume as shown in Fig. 38. The correlation coefficient (r^2 = 0.83) and the root mean square error (RMSE = 6.3233) for the training data and the correlation coefficient (r^2 = 0.85) and the root mean square error (RMSE = 6.7857) for the tested data are still significant. Fig. 58 shows the results of the tested data on the three reservoirs for the period 1993 and 2004 for the Hartbeespoort, Roodeplaat and Rietvlei reservoirs. It is clear that the rule set fits the Hartbeespoort Reservoir better than the Roodeplaat and the Rietvlei data, where under and over predictions were found. However, the magnitudes of the maximum *Ceratium* biovolume peaks were predicted quite well in all three the reservoirs.

Table 27 Summary of the average actual error (AE), the average mean square error (MSE) and the relative tolerance of the real time training and testing data sets of the *Ceratium* biovolume rule set development.

	Training set	**Test set**
# of rows:	13148	2193
Average AE:	-0.59789	-0.63201
Average MSE:	5.763118	6.593074
Tolerance type:	Relative	Relative
Tolerance:	10%	30%
Good predictions:	78.4%	85.5%
Bad predictions:	21.6%	14.5%

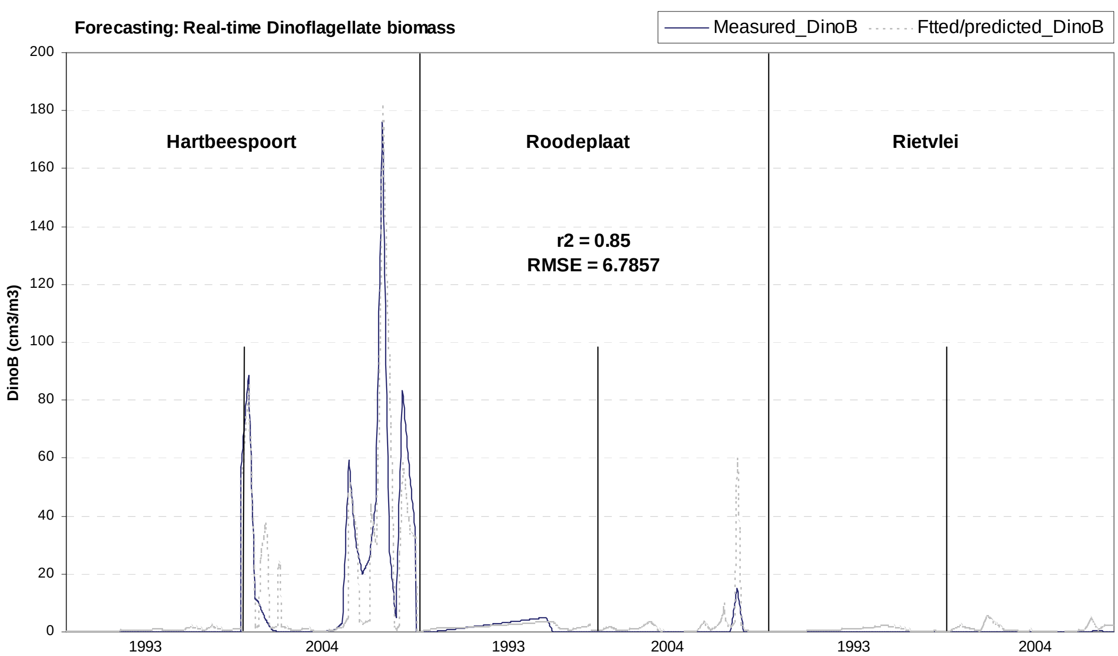


Figure 58 Testing results of the real-time forecasting of *Ceratium* biovolume (DinoB), in the Hartbeespoort, Roodeplaat and Rietvlei reservoirs using the rule set as shown in Figure 59, including Chl *a* as an environmental factor.

Further validation shows that the Relative Tolerance of 10% does give an extremely good outcome of 78.4% good predictions for the training data set. The Relative Tolerance of 30% for the testing data set shows an outcome of 85.5% good predictions (Table 27). The increase in MSE found between the training and the testing data set show that the predicting capability of the RULE set decreased from the training to the testing data set.

The conditions for the rule set included TP and Chl *a* concentrations that were used to determine if the THEN branch or the ELSE branch of the rule set was to be used for forecasting the *Ceratium* biovolume. The THEN branch is applicable to situations when the Chl *a* concentrations and the Dinoflagellate biovolume are very high (Fig. 40). The sensitivity analysis that was done on the real-time testing data for the three reservoirs to determine the *Ceratium* biovolume shows that with the THEN branch of the rule set Chl *a*, TN and TP are the variables that the Dinoflagellate biovolume is most sensitive to. The TN concentrations vary from 2.1 mg/L to 4.53 mg/L and TP concentrations vary between 110.86 ug/l and 272 ug/l. Under these high nutrient conditions, other variables were not important in the forecasting of the *Ceratium* biovolume.

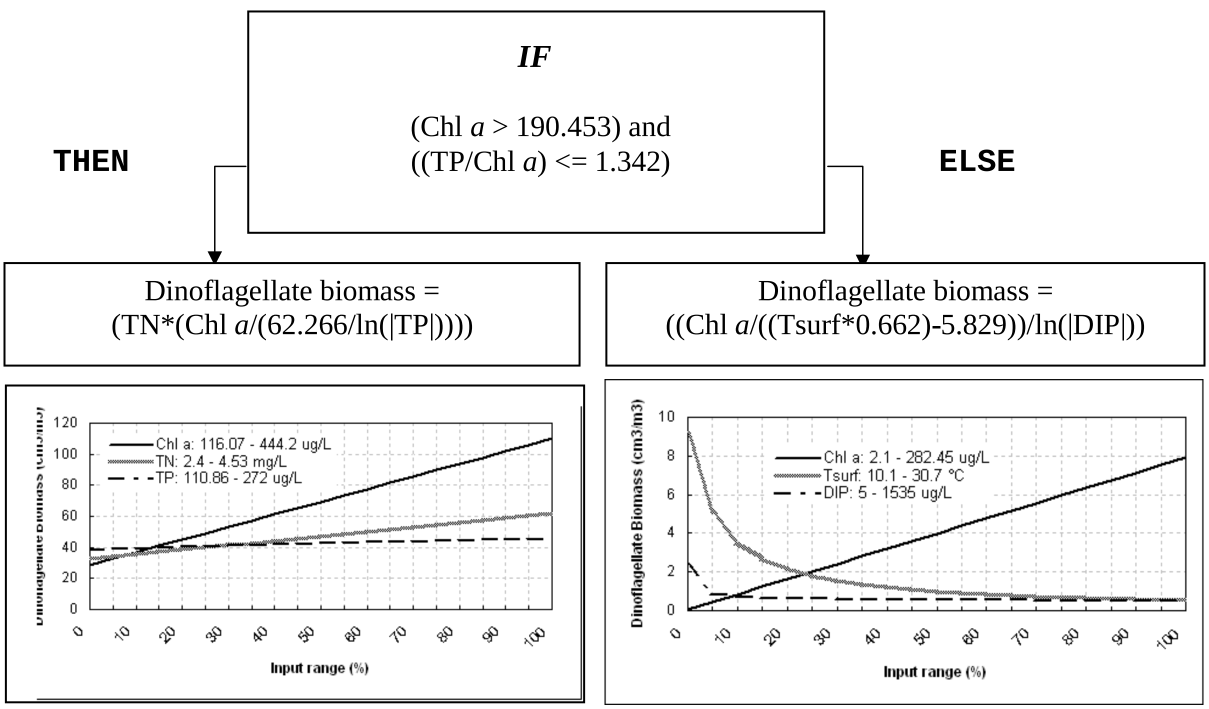


Figure 59 Sensitivity analysis of the input data for the THEN-branch (left) and the ELSE-branch (right) of the rule set for real-time Dinoflagellate biovolume forecasting.

The ELSE branch of the rule set is used when Chl *a* concentrations varied between 2.1 ug/l and 282.45 ug/l and the *Ceratium* biovolume was below 10 cm^3/m^3. The temperature change of the surface water is important in determining the *Ceratium* biovolume. Increases in the temperature input were important in the decrease of the *Ceratium* biovolume (Fig. 59). This showed that the optimum growth temperature that ranged from 5°C to 30°C according to Buck (1989) is only important under low Chl *a* concentrations and up to 17°C. Temperatures higher than 17°C showed no significance on the dinoflagellate biovolume. Higher *Ceratium* biovolume is more regulated by the availability of sufficient nutrients (Reynolds, 1978; Buck, 1989) within the water body as shown by the THEN rule set. Under lower Chl *a* concentrations, the availability of DIP was important up to 82 ug/l after which the effect of the change in input on the determination of the *Ceratium* biovolume was insignificant.

Real-time rule-set for Ceratium biovolume testing in Bon Accord and Klipvoor Reservoirs

Five years of data from both the Bon Accord and Klipvoor Reservoirs were used to test the applicability of the rule set to unseen data. The correlation of the measured and predicted *Ceratium* biovolume in the Bon Accord Reservoir (Fig. 60) was 0.62, which is statistically highly significant ($P < 0.001$). The RMSE of 6.803 also indicates that the results were significant. The extent of the peaks were under-predicted or over-predicted in certain instances, but all the peaks were predicted.

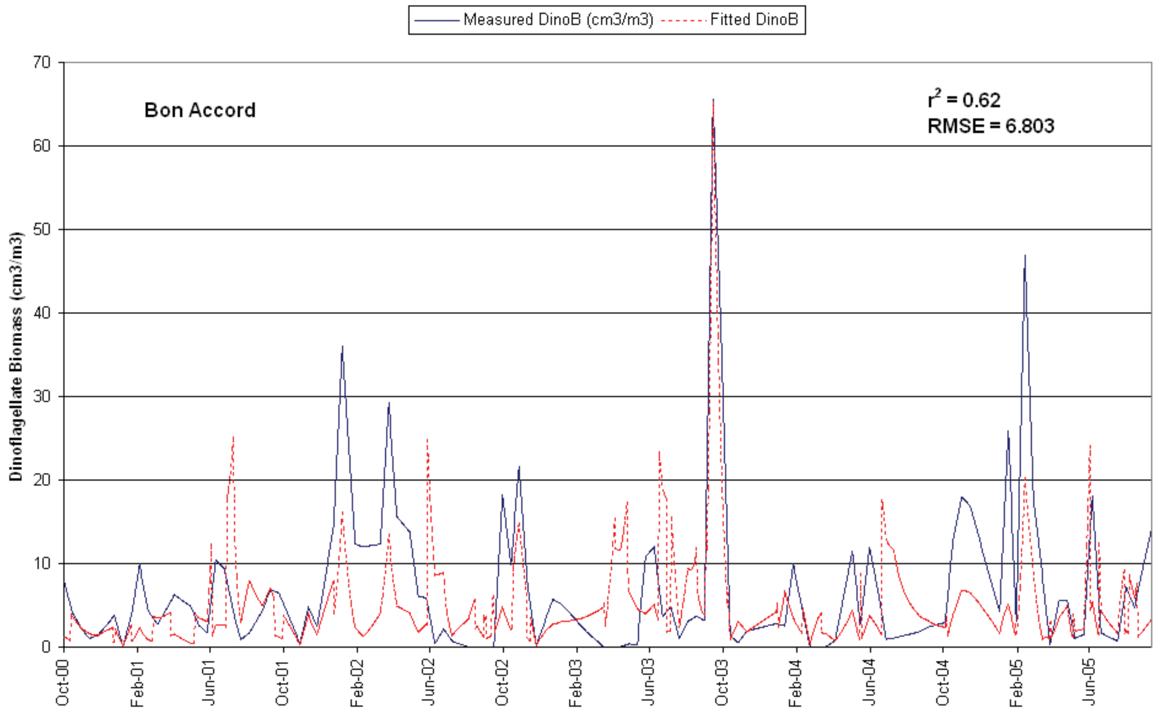


Figure 60 Testing of the developed rule set on Bon Accord Dam for real-time Dinoflagellate (*Ceratium*) biovolume forecasting.

On two occasions, peaks were predicted that did not occur (Autumn 2003 and Spring 2004). This may be due to the occurrence of other phytoplankton taxa (e.g. *Microcystis*) that dominated the community and the rule set used the Chl *a* concentration in determining the predicted biovolume of the *Ceratium* in the Bon Accord Reservoir. The maximum peak of *Ceratium* biovolume in the spring of 2004 was predicted very well.

In the Klipvoor Reservoir (Fig. 61), the correlation of the measured and predicted *Ceratium* biovolume was 0.48, which is significant ($P < 0.001$). Although the correlation coefficient is less than for Bon Accord the results is still statistically significant. The RMSE, as an ‘estimation’ of the standard deviation, of 2.53 also indicated that results were significant. The extents of the peaks were under-predicted or over-predicted, but all the peaks were predicted. Peaks were predicted in the spring of 2002 and the autumn of 2003, which did not occur.

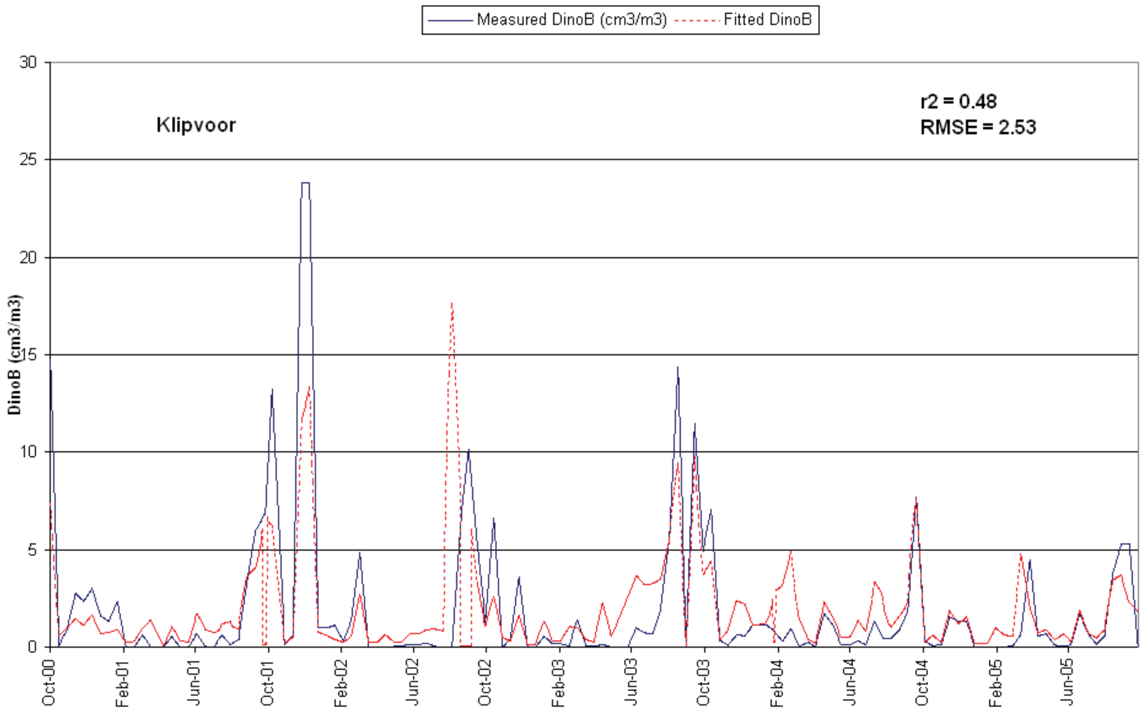


Figure 61 Testing of the developed rule set on Klipvoor Dam, for real-time *Ceratium* biovolume (DinoB) forecasting.

These results indicate that the RULE set developed on hypertrophic reservoirs in the summer rainfall and temperate region of South Africa is applicable to reservoirs within the same climatic region and of the same hypertrophic status. The methods used may further be investigated for applicability in other climatic regions of South Africa and on reservoirs with different trophic status to determine if a separate RULE set needs to be developed for different climatic zones or for reservoirs of different trophic status.

The developed RULE sets made use of the most important environmental variables as have been determined through years of limnological research (Table 28). For the *Microcystis* RULE Set development, the inclusion of the Chl *a* concentrations gave the best results. The most important environmental variables that were used in determining the final most applicable RULE sets for the different experiments are the existing biovolume that are measured as Chl *a*, Tsurf, TP, DIP, Secchi (as indication of light conditions), TN and lastly pH. In no circumstances was DIN used in the most applicable RULE sets for the prediction of *Microcystis* or in the prediction of *Ceratium*. This may indicate that although DIN is the food source, the TN is more important and determine the eventual availability of nitrogen and contribution to growth.

Table 28 The summarised results from the HEA Experiments, showing the correlation coefficient (r^2), Root Mean Square Error (RMSE), the relative tolerances (10% for training and 30% for testing), the Environmental Variables important in Conditions to apply the THEN or ELSE Rule set, and the Environmental variables (in order of importance) that were used in the developed RULE sets. Experiment 1-6 was the development of RULE sets for *Microcystis*, and Experiment 7 was done for the development of a RULE set for the dinoflagellate, *Ceratium*.

Experiment	**r^2**	**RMSE**	**Relative Tolerance**	**Environmental Conditions**	**Environmental Variables Used**	
					THEN	**ELSE**
Experiment 1: Real time + Chl *a* Training: Testing	 0.88 0.73	 9.3357 7.4120	 38.7% 44.2%	TP Chl *a*	1. Tsurf 2. TN (neg)	1. Chl *a* 2. Tsurf 3. pH
Experiment 2: Real time – Chl *a* Training: Testing	 0.81 0.46	 11.7002 10.3676	 42.3% 62.9%	TN Secchi	1. TP 2. TN 3. Tsurf 4. pH	1. Secchi (neg) 2. pH
Experiment 3: 7 days forward Training: Testing	 0.69 0.52	 14.9208 9.3582	 53.9% 70.3%	Chl *a*	1. Chl *a* 2. Tsurf	1. TP
Experiment 4: 14 days forward Training: Testing	 0.64 0.29	 16.1432 11.0916	 55.4% 67.5%	Chl *a* DIP	1. Chl *a* 2. Secchi	1. Secchi 2. Chl *a* 3. pH
Experiment 5: 21 days forward Training: Testing	 0.56 0.15	 17.9575 12.0300	 55.4% 64.6%	TN Chl *a*	1. Chl *a* 2. Tsurf	1. Chl *a* 2. TP 3. TN
Experiment 6: 28 days forward Training: Testing	 0.47 0.20	 19.6989 12.0657	 53.6% 55.5%	DIP Chl *a*	1. Secchi 2. TP 3. DIP 4. Tsurf	1. Tsurf 2. Secchi (neg)
Experiment 7: Real time + Chl *a* Training: Testing 1 Testing 2 Testing 3	 0.83 0.85 0.62 0.48	 6.3233 6.7857 6.8030 2.5300	 78.4% 85.5% 43.2% 70.1%	Chl *a* TP	1. Chl *a* 2. TN 3. TP	1. Chl *a* 2. Tsurf 3. DIP

For the dinoflagellate, *Ceratium*, it was shown that a temperature range of 5°C to 17°C and DIP concentrations below 82 ug/L are important environmental conditions during the development of the initial low Dinoflagellate biovolume. In the development of excessive Dinoflagellate blooms TN is the most important variable in determining the extent of the Dinoflagellate bloom.

In all the cases where pH was used in the developed RULE set, the change in pH input had little effect on the output algal biovolume, and it can be considered to be not a major contributor to the final results. Tsurf seems to be one of the most important environmental variables together with the nutrient concentrations (Table 28). TP and DIP are the most important nutrients in determining the outcome of the algal biovolume. TN when used has mostly a negative impact on the algal biovolume output of the model.

It is interesting, that for the forward prediction of *Microcystis* the 7-days ahead forecasting gave the best results (Table 28), followed shortly by the 14-days, the 21-days and the 28-days ahead forecasting. The worst predictions (28-days), as found with the real time results, can be explained by the fact that real time environmental conditions are not causing the biovolume, but are rather the result of the biovolume.

From these results, it is shown that the existing biovolume, temperature, nutrients specifically phosphorous, and the existing light conditions are the most important environmental variables in the determination or prediction of the algal biovolume of *Microcystis*. In the case of *Ceratium* the nitrogen and temperature are the most important environmental variables in determining the predicted biovolume.

3.5 Conclusions and Evaluation

Five modelling techniques were included in the study and tested on hypertrophic reservoirs in South Africa. The data and results generated with the different models showed variable successes to predict chlorophyll *a* (Chl *a*), phosphorous, algal groups and specific species. The testing of management options in some of the models proved to be quite useful.

Firstly, the relatively simple Vollenweider Model, a well-known and widely tested model was used. The Vollenweider model (Vollenweider, 1976) was applied in South Africa on a number of occasions (Thornton and Walmsley, 1981; Grobler and Silberbauer, 1984; Grobler, 1985). This model was originally developed as an eutrophication management tool. It did not provide information on the algal or cyanobacterial species that may pose a problem in the system. The ease of application of the model using total phosphorus as major input to determine the Chl *a* outcome still makes this model a favourite with managers as the effect of decreases or increases in total phosphorus does give a quick result for management purposes. It does, however, give no information on the phytoplankton species that may be present in the system and hence management problems.

The model does not take any of the complex characteristics of a freshwater system into consideration but uses a simple linear correlation that exist between the TP concentrations in a system and the potential to develop phytoplankton biovolume, as measured by Chl *a*. This model is giving the manager a quick reference on the trophic conditions within the system. It supplies the manager with an easy to use tool, for possible consideration of potential management options for phosphorous removal.

The second model tested is the SALMO-OO model, a complex deterministic model that takes growth equations of the different algal groups into consideration and that takes the main impacting factors like inflow and nutrient loads, as inputs, into consideration. The simulation library SALMO-OO has been developed by the object-oriented implementation of the lake ecosystem model SALMO (Recknagel and Benndorf, 1982; Benndorf and Recknagel, 1982; Recknagel *et al.,* 1995) as the core of a lake simulation library by means of JAVA. It provides optional access to alternative causal representations of ecological processes in lakes such as: a) photosynthesis and respiration of diatoms, green algae and cyanobacteria; b) grazing of diatoms, green algae and cyanobacteria by zooplankton; c) growth of herbivorous zooplankton; and d) predation of zooplankton by planktivorous fish. Alternative process representations were adopted from published lake ecosystem models different to SALMO-OO such as Park *et al*. (1974), Hongqing and Jianyi (2002) and Arhonditsis and Brett (2005) to test applicability in hypertrophic reservoirs of South Africa.

SALMO-OO was tested on data from 2003 to 2004 on three hypertrophic reservoirs, Hartbeespoort, Klipvoor and Roodeplaat with regards to the simulation of seasonal abundances of diatoms, green algae and cynaobacteria. It proved to be valid for the temperate hypertrophic lakes and it can assist in optimising eutrophication control of these lakes based on complex management scenario analysis. The one problem foreseen with this model is the fact that it does not make provision for dinoflagellates, which are becoming more dominant in the hypertrophic systems of South Africa.

The nutrient loads are used in the model to predict the outcomes. The model is designed to test the application of different potential management options, which make it applicable for use by mangers that need to determine management options.

The predicted outcomes of the method are not quite as accurate as for lakes in the literature, but do predict the highs and lows of bloom development to a certain degree of accuracy. Discrepancies in the predictions may be because not all algal groups are included in the model. Especially the Dinoflagellate group is not included, probably because major blooms was not pronounced during the development of SALMO-OO, and may account for the discrepancies in the predictions, as all five the reservoirs did experience dinoflagellate blooms during the study period.

Thirdly, the Artificial Neural Network modelling methods tested for the study included two techniques. Firstly, the multilayered fast-forward neural network model (MFNN), Forecaster XL, and secondly, a Self Organising Mapping (SOM) technique were used to determine if it is applicable for usage in South African conditions.

The results achieved with Forecaster XL gave an output that shows the successes and failures of the results. The percentage tolerance of the modelling package with the training data set is 10% and with the testing data set 30%. The model is, therefore, quite strict with itself, in accepting the efficiency of the model. The modelling results did not show very high successes, however, the user friendliness of the program makes it a good choice for further use and testing. Because of the hidden layer of the ANN modelling technique the main problem of the program is that it does not provide the user with the mathematical methods used within the model for easy application on new data for prediction purposes.

The MFNN model, Forecaster XL, is easy to use and fits well within the wide use of Microsoft Excel as background. Data import, and the output from the model make this model very user friendly. The output does give one results that show the success and failures of the model. The two negative features of the model are:

a) The modeller does not know what algorithms were used to determine the output,

b) The methods to determine the tolerance of the results within the model are unknown.

The SOM modelling method, which is not a forward predictive modelling technique, but rather gives insight into historical events, showed potential for further use in South Africa as it can be used to:

- Investigate the before and after situations,
- To determine the potential causes of management actions,
- To determine changes in environmental conditions.

The SOM method is not a prediction method but is an ecological informatics method that can be used to determine cause and effect of changes that occur within a reservoir or catchment system. This method may need to be tested more intensively in South Africa for applicability to other systems and data sets. Using SOM, to test the impact of management and environmental changes that may have occurred within a catchment, reservoir or other system is highly applicable to this method.

Lastly, with the hybrid evolutionary algorithm (HEA) development, a number of tests were done to develop real time RULE agents for the prediction of *Microcystis* spp. and the Dinoflagellate (*Ceratium hirundinella*) bloom events in South African hypertrophic reservoirs. Validation of the results was done on the limnological time-series data. The tests to develop a prediction tool for *Microcystis* spp. was done with real time prediction, 7-days forward, 14-days forward, 21-days forward and 28-days forward predictions. The 7 day-forward prediction rule-based agent for *Microcystis* spp. has proven to be most accurate. The HEA was designed to assemble and optimise both the structure and parameters of predictive rules using genetic programming and evolutionary computation. In order to develop the rule-based agent for *Microcystis* and the Dinoflagellate group, merged limnological time-series data of the hypertrophic reservoirs Hartbeespoort, Rietvlei and Roodeplaat dams have been used for training. Rigorous leave-*k*-out cross-validation for a total of 36 years (12 years from each reservoir during the period 1991-2004) of data was used to do the rule based development training, excluding the years 1993 and 2004 (from each reservoir) to use for testing the developed rule.

The developed RULE sets of the hybrid evolutionary algorithms (HEA) for forecasting *Microcystis* and the dinoflagellate (*Ceratium*) biovolume proved to be highly applicable to complex unseen ecological data of South African Reservoirs with the same trophic status as the reservoirs that were used to develop the RULE Set. The five reservoirs used for the testing of the RULE Set are all within the same temperate climatic region of South Africa and all reservoirs had the presence and dominance of either *Microcystis* or the dinoflagellate, *Ceratium*, during the study period, even though the sizes and other limnological characteristics differed between the reservoirs.

The sensitivity analysis and the best RULE set correspond well with theoretical hypotheses and experimental findings in previous studies. It can also refine ranges of variables that are deterministic in the development of the Dinoflagellate biovolume. This study indicates that the HEA methods for the development of RULE sets by machine learning of complex ecosystems such as manmade Reservoirs is extremely applicable. The method should also be tested for further application in other ecological environments within South Africa.

CHAPTER 4

CONCLUSIONS AND RECOMMENDATIONS

4.1 Summary of Conclusions

The main aim of this project was to investigate the applicability of ecological infomatics modelling techniques to develop a predictive tool for harmful algal blooms in South Africa.

The Reservoirs studied are hypertrophic systems and are situated downstream of the largest urban development in the summer rainfall area of South Africa. These systems are subjected to severe algal blooms, dominated primarily by Cyanobacteria (*Microcystis*) and lately, also Dinoflagellates (*Ceratium hirundinella*).

The results from this study show that the cyanobacterial blooms in the Crocodile West/Marico Water Management Area are dominated by *Microcystis*, and although *Anabaena* and *Oscillatoria* are found occasionally in large numbers, they do form only a negligibly small component of the annual phytoplankton community. Furthermore, it was found that *Microcystis* is the most important cyanobacterial species, associated with the presence of cyanobacterial toxins in the five reservoirs. However, *Anabaena* & *Oscillatoria* are both also known TM producers and could contribute to the toxin production in all the reservoirs.

All the sites showed regular cyanobacterial, and increasingly dinoflagellate, blooms. The dinoflagellate blooms are exclusively *Ceratium hirundinella* and these dinoflagellate blooms are associated with extremely high Chl *a* concentrations in the five Reservoirs. *Ceratium* dominated Bon Accord and Klipvoor Dams during the 5-year study period, while Hartbeespoort and Rietvlei experienced *Ceratium* blooms during 2000 and again in 2005. Roodeplaat Dam experienced for the first time a *Ceratium* bloom in 2005.

The PCA of CANOCO indicated that the reservoirs are similar in both algal community and physico-chemical variables. This support the assumption that there are no major differences between the reservoirs and that the data could be combined in the modelling exercises that followed. The assumption that a reservoir is one site, and taking samples at five different sites as compared to the regular sampling in the reservoir, to determine toxin presence, may have led to discrepancies in the cyanobacteria association with toxin results. However, it does give one a better perspective of when to potentially expect cyanobacterial toxins to be present in these hypertrophic reservoirs. This will enable Management to issue warnings in time, regarding the potential health risk that cyanobacterial blooms may pose to recreational users.

The multivariate analysis shows that of the environmental factors, temperature is the most important factor in the development of cyanobacteria in these hypertrophic systems. Temperature is, therefore, one of the main driving forces of the blooms and is a good indicator of climate and weather impacts on a system. According to the multivariate analysis, the main driving force that correlates quite well with the TM is the DIP concentrations in these systems. This variable will thus play an important role in the prediction of the cyanobacterial toxin production (TM).

The depth distribution of the toxins measured in the Hartbeespoort and Roodeplaat Reservoirs indicated that during the periods of excessive *Microcystis* biovolume, toxins are often found all the way through the water column. This may necessitate WCWs that produce potable water, to monitor at different depths, on the condition that they have the option to withdraw water at different depths, as is the case at the Roodeplaat Reservoir.

Since the multivariate statistical analysis with the CANOCO program showed that the five reservoirs were so similar that it enabled us to combine all the data for further use in applying the modelling techniques, especially the Artificial Neural Network modelling technique and the Hybrid Evolutionary Algorithm development technique. The most important environmental variables that were also used in further predictive capability development were water surface temperature (Tsurf), nutrients (TP, TN, DIP &DIN), underwater light conditions (Secchi depth readings) and existing biovolume (Chl *a*).

A number of different types of models were tested to determine the applicability to South African conditions:

(1) The relatively simple Vollenweider model was tested for Hartbeespoort, Klipvoor and Roodeplaat reservoirs. This model is easy to apply and provide a manager with a quick answer and relatively little information is needed to apply the model. It also provides the manager with the possibility of testing different management scenarios. However, over

and under predictions of 30% to 300% (IETC, 2000) is possible and acceptable within the context of the model.

(2) The simulation library, SALMO-OO, allowing forecasting abundances of blue-green algae, green algae and diatoms in response to eutrophication control scenarios for Hartbeespoort, Klipvoor and Roodeplaat reservoirs. The model is data intensive as it works with a ten-day time step and inflow and outflow data are necessary to apply the model. This information was not available for the Bon Accord and Rietvlei reservoirs. This model takes the complex limnological characteristics of reservoirs into consideration and it supplies the manager with a tool to test different management scenarios to assist in decision-making. The results were, however, only partly successful with large over and under predictions, even after the growth equations were adapted.

(3) With the Artificial Neural Network modelling techniques, both the supervised multilayered feed forward neural network and the non-supervised self-organising map methods were tested. The Software Package Forecaster XL was used to predict the biovolume of the non-cyanotoxin producing group and the cyanotoxin producing group of algae. The five-year data set was used. The model provides visual successes but the strict tolerances, set by the model, to determine acceptable prediction as part of the outcome of the model, may be a problem to validate the results and ensure that an acceptable number of good predictions were found. The main disadvantage of the Forester XL model is that the outcomes do not provide the modeller with the algorithms and validation methods used, because of the black box nature of the technique.

The Self Organising Mapping (SOM) method was used on the Roodeplaat Dam data for a period of 20 years. This was done to determine the differences of the before and after conditions of the influence of the Zeekoegat WCW. The seasonal changes and increases in nutrients and Chl *a* concentration are pronounced. This modelling technique is thus applicable to investigate before and after scenarios. This is more of a knowledge development tool than a predictive tool. Only one test was done and the applicability to the impacts of other environmental variables on the development of harmful algal blooms needs to be further investigated.

(4) The RULE set discovery by Hybrid Evolutionary Algorithm (HEA) was tested on different scenarios of real time and 7-days forward, 14-days forward, 21-days forward and 28-days forward forecasting of the abundance of the cyanobacterium, *Microcystis* in the Hartbeespoort, Rietvlei and Roodeplaat reservoirs. The developed rule sets are highly applicable to the hypertrophic reservoirs of South Africa. These methods need, however, to be tested in other reservoirs to determine the applicability under different trophic status and different climatic conditions.

The same method was used to develop a real time algorithm for the dinoflagellate, *Ceratium hirundinella*, for the Hartbeespoort, Rietvlei and Roodeplaat reservoirs. The developed RULE set was then tested on the Bon Accord and Klipvoor Reservoirs that both experienced extreme blooms during the study period. This application was highly applicable to these reservoirs. This further suggests that the developed RULE set may potentially be applicable to reservoirs in other climatic areas of South Africa. This needs further investigation.

4.2 Recommendations

The study showed that eutrophication and the associated problems is a real threat to South African fresh water resources. The list of recommendations need to be taken further by a number of stakeholders, e.g. the Department of Water Affairs and Forestry, future CMAs, Universities and other researchers:

a) Monitor all the necessary variables for future modelling exercises. These include temperature and volumes at inflow. Some of the reservoirs lacked essential variables and certain models, e.g. SALMO-OO could not be tested on Bon Accord and Rietvlei reservoirs due to a lack of flow data. WST is one of the most important variables to measure in-lake and should be included in all monitoring programmes, in addition to the regular chemical and biological monitoring.

b) Include TMs monitoring in impacted fresh water resources at least during the summer periods to enable resource managers to issue warnings to all potential impacted stakeholders and also to provide data for future modelling exercises.

c) Initiate and test available management options to minimise the serious eutrophication levels in the Crocodile-West/Marico Water Management Area. Information and data collected during this testing should be available on the DWAF database for future use.

d) The cause and effects for the changing composition of the phytoplankton of these five reservoirs, which was previously dominated by *Microcystis* during summer periods and by diatoms during winter periods to change to *Ceratium* dominance need to be investigated.

e) Reservoirs that have the option of extracting water at different depths and that are subject to eutrophication related problems should monitor regularly at different depths, to determine the best depth for abstraction. This will enable them to abstract the best quality water and it will minimise the associated financial implications of treating water with potentially bad quality.

f) Of all the modelling methods used the Hybrid Evolutionary Algorithm (HEA) RULE set development proved to very effective. It is recommended that capacity is developed in South Africa regarding the use of this technique. Funding should be made available for the implementation and use of this technique in all research spheres, as the method is applicable to any type of numerical data.

g) Manage the risk imposed by the cyanobacterial blooms and the associated toxins produced in the water resources, on drinking water facilities and the health of recreational users.

h) In view of the successes of the modelling results the next step would be to develop short-term forecasting tools, for the algal blooms of *Microcystis* and *Ceratium,* with on-line water quality monitoring for early-warning and real-time forecasting for reservoir managers.

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