

**Investigating integrated catchment management using a simple water quantity and quality model: A case study of the Crocodile River Catchment, South Africa**

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## **Abstract**

Internationally, water resources are facing increasing pressure due to over-exploitation and pollution. Integrated Water Resource Management (IWRM) has been accepted internationally as a paradigm for integrative and sustainable management of water resources. However, in practice, the implementation and success of IWRM policies has been hampered by the lack of availability of integrative decision support tools, especially within the context of limited resources and observed data. This is true for the Crocodile River Catchment (CRC), located within the Mpumalanga Province of South Africa. The catchment has been experiencing a decline in water quality as a result of the point source input of a cocktail of pollutants, which are discharged from industrial and municipal wastewater treatment plants, as well as diffuse source runoff and return flows from the extensive areas of irrigated agriculture and mining sites. The decline in water quality has profound implications for a range of stakeholders across the catchment including increased treatment costs and reduced crop yields.

The combination of deteriorating water quality and the lack of understanding of the relationships between water quantity and quality for determining compliance/non-compliance in the CRC have resulted in collaboration between stakeholders, willing to work in a participatory and transparent manner to create an Integrated Water Quality Management Plan (IWQMP). This project aimed to model water quality, (combined water quality and quantity), to facilitate the IWQMP aiding in the understanding of the relationship between water quantity and quality in the CRC. A relatively simple water quality model (WQSAM) was used that receives inputs from established water quantity systems models, and was designed to be a water quality decision support tool for South African catchments.

The model was applied to the CRC, achieving acceptable simulations of total dissolved solids (used as a surrogate for salinity) and nutrients (including orthophosphates, nitrates +nitrites and ammonium) for historical conditions. Validation results revealed that there is little consistency within the catchment, attributed to the non-stationary nature of water quality at many of the sites in the CRC. The analyses of the results using a number of representations including, seasonal load distributions, load duration curves and load flow plots, confirmed that the WQSAM model was able to capture the variability of relationships between water quantity and quality, provided that simulated hydrology was sufficiently accurate. The outputs produced by WQSAM was seen as useful for the CRC, with the Inkomati-Usuthu

## Abstract

Catchment Management Agency (IUCMA) planning to operationalise the model in 2015. The ability of WQSAM to simulate water quality in data scarce catchments, with constituents that are appropriate for the needs of water resource management within South Africa, is highly beneficial.

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## **List of Acronyms**

BASINS	Better Assessment Science Integrating Point and Non-Point Sources
BMP	Best Management Practices
CMS	Catchment Management Strategy
CSM	Core Stakeholder Meetings
CRC	Crocodile River Catchment
CSTRs	Completely Stirred Tank Reactors
DOM	Dissolved Organic Matter
DWS	Department of Water and Sanitation
EC	Electron Conductivity
FDC	Flow Duration Curve
GIS	Geographical Information Systems
HSPF	Hydrological Simulation Program-Fortran
INCA	Integrated Nitrogen in Catchments model
IMPAQ	Impoundment/River Management and Planning Assessment tool for water Quality simulation
IWQMP	integrated water quality management process
IWRM	Integrated Water Resource Management
IUCMA	Inkomati-Usuthu Catchment Management Agency
KNP	Kruger National Park
LDC	Load Duration Curves
MAE	Mean Annual Evaporation
MAP	Mean Annual Precipitation
MAR	Mean Annual Runoff
MYA	Million Years Ago
NOAA	National Oceanic and Atmospheric Administration
NSE	Nash-Sutcliffe efficiency

## List of Acronyms

POM	Particulate Organic Matter
TPC	Thresholds of Probable Concern
QUAL2K	Stream Water Quality Model
USA	United States of America
USEPA	United States Environmental Protection Agency
RQO	Resource Quality Objectives
RTC	Recommended Target Concentration
RWQO	Resource Water Quality Objectives
SAWS	South African Weather Services
SPATSIM	Spatial and Time Series Information Modelling framework
SRP	Soluble Reactive Phosphorus
SWAT	Soil and Water Assessment Tool
TIN	Total Inorganic Nitrogen
TWQR	Target Water Quality Range
TDS	Total Dissolved Solids
TMDL	Total Maximum Daily Load
WASP5	Water Quality Analysis Simulation Program
WEAP	Water Evaluation and Planning model
WMA	Water Management Area
WQSAM	Water Quality Systems Assessment Model
WReMP	Water Resources Modelling Platform
WRYM	Water Resources Yield Model
WWTW	Waste Water Treatment Works

## **Dedication**

I would like to dedicate this dissertation to my loving oupa Chris van Aardt and Grandfather Neil Retief, the life lessons, support and continuous reminders “to keep studying” kept me going. I can only wish to become half the great-grandfathers, grandfathers and fathers you two have been. Oupa, while you are not with us anymore, your passion and your stance towards the importance of education most certainly motivated me to get this far.

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## **Chapter 1: General Introduction**

The rapid expansion in the human population has led to natural resources being over exploited on almost every continent. Freshwater fit for social and economic consumption is one vitally important resource that is becoming increasingly limiting to human development. The pressure placed on this resource in the near future is expected to increase as the global human population is expected to grow to 8.9 billion by 2050 (Cohen, 2003).

### **1.1. Current water quantity and quality situation in South Africa**

South Africa is a semi-arid country, with limited fresh water resources that are under increasing threat from pressure due to population growth and an expanding economy (von der Meden *et al.*, 2005). Scarcity of fresh water is aggravated by the alarming increase in pollution caused by industry, urbanisation, afforestation, mining, agriculture and power generation (Nyenje *et al.*, 2010). According to Oberholster and Ashton (2008), if current and anticipated trends of population and socio-economic growth in South Africa persist, it is highly unlikely that South Africa's water resources will be able to sustain future expected water use and waste discharge, with the estimated threshold being reached by 2030.

### **1.2. Why we need water quality models**

While water quantity is routinely measured and well represented in most countries, the contrary is true for water quality. In South Africa, water quality datasets are often incomplete or unreliable and the number of water quality variables measured is also limited. This means that water resource managers in South Africa are often faced with making management decisions within complex systems based on highly uncertain data (Slaughter, 2011a). Water quality data can be of low resolution on both temporal and spatial scales, as measurement of most water quality variables can be time consuming and expensive. Water quality models can be used to complete the spatial and temporal gaps evident within observed data. Water quality models also allow the conceptualisation of processes affecting water quality, and the testing of the validity of these conceptualisations. Finally, water quality models are useful for investigating water quality scenarios where the predictions of water quality outcomes of changing land use, pollutant loading and water extraction for example can be useful for water resources management (Lindenschmidt, 2005; Wang *et al.*, 2013).

### 1.3. Simple versus complex models

Models can be characterised by being highly complex or extremely simple or any gradient of intermediate complexity. Typically, the more complex models have several common characteristics. Complex models usually attempt to model a large number of water quality variables, and therefore, represent a large number of processes affecting these variables. Logically, one could conclude that more complex water quality models would be preferable to simpler models as their simulations are more likely to mimic reality. However, in practice, complex water quality models are prone to several problems. Complex models require a wide range and extent of observed data for calibration purposes and are usually associated with a large number of parameters that represent the rate of the processes conceptualised within the model. This large data requirement means that complex models are not suitable for application within data poor catchments. In addition, the large numbers of parameters associated with complex models make them prone to equifinality (Beven, 1992). While simpler models usually simulate fewer water quality variables and represent fewer processes, they are not necessarily less accurate than complex models. By recognising requisite simplicity (Stirzaker *et al.*, 2010), a simpler model can be constructed by identifying the required level of process complexity required to reasonably/reliably capture variability of a particular variable. Simple models can be developed to conceptually represent the most critical processes affecting water quality, and therefore, require more limited observed data and fewer parameters. Furthermore, as water resource managers are more concerned with the risk associated with management decisions, rather than highly accurate model predictions of water quality on fine spatial and temporal scales, simpler models that provide a frequency distribution of model simulations may be more appropriate. The links between accuracy/uncertainty and requirements for decision making informs the links between data availability, model structure, process understanding and the output requirements. Therefore, in South Africa, the requisite for simplicity or complexity may be driven by the scale at which implementation is required. At a catchment scale, complex models are not supported by the available data and highly accurate time series outputs are not needed for critical decisions based on thresholds of probable concern (TPC). However, if an overly parsimonious modelling approach is taken and the model becomes too simple, critical processes may be missed.

#### **1.4. Background to the WQSAM model**

Hughes *et al.* (2011) investigated the effects of climate change and development on water quantity and quality for the Buffalo River Catchment, in the Eastern Cape of South Africa. The Water Evaluation and Planning (WEAP) model was chosen after an extensive evaluation of other models available. One key outcome of this study was that the WEAP model would not be readily accepted by water resource managers for water quality management due to the inability of WEAP to model water quality of reservoirs, and the simplistic manner in which non-conservative water quality constituents are simulated. No other models assessed could meet the requirements, with most being too complex for the limited data available. Consequently, it was proposed that a new model should be developed for South African conditions and water resource management requirements.

The Water Quality Systems Assessment Model (WQSAM) (Slaughter *et al.*, 2011b), was proposed and is currently being developed to integrate closely with the existing yield models. Water quantity models are well established in South Africa and therefore, WQSAM was designed to integrate water quality components with an existing quantity model. WQSAM directly inputs the water quantity output (storage, abstraction, return flows, incremental and cumulative flows) from a water resources system model (the Water Resources Yield Model: WRYM or the Water resources Modelling Platform: WReMP) (Wimberley and Coleman, 2005; Sieber and Purkey, 2007). The natural flows used within the yield models are typically simulated by the Pitman Model (Pitman, 1973). WQSAM aims to address management requirements for water quality management by utilising existing routinely observed data, integrating with existing yield (quantity) models and providing estimates of risk associated with management scenarios. The procedures used within WQSAM extensively use the relationships between flow and water quality to simulate water quality variable loads. Many procedures used within WQSAM for simulating water quality have been adopted from established international water quality models, such as CE-QUAL-W2 (Cole and Wells, 2008) and QUAL2K (Pelletier *et al.*, 2005), but simplified in order to use the existing observed data. WQSAM also includes a simplified reservoir water quality modelling component.

### **1.5. WQSAM applied to the Crocodile River Catchment and the IWQMP**

The Crocodile River Catchment, located within Mpumalanga Province of South Africa, has been experiencing a decline in water quality as a result of point source inputs of a mixture of pollutants, which are discharged from industrial and municipal wastewater treatment plants, as well as from diffuse source runoff and return flows from the extensive areas of irrigated agriculture and mining sites (Deksissa *et al.*, 2004). The decline in water quality has profound implications for a range of stakeholders across the catchment. The major implication is the financial cost incurred by stakeholders, particularly those that rely on good water quality for production, as they face increased costs of treating water extracted from the Crocodile River. Even more importantly, the Crocodile River flows into neighbouring Mozambique, and South Africa is governed by international treaties to regulate the quantity and quality of river flow leaving South Africa (Palmer *et al.*, 2013).

One of the research requirements concerning the status of water quality in the Crocodile River Catchment (CRC), is that there is a need for understanding the relationship between flow and water quality to be able to determine water quality compliance (or non-compliance) of water users within the catchment (Palmer *et al.*, 2013). Therefore, this research project was designed to contribute to understanding the relationships between quantity and quality of surface water in the CRC with the use of WQSAM. This research will contribute to a larger project with the aim of developing and implementing a co-operative and integrated water quality management process (IWQMP) in the CRC. Furthermore, the application of WQSAM to the CRC represents an opportunity to test the capabilities of WQSAM within a large, extensively exploited catchment and specifically assessing the model on two fronts:

1. Whether the simplified water quality processes represented within WQSAM can generate water quality outputs that are appropriate and reliable enough for management requirements.
2. Whether the outputs of WQSAM can be used for future scenario analysis to facilitate water quality management planning within the CRC.

### **1.6. Aims and objectives**

This research aims to model water quality, (combined water quality and quantity), to facilitate a co-operative management plan that will decrease pollutant concentrations and effectively work towards improving source (in-stream) water quality using the CRC as a case study. The objective of this study was to test WQSAM to determine if it can adequately

## Chapter 1: General Introduction

capture the variability of relationships between water quantity and quality, and if it can generate relevant water quality information that can be used for the IWQMP within the CRC.

The specific research questions to be explored are:

1. Is it acceptable to link existing water quantity models to WQSAM?
2. Are the water quality constituents modelled by WQSAM appropriate to management requirements?
3. Does the available data in the CRC meet WQSAM's minimum data requirements?
4. Does WQSAM produce water quality information that is appropriate for the development of the IWQMP?

To answer the above questions, the following tasks were undertaken: all relevant existing data were collated for the study area, all major point and diffuse sources of pollution were identified, key water quality variables to be modelled were identified and the minimum data requirements of WQSAM were determined.

## **Chapter 2: Literature Review**

### **2.1. Integrated Water Resources Management**

Internationally, water resources are facing increasing pressure due to over-exploitation and pollution which, together with natural variability, makes planning and management of water resources a very complex and difficult task (Biswas, 2008). Integrated Water Resource Management (IWRM) has attracted increasing interest globally as a paradigm for integrative and sustainable management of water resources (Ballweber, 2006). IWRM, according to Giordano and Shah (2014), is designed “to consider water holistically, to manage it across sectors, and to ensure wide participation in decision making”. However, in practice, the implementation of IWRM policies has been hampered by the limited availability of integrative decision support tools, limited human resources and insufficient observed data (Ballweber, 2006). Jeffery and Geary (2006) suggest that there is no evidence that IWRM has actually worked, while Ballweber (2006) states that there are a growing number of individual IWRM successes on a regional or local scale, despite the lack of success at national levels.

In South Africa, the new constitution of 1996 contained the principles of IWRM by embracing environmentally sound, sustainable economic and social development policies (Ballweber, 2006). This was expanded in the National Water Act (Act 36 of 1998) that is internationally recognised as legislation that promotes excellent water management. Ballweber (2006) describes South Africa as taking a bold leap in attempting to apply IWRM with a top down approach, while other countries such as the United States of America applied the bottom up approach. However, these ambitions have not always been achieved in the practical management of South African water resources. According to Palmer *et al.* (2013), there is a notable failure within the implementation of water resource management policies resulting in the decline of surface water quality.

### **2.2. Water quality models tools for IWRM**

A critical component of IWRM is the integration of water quantity and quality management, with all water users depending on a certain standard of water quality and quantity (Garcia, 2008). Available water quantity is decreasing due to the increased demands from growing economies and populations, and this scarcity is being exacerbated by poor water quality

(Cohen, 2003). Consequently, increased financial investments are being made in order to protect water quality and ensure ecological water requirements are met. Traditionally, water quality analyses within water resource systems have been performed through the use of historical observed data. However, the limits to this approach have been highlighted in recent years. Loucks and Beek (2005) suggest that modelling can be used in conjunction with monitoring data, or even in their absence, for making management decisions for several reasons including: “1) modelling can be a more feasible option due to lack of observed data or financial costs of monitoring; 2) integrated monitoring and modelling systems could provide better information than one or the other alone for the same total cost; 3) modelling can be used to predict future water quality based on scenarios”. Due to financial constraints, water resource managers usually have access to observed data of low temporal and spatial resolution. Depending on the scale and data constraints, a model can be used to bridge data gaps, both temporally and spatially, providing information to managers for appropriate decision making (Borah and Bera, 2003).

The scale at which models can be applied for water quality management is dependent on the characteristics of the model or more specifically the data requirements. A localised model such as the Stream Water Quality Model (QUAL2K) (Pelletier et al., 2006) operates on an hourly time step and simulates many variables (data intensive) (Wimberley and Coleman, 2005). This limits the scale at which it can be applied to short sections of a river reach (Wimberley and Coleman, 2005). The QUAL2K model has been utilised worldwide and South Africa is no exception (Venter *et al.*, 1997; Malan and Day, 2003). According to Tsakiris and Alexakis (2012), the main advantage of the QUAL2K model is the capability of simulating algae (chlorophyll-a). However, the QUAL2K model is not an ideal tool to support IWRM, as it cannot be applied at a catchment scale and cannot simulate reservoir processes.

The Soil and Water Assessment Tool (SWAT) (Arnold *et al.*, 1998) model can be applied at a catchment scale, simulates catchment in-stream processes at high levels of spatial detail and can be used to simulate long term trends on a daily time step (Borah and Bera, 2003). Santhi *et al.* (2002) applied the SWAT model in the North Bosque River Watershed in Texas, USA, to support the Total Maximum Daily Load (TMDL) program, and found that the modelling approach was relevant and could be adapted for other areas of concern in USA. The strength of the model is that it can be used to separate diffuse and point source loading to a system, and water managers can determine load reductions to ensure water quality standards are not

exceeded (DePinto *et al.*, 2004; Santhi *et al.*, 2006). The Better Assessment Science Integrating Point and Non-Point Sources (BASINS) (Lahlou *et al.*, 1998) model developed by the United States Environmental Protection Agency (USEPA), incorporates SWAT and the Hydrological Simulation Program-Fortran (HSPF) rainfall-runoff model (Borah and Bera, 2003). BASINS was designed to investigate Best Management Practices (BMP) and to help in the development of TMDL standards in the US (Borah and Bera, 2003). This is now used routinely in the TMDL process to simulate different management scenarios of point and diffuse loading to a system (Arnold *et al.*, 1998; DePinto *et al.*, 2004, Jayakrishnan, 2005).

It is not uncommon for existing hydrological models to be incorporated with water quality models. Wilby *et al.* (2006) investigated climate change impact scenarios of water quality by incorporating CATCHMOD (a hydrological model) and the Integrated Nitrogen in Catchments (INCA) model in a single framework. The INCA model was developed for European catchments to integrate catchment and river processes related to nitrogen dynamics (Whitehead *et al.*, 1998; Jarvie *et al.*, 2002; Wade *et al.*, 2002). The limitations of the model are that it only simulates nitrogen and according to Jarvie *et al.* (2002), the INCA model could simulate long term trends but was less accurate when simulating short term trends. In South Africa, the Impoundment/River Management and Planning Assessment tool for water Quality simulation (IMPAQ) has been used in conjunction with the Water Resource Yield Model (WRYM) to simulate conservative and non-conservative pollutants in a number of catchments (Wimberley and Coleman, 2005). The IMPAQ model functions on a monthly time step which is not optimal for water quality modelling, as water quality is influenced by transient events. The Water Evaluation and Planning (WEAP) model (Sieber and Purkey, 2007) was developed by the Stockholm Environment Institute (SEI) as a robust tool for integrated water resource planning. The WEAP model is a watershed model with a dedicated systems model for quantity and is simple to use. Slaughter and Hughes (2013b), used the WEAP model to simulate climate change scenarios for the Buffalo River Catchment in the Eastern Cape, South Africa. They found the WEAP model to be too simplistic in modelling non-conservative pollutants, as the model represents multiple in-stream processes by a single parameter and does not simulate water quality in reservoirs (Assaf and Saadeh, 2008). Catchment scale water quality models have therefore had to make compromises (reducing the number of parameters and variables simulated etc.) to be applicable at this scale. However, the compromise should not entail neglecting critical processes influencing water quality as was identified in the WEAP model (Slaughter and Hughes, 2013). While water quality



models are highly useful, it is important to note that models are a simplified representation of reality regardless of the complexity of the model. Therefore, it is critical that the assumptions made, processes represented and shortcomings within a model are made completely transparent (Loucks and Beek, 2005).

### **2.2.1. Complex versus simple models**

One broad classification of models is by model complexity, and traditionally complex models have been favoured over simpler models to give more reliable simulations. Complex models include more processes and therefore, simulated results should be a more accurate representation of true conditions. However, experience has shown that the value of complex models is subject to several constraints. Complex models typically require more observed data, more financial resources and greater technical expertise. It is difficult to obtain reliable simulations within data-poor catchments, when the model parameterisation is hampered by a lack of calibration data. Complex models typically have more parameters, making these models susceptible to equifinality. Equifinality in a modelling context refers to the likelihood that multiple parameter value sets can generate similar model outputs (Bevan, 2006) and determining which model setup is providing the correct representation of processes can be difficult or even impossible.

Snowling and Kramer (2001) suggested a model uncertainty-complexity relationship, where error decreases with complexity but results in a higher sensitivity. This conceptual relationship was tested by Lindenschmidt (2006) using the Water Quality Analysis Simulation Program (WASP5) of five varying complexity structures applied to a study catchment. They calculated the error and sensitivity of each model structure as well as scoring the overall usefulness of the five models. While they found the Snowling and Kramer (2001) hypothesis to be true; they also found that the models with the greatest utility were intermediate in complexity (Figure 2.1), with very simple and very complex models showing lower utility scores.

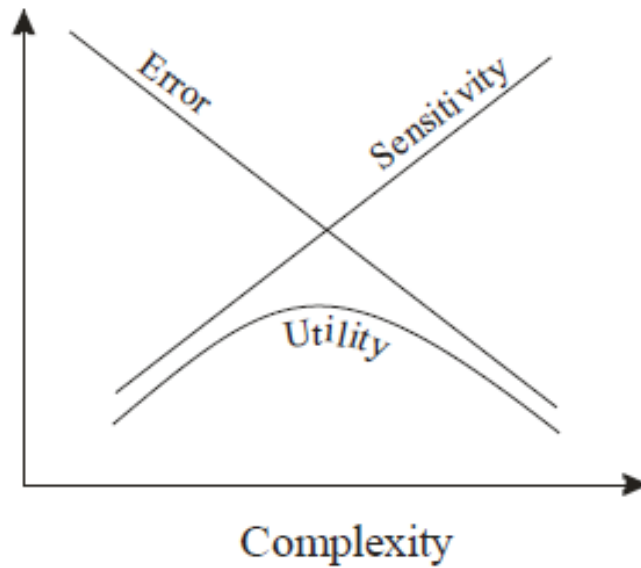


Figure 2.1 Snowling and Kramer’s (2001) hypothetical uncertainty-complexity relationship with Lindenschmidt’s (2006) added utility representation.

The ‘accuracy’ requirement of model simulations is dependent on the aims of specific studies. This is illustrated by Snowling and Kramer’s (2001) acknowledgement that the choice of model complexity should be driven by the model’s intended use. For example, complex models may be more suitable for scientific research purposes, whereas simpler models may be more useful for management. Snowling and Kramer (2001) represent the intended use along a model complexity spectrum (Figure 2.2).

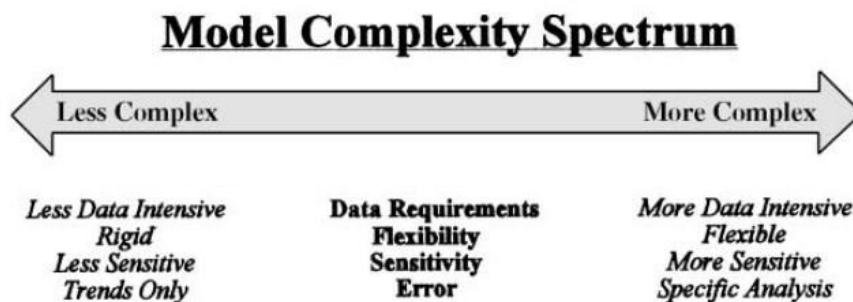


Figure 2. 2 Model complexity spectrum (taken from Snowling and Kramer, 2001)

McIntyre *et al.* (2003), suggests that while additional complexity may improve the precision of model results, the added complexity hinders the formal evaluation of uncertainty. This is primarily due to the increased number of uncertain model components that would need to be simultaneously analysed (Snowling and Kramer, 2001; McIntyre *et al.*, 2003; Lindenschmidt, 2006). According to McIntyre *et al.* (2003), “water quality policy must take account of the uncertainties associated with both the validity of the models and the driving forces”. Therefore, the reduced ability to estimate uncertainty in complex models may be a compromise to their usefulness for management. This is especially true for South Africa as resource managers are likely to be less concerned about highly accurate time series simulations, and more concerned with identifying water quality risks associated with different water use and pollution scenarios.

Based on the available literature, there are a number of minimum criteria that should be met for a model to be useful as a tool supporting IWRM. These include:

1. functions on a daily time step (minimum);
2. simulates critical processes and variables of concern;
3. applicable at a catchment scale;
4. simulates water quality for rivers and reservoirs and;
5. a level of requisite simplicity should be maintained.

### **2.3. Water quality constituents commonly simulated by models**

#### **2.3.1. Total dissolved solids (abbreviated TDS) as an indication of salinity**

TDS is the measure of the combined content of all inorganic substances contained in a liquid in molecular, ionized or micro-granular suspended form (Webber-Scannell and Duffy, 2007). This includes all minerals, salts, metals, cations or anions (Table 4.4) dissolved in water. A measurement of TDS cannot differentiate among ions (Webber-Scannell and Duffy, 2007), and TDS concentrations can be determined by the sum of the cations and anions in the water. Traditionally TDS concentrations were determined through filtering the sample through a 2 µm pore sized filter, evaporating the remaining filtrate and then drying the remains at 180 °C. More common today, which is seen to be slightly less accurate, is calculating TDS concentration based on the Electrical Conductivity (EC) reading as:

$$TDS = k_e E \quad \text{Equation 2.1}$$

Where TDS is expressed in mg ℓ<sup>-1</sup> and EC is the electrical conductivity in µS cm<sup>-1</sup> at 25 °C. The correlation factor  $k_e$  varies between 0.55 and 0.8. In South Africa, electrical conductivity

is most commonly reported in  $\text{mS m}^{-1}$ , and the correlation factor  $k_e$  ranges from 5.5 to 7.5 (van Niekerk *et al.*, 2014). The average conversion factor in South Africa for most waters has been identified to be 6.5, and is used in this study to calculate TDS concentrations from measured electrical conductivity readings as there is a lack of observed TDS measurements (van Niekerk *et al.*, 2014). TDS is used within water quality modelling because it represents a mass-based measure that be used within a mass-balance modelling approach.

Table 2.1 Examples of cations and anions found commonly in water that influence TDS concentrations

<b>Cations</b>	<b>Anions</b>
<b>Calcium Ca ++</b>	Bicarbonate $\text{CHO}_3^-$
<b>Magnesium Mg ++</b>	Chloride $\text{Cl}^-$
<b>Sodium Na+</b>	Sulphate $\text{SO}^-$
<b>Iron Fe ++</b>	Nitrate $\text{NO}^-$
<b>Manganese Mn ++</b>	Carbonate, $\text{CO}^-$

### 2.3.2. Nutrients

The chemical species nitrogen and phosphorus are classified as nutrients that influence the productivity of all ecosystems, and are key indicators of water quality (Slaughter, 2011a). Aquatic flora (algae, macrophytes and phytoplankton) require many nutrients (e.g. carbon, nitrogen, phosphorus, oxygen, silica, magnesium, potassium, calcium, iron, zinc, copper). Of these, the most essential for the growth of flora, are phosphorus and nitrogen. Under natural conditions, these nutrients are often in short supply, both on land and in water bodies. Therefore, fertilisers are applied regularly for increased crop and fodder yields (Mann, 2000). This often leads to the leaching of nutrients through interflow and ground water contamination, and transport through surface runoff, resulting in increased or excess nutrients in surface water. Also contributing to excess nutrients in surface waters are inputs from point sources such as waste water treatment plants. Nitrogen is one of the key elements that influence water quality, as biological processes can only occur in the presence of sufficient nitrogen (Tebbutt, 1988). Nitrogen can be found within water bodies in four major forms, organic nitrogen, nitrite, nitrate and ammonia (nitrogen salts as ammonium or free ammonia) (Tebbutt, 1988; Chapra, 1997). Chapra (1997) groups water quality problems arising from nitrogen in two major categories. The first category encompasses the secondary effects of

nutrient enrichment including eutrophication. The second category encompasses the actual direct toxicity effects of nutrients themselves and includes nitrate pollution and ammonia toxicity. These groups are however interconnected as seen in the nitrogen cycle depicted in Figure 2.3 (Chapra, 1997).

### 2.3.2.1. Nitrate and nitrite

Aerobic nitrification is the biological oxidation of ammonia in the presence of oxygen in a two-step process to form nitrite (Equation 2.2) and/or then oxidising of nitrites to form nitrates (Equation 2.3) (Chapra, 1997; Kuai and Verstraete, 1998). Denitrification is a microbial facilitated process of reduction occurring in anoxic conditions. The nitrification processes consumes oxygen, as the oxygen atoms act as the electron acceptors, and ultimately leads to decreased dissolved oxygen concentrations.

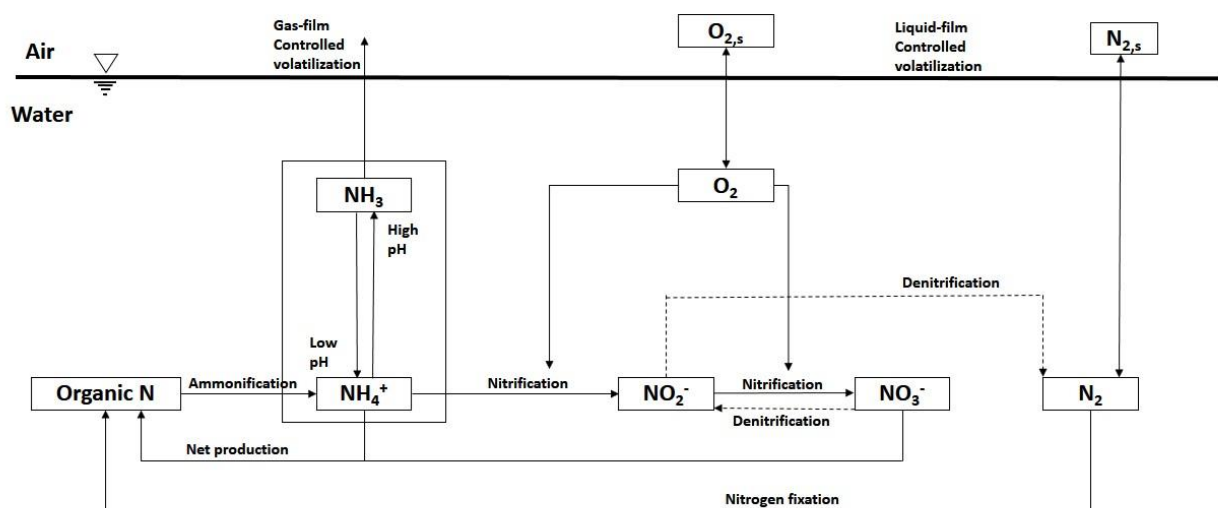
*Step 1 of nitrification to form nitrites:*



*Step 2 of nitrification to form nitrates*



Denitrification occurs under special conditions, generally when oxygen is depleted, leading to bacteria respiring nitrate (Chapra, 1997). When there are sufficient quantities of nitrates and the oxygen consumption exceeds the oxygen supply, the reduction of nitrates and nitrites



occurs with ammonium acting as the electron donor (Equation 2.4).



Figure 2.3 The nitrogen cycle in natural waters (taken from Chapra, 1997). Dashed arrows indicate denitrification reactions taking place under anaerobic conditions

### 2.3.2.2. Ammonia

Ammonia can be found in aquatic ecosystems in two forms, namely as ammonium ions ( $\text{NH}_4^+$ ) and ammonia gas ( $\text{NH}_3$ ), with the equilibrium between the two forms governed predominantly by pH and temperature (Chapra, 1997). Found in all natural waters, even if only in low concentrations, together they form total ammonia. Measuring the un-ionised form of ammonia ( $\text{NH}_3$ ) is extremely difficult and therefore, in South Africa, the ionised form  $\text{NH}_4^+$  is most commonly measured.

Ammonia is derived from the breakdown of organic nitrogen or by the reduction of nitrate in the process of denitrification (Figure 2.3). The formation of  $\text{NH}_3$  is favoured at high pH levels (>8), but is influenced by temperature as well. This means that even though the in-stream total ammonia may remain constant the concentrations of the two forms may vary. In high concentrations, ammonium can stimulate the growth of algae and aquatic plants. In the presence of bacteria, ammonium can be converted to nitrate ( $\text{NO}_3^-$ ) through the process of nitrification (Chapra, 1997).

### 2.3.2.3. Phosphorus

Phosphorus is one of the key elements essential to all life, being necessary for the growth of plants and animals, and plays a critical role in genetic systems and the storage and transfer of cell energy as well (Chapra, 1997; Novotny, 2003; McDowell *et al.*, 2004). In terms of water quality, phosphorus is important as it is usually in short supply in comparison to other macronutrients (Chapra, 1997). Phosphate exists in three forms, namely orthophosphate, metaphosphate and organically bound phosphate (each compound contains phosphorus bound in different chemical arrangements) (Chapra, 1997). Chapra (1997) suggests that phosphate scarcity is due to three major factors:

1. the element phosphorus is not abundant in the Earth's crust and its mineralised forms are not very soluble in water;
2. unlike nitrogen, phosphorus does not exist in a gaseous form, therefore, no phosphorus is transferred from the atmosphere into the aquatic environment and;
3. phosphates adsorb strongly to fine-grained sediments in natural conditions. This removes bioavailable phosphates from the water column to sediment sinks.

The loss/storage of phosphates within a system can be influenced by several factors as described by Novotny (2003):

1. aluminium and iron oxides are responsible for the retention of phosphates in acidic soils;

2. calcium compounds influence the solubility of phosphates in calcareous soils and;
3. organic matter contributes to phosphate adsorption.

The three forms of phosphates are further divided for natural waters by Chapra (1997) into soluble reactive phosphorus (SRP), also referred to as orthophosphate or soluble inorganic phosphorus (this form is readily available to plants), particulate organic phosphorus (consists of mainly living aquatic organisms), non-particulate organic phosphorous (originates from the decomposition of particulate organic phosphorus), particulate inorganic phosphorus (e.g. phosphate minerals, adsorbed orthophosphate and phosphate complexed with solid matter) and non-particulate inorganic phosphorus (condensed phosphates). Chapra's (1997) figure representing phosphorus in natural waters sums up the processes of decomposition and production of phosphates in natural waters (Figure 2.4).

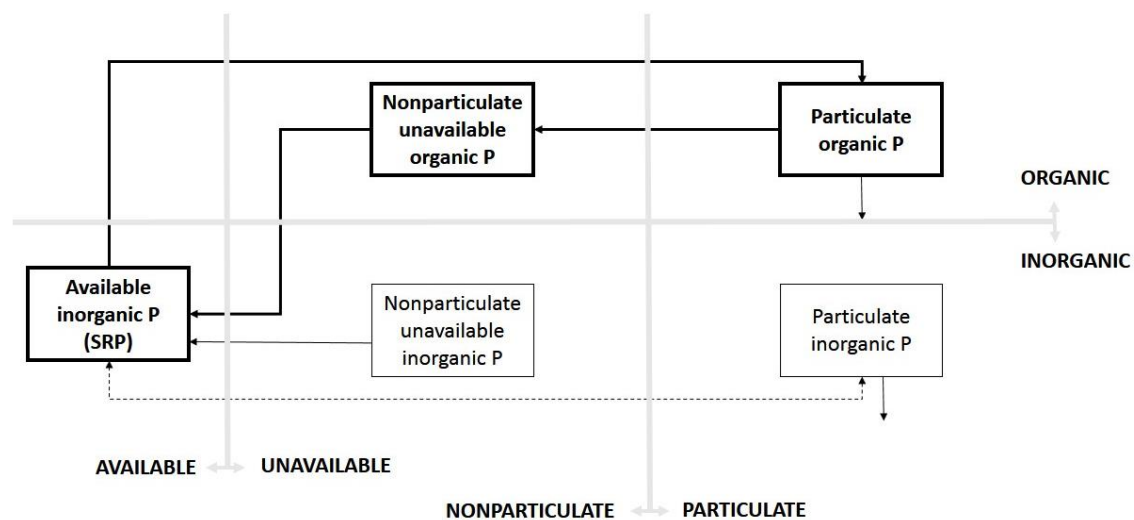


Figure 2.4 Forms of phosphorus found in natural waters (taken from Chapra, 1997). The principal forms involved in the production/decomposition life cycle are shown in bold.

## 2.4. Processes represented within water quality modelling

### 2.4.1. Relationship between flow and water quality

The primary driver of all water quality constituents is the movement of water through porous media (soils and rock), over the land surface and as flow in channels. These hydrological processes were poorly understood in the past, however, with advances in geochemical and isotopic tracer studies, important insights have been gained into catchment hydrological processes, ranging from geographical sourcing of water, to assessing source contributions to stream flow (Soulsby *et al.*, 2007). These hydrological processes determine flow pathways which can strongly influence the chemical and physical properties of river flow (Sear *et al.*,

1999). Water quality and quantity relationships differ amongst water quality constituents and are influenced by the prevailing physical characteristics (topography, soils, geology, vegetation and land cover) of a catchment and the way in which these affect hydrological processes (Malan and Day, 2003; Soulsby *et al.*, 2006; Slaughter, 2011a). Contributions to natural stream flows can be broadly classified into three components on the basis of the hydrological processes through which rainfall is translated into runoff, namely surface flow, interflow and groundwater (Figure 2.5) (Hughes *et al.*, 2003; Soulsby *et al.*, 2006), which follow different pathways, have different residence times and consequently are expected to have different natural water quality signatures. As described by Hughes *et al.* (2003), total stream flow is derived from runoff processes, with surface runoff being the most rapidly reacting source (primarily associated with transient events), interflow being slower to react and the slowest being discharge from groundwater. As volumes of water travel through the catchment within the various flow pathways, the chemistry changes as they come into contact with various substrates (surface land-use structure, soils and geology). The methods used to account for these flow contributions vary amongst models, for example, the SWAT model estimates runoff volume using curve numbers, subsurface flow is calculated using the kinematic storage model and groundwater flow using empirical relations (Borah and Bera, 2003).

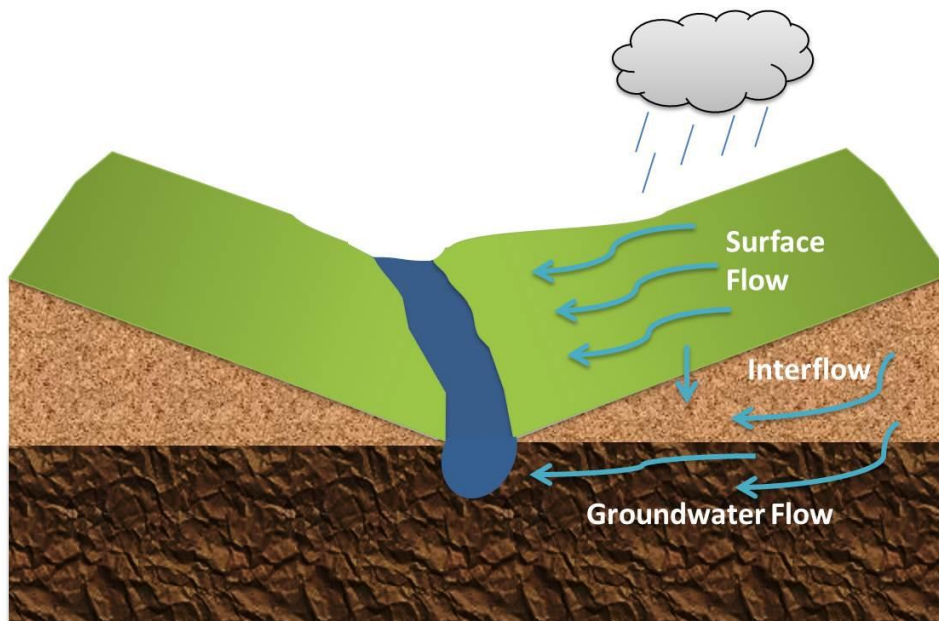


Figure 2.5 Water flow paths contributing to in-stream flow and the natural mode of travel for various water quality constituents



#### **2.4.1.1. Transient events**

Whitefield and Wade (1996) investigated the influence of transient events on the water quality of British Columbian coastal streams and found that urbanised areas have a direct influence on in-stream water quality during a transient event. While it is important to take account of transient event influence on in-stream water quality, acquiring data for these events is extremely intensive and often electronic data loggers are used, but are limited to measuring a few water quality variables. Models such as the IMPAQ and WEAP simulate water quality on a monthly time step, and neglect to take into account transient events that would influence in-stream water quality such as rapidly reacting surface runoff loads (Hughes *et al.*, 2003). Simpson and Stone (1988) found that following a dry spell in an urban catchment, runoff was excessively loaded with nutrients (first-flush event). This could only be captured if you were considering transient flow events on water quality. The more complex model QUAL2K functions on an hourly time step, whereas catchment scale models such as the BASINS, SWAT and CATCHMOD function on a daily time step (Lahlou *et al.*, 1998; Borah and Bera, 2003; Wimberley and Coleman, 2005). In South Africa there is access to daily flow and rainfall data, which allows models to operate on a daily time step. The availability of water quality data are however usually too little and contributes to uncertainty.

#### **2.4.1.2. Residence time**

The residence time of quality constituents plays a critical role in overall water quality and ecosystem dynamics. The extended presence of water quality constituents within any water body increases the overall effect on water quality, for example, allowing increased plant growth in the case of nutrients, or allowing increasing exposure of toxicants such as toxic metals to biota. Brion *et al.* (2000) found that in the Seine River (France), because of short residence times, slower growing nitrifying bacteria populations did not have enough time to develop sufficiently to nitrify available ammonium. Nutrients trapped in slow moving or lotic rivers, or lotic impoundments, are more bioavailable for adsorption by macrophytes or to settle and be bound to sediments. This is illustrated by the presence of dense hyacinth growth in some of the slower-moving stretches of the Crocodile River (Deksissa *et al.*, 2004)

#### **2.4.2. Natural processes**

Sear *et al.* (1999) states that “the form and concentration of dissolved materials in stream water depends on its history of contact”. The water quality in surface waters is influenced by a number of processes as a result of contact between water and a number of natural elements

that may influence in-stream water quality independently or concurrently. These elements include the climatic conditions in a catchment (geomorphological, geological, soils and vegetation), hydrological conditions (flow regime) and hydrodynamic conditions (rate of river flow) (Soulsby *et al.*, 2006). The resulting processes influence the input of minerals and organic matter (e.g. soils, minerals from groundwater flow, organisms etc.) and determine the conditions (climate, relief and stream-flow regime) for in-stream chemical reactions (Sear *et al.*, 1999).

According to Day *et al.* (1998), underlying geology in South Africa can influence in-stream water quality. The geological formations found across a catchment can vary greatly both in age and composition. In South Africa, predominant underlying geological formations are sedimentary of marine origin (Day *et al.*, 1998; Slaughter, 2011a). It has been found that geological formations of igneous origin (e.g. basalt, andesite, rhyolite, granite and diorite etc.) are far less susceptible to weathering due to their composition, and associated water quality signatures are typically lower (generally  $< 65 \text{ mg } \ell^{-1}$  for TDS) (Health Canada, 1991). Geological formations of sedimentary origin comprising shale (with high  $\text{CaCO}_3$  composition) for example (Railsback, 1993), are more susceptible to weathering, and flow through these rock formations tends to be associated with higher water quality concentrations (e.g. TDS ranging from 195 to 1 100  $\text{mg } \ell^{-1}$ ) (Health Canada, 1991).

The type of soil found within a catchment can have a profound influence on surface runoff, interflow and groundwater water quality concentrations (Bronick and Lal, 2005). Both inorganic and organic soil particles have negative charges on their surfaces (Carter and Gregorich, 2008). This allows the adsorption of mineral cations to soil particles (Bronick and Lal, 2005; Carter and Gregorich, 2008), which are not easily leached out during vertical (recharge) or lateral (interflow) drainage processes (Carter and Gregorich, 2008). The soil's ability to attract, retain and exchange cations is known as the Cation Exchange Capacity (CEC), and soils with high clay composition have higher CECs and a greater ability to hold onto nutrients (Figure 2.6) (Carter and Gregorich, 2008).

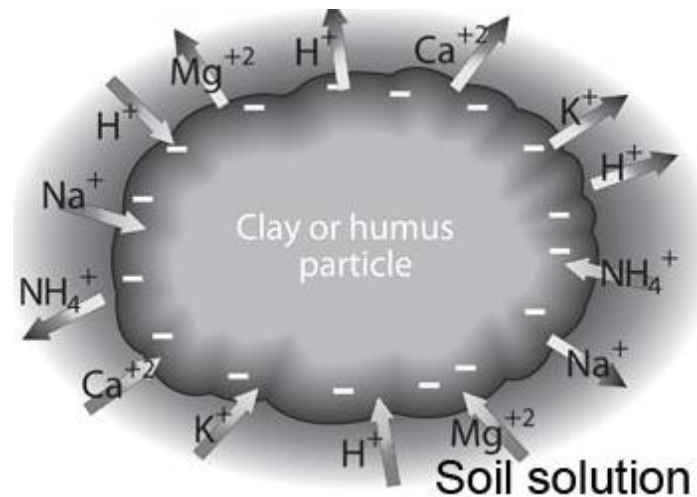


Figure 2.6 Diagram representing exchangeable nutrient cations adsorbed on soil particles (taken from Nathan, 2009)

### 2.4.3. Anthropogenic processes

Pollutants from anthropogenic activities enter lentic or lotic water bodies at a specific location within a catchment, but have a range of possible scale outcomes, from localised to first order catchment level responses (Johnson *et al.*, 1997). The mode in which pollutants enter water bodies varies but can be broadly classified as point sources or diffuse sources. A point source represents polluted effluent that travels directly from source to water body through a conduit of restricted spatial extent (e.g. from a factory via a pipeline to a nearby water body). Diffuse sources represent pollutant sources where there is no direct point of input and are often mobilised and transported by natural hydrological processes (Muir, 2011).

#### 2.4.3.1. Point sources

Point source pollution is frequently assumed to be highly predictable due to strict discharge licensing regulations. Therefore, it is assumed that point source contributions would be constant over time. Bowes *et al.* (2008) found a decrease in phosphorus concentrations with increasing flow in catchments dominated by point sources that can be attributed to a constant input of a pollutant during all flow conditions and therefore, diluted during high flow events. However, Hughes and Slaughter (2013a) noted a great deal of scatter in in-stream nutrient concentrations at low flows, which was attributed to temporally variable effluent releases and effluent concentrations from waste water treatment works (WWTWs) in South Africa.

#### **2.4.3.2. Diffuse sources**

Diffuse sources are extremely difficult to measure and regulate, and the pollutant load associated with diffuse sources usually varies spatially and temporarily with season, precipitation and other transient events (Malan *et al.*, 2003; Slaughter, 2011a). Anthropogenic diffuse sources include agricultural activities that may result in surface runoff loads and/or leaching from the use of manure and nitrogenous based fertilisers and the cultivation of nitrogen fixing crops. Other sources falling under the broad category of urban runoff include failed septic tanks and runoff from construction sites and abandoned mines, where mine waste water will eventually make its way into nearby water bodies (Oberholster and Ashton, 2008). Flow rate and volume have an influence on in-stream water quality concentrations through mobilisation, dilution and/or residence time. Bowes *et al.* (2008) found that rivers dominated by diffuse sources of phosphorus experience increased water quality concentrations during high flow periods. This is because the mobilisation of phosphorus is dependent on flow processes, including runoff from urban areas (e.g. first-flush events), and/or surface waters draining soils of agricultural areas and entering rivers as interflow with large phosphorus loads (Simpson and Stone, 1988; Hughes and van Ginkel, 1994; Slaughter and Hughes, 2013a). Slaughter and Hughes (2013a) found that for South African conditions, there are frequently increasing concentrations of nitrates, nitrites and phosphates with increasing flows similar to that noted by Bowes *et al.* (2008). However, the relationship was found to be highly scattered.

#### **2.4.4. In-stream processes**

Once water quality constituents have entered a river channel, they are exposed to a number of processes that will determine their environmental fate. The in-stream processes can be broadly classified into hydrophysical, hydrochemical and hydrobiological. These are represented in models at varying levels of detail dependent on the model's complexity. The QUAL2K model is classified as a complex localised model representing in-stream processes to a relatively large degree of detail (Table 2.1). It is used here to illustrate complex representation of in-stream water quality processes (conceptual model component diagrams from the CE-QUAL-W2 user manual are presented in figures 2.7 and 2.8, but represent similar processes to those represented within the QUAL2K model).

Hydrophysical processes influence the transportation of water quality constituents through the processes of convection and diffusion. Tsakiris and Alexakis (2012) describe the

QUAL2K model's water quality constituent transportation assumptions as: "a) the advective transport is based on mean flow; b) the water quality indicators are completely mixed over the river cross-section and; c) the dispersive transport is correlated with the concentration gradient". Hydrochemical processes influencing in-stream water quality include dissolving of constituents, sedimentation and adsorption. Models commonly use a mass balance approach to simulate the process of dilution (Chapra, 1997). The QUAL2K model simulates adsorption and settling of algae, phosphates and detritus to sediments (Figure 2.7), and the anaerobic release of adsorbed/settled phosphates (Figure 2.8) (Cole and Buchak, 1995).

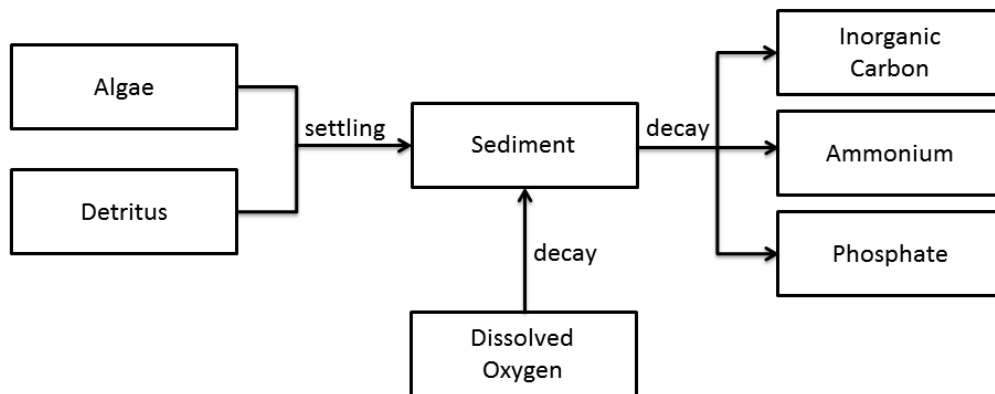


Figure 2.7 Conceptual sediment model component of the CE-QUAL-W2/QUAL2K model (Cole and Buchak, 1995)

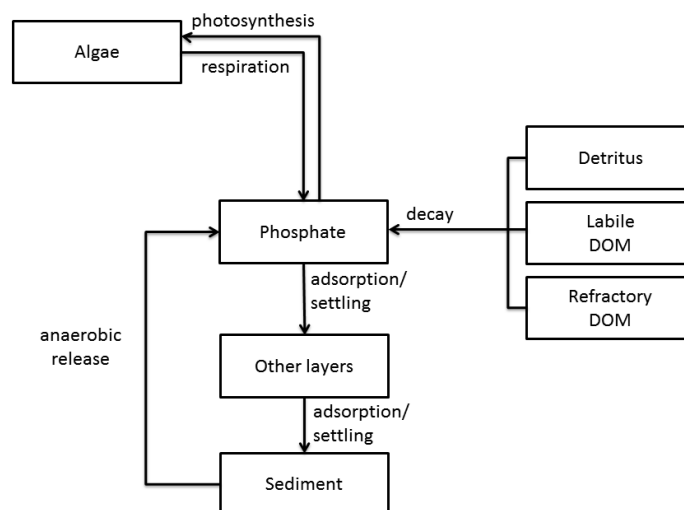


Figure 2.8 Conceptual phosphate model component of the CE-QUAL-W2/QUAL2K model (Cole and Buchak, 1995)

## Chapter 2: Literature Review

Organisms in the water strongly influence water quality through hydrobiological processes. Algae in fresh water systems are major primary producers and play a critical role in the nutrient dynamics of streams. The QUAL2K conceptual algal component (Figure 2.9) shows that the model takes account of the processes between dissolved oxygen and algae (respiration and photosynthesis), nutrient cycling through respiration and photosynthesis, excretion, mortality and settling on sediments (Cole and Buchak, 2005). Simulation of dissolved oxygen dynamics increases model complexity drastically (Figure 2.10) and the algorithms are difficult to validate in South African due to lack of data. The QUAL2K dissolved oxygen model component accounts for loss of oxygen due to respiration, decay and nitrification and gain from aeration and photosynthesis (Figure 2.10).

While all the processes affecting water quality are important, some have a more pronounced effect. Simpler models attempt to decrease the number of processes simulated while attempting to maintain a level of requisite simplicity. This entails simulating key processes, while removing more complex processes such as the QUAL2K dissolved oxygen modelling component.

Table 2.2 In-stream processes represented by the QUAL2K model

Processes				
Mortality	Excretion	Decay	Settling/adsorption	Photosynthesis
Respiration	Anaerobic	Release	Nitrification/Denitrification	Rearation

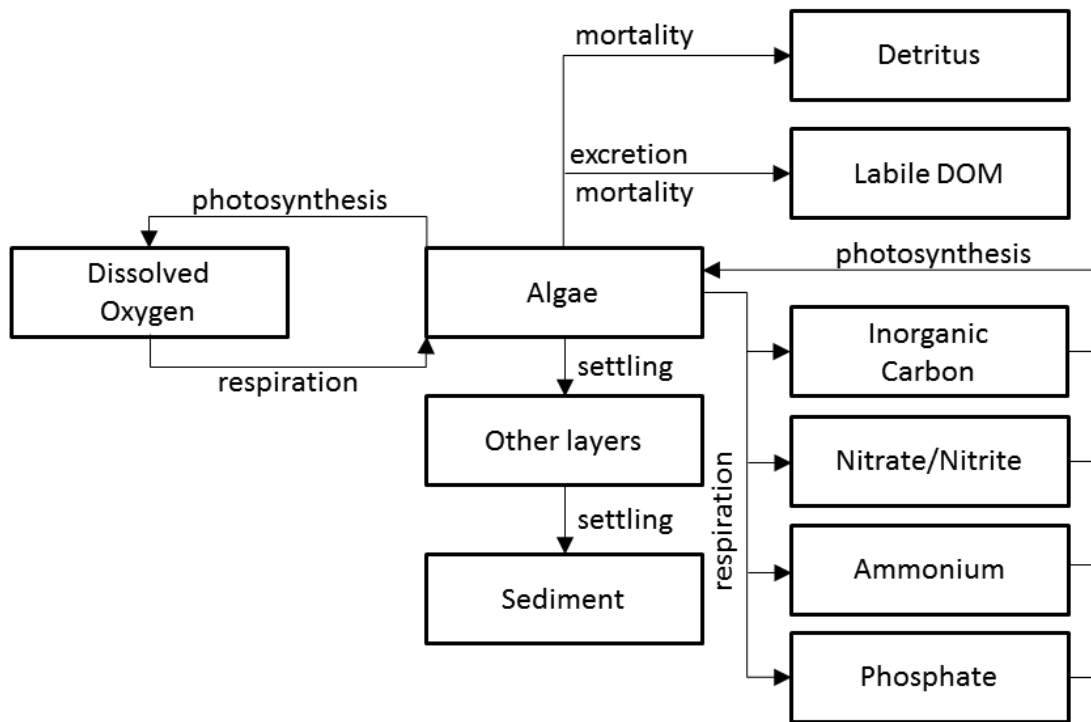


Figure 2.9 Conceptual algal model component of the CE-QUAL-W2/QUAL2K model (Cole and Buchak, 1995)

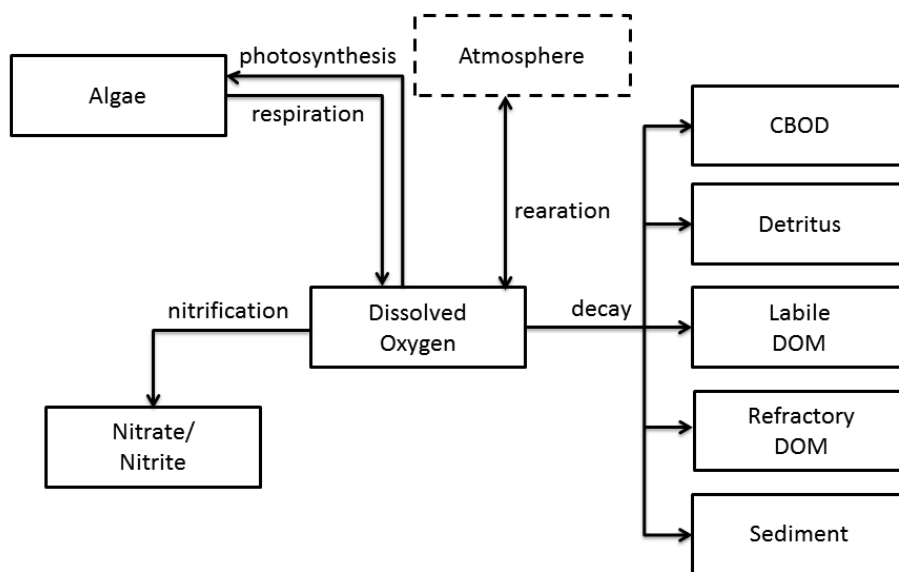


Figure 2.10 Conceptual dissolved oxygen model component of the CE-QUAL-W2/QUAL2K model (Cole and Buchak, 1995)

#### **2.4.5. Reservoir processes**

A number of processes occur within a reservoir that may influence water quality. Slaughter and Hughes (2013b) list some of these processes as:

- 1) stratification;
- 2) changing surface area and depth;
- 3) increased residence time;
- 4) eutrophication and algal blooms and;
- 5) sediment uptake and release of pollutants.

Stratification occurs when temperature differences occur at varying depths, creating water quality boundaries for water quality constituents such as oxygen and salinity, commonly referred to as a reservoir's temperature profile (Palma *et al.*, 2014). Palma *et al.* (2014), found that the temperature profile in the Alqueva Reservoir in southern Portugal varied seasonally, with well- defined stratification during the dry season and complete mixing in the wet season, attributed to cold temperatures and strong winds (Palma *et al.*, 2014). In South Africa stratification has been recorded in a number of large reservoirs (namely: Roodepoort, Laing, Berg River etc.) and successfully simulated with CE-QUAL-W2 and DYRESM. The CE-QUAL-W2 model uses a combination of topographic maps, sediment range surveys and volume-area-elevation tables to generate bathymetric cross-sections for the water body being investigated (Cole and Buchak, 1995). A computational grid is constructed, and initial conditions are specified (start time, temperatures and concentrations etc.)(Cole and Buchak, 1995). This allows the model to simulate water quality in two dimensions and account for stratification. Simulating stratification in reservoirs is complex and requires bathymetry data and complex grid model setups (Cole and Buchak, 1995; Slaughter and Hughes, 2013b). In South Africa, the data required to calibrate and assess simulations of stratification are not included within routine monitoring water quality data sets, therefore, additional sampling would be required.

#### **2.5. Typical modelling procedure**

When selecting a water quality model for management, it should be appropriate to the complexity of the situation, and a number of questions need to be addressed before selecting a model (Loucks and Beek, 2005):

1. how much historical data are available;



2. is the model flexible enough to allow updates and improvements;
3. do stakeholders accept the model proposed and;
4. is the cost of maintaining and updating the model acceptable?

Once a model has been selected on the basis of meeting a set of criteria, the next step is to plan the implementation of the model. This includes identifying all inputs required, the time periods to be simulated and the expected quality of the results (Loucks and Beek, 2005).

Data collection (Figure 2.11) may consist of gathering all historical monitoring data or field sampling. While the Department of Water Affairs and Sanitation (DWS) have historical data sets of water quality, they are often limited both spatially and temporally, as well as in the range of water quality constituents tested (Slaughter, 2011a). The DWS historical records for flow are relatively complete compared to that of water quality however, flow is usually only measured for the larger rivers in South Africa. Other data required for water quality modelling include Geographical Information Systems (GIS) based products such as land use, soil, geology, topography and climate, all of which are used for understanding the system, assigning parameter values and calculating values such as reach lengths.

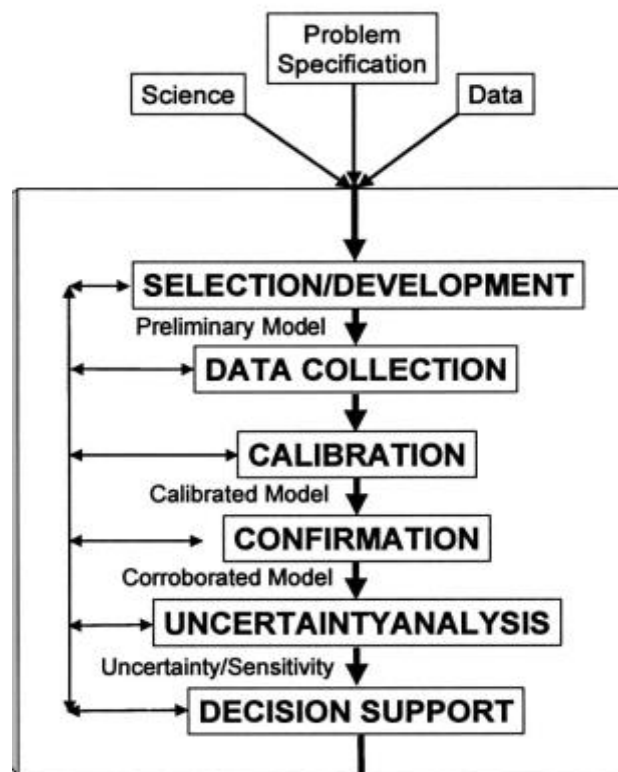


Figure 2. 11 Modelling procedure conceptualisation (taken from Chapra, 2003)

A rigorous formal calibration procedure (Figure 2.12) is vital to the usefulness of a model's result (Janssen and Heuberger, 1995). The difficulties associated with model calibration depend on the nature of the model and the purpose for which it is being used. Models that simulate water quality (or any other environmental variable) reduce complex environmental processes to sets of mathematical equations (Beven, 1989; Hill, 1998). Typically, process rates are represented by model parameter values (e.g. rate of decay). Beven and Binley (1992) point out that when calibrating a model, there will always be some degree of error associated with the observed data or the lack of understanding of physical processes. Therefore, no model calibration can be seen as a true representation of the physical processes. In most cases, parameter value sets represent simple, conceptual or complex physical processes that often cannot be measured and are therefore, calibrated against observed data representing the collective outcome of a number of processes. As a result, the calibration process comprises assigning numerical values to the various parameters to allow the model to produce outputs that represents observed data as closely as possible. While the model calibration can be guided by visual goodness of fit, a more rigorous approach is to use goodness of fit statistics, such as the Nash-Sutcliffe efficiency (Nash and Sutcliffe, 1970).

The methods used to assign these numerical values range quite drastically, but are all based on the same principal. This is described best by Janssen and Heuberger (1995): “the approach for model calibration is guided by the intended model use, which is supported by adequate techniques, prior knowledge and expert judgement”. However, as previously mentioned in Chapter 1, one of the major challenges to modelling in South Africa is access to reliable and consistent observed data with which to calibrate models at a catchment scale. In addition to the data constraints, the success of calibrating a model at any scale can be hindered by the availability of time and computer power, adequate expertise and financial resources (Janssen and Heuberger, 1995). In the context of situations with limited monitoring data for both flow and water quality, the calibration should be based on both empirical data and expert knowledge of catchment processes that influence in-stream water quality. While there may be no observed data related to certain parameters, previous studies can be used to constrain parameters that are not commonly measured. Examples of these are the rates, constants and kinetic values reviewed by Bowie *et al.* (1985). Using these parameter value ranges as a guide would reduce the risk of equifinality during the calibration procedure.

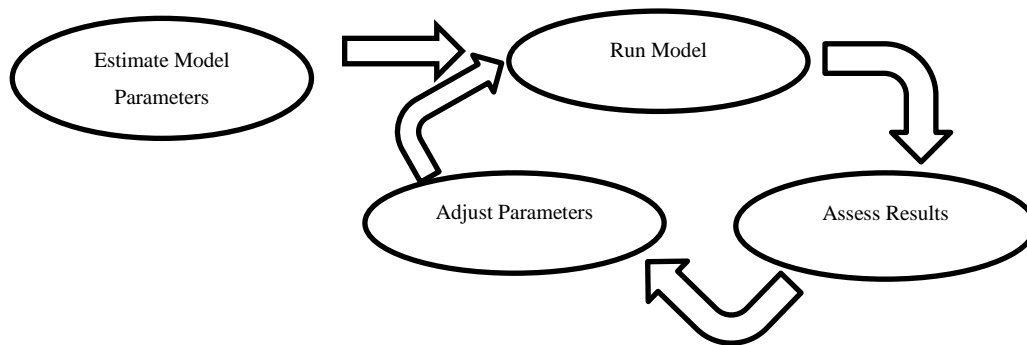


Figure 2.12 Flow diagram representing a simple model calibration process

## 2.6. Water quality situation in the CRC

Water quality in the CRC is influenced by natural phenomena (climate and geology) as well as a result of a number of anthropogenic activities. The latter include discharge of waste water effluent, agricultural return flows (especially during low flow conditions) from farmland used for intensively irrigated sugar cane and subtropical fruits and pollutant inputs from urban areas and old gold mining activities (DWAF, 2003b; DWAF, 2008; DWAF, 2009; DWAF, 2010). One major driver of water pollution is industrial and domestic waste water disposal (Deksissa *et al.*, 2004), with some 30 sewage treatment works discharging effluent directly into the middle reaches of the Crocodile River and its tributaries. According to Deksissa *et al.* (2004), this has had significant influence on the downstream reaches of the Crocodile River, leading to serious water quality issues.

### 2.6.1. Variables of concern

According to the DWS (DWAF, 2010; DWA, 2011), the water quality in the upper CRC is relatively good. However, quality deteriorates in the lower regions of the catchment below the Kaap River confluence with the Crocodile River and its tributaries, showing unacceptable salt values (electrical conductivity), turbidity, pH, nitrates, ammonia, phosphates and the presence of heavy metals. In the slower flowing reaches of the CRC, water hyacinth (*Eichhornia crassipes*) and algae populations have established and are spreading rapidly, taking advantage of the escalating anthropogenically induced nutrient levels in the water, resulting in increased pH levels of surface waters (DWA, 2011).

## **Chapter 3: Description and water quality analysis of the Crocodile River Catchment**

### **3.1. Location**

The CRC is located in the Mpumalanga Province (Figure 3.1) of South Africa, occupying 1.2% of the country's land surface area (Deksissa *et al.*, 2004), and is part of the Inkomati Water Management Area (WMA). The Crocodile River is  $\pm 320$  km in length and flows west to east across the centre of the catchment draining some 35 quaternary catchments and an area of  $\sim 10\,440$  km<sup>2</sup> (Deksissa *et al.*, 2004). The Crocodile River crosses the border with Mozambique at Komatipoort, and finally drains into the Indian Ocean via the Inkomati River.

### **3.2. Geology, soils and topography**

#### **3.2.1. Geology**

The underlying geology of the catchment inherently determines the geomorphology and soils which in turn influence the water quality constituent concentrations (natural background concentrations) found in water bodies. The western upper reaches of the CRC are underlain predominantly by sedimentary rocks belonging to the Transvaal Super Group which includes the Pretoria Group (Figure 3.2). This area's lithology is dominated by shale, andesite, arenite, quartzite and hornfels, with the majority being laid down from the start of the Cambrian period ( $< 541$  MYA) and onwards (Figure 3.3, and 3.4). The remaining areas of the catchment are predominantly underlain by rocks formed in the Pre-Cambrian ( $> 541$  MYA) period, with the lithology comprising of less weatherable: lutaceous arenite, arenite, dolomite, gneiss and granite (Figure 3.4; Table 3.1). The outlet of the catchment is underlain by sedimentary rock formations of the Lebombo Group belonging to the Karoo Super Group, comprising arenite, rhyolite and basalt.

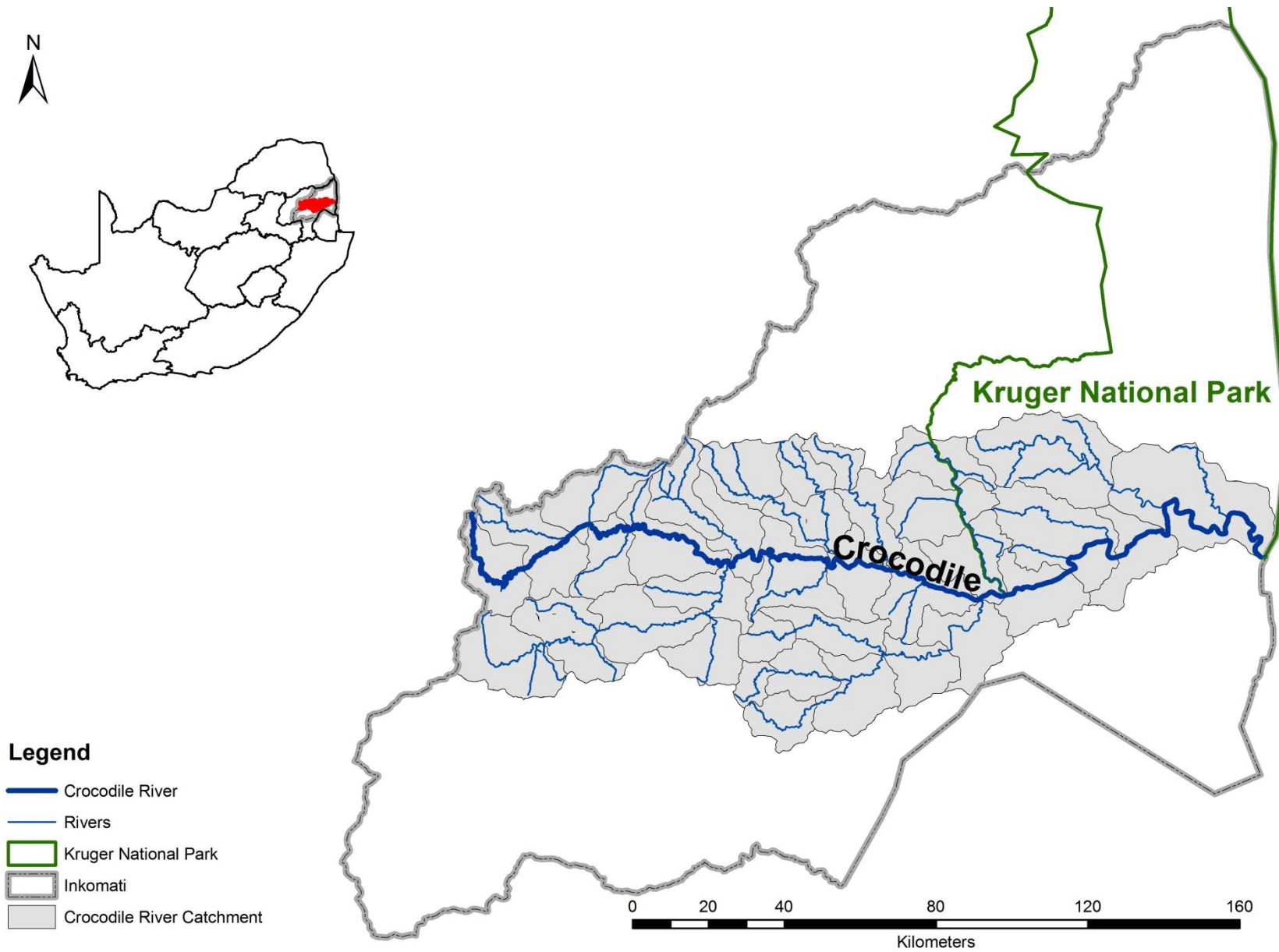


Figure 3.1 Map of the Crocodile River Catchment in relation to the Inkomati Management Area and South Africa

Table 3. 1 Age of lithology in the Crocodile River Catchment

<b>Pre Cambrian (&gt;541 MYA)</b>	<b>&lt;541 MYA</b>
<b>Dolomite</b>	<b>Rhyolite</b>
<b>Granite</b>	<b>Basalt</b>
<b>Quartzite</b>	<b>Shale</b>
<b>Andesite</b>	<b>Sedimentary</b>
<b>Hornfels</b>	<b>Dolerite</b>
<b>Gneiss</b>	<b>Arenite</b>
<b>Lutaceous Arenite</b>	<b>Gabbro</b>
<b>Granodiorite</b>	<b>Ultramafic Rocks</b>
<b>Lava</b>	

### 3.2.2. Soils

The three dominant soil types found in the CRC are Orthic Acrisols (Ao) in the western high-lying areas, Rhodic Ferralsols (Fr) on the northern and southern high-lying areas and Chromic Luvisols (Lc) in the low lying areas (Figure 3.5). Orthic Acrisols (Ao) soils are acidic clay accumulations with low cation exchange capacities (Table 3.2). These are inherently infertile soils and can rapidly become chemically and organically degraded when utilised (Soil Map of the World edition, 1974; Fey, 2010). Rhodic Ferralsols (Fr) soils are red in colour due to high levels of iron. These soils have limited nutrient holding capacities due to low cation exchange capacities and are acidic (Fey, 2010). Rhodic Ferralsols (Fr) soils are impacted greatly by erosion, easily losing their topsoil organic matter. Chromic Luvisols (Lc) soils are one of the preferred soils for cultivation, containing clays with high cation exchange capacities, thereby concentrating nutrients in the topsoil (Fey, 2010). Chromic Luvisols (Lc) soils have low levels of organic matter and have a moderate resilience to degradation (Fey, 2010).



## Legend

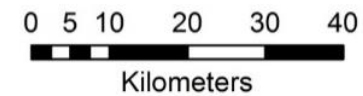


Figure 3.2 Geology of the Crocodile River Catchment

Chapter 3: Description and water quality analysis of the Crocodile River Catchment

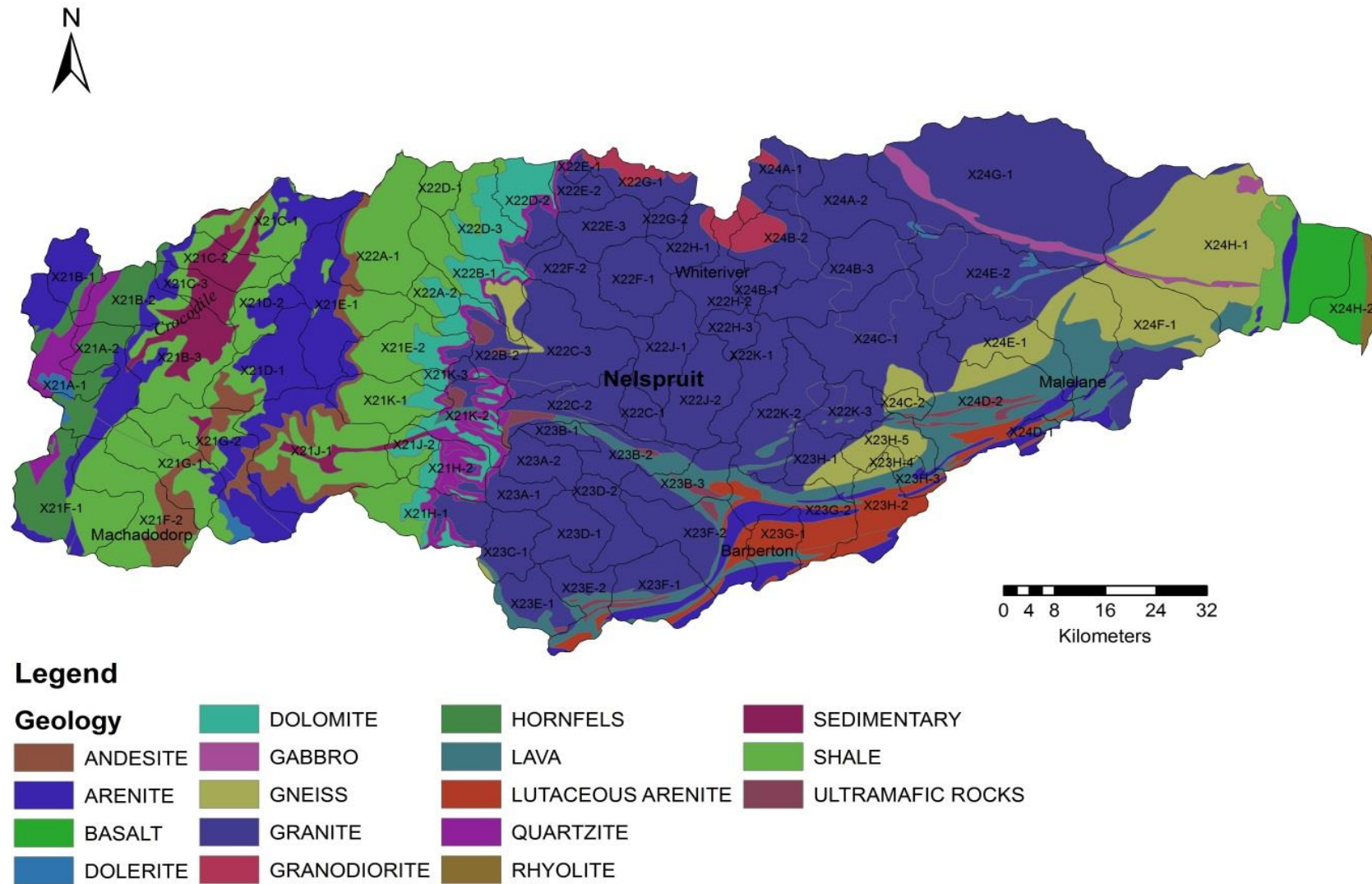


Figure 3.3 Dominant lithology of the Crocodile River Catchment



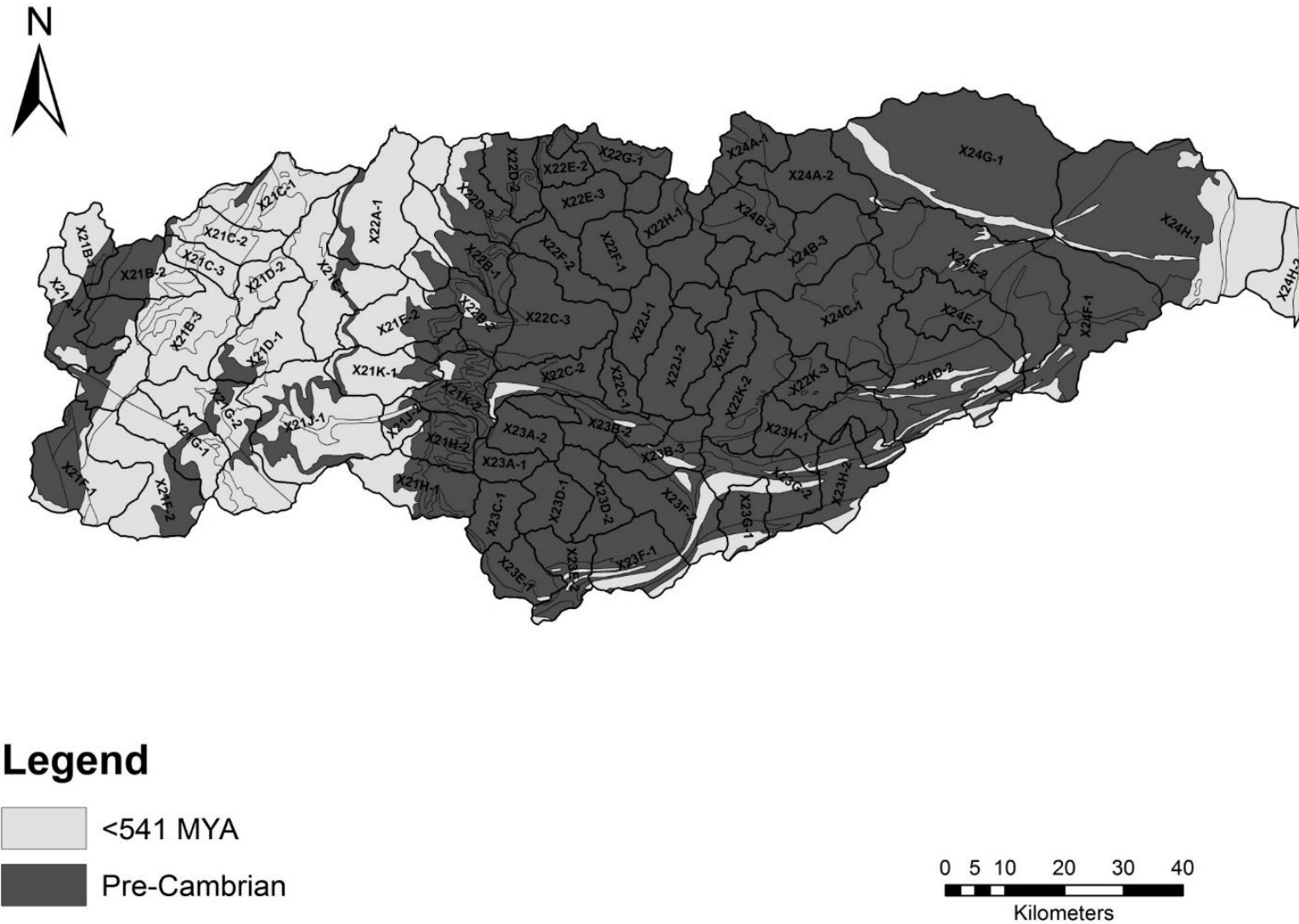


Figure 3.4 Separation of dominant lithology according to age of formation

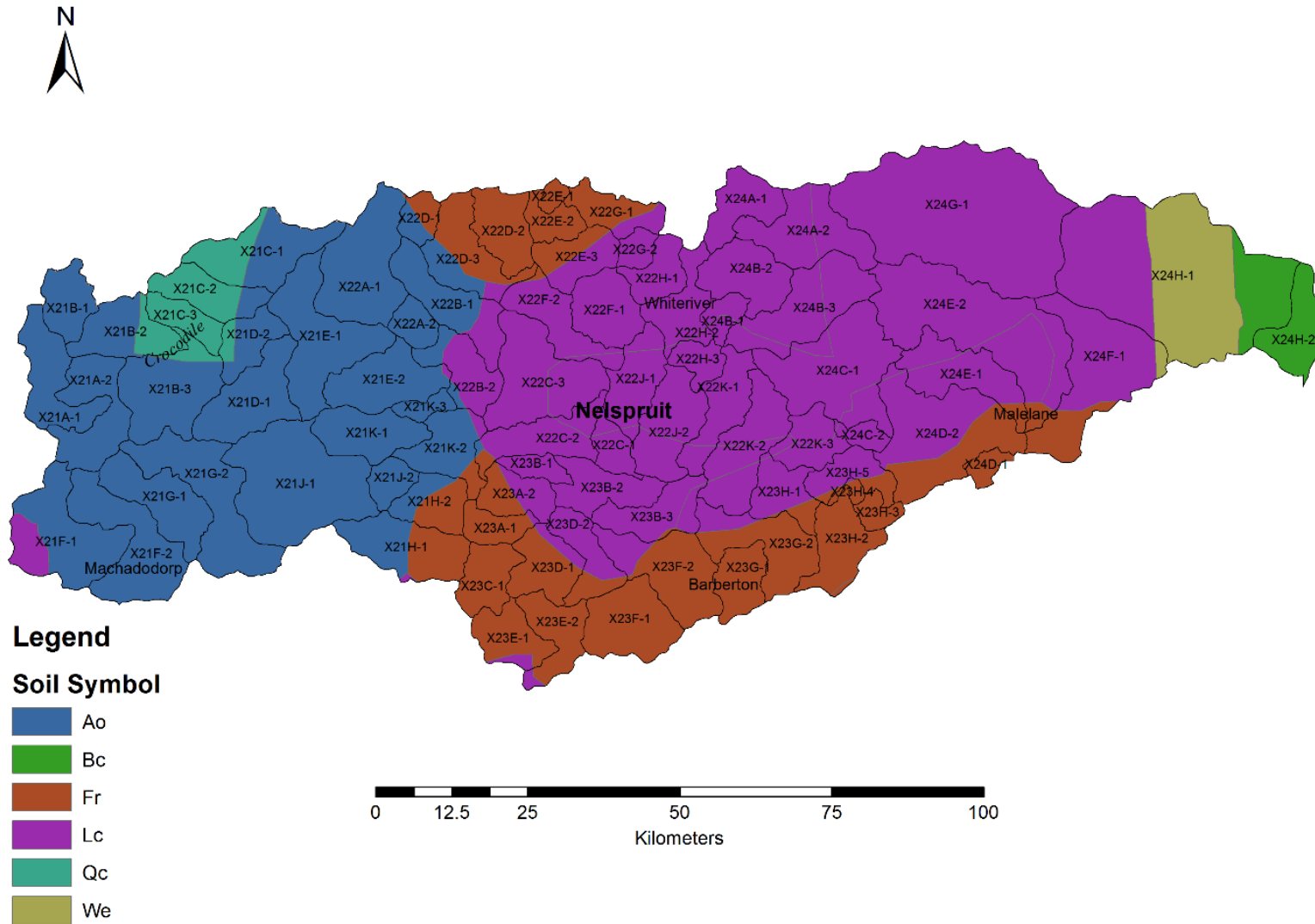


Figure 3.5 Map of soil types found in the CRC

Chapter 3: Description and water quality analysis of the Crocodile River Catchment

Table 3.2 Index for soil symbols represented in Figure 3.5 (based on descriptions from the Soil Map of the World, 1974)

<b>SYMBOL</b>	<b>SOIL TYPE</b>	<b>COMMENT</b>	<b>CEC TOPSOIL</b>	<b>CEC SUBSOIL</b>
<b>AO</b>	Orthic Acrisols	Acidic soils with a layer of clay accumulation. This class consists only of clays with low cation exchange capacity.	7.6	7.5
<b>BC</b>	Chromic Cambisols	Soils with slight profile development that is not dark in colour.	15.7	18.9
<b>FR</b>	Rhodic Ferralsols	Highly weathered soils rich in sesquioxide clays and with low cation exchange capacities.	8.6	4.9
<b>LC</b>	Chromic Luvisols	Soils with strong accumulation of clay in the B-horizon and not dark in colour. These soils have clays with high cation exchange capacity.	13.1	14.7
<b>QC</b>	Cambic Arenosols	Soils with a strongly bleached layer and a layer of iron or aluminium cemented organic matter.	3.5	3
<b>WE</b>	Eutric Planosols	Soils with a light coloured layer over a soil layer that restricts water drainage.	8.4	14

### 3.2.3. Topography/Drainage

The CRC is located within the eastern escarpment of southern Africa, characteristic of rivers draining steep escarpment slopes, then flowing across more gently sloping lowveld terrain (Figure 3.6). The topography and drainage characteristics of the CRC influence residence time of water quality constituents.

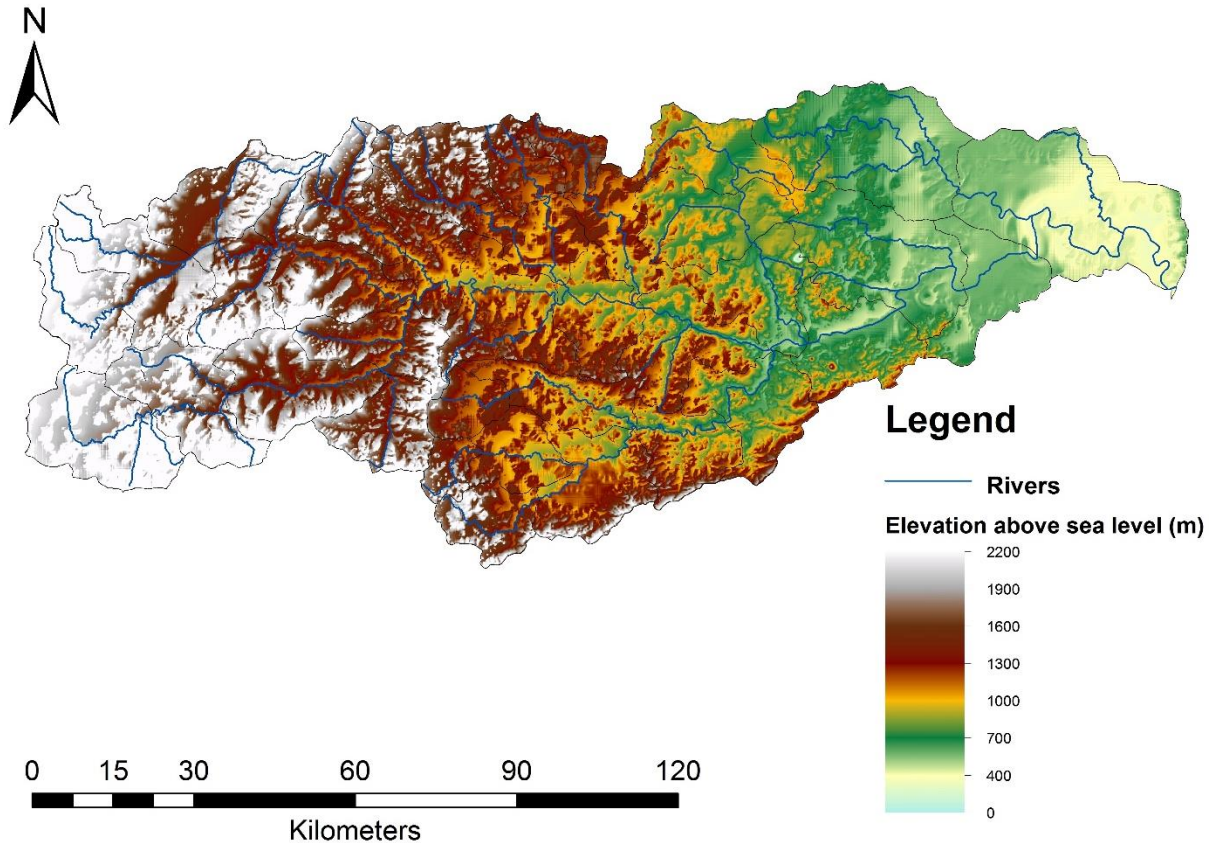


Figure 3. 6 Topography and drainage map of the Crocodile River Catchment

### 3.3. Climate

Mean Annual Precipitation (MAP) varies across the catchment, ranging from 1 200 mm in the western regions to 600 mm in the lower eastern parts of the catchment. The overall MAP across the catchment is  $\pm 880$  mm, with the majority of rainfall received during the hot summer months of November–April. The mean annual runoff (MAR) for the entire catchment according to Deksissa *et al.* (2003), is  $1\,446 \times 10^6 \text{ m}^3$ . Mean annual potential evaporation losses for the CRC range from 1 800 to 2 000 mm, which greatly exceeds the MAP for the drier areas of the upper most parts of the catchment and the lower parts (Figure 3.7) (Deksissa *et al.*, 2003). Average annual temperatures differ across the catchment, with the upper catchment being the coldest ( $13.2\text{--}16.1 \text{ C}^\circ$ ) and the lower parts of the catchment being much warmer ( $20.2\text{--}22.7 \text{ C}^\circ$ ) as seen in Figure 3.8.

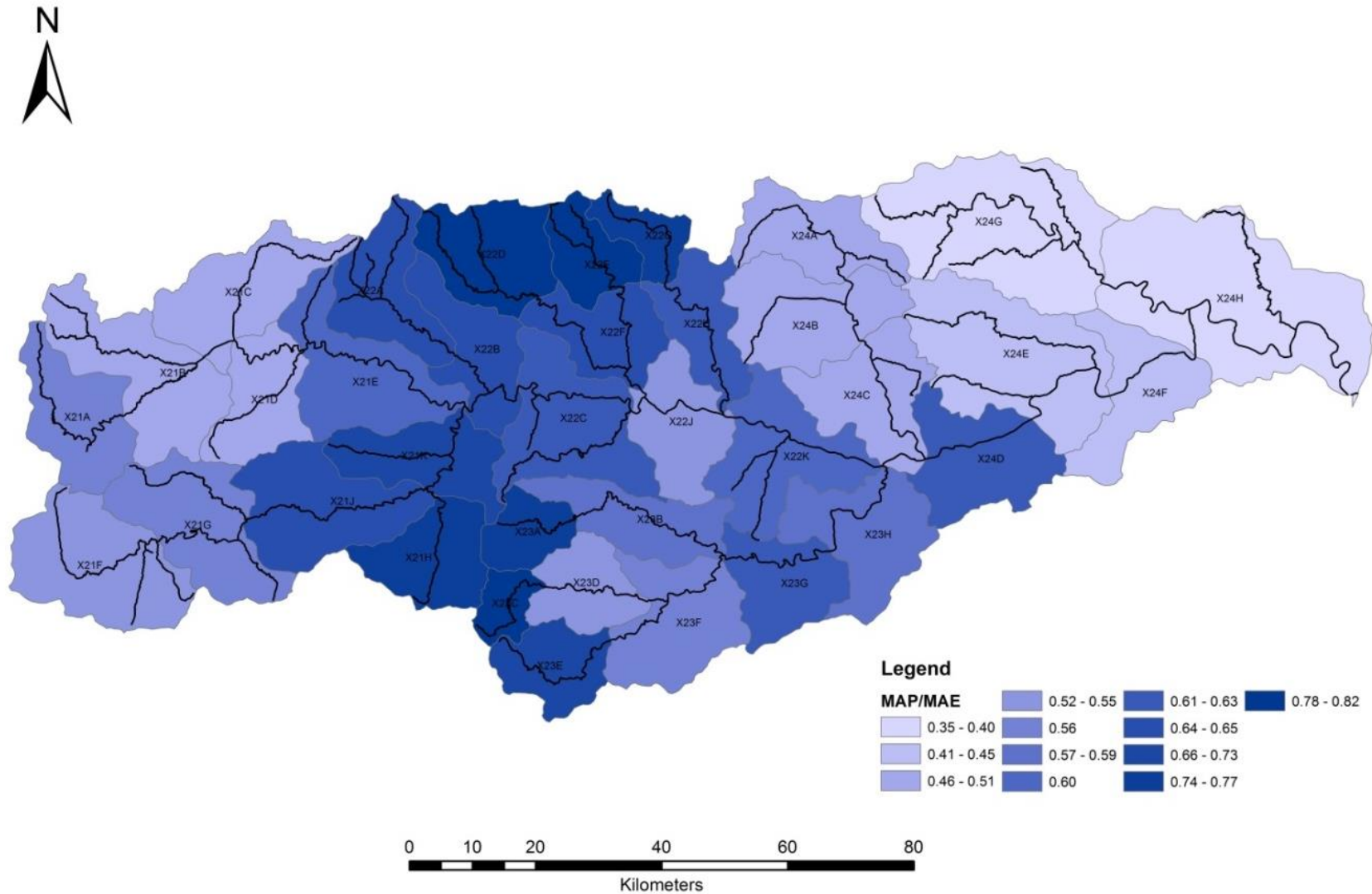


Figure 3.7 Aridity represented as a ratio of Mean Annual Precipitation (MAP) and Mean Annual Evaporation (MAE)

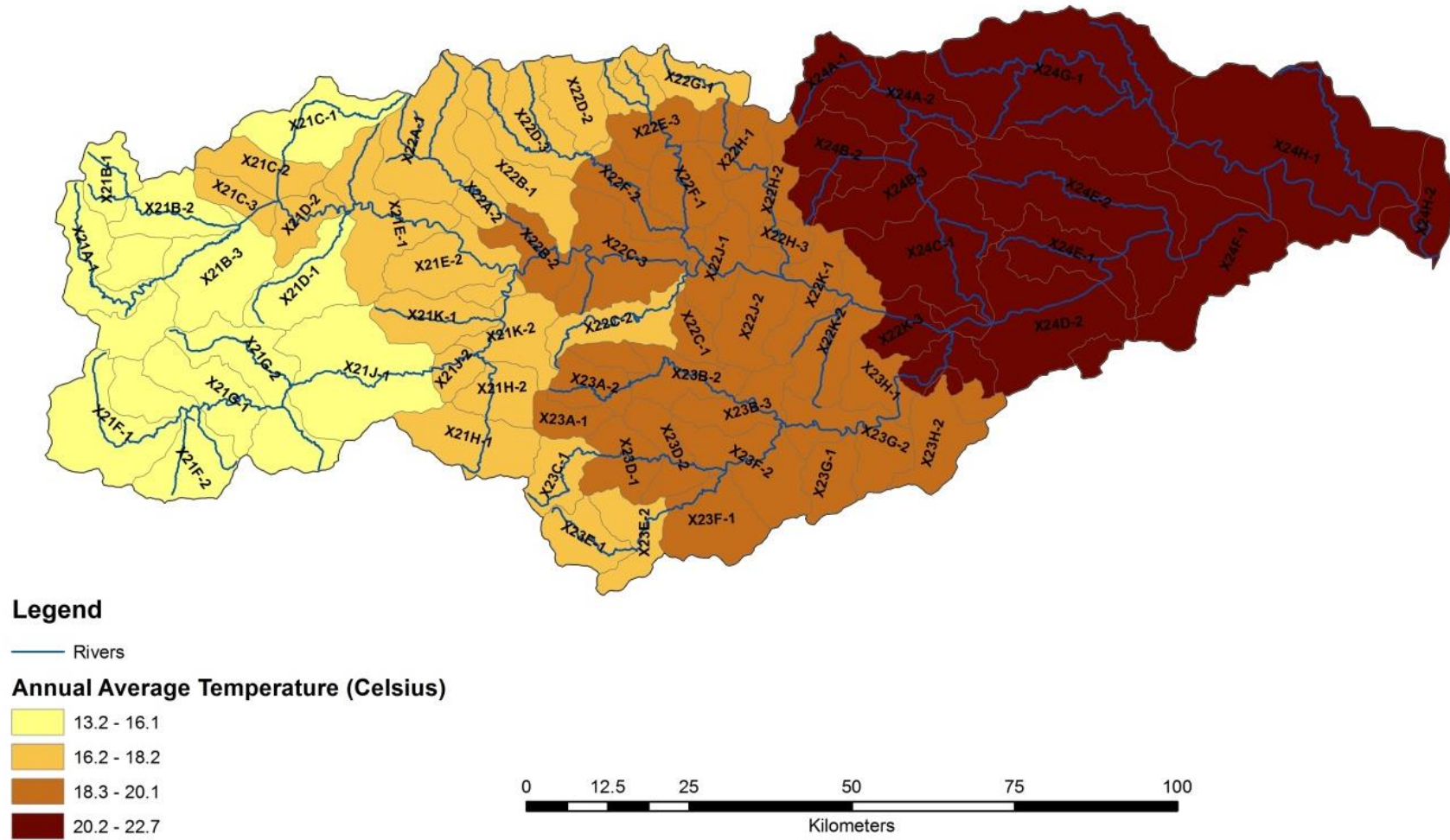


Figure 3.8 Annual average air temperature (C°)

### 3.4. Vegetation

There are three biomes present within the catchment, namely forests, grasslands and savannah (Figure 3.9) with savannah being the predominant catchment biome. These biomes support Lydenburg Montane Grassland in the western regions, Legogote Sour Bushveld in the mid region and the Granite Lowveld in the eastern regions.

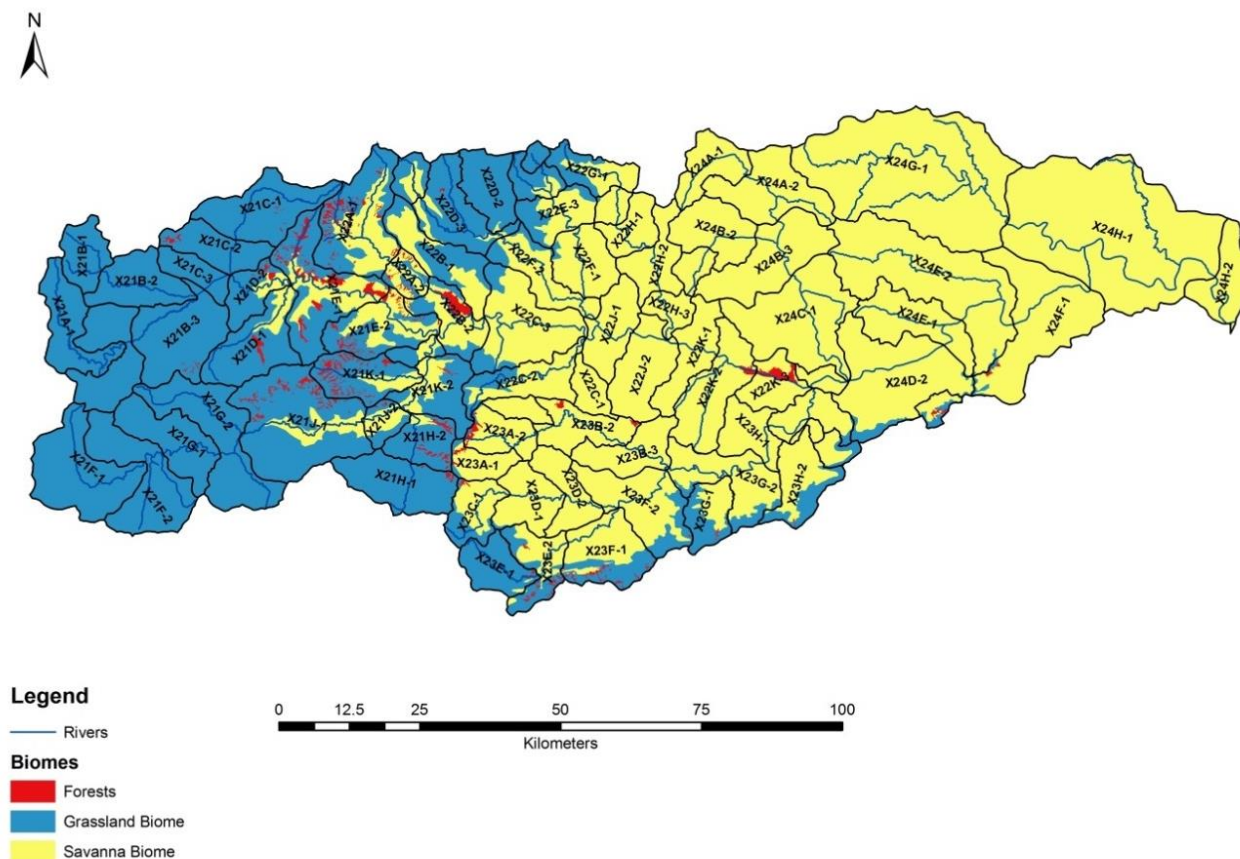


Figure 3.9 Biomes present in the Crocodile River Catchment

### 3.5. Land Use

Agricultural activities within the CRC range from forestry, wheat and maize farming in the western regions to cattle, game farming and sugar cane cultivation in the eastern regions (Figure 3.10). The CRC supports South Africa’s largest irrigation area ( $\pm 42\,300$  ha, DWAF, 2004), with farmers and industries abstracting large quantities of water to support water intensive crop species and industrial applications (Roux *et al.*, 1994). Water flow is further decreased by extensive afforestation (19% of the catchment, Figure 3.10), and a low precipitation to evaporation ratio, leading to significant decreases in flow in the Crocodile River and the lower tributaries during the winter months (Figure 3.7). Apart from the

agricultural economic importance, the Crocodile River also forms the southern boundary of the internationally renowned Kruger National Park (KNP) (Figure 3.10).

### **3.6. Demographics**

The CRC encompasses one moderately large city, Nelspruit, situated in the centre of the catchment, with a few towns and many rural settlements distributed across the catchment (Figure 3.11). The majority of the urban and rural populations are situated within close proximity of the Crocodile River or its major tributaries. The population for the CRC in 2003 according to the DWAF (2003a) report was estimated at 479 700 people, with just over 76% residing in urban areas (Deksissa *et al.*, 2004). The catchment falls within the boundaries of three district municipalities, and is further sub-divided into six local municipalities with the largest being Mbombela.

### **3.7. Analysis of Water Quality in the CRC**

In Chapter 2, the relationships between flow and water quality were described, showing how flow has a major influence on the concentration and residence time of water quality constituents in a catchment. Therefore, in this section, water quality and flow data are analysed together in the form of water quality loads. This provides an indication of source loading as well as dilution capacity of major reaches of the CRC and helps to identify flow conditions in which water quality guideline indicators are exceeded.

Water quality and flow data for six DWS stations were downloaded from the Resource Quality Services website (<http://www.dwaf.gov.za/iwqs/>, accessed 25 July 2013). The stations were selected based on their positioning within the catchment, so that the selected stations give a spatially representative overview of the water quality status of the catchment. Only stations containing both flow and greater than 50 samples of water quality data for analyses were selected (see Figure 3.13). The water quality concentrations for total dissolved solids (TDS), orthophosphates (PO<sub>4</sub>-P), ammonium (NH<sub>4</sub>-N) and nitrates + nitrites (NO<sub>3</sub>-N + NO<sub>2</sub>-N) were used in conjunction with daily flow data to create load duration curves (LDCs) seen in Figures 3.14–3.19. LDCs are a method of representing observed loads as frequency of exceedance distributions, and are based on ranking loads according to observed flow rates.



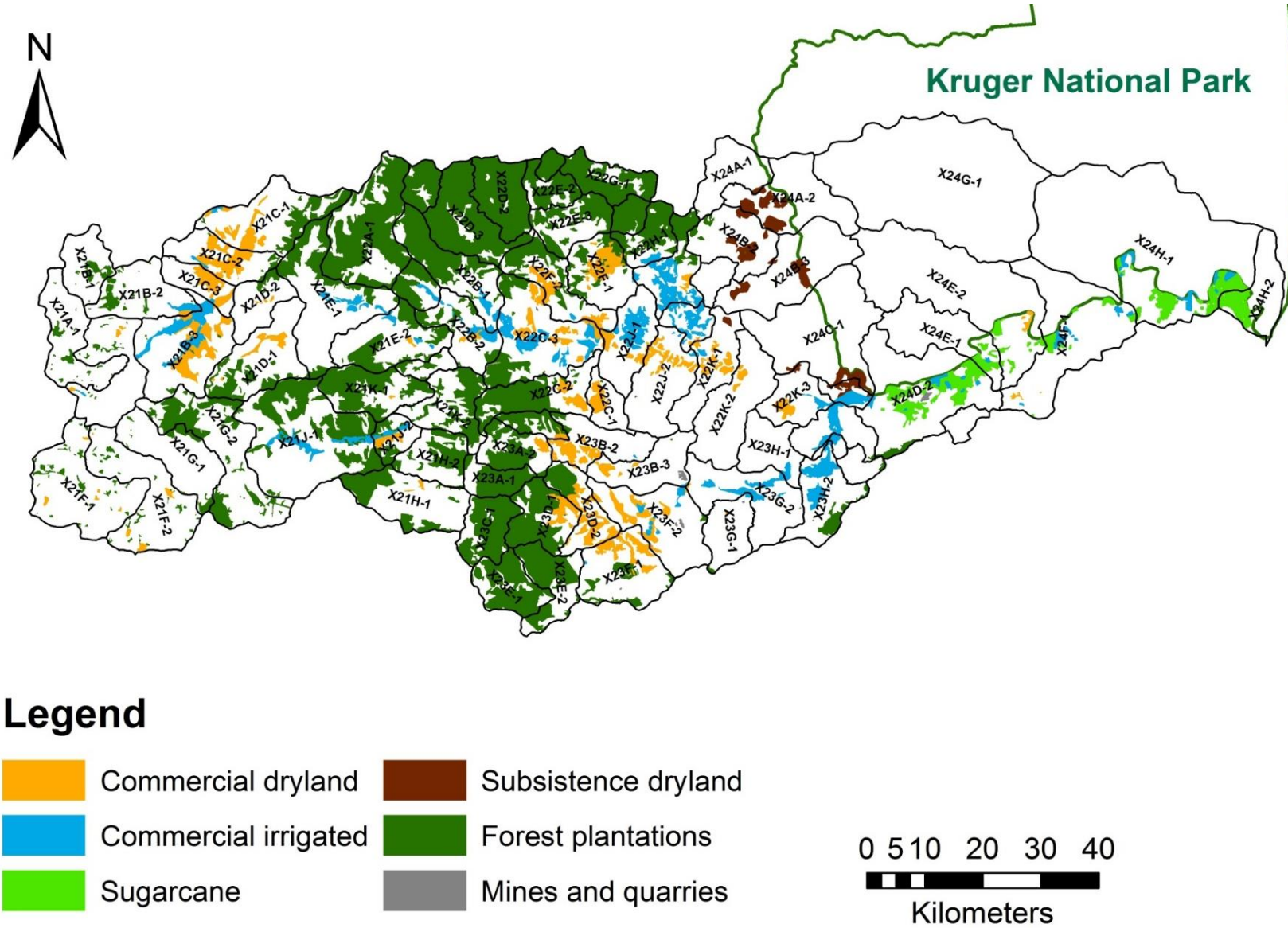


Figure 3.10 Anthropogenic land use in the Crocodile River Catchment

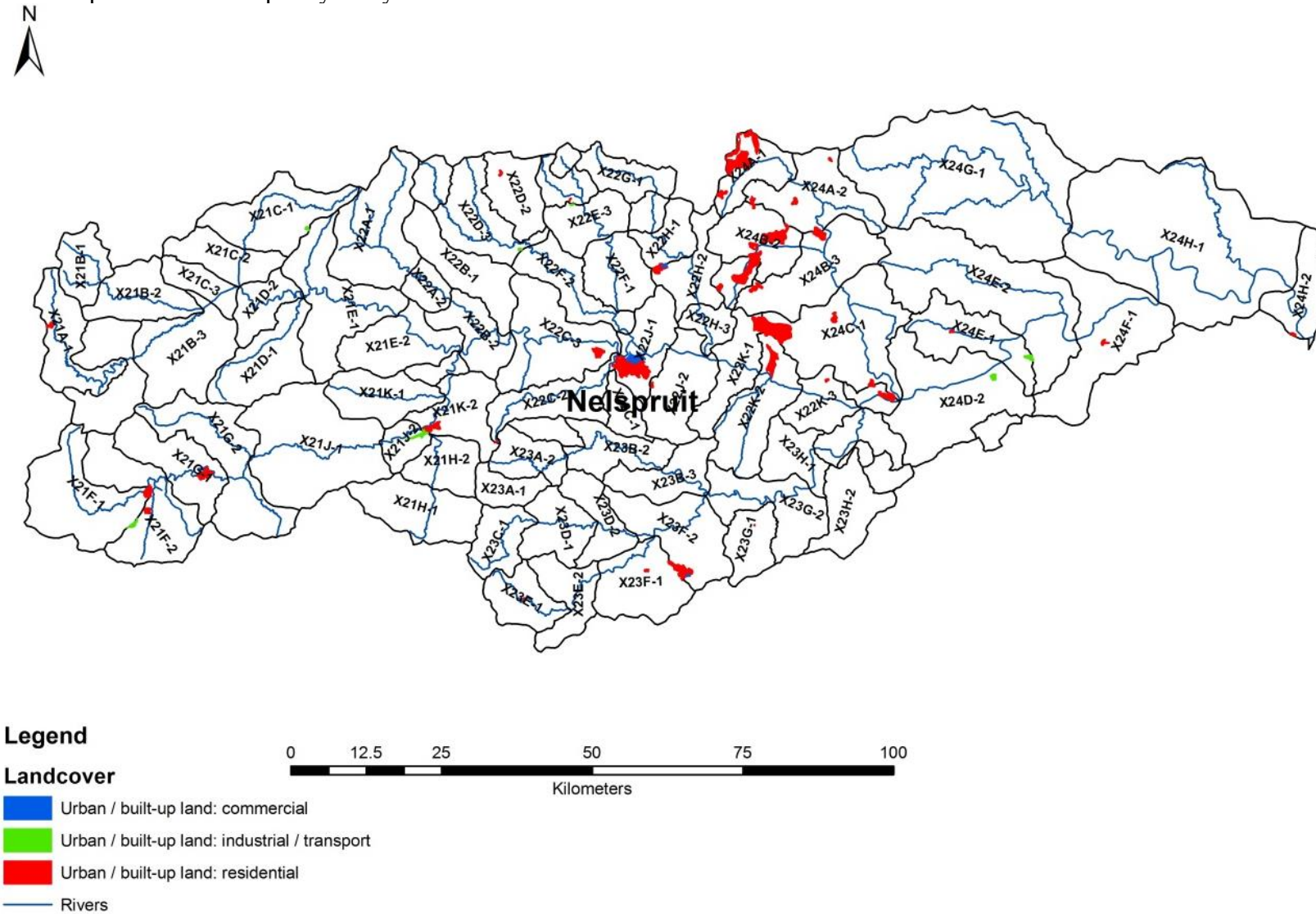


Figure 3.11 Map showing the urban areas of the Crocodile River Catchment

LDCs are useful tools for analysing the spatial variability of water quality across the catchment and represent the flow conditions in which the water quality sample was taken. The flow component inherently provides a seasonality signature to the water quality observations, and in addition, can help identify the type of source loading to the system (diffuse or point source). Using LDCs, a guideline water quality concentration (related to human use or ecological requirements) can be expressed as threshold loads (mass) across the entire flow frequency distribution. In this way, LDCs allow the link to be made between a threshold water quality concentration and the load at different flow rates (and therefore different dilution capacities) before the threshold concentration is exceeded. Bonta and Cleland (2003) suggest that LDCs can be used as a water resource management tool in the TMDL allocation process, as LDCs provide an indication of the load a polluter can release to a river, taking into account variable dilution capacities of the river at different flow rates. The water quality thresholds are defined by the generic Resource Water Quality Objectives (RWQO) at a national level for South Africa (DWA, 2011) (see Appendix A, Table A1).

The national RWQOs were used in this analysis and may not be applicable to the CRC. However, the RWQOs specific to the CRC were still being determined at the time of the study. However, LDCs are still helpful regardless of whether the water quality targets are applicable, as they help to give an overview of pollutant dilution capacities of rivers and possible sources of pollutant loading to the river.

The dominant water quality constituents analysed that are of concern are orthophosphates and ammonium, which appear to exceed the tolerable thresholds at all monitoring points (see Tables 3.5 and 3.6). The LDCs indicate that the pollutant loading sources for these nutrients are both point and diffuse in nature, as observed loads exceed the tolerable range in all flow conditions (as shown in Figures 3.17B and D). One major driver of point source water pollution in the CRC is industrial and domestic waste water disposal (Deksissa *et al.*, 2004), with many sewage treatment works discharging effluent directly into the middle reaches of the Crocodile River and its tributaries. Diffuse contribution of ammonium and orthophosphates may be attributed to surface runoff from agriculture and urban areas.

While TDS loads never exceeded the tolerable range except for gauge X2H017 (see Table 3.3), there is a notable change in TDS loads when moving from the upper reach of the Crocodile River towards the lower reaches. The two major tributaries influencing the TDS loads in the Crocodile River are the Elands and Kaap River reaches (see Table 3.3). The LDCs indicate that major sources of TDS in the CRC are point source dominated, exceeding

thresholds in lower flow conditions, which may be attributed to the extensive mining and industrial activities that occur across the catchment. Higher TDS at lower flows may also be due to lower dilution capacity, dominance of more saline ground water and evaporation.

The main sources of nitrates and nitrites in the CRC are from WWTWs and agricultural runoff. Although nitrates and nitrites do not exceed the RWQOs (see Table 3.4), they play a critical role in water quality.

Malan and Day (2005) investigated DWS water quality guidelines specified for nutrients by analysing water quality for reference sites across South Africa. They found that the Target Water Quality Range (TWQR) of  $0.005 \text{ mg } \ell^{-1}$  for inorganic phosphate was too conservative and that the  $0.5 \text{ mg } \ell^{-1}$  target for Total Inorganic Nitrogen (TIN) to be too lenient (Malan and Day, 2005). Two of the reference sites they used are located within the CRC (gauges X2H010 and X2H014). They used these gauges with two others to determine the 75<sup>th</sup> percentile for TIN ( $0.12 \text{ mg } \ell^{-1}$ ) and Soluble Reactive Phosphorus (SRP) ( $0.018 \text{ mg } \ell^{-1}$ ), and proposed these values as the Recommended Target Concentration (RTC) thresholds. Therefore, to assess the trophic status of the CRC, the RTCs were assessed against observed water quality data for all water quality monitoring sites that are still active and have more than fifty samples (Table 3.7).

The upper Crocodile River at Montrose Falls (gauge X2H013) has a mean TIN concentration of  $0.177 \pm 0.276 \text{ mg } \ell^{-1}$  and SRP mean concentration of  $0.028 \pm 0.08 \text{ mg } \ell^{-1}$ . The RTCs are exceeded 53.2% and 2.5% for TIN and SRP, respectively. The middle Crocodile River (gauge X2H032) has a mean TIN concentration of  $0.742 \pm 0.560 \text{ mg } \ell^{-1}$  and a mean SRP concentration of  $0.060 \pm 0.08 \text{ mg } \ell^{-1}$ . RTCs for TIN and SRP are exceeded 92.5% and 2.5% of the time, respectively. At gauge X2H017, representing the lower Crocodile River, the mean concentrations are  $0.615 \pm 0.428 \text{ mg } \ell^{-1}$  and  $0.028 \pm 0.02 \text{ mg } \ell^{-1}$  for TIN and SRP, respectively, exceeding the RTCs 88.6 and 3.8% of the time. Figure 3.12 shows that SRP and TIN concentrations increase considerably from the upper to the middle catchment, and then decrease slightly from middle to the lower reaches of the CRC. There is extensive sugar cane cultivation (Figure 3.10) in the lower areas of the CRC which may be influencing the retention of nutrients from irrigated water. This area is also a low seasonal rainfall area and therefore may be less prone to transient rainfall-runoff events.

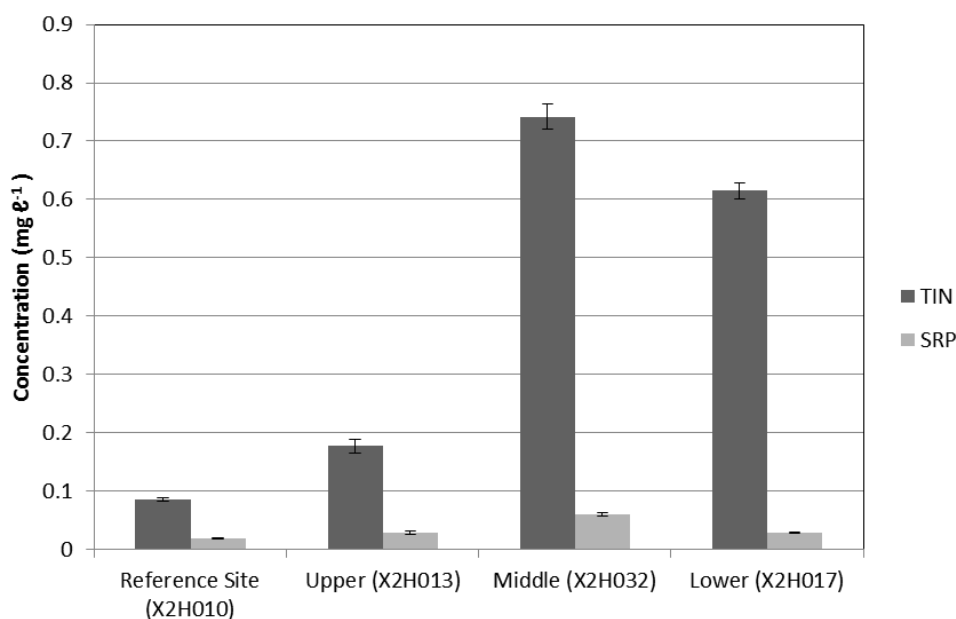


Figure 3.12 Mean concentration with standard error bars showing Total Inorganic Nitrogen (TIN) and Soluble Reactive Phosphorus (SRP) for the reference site and the upper, middle and lower reaches of the Crocodile River

The results of the trophic assessment for the CRC (Table 3.7) indicate that the median TIN concentration is 0.17 mg l<sup>-1</sup> which is greater than the RTC of 0.12 mg l<sup>-1</sup> with observed concentrations exceeding the RTC 65.2% of the time. The SRP median concentration is 0.016 mg l<sup>-1</sup> which is less than the RTC of 0.018 mg l<sup>-1</sup> with observed concentrations exceeding the RTC 2.8% of the time. A summary of the statistical parameters for all monitoring sites considered are given in Appendix A, Tables A2 to A27. While the RTC for TIN is exceeded, SRP concentrations in the CRC fared a lot better. Phosphates play a critical role in limiting eutrophication (Malan and Day, 2005) and therefore, the general trophic status of the CRC is relatively good. However, TIN concentrations should be addressed through management of WWTW discharge and agricultural runoff.

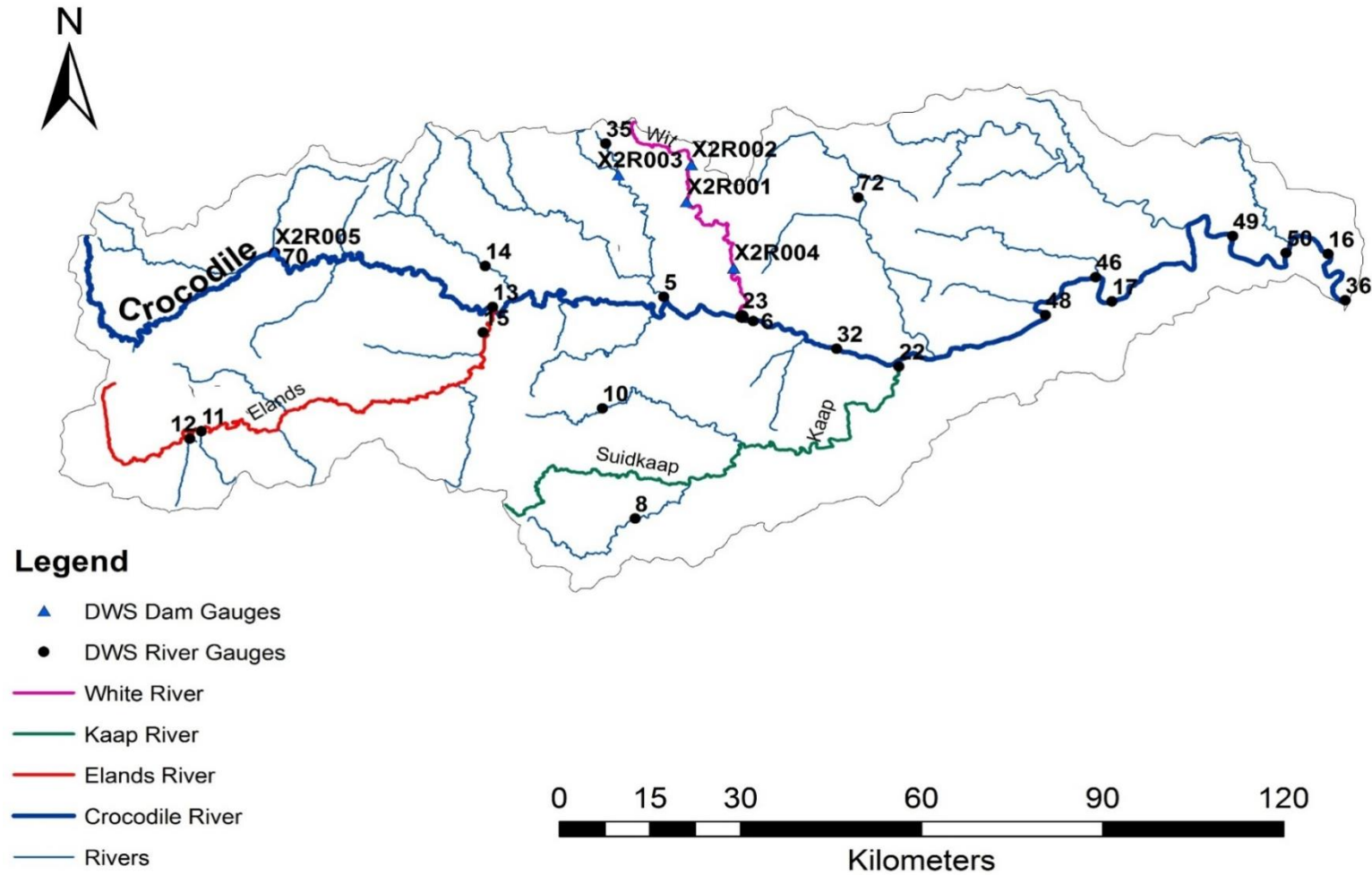


Figure 3.13 Active DWS River and Dam monitoring stations in the CRC. All river stations have been abbreviated to a number that for example 12 represents X2H012

Chapter 3: Description and water quality analysis of the Crocodile River Catchment

Table 3.3 Percentage of observed TDS readings within each National RWQO category

WQ Constituent	TDS			
	Ideal	Acceptable	Tolerable	Unacceptable
DWS Gauge				
X2H013	100.0	0.0	0.0	0.0
X2H015	73.8	20.1	6.1	0.0
X2H023	97.1	2.9	0.0	0.0
X2H032	95.7	3.9	0.3	0.0
X2H022	10.8	45.1	44.1	0.0
X2H017	40.8	54.0	5.1	0.1

Table 3.4 Percentage of observed NO<sub>3</sub>-N + NO<sub>2</sub>-N readings within each National RWQO category

WQ Constituent	NO <sub>3</sub> -N + NO <sub>2</sub> -N			
	Ideal	Acceptable	Tolerable	Unacceptable
DWS Gauge				
X2H013	100.0	0.0	0.0	0.0
X2H015	100.0	0.0	0.0	0.0
X2H023	100.0	0.0	0.0	0.0
X2H032	99.9	0.1	0.0	0.0
X2H022	99.8	0.2	0.0	0.0
X2H017	100.0	0.0	0.0	0.0

Table 3.5 Percentage of observed NH<sub>4</sub>-N readings within each National RWQO category

WQ Constituent	NH <sub>4</sub> -N			
	Ideal	Acceptable	Tolerable	Unacceptable
DWS Gauge				
X2H013	0.3	23.8	17.6	58.2
X2H015	0.0	21.9	11.2	66.9
X2H023	0.0	47.7	12.8	39.4
X2H032	0.1	5.2	2.5	92.1
X2H022	0.0	5.6	2.1	92.3
X2H017	0.1	8.5	4.5	86.9

Table 3.6 Percentage of observed PO<sub>4</sub>-P readings within each National RWQO category

WQ Constituent	PO <sub>4</sub> -P			
	Ideal	Acceptable	Tolerable	Unacceptable
DWS Gauge	11.7	43.5	24.2	20.6
X2H013	10.7	39.2	28.9	21.3
X2H023	28.2	53.4	9.2	9.2
X2H032	4.3	12.3	14.8	68.6
X2H022	6.6	22.9	31.0	39.5
X2H017	8.1	24.7	25.2	42.1



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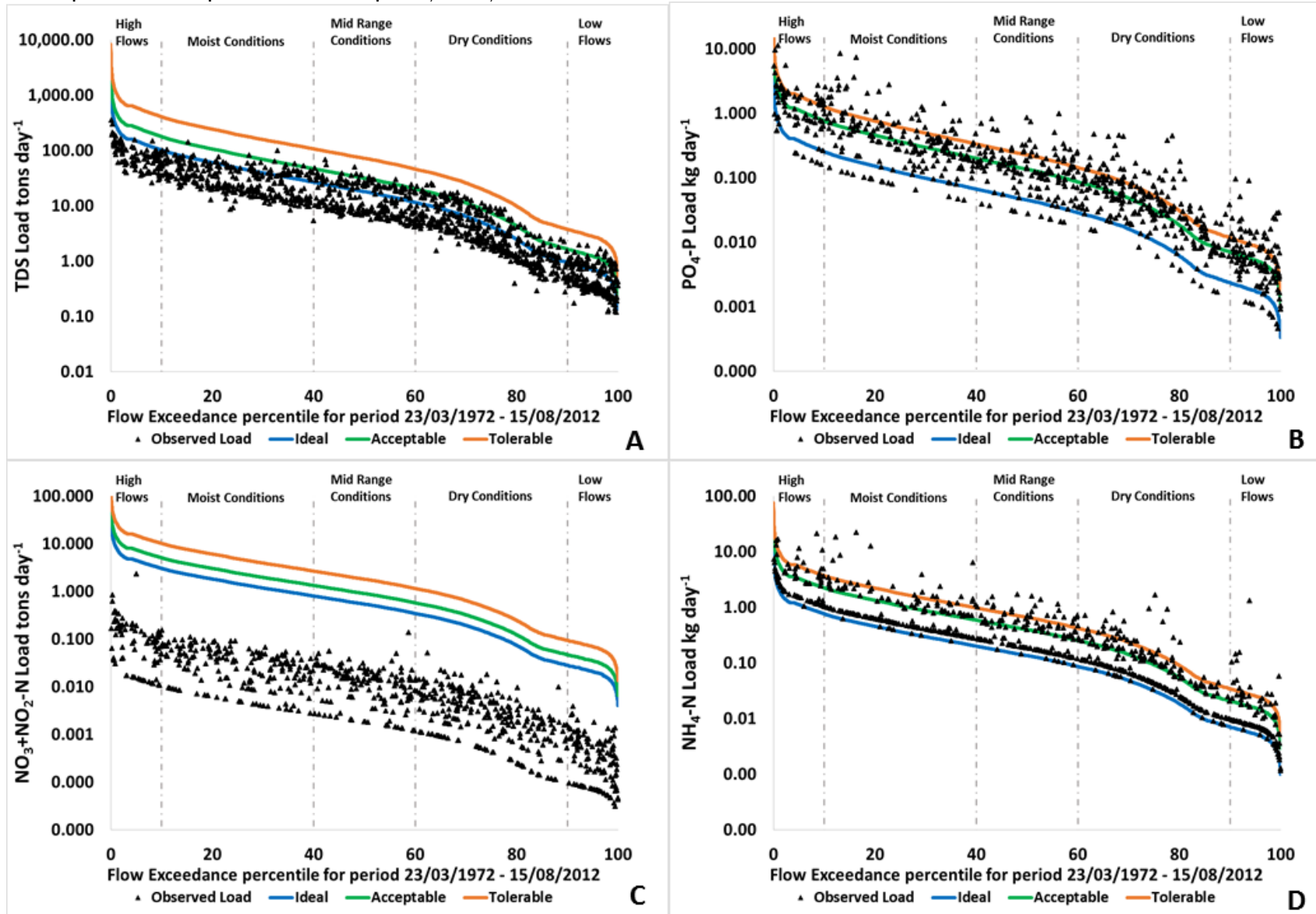


Figure 3.14 Load Duration Curves for gauge X2H015 situated along the Elands River. *A: TDS, B: PO<sub>4</sub>-P, C: NO<sub>3</sub>-N + NO<sub>2</sub>-N, D: NH<sub>4</sub>-N*

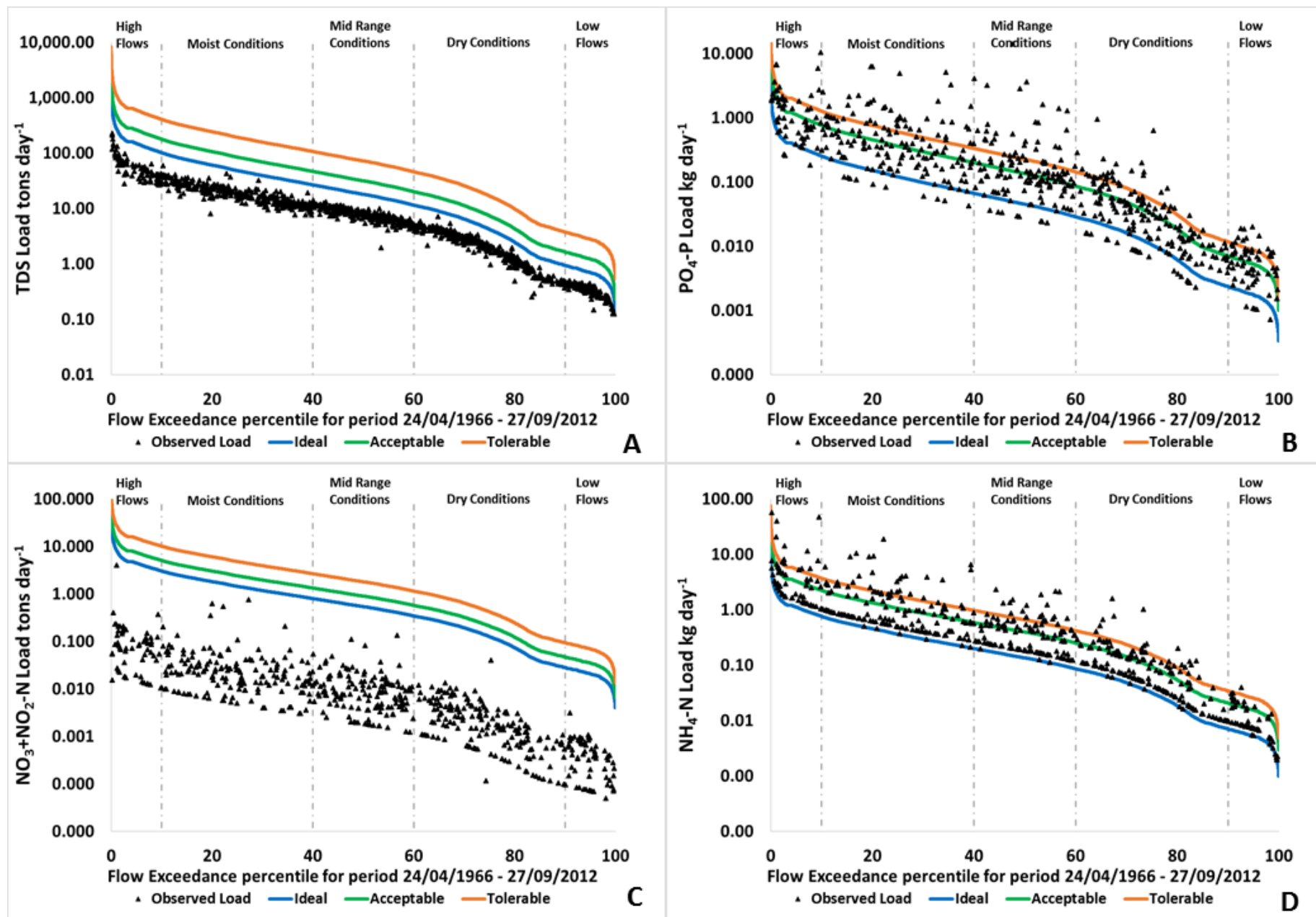


Figure 3.15 Load Duration Curves for gauge X2H013 situated along the Crocodile River. *A*: TDS, *B*: PO<sub>4</sub>-P, *C*: NO<sub>3</sub>-N + NO<sub>2</sub>-N, *D*: NH<sub>4</sub>-N

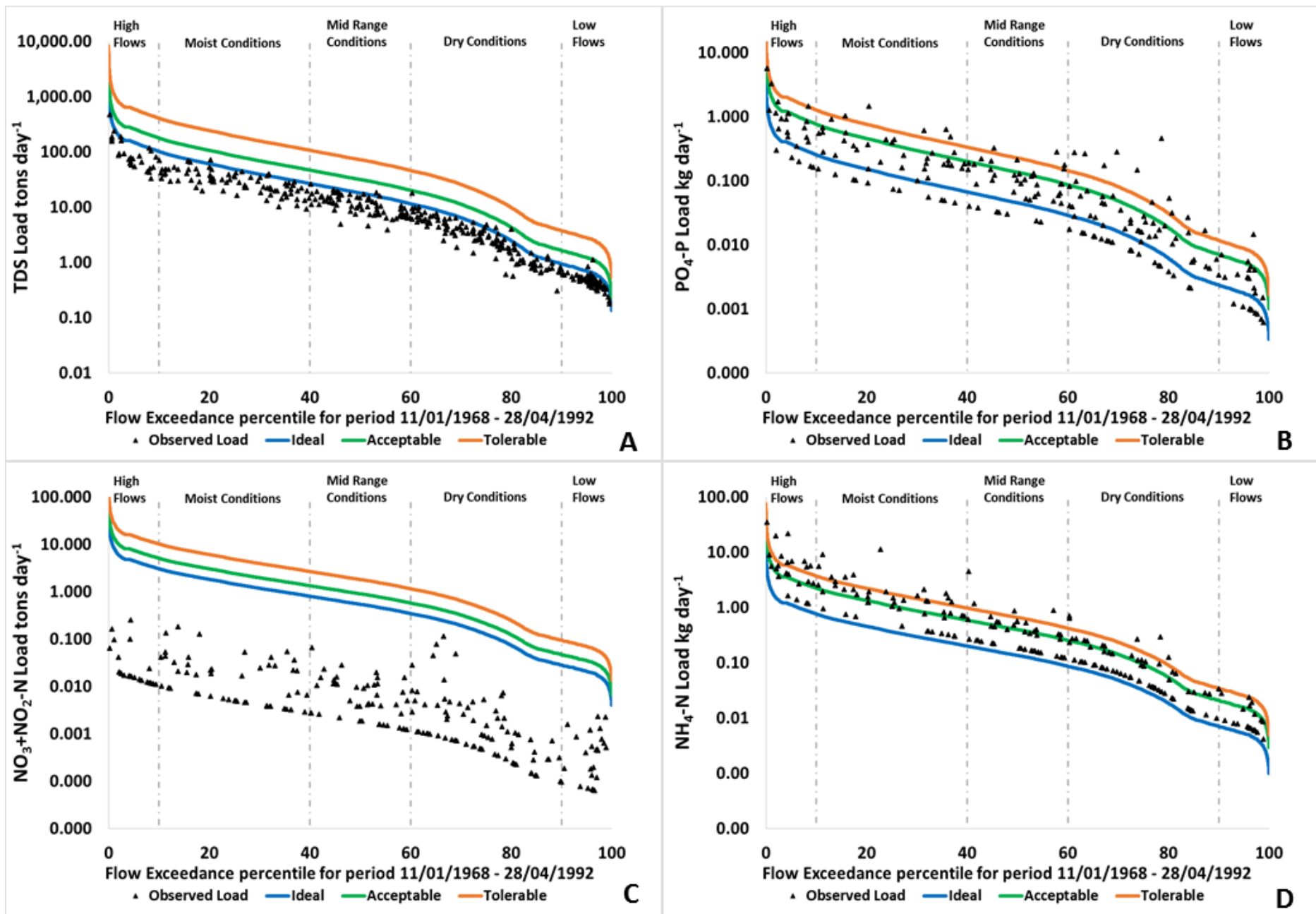


Figure 3.16 Load Duration Curves for gauge X2H023 situated along the White River. *A*: TDS, *B*: PO<sub>4</sub>-P, *C*: NO<sub>3</sub>-N + NO<sub>2</sub>-N, *D*: NH<sub>4</sub>-N

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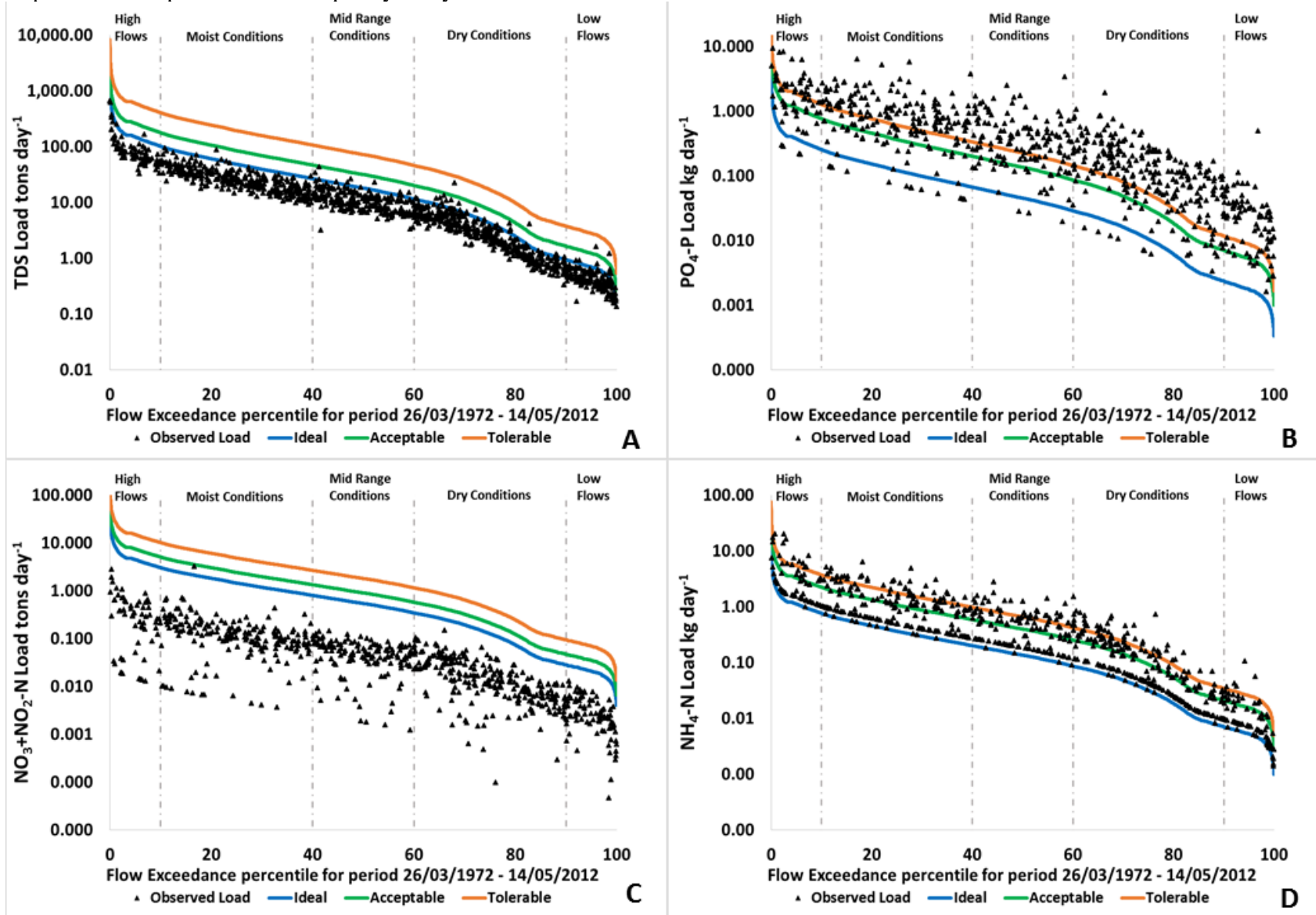


Figure 3.17 Load Duration Curves for gauge X2H032 situated along Crocodile River. A: TDS, B:  $\text{PO}_4\text{-P}$ , C:  $\text{NO}_3\text{-N} + \text{NO}_2\text{-N}$ , D:  $\text{NH}_4\text{-N}$

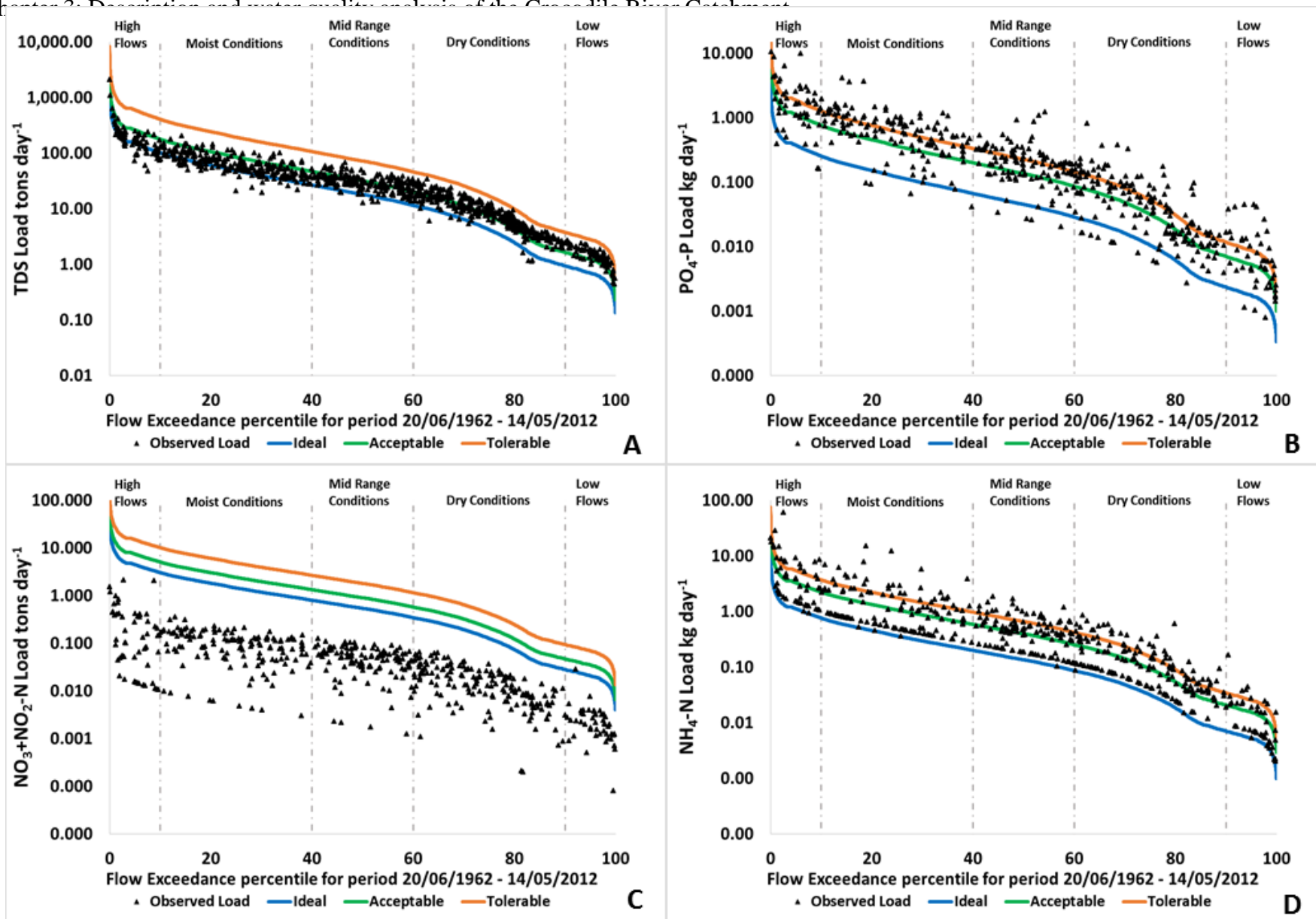


Figure 3.18 Load Duration Curves for gauge X2H022 situated along the Kaap River. *A*: TDS, *B*: PO<sub>4</sub>-P, *C*: NO<sub>3</sub>-N + NO<sub>2</sub>-N, *D*: NH<sub>4</sub>-N

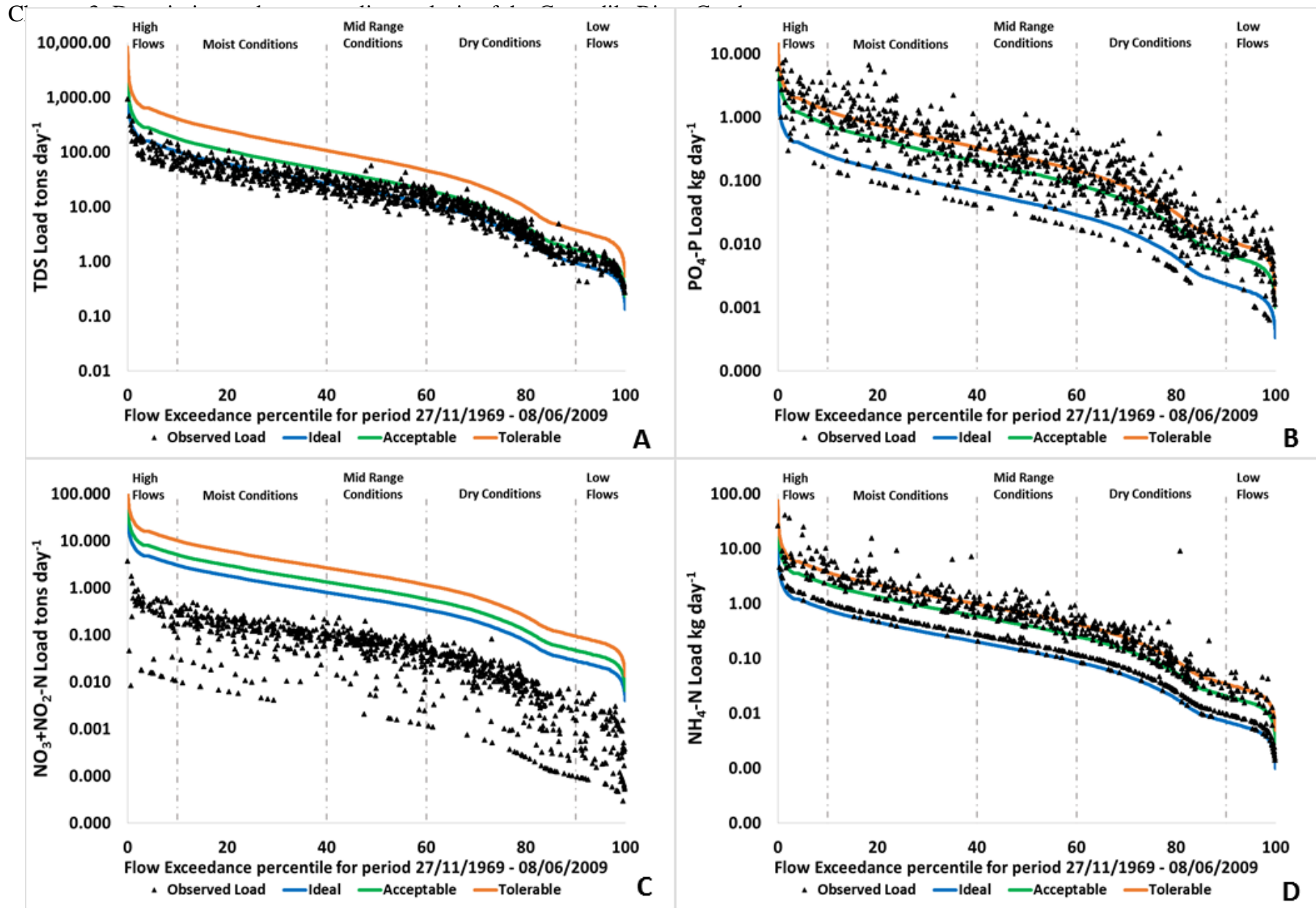


Figure 3.19 Load Duration Curves for gauge X2H017 situated along the Crocodile River. *A*: TDS, *B*: PO<sub>4</sub>-P, *C*: NO<sub>3</sub>-N + NO<sub>2</sub>-N, *D*: NH<sub>4</sub>-N

Table 3.7 A summary table of the median and percentage measurements exceeding Recommended Target Concentrations (RTCs) (method based on Malan and Day, 2005) for all active monitoring sites in the CRC

DWS Station	Total Inorganic Nitrogen		Soluble Reactive Phosphorus	
	Median	% TIN > 0.12	Median	%SRP > 0.018
X2H005	0.18	68.2	0.014	3.6
X2H006	0.65	92.6	0.029	2.8
X2H008	0.11	44.6	0.014	4
X2H010	0.07	15.4	0.015	4.4
X2H011	0.17	63.3	0.018	5.2
X2H012	0.14	56.3	0.018	4.4
X2H013	0.13	53.2	0.014	2.5
X2H014	0.12	47.9	0.011	3.7
X2H015	0.17	64.6	0.016	2.9
X2H016	0.5	89	0.02	3.6
X2H017	0.62	88.6	0.022	3.8
X2H022	0.58	92.5	0.022	3.1
X2H032	0.64	92.5	0.041	2.5
X2H035	0.08	30.2	0.01	1.9
X2H036	0.43	86.5	0.022	2.7
X2H046	0.62	89.7	0.031	1.8
X2H048	0.62	84.3	0.024	2.4
X2H049	0.58	93	0.018	3.2
X2H050	0.53	90.9	0.015	2.8
X2H070	0.2	81.6	0.015	1.8
X2H072	0.14	52.9	0.019	1
X2R001	0.09	32.4	0.013	2.3
X2R002	0.09	24.4	0.013	2.7
X2R003	0.1	32.7	0.012	1.8
X2R004	0.1	41.4	0.016	2
X2R005	0.15	65.8	0.015	3.2
Median	0.17	65.2	0.016	2.8

## **Chapter 4: Model Procedure**

### **4.1. Model Description**

WQSAM has been developed as a model linked to the SPATSIM (Spatial and Time Series Information Modelling) framework (Hughes *et al.*, 2000; Slaughter *et al.*, 2011b). Hydrological models such as the Pitman Model and other models can be run from within the SPATSIM environment. SPATSIM includes a simple Geographical Information Systems (GIS) interface which facilitates the representation and storage of study catchment attributes (e.g. observed and simulated values and model parameters).

### **4.2. Process representation within WQSAM**

#### **4.2.1. Requisite simplicity model design**

As noted in Chapter 1, data availability is one of the key issues for the effective management of water quality in South Africa (Wimberley and Coleman, 2005). While water quality models can be used to bridge the gaps in water quality datasets, the model is still limited to simulating variables of concern that are well represented in the observed water quality data sets, to ensure the effective calibration and validation of the model. Therefore, for a water quality model to be useful in a South African context, the model should be applicable at a catchment scale utilising limited existing observed data and integrating with existing yield models. The WQSAM model aims to address these South African management requirements and uses the relationship between flow and water quality to simulate water quality variable loads.

#### **4.2.2. Flow**

While point source contributions are often considered relatively constant over time, diffuse contributions vary temporally and spatially as a result of variations in rainfall runoff. Therefore, modelling at a monthly time step would not represent the transient events affecting water quality, and the peaks of some water quality concentrations would not be represented in the simulated data. It was therefore decided that WQSAM would have to function on a daily time step to account for transient events (Slaughter and Hughes, 2013b). WQSAM relies on the input of simulated flow volumes from a yield model which is routinely used within water quantity management in South Africa. The yield models, however, operate at a monthly time step, which is generally regarded as being of sufficient temporal resolution for water quantity management requirements. A monthly to daily disaggregation method was therefore



necessary to disaggregate monthly simulated flows to daily simulated flows (Slaughter *et al.*, 2015).

#### **4.2.2.1. Diffuse loading through hydrological flow pathways**

Acknowledging that natural and anthropogenic sources can be characterised by different water quality signatures, a base flow separation method is used to quantify the volumes of water within the three flow pathways (surface runoff, interflow and groundwater discharge), and each flow fraction is assigned a water quality signature for each water quality variable.

#### **4.2.2.2. Point sources**

Point source contributions are modelled in WQSAM by assigning a constant water quality signature to the yield model return flows (e.g. Agricultural return flows, WWTW etc. ). It has been noted that point source effluent concentrations and flow vary temporally (Slaughter and Hughes, 2013b), and in the future WQSAM may be adapted to represent this. WQSAM uses mass-balance modelling, and therefore, in-stream pollutants entering through point sources are diluted by the flow in the channel at that point in the system.

#### **4.2.3. Simplified in-stream and reservoir processes**

The overall aim of WQSAM was to represent processes as simply as possible in order to reduce observed data requirements. Therefore, reservoirs are simulated as modified Completely Stirred Tank Reactors (CSTRs) (see Figure 4.1), where stratification within reservoirs is not considered (Slaughter and Hughes, 2013b), as complete mixing of the reservoir is assumed (Chapra, 1997).

WQSAM models the most critical processes influencing water quality in-stream and in reservoirs while attempting to remain as simple as possible (Figure 4.2). Importantly, Figure 4.2 also represents the processes simulated for river nodes, except settling is not considered and attached periphyton are modelled instead of algae suspended in the water column. In addition, hyacinth growth is only modelled in reservoirs at this stage.  $\text{NH}_4/\text{NH}_3$  can be converted to  $\text{NO}_2/\text{NO}_3$  through nitrification (Chapra, 1997).

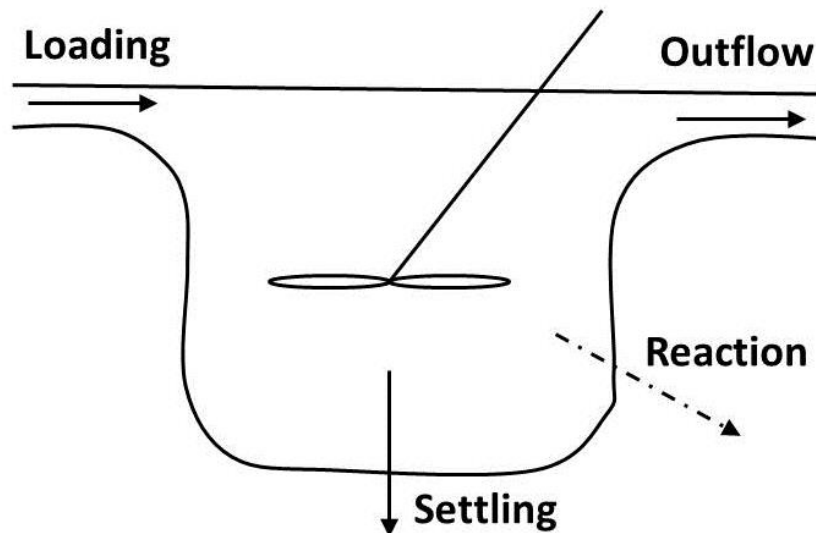


Figure 4.1 Conceptual process model of a Completely Stirred Tank Reactor (CSTR) taken from Chapra (1997)

Denitrification can occur under anoxic conditions (Chapra, 1997), but since WQSAM does not simulate oxygen, and there is an assumption of complete mixing within reservoirs, denitrification is not simulated in WQSAM. Hyacinth and algae take up nutrients with growth. This uptake with growth is modelled by assuming that a portion of organic algal biomass is made up of nitrogen and phosphorus. Algal and hyacinth growth may preferentially take up  $\text{NH}_4/\text{NH}_3$  instead of  $\text{NO}_2/\text{NO}_3$  (Berman et al., 1984), and this is facilitated within WQSAM. Algae and hyacinth release particulate organic matter (POM) and dissolved organic matter (DOM) through excretion and death. Within some models such as CE-QUAL-W2 (Cole and Buchak, 1995), a distinction is made between refractory and labile POM and DOM, with refractory organic matter decaying at a slower rate. Within WQSAM, no distinction is made between refractory and labile organic matter, with the same decomposition rate applied to all organic matter within a particular node. POM and DOM within WQSAM are simulated as transition variables, as the decomposition process of organic matter releases nutrients back in to the water column. Generally, POM and DOM are not measured within water quality monitoring programs, and therefore, it is difficult to validate WQSAM's simulations of organic matter. Some of the POM simulated within WQSAM is assumed to settle to the bottom of reservoirs, and WQSAM assumes a portion of the total organic matter within the sediment is buried within each model time step. This functionality serves as a nutrient sink within reservoirs. The rest of the organic matter within

the sediments, as well as POM and DOM, decompose to release nutrients back into the water column.

#### **4.2.4. Eutrophication**

Eutrophication occurs when a water body receives excessive loadings of nutrients which in turn stimulate excessive plant growth. Nyenje *et al.* (2010) broadly classifies the possible outcomes of excessive nutrients with four major adverse effects: 1) increased phytoplankton primary production with cyanobacteria replacing diatoms as the dominant group of planktonic algae; 2). rapid growth of phytoplankton species and aquatic macrophytes, which in extreme cases can lead to the dominance of mono-specific blooms which are often associated with heavy biomass accumulation leading to harmful cyanobacteria; 3) an alteration of ecological integrity of fresh water resources leading to a decline in macro invertebrate abundance and diversity (Oberholster and Ashton, 2008; Oberholster *et al.*, 2009) and; 4) the complete depletion of oxygen associated with the accumulation of dead algal or macrophyte debris, where the anoxic conditions suffocate macro invertebrates and fish species, with immobile benthic species dying off completely.

Water quality models represent the effects of eutrophication by simulating algal growth and mortality and the resulting effects on nutrients (dissolved oxygen etc.). Complexity increases with increasing number of variables related to eutrophication simulated. Complex models such as QUAL2K (the modernised version of QUAL2E) (Brown and Barnwell, 1987), and CE-QUAL-W2 (Cole and Buchak, 1995) simulate a multitude of water quality variables related to eutrophication. When comparing WQSAM (a relatively simple model) to CE-QUAL-W2 (a complex model), there is a trade-off between the number of water quality variables (and therefore processes) represented within the model and the complexity of the model. Important water quality processes must be identified that will allow for the simulation of the most important water quality variables and will explain the majority of the temporal and spatial variation of the chosen variables. Figure 4.3 conceptually represents the single algal model compartment of CE-QUAL-W2 that simulates the interactions between nutrients, algae and dissolved oxygen (Cole and Buchak, 1995). WQSAM does not model oxygen, inorganic carbon and other layers for various reasons including: 1) this would drastically increase the complexity of the model and would amplify the data requirements; 2) some of the excluded variables are not regarded as important from a management perspective and; 3) there are no available observed data to validate the simulations.

Chapter 4: Model Procedure

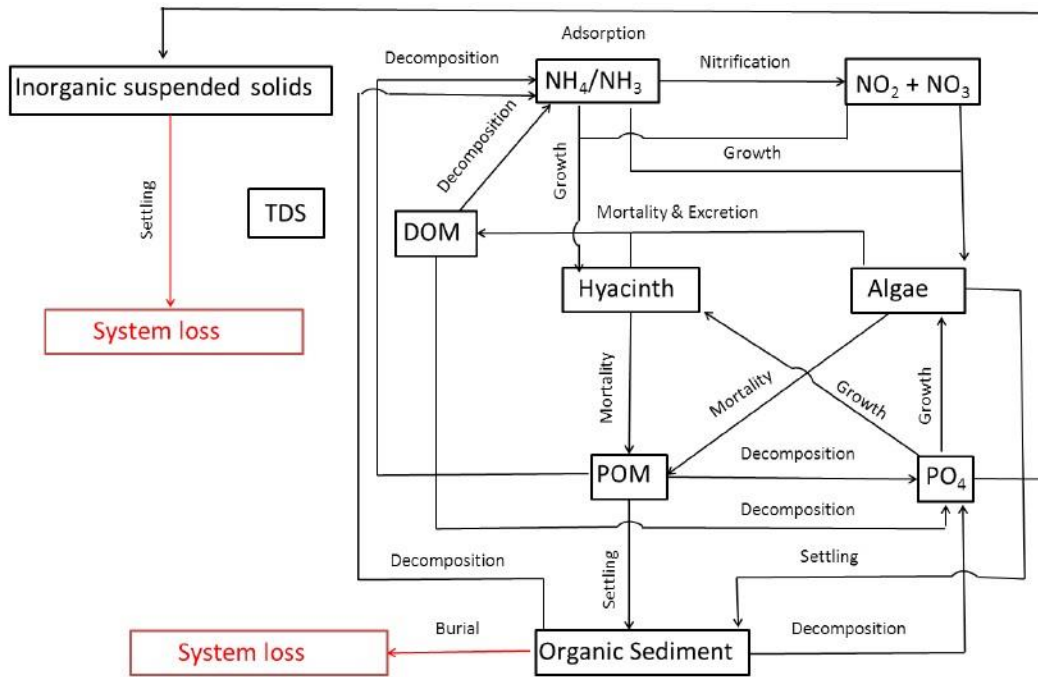


Figure 4.2 Conceptual modelling framework for simulation of water quality variables for reservoirs within WQSAM (Slaughter and Hughes, 2013b)

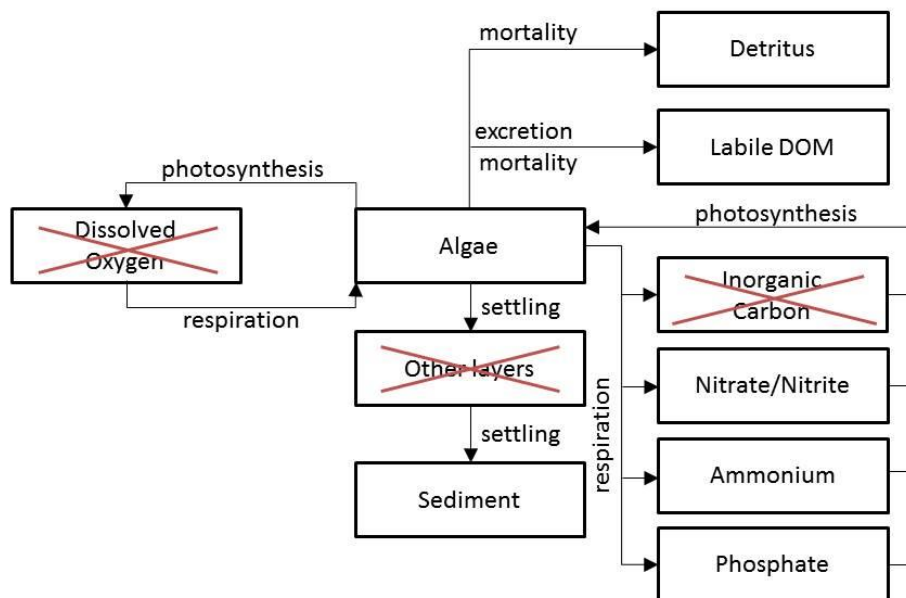


Figure 4.3 Conceptual diagram representing the CE-QUAL-W2 algal model and the processes represented. Red crosses have been placed through the variables that WQSAM does not simulate

Algal and hyacinth growth is considered within WQSAM as these processes affect the concentrations of nutrients. WQSAM models the nitrogen based nutrients  $\text{NH}_4/\text{NH}_3$  and  $\text{NO}_2 + \text{NO}_3$  as well as  $\text{PO}_4$ . WQSAM does not differentiate between  $\text{NH}_4$  and  $\text{NH}_3$  fractions as pH is not simulated, and pH is required to determine the species fractions (Chapra, 1997). Models such as CE-QUAL-W2 and QUAL2K allow algae to adsorb certain nutrient species before others, called ‘preferential uptake’ (Cole and Buchak, 1995; Pelletier et al., 2006). This is to allow algae to adsorb preferential nutrient species, such as ammonia, before nitrates/nitrites for growth which has been demonstrated in the literature (e.g. Berman *et al.*, 1984). This staggered preferential uptake is represented within WQSAM, which also models water temperature, as temperature has a regulating effect on the rate of processes affecting nutrients, including algal growth (Chapra, 1997). This is due to the fact that for a chemical reaction to occur, there is a limiting required energy known as the activation energy. Generally, the reaction rate increases with temperature (to a threshold limit) (Grafton and Hussey, 2011). Chapra (1997) has stated that generally, a process rate will approximately double for a temperature rise of 10 °C. In WQSAM, temperature regulation of algal growth is simulated using the Optimal Model (Chapra, 1997), where minimum, optimal and maximum temperatures are considered within algal growth. Unlike more complex models such as CE-QUALW2 and QUAL2K, the algae model used in WQSAM does not differentiate between algal species and rather lumps all species into one variable (Slaughter and Hughes, 2013b). Certainly, certain algal species, such as blue-green algae (*Microcystis*), are more of a water quality problem than others, while different species may affect variable nutrient uptake rates. Therefore, increased functionality may be incorporated into WQSAM in the future to consider some of these processes.

### 4.3. Data for Modelling

The WQSAM model requires a yield model to generate non-naturalised flow, abstraction, return flows and reservoir yields, and in this case, the Water Resources Modelling Platform (WReMP) model (Mallory and van Vuuren, 2007) was used, which has been well established and used extensively for simulation purposes in the Crocodile River Catchment (Louw and Mallory, 2010). The WReMP model is a stand-alone executable program with a dedicated modelling platform, and currently cannot be run within SPATSIM. Therefore, the output of the WReMP model is imported into SPATSIM attributes, a process facilitated by the first

level of the WQSAM model which creates an interface with outputs from the yield model (Figure 4.4A).

The system setup of the WReMP model (Figure 4.5A) is replicated within SPATSIM by recreating the nodes within the SPATSIM GIS interface as SPATSIM point features (Figure 4.5B and 4.5C). Observed water quality data sets can then be associated with the nodal point features in SPATSIM by associating spatially proximate water quality stations with particular nodes (Figure 4.5D and A). To facilitate the modelling of in-stream and reservoir processes, WQSAM requires additional data, some of which could possibly be obtained from observed historical data (see Table 4.1), and some of which will have to be inferred from land-use practices.

A number of hydrological and water quality data sets are required for setting up and running the WQSAM model. Figure 4.5D below represents the most common data sets of both water quality and quantity available that are processed, linked to specific model nodes and stored in SPATSIM as attributes. The model's data requirements can be separated into two major components, namely water quantity and quality. Both are equally important to the modelling process.

Table 4.1 DWS water quality gauging stations linked to WReMP nodes

WReMP Node	River Name	WQ Gauging Station	WQ Data	
			From:	To:
X21F-2	Elands	X2H011	1972	2009
KwenaDam	Kwena (Crocodile)	X2R05	1984	2012
X21D-2	Crocodile	X2H033	1977	1992
X22A-1	Blystaanspruit	X2H027	1966	1981
X21H-1	Ngodwana	X2H034	1972	1983
X21K-2	Elands	X2H015	1972	2012
X22A-2	Houtbosloop	X2H014	1966	2012
MontroseFalls	Crocodile	X2H013	1966	2012
X23C-2	Suidkaap	X2H024	1972	1996
X23A-2	Noordkaap	X2H010	1972	2012
X22E-1	Kruisfonteinspruit	X2H035	1984	2011
WitklipDam	Witklip (Sand)	X2R03	1975	2012
X23E-2	Queens	X2H008	1969	2012
X22CTributary	Rietspruit	X2H031	1966	2012
X22F-2	Nels	X2H005	1969	2012
X23D-2	Suidkaap	X2H031	1966	2012
LongmereDam	Longmere Dam (Witrivier)	X2R01	1968	2011

Table 4.1 continued. DWS water quality gauging stations linked to WReMP nodes

WReMP Node	River Name	WQ Gauging Station	WQ Data	
			From:	To:
KlipkoppieDam	Klipkopjes (Wit)	X2R02	1981	2012
PrimkopDam	Primkop (Wit)	X2R04	1972	2012
X22H-3	Wit	X2H023	1968	1992
X22J-2	Crocodile	X2H006	1969	2012
X22K-2	Crocodile	X2H032	1972	2012
X24A-2	Nsikazi	X2H072	1990	2001
X23HGuage	Kaap	X2H022	1969	2012
X24E-2	Crocodile	X2H017	1969	2009
X24H-1	Crocodile	X2H016	1970	2011

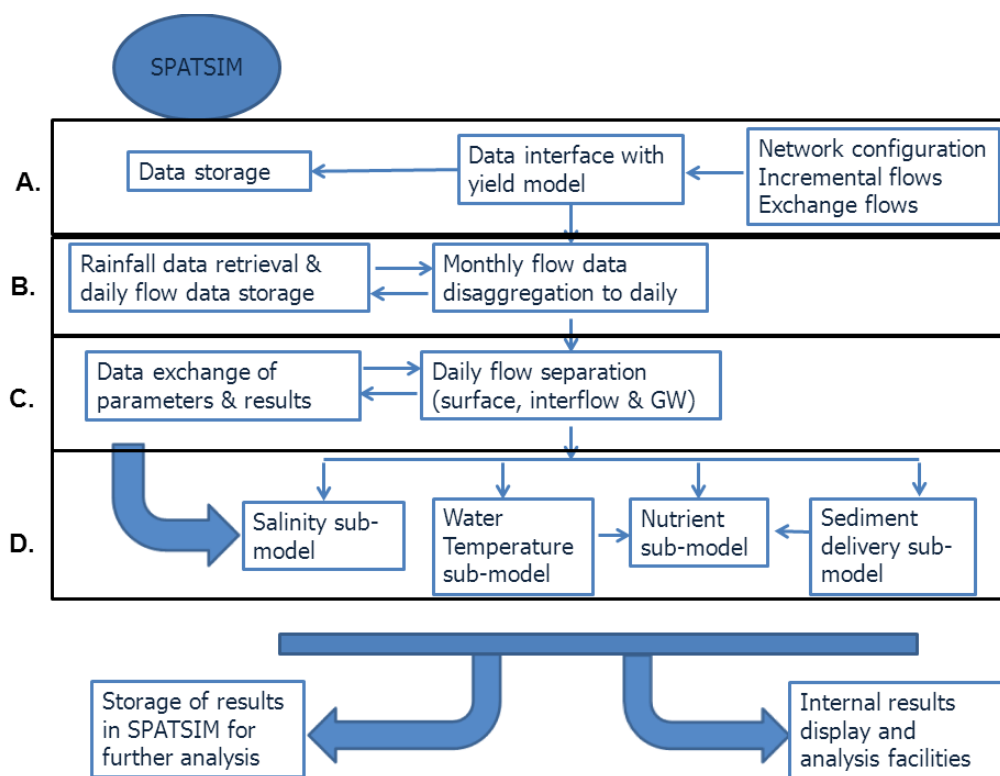


Figure 4.4 Conceptual representation of WQSAM model components (Slaughter and Hughes, 2013)

Rainfall data sets in conjunction with daily flow are used in a disaggregation sub-model (Figure 4.4B). As water quality can be influenced by transient events such as rainfall-runoff events, modelling at a monthly time step may miss important temporal variation in water quality. Therefore, monthly incremental flow outputs from the yield model are disaggregated to daily simulated flows. Furthermore, the simulated disaggregated daily incremental flow

time-series are separated into three major flow components: 1) surface; 2) interflow and; 3) groundwater flow (Figure 4.4C). Observed water quality datasets are used in the calibration of the water temperature sub-model, salinity sub-model and nutrient sub-model (Figure 4.4D). The data for modelling and the sub-model processes will be dealt with in further detail in the sections below.

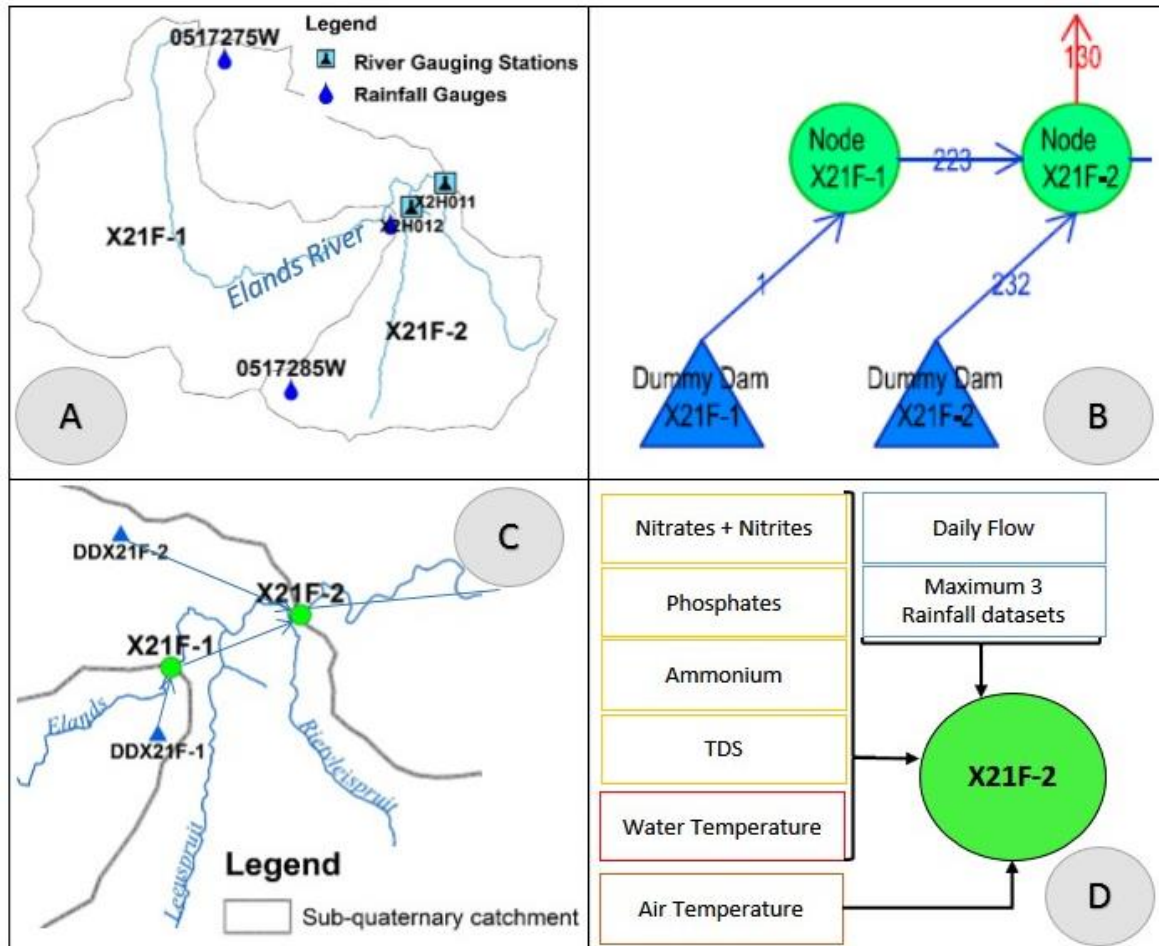


Figure 4.5 Model structure and data for modelling and linking to WReMP nodes

Yield models such as WReMP represent a catchment’s hydrological system (A) as a network of nodes, channels and dams (B). The structure of the WReMP yield model (B) is translated in SPATSIM with nodes being positioned geographically (C). All available water quality, hydrological and meteorological data (A) are linked to nodes (D).

### 4.3.1. Water quantity sub-model requirements

#### 4.3.1.1. Flow data requirements

WQSAM requires monthly inflow and outflow data, as well as reservoir storage data, which is generated by the WReMP model (Slaughter *et al.*, 2011b). As mentioned above, the nodal



structure of the WReMP model is replicated in SPATSIM and in WQSAM (run-time model execution) to ensure that all data exported from the WReMP outputs for each specific node matches that of the corresponding node within WQSAM.

These WReMP output data required include:

1. nodal incremental flows;
2. nodal inflows (from upstream nodes, as well as return flows);
3. nodal outflows (to downstream nodes and abstraction for irrigation or urban use);
4. evaporation;
5. monthly reservoir storage;
6. stream flow reduction.

Daily flow data sets for the entire catchment were acquired from the DWS hydrological services website (<http://www.dwaf.gov.za/hydrology/>). The daily flows are used to determine the scaling parameters required to scale yield model monthly flow duration curves (FDC) to daily FDCs as part of the disaggregation process (see Slaughter *et al.*, 2015).

### **4.3.1.2. Rainfall data sets**

One of the most important data inputs into a hydrological model is precipitation, which is the driving force behind catchment hydrology along with evapotranspiration. Within WQSAM, daily rainfall data are used to disaggregate the input simulated monthly incremental flows to daily incremental flows. A maximum of three rainfall gauges can be used to collate a continuous time series of daily rainfall, representative of precipitation that occurred within the incremental catchment area of the node (see Figure 4.5A). A national database of observed daily rainfall data is readily available, however, the existing collated database only covers rainfall up until mid-June 2000 (Lynch, 2004). Three available ground based rainfall time series were assigned to each node. However, to disaggregate monthly incremental flows up to the end date of the WReMP simulation (2004), rainfall data had to be additionally extracted from satellite data after year 2000. The National Oceanic and Atmospheric Administration Rainfall Estimation 1 (RFE 1) daily rainfall satellite data were utilised to bridge the gap with a single time series of satellite data being assigned to each node. It is recognised that satellite estimates of rainfall may differ substantially from ground based rainfall measures, with complications arising from spatial resolution, satellite technology used and topographical effects (Thiemig *et al.*, 2012), but assessing these limitations is beyond the scope of this study. Differences between satellite rainfall and ground based

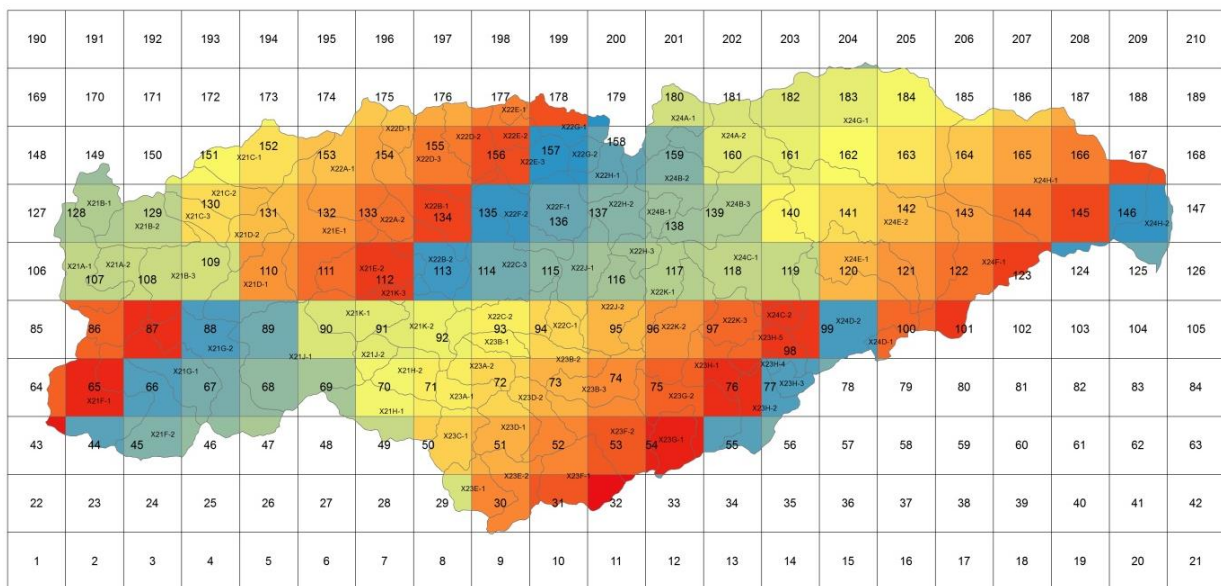
## Chapter 4: Model Procedure

rainfall would only manifest as daily flow frequency in this study, as final volumes of flow are corrected to monthly volumes obtained from the yield model.

The daily rainfall datasets were acquired from a secure file transfer protocol (FTP) site. Each daily file downloaded from the secure NOAA FTP site contains daily rainfall estimates for a 0.1 degree cell based on a global grid. Knowing this, a partial hypertext pre-processor (PHP) program was used to extract rainfall for cells forming part of a grid that expands across the Crocodile River Catchment (Figure 4.6). Using ESRI's ArcView 10.1, a grid Shapefile was intersected with the underlying sub-quaternary shapefile. The intersected output shapefile was projected and the area of the sub-quaternary in relation to the grid number was calculated (Table 4.2). These areas were summed and a grid weighting factor for each grid number in relation to a sub-quaternary catchment was calculated. Using the grid weighting factors, an average rainfall for each sub-quaternary was calculated and exported and linked to the nodes.

Table 4.2 Example of intersect function output

Grid Number	Sub-quaternary Catchment	Area (Km <sup>2</sup> )
85	X21A-1	0.23
86	X21A-1	15.22
106	X21A-1	5.51



### 4.3.2. Water quality related data sets

#### 4.3.2.1. Observed water quality time series

In this study, salinity (TDS), nitrates+nitrites, ammonia, and phosphates were the water quality variables of concern simulated by WQSAM. The historical monitoring data, which includes observed values for the identified water quality variables of interest, can be found at the Department of Water and Sanitation (DWS) Resource Quality Services website (<http://www.dwaf.gov.za/iwqs/report.aspx>; accessed 20 September 2014). The observed water quality data within the catchment were used to calibrate the water quality parameters within WQSAM, and to benchmark the reliability of the model. Water quality data for all waste water treatment works (WWTW) were collected and associated with nodes (see Figure 4.7); the data are used for assigning water quality signatures to return flows.

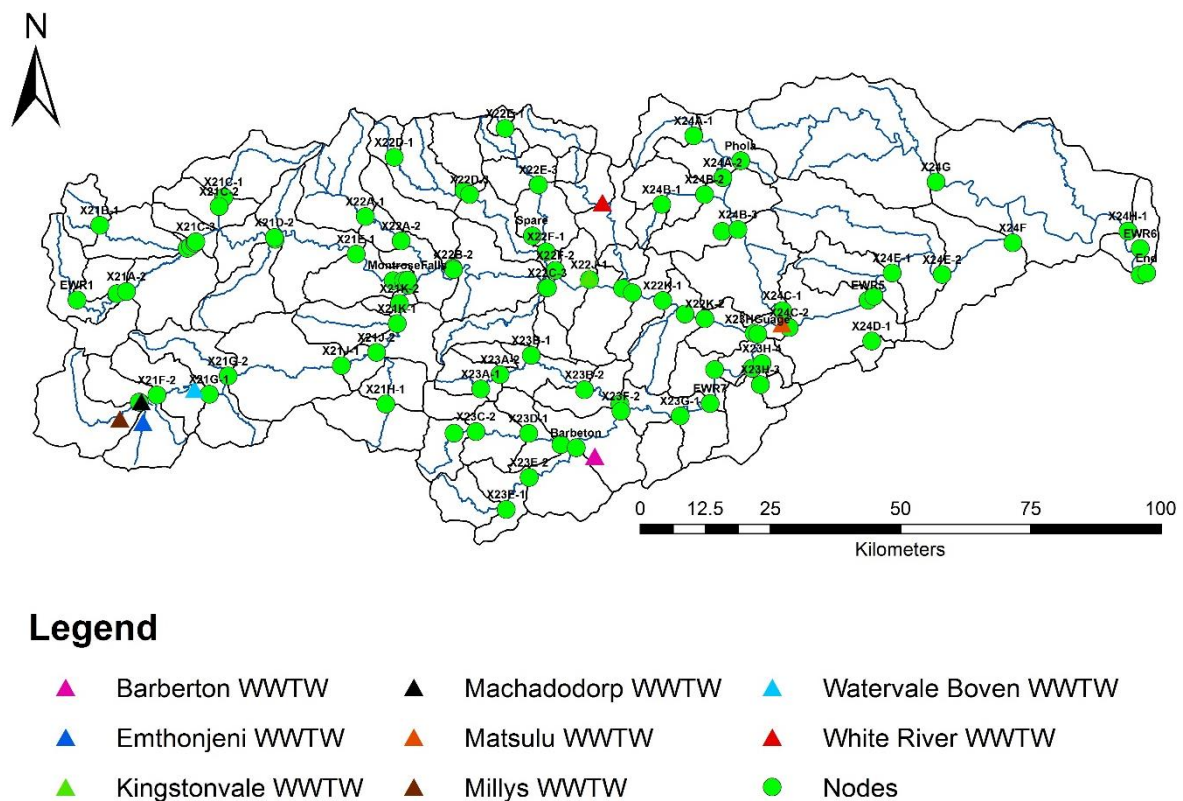


Figure 4.7 Map showing the replicated nodes based on the WReMP yield model structure overlain with WWTWs in the CRC

#### **4.3.2.2. Land use data**

Land use practices play a critical role within a catchment, with various land use practices affecting water quality through the input of diffuse source pollution (e.g. permanently irrigated cultivation practices) and sediment load variations. The model's nodes and water quality stations are overlain on the land use polygon (Fairbanks *et al.*, 2000). This process allows the user to identify water quality observation stations that can be used to assess the water quality simulations of model nodes. Land-use maps are used to provide guidance in assigning water quality signatures given to surface flow, interflow and groundwater flow components at the nodes. The allocation of signatures to the flow components is a model calibration exercise, guided by land use information, and benchmarked against observed data.

#### **4.3.2.3. Temperature**

Water temperature within rivers is required to model rate processes (e.g. biological degradation and chemical speciation), phytoplankton and macrophytes growth and respiration rates. While the DWS does not routinely measure water temperature, it can be simulated using the water temperature sub-model (Rivers-Moore *et al.*, 2008) which uses air temperature extracted from a consolidated database (Schulze and Maharaj,, 2004). Observed water temperature data sets that do exist are used in the calibration of the temperature sub-model.

#### **4.3.2.4. POM and DOM**

Within the modelling of in-stream processes, some indication of dissolved organic matter (DOM), and particulate organic matter (POM) concentrations are required. This is because POM and DOM are important transitional water quality variables that affect the variables of interest, such as ammonia and phosphates. For example, hyacinth death produces POM which settles to form organic sediment which in turn degrades to release ammonia and phosphates. While DOM and POM is not routinely measured by the DWS, concentration ranges could be inferred by land use practices within a catchment. Some indication of phytoplankton concentrations and data on water hyacinth growth in the modelled rivers and reservoirs would be useful from a model calibration and validation perspective. WQSAM also models inorganic sediment as a surface water signature, with a proportion of suspended sediment settling to form bottom sediment in reservoirs within each time step. It is envisaged that more mechanistic sediment modelling routines will be incorporated in the near future. Potentially, sediment modelling could give useful indications of reservoir sedimentation, which negatively affects reservoir capacity over time.

#### **4.4. Data pre-processing requirements**

A database of all the DWS water quality and quantity data was created using Microsoft Excel, and all the data outliers removed. All DWS water quality and quantity stations that had >50 sample were processed into text files that only include a single water component (i.e. flow, temperature, salinity (TDS), nitrites + nitrates, phosphates and ammonia). All data are imported into SPATSIM as a time series and in a continuous text format with the value -9.9 representing missing data.

#### **4.5. WQSAM sub-model components**

##### **4.5.1. Disaggregation sub-model overview**

The WReMP output data for incremental nodal flow is represented as monthly incremental flow as volumes in million cubic meters. The WQSAM model requires that the incremental flow be represented at a daily time step in  $\text{m}^3 \cdot \text{s}^{-1}$  for the purpose of water quality modelling. Therefore, a component to disaggregate monthly simulated incremental flows is included. The conceptual diagram taken from Slaughter *et al.* (2015) shows the disaggregation process (Figure 4.8). Observed flows within the region are used to determine the relationship between the monthly and daily flow duration curves as a scaling equation. Monthly incremental flows obtained from the WReMP model (Figure 4.8 Step 1) and the scaling equation is used to scale the monthly duration curve to a daily duration curve (Figure 4.8 Step 2). Multiple time series of daily rainfall (up to three) for a particular catchment are converted to a single timeseries of antecedent rainfall (Figure 4.8 Step 3). The antecedent rainfall takes into account that rainfall causing runoff on any particular day is influenced by rainfall that occurred in the near past, and that a threshold of rainfall must be exceeded before runoff occurs. The time series of antecedent rainfall is used to construct a daily antecedent rainfall exceedance frequency curve (Figure 4.8 Step 4). The model steps through the daily antecedent rainfall, finds the corresponding frequency of exceedance, and the initial daily flow is determined from the equitable frequency on the daily flow duration curve (Figure 4.8 Step 5). Finally, the time series of daily flows are volume corrected against monthly simulated incremental flow volumes (Figure 4.8 Step 6); to form the final time series of daily flows (Slaughter *et al.*, 2015).

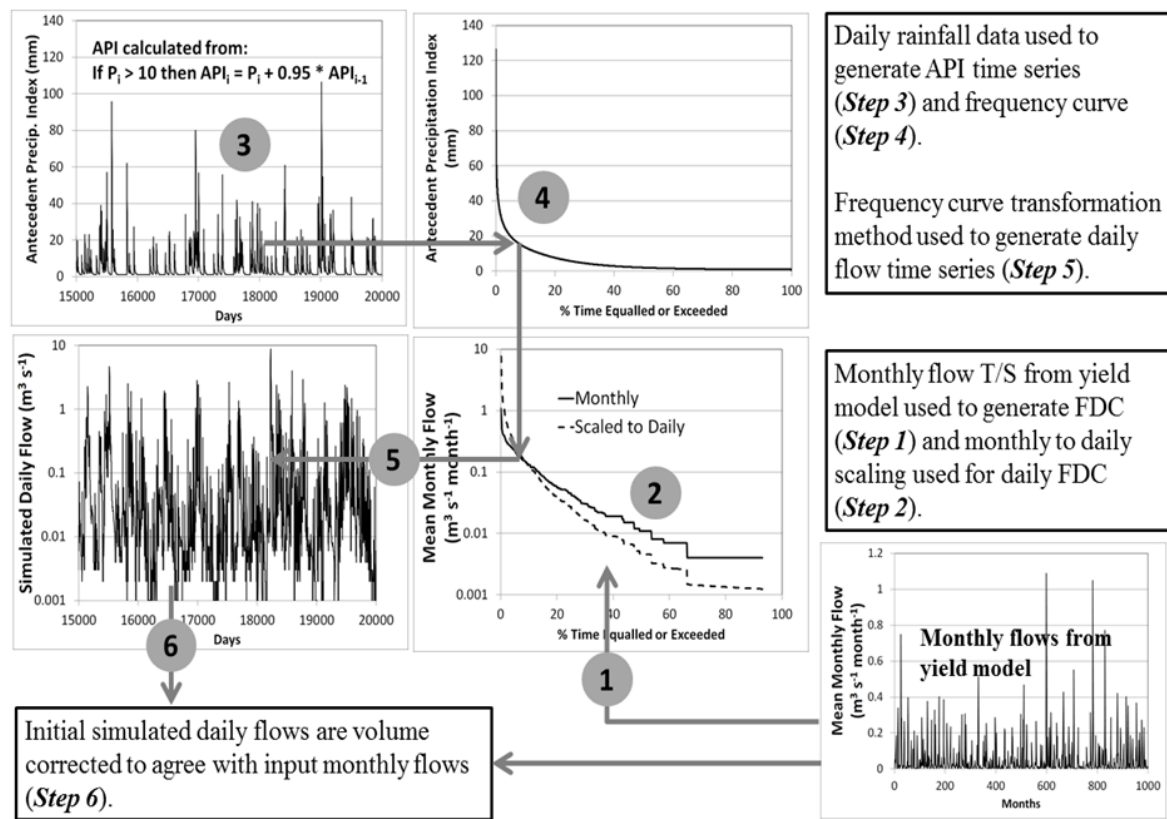


Figure 4.8 Conceptual diagram of the process of disaggregating monthly incremental flows to daily as used in the Water Quality Systems Assessment model (Slaughter *et al.*, 2015)

#### 4.5.2. Separation of daily incremental stream flows into flow fractions (baseflow separation)

Natural stream flows can be separated into three main components: surface flow, interflow and groundwater flow, each of these associated with different water quality signatures influenced by land use practices or geology within a particular catchment (Slaughter and Hughes, 2013a). For example, land-use dominated by urban areas would indicate that the surface incremental flow should be associated with elevated nutrient signatures in the surface flow, and to a lesser extent the interflow and groundwater flow components. Agricultural land-use practices would indicate an elevated signature of nitrates in surface flow, and to a lesser extent in interflow and groundwater flow. Generally, phosphates bind to inorganic sediment, and do not filter down into subsurface flow. Nitrates become dissolved and do infiltrate to add to interflow and groundwater flow quality signatures. Therefore, disaggregated daily incremental stream flows are separated into surface, interflow and

groundwater flow using a simple statistical baseflow separation sub-model within WQSAM (Hughes *et al.*, 2003). The parameters used for the baseflow separation technique have been fixed in this study using the values determined by Hughes *et al.* (2003). Calibration could be done if more information were available from field or modelling studies.

### **4.5.3. Water temperature sub-model**

As previously mentioned, water temperature is important for water quality modelling. Unfortunately, observed historical data sets are often scarce. WQSAM has adopted the Rivers-Moore *et al.* (2008) regression model, which uses air temperature to simulate in-stream water temperature. While there is a consolidated database of air temperature (Schulze and Maharaj, 2004), there are only data available for the period 1950–2000, restricting the simulation time periods. Therefore, WQSAM uses daily air temperatures when they exist, and monthly observed water temperature averages for other periods.

### **4.6. Assigning parameter values to WQSAM sub-model components**

When calibrating water quality parameters, it is vitally important that the modeller understands the characteristics and relationships of the water quality constituents being simulated and the parameters involved. There are two major factors limiting the range of variables simulated within WQSAM: 1) the availability of historical water quality data and; 2) the requisite simplicity of WQSAM. While there may be historical data available within a catchment, the data are often limited spatially and temporally, with a narrow range of water quality constituents being represented. These limit the calibration capabilities as there often are no water quality data sets available to calibrate process parameters, leading to increased uncertainty. Therefore, WQSAM has been developed on the basis of requisite simplicity and models only the key processes effecting water quality. While this limits the number of water quality constituents that can be modelled, it is more appropriate from a management perspective as it allows an entire catchment to be modelled with limited available data. This section provides an overview of the approach adopted for quantifying the model component parameters and the water quality constituents modelled that can be calibrated against observed historical DWS data.

#### **4.6.1. Water quantity parameters**

Slaughter *et al.* (2015) developed and tested the monthly to daily flow disaggregation method. Near perfect monthly flows (observed daily flows summed to monthly volumes where missing data were patched with simulated flow from the Pitman model) were used, and

disaggregated daily flows were assessed against the observed daily flows. A number of quaternary catchments used by Slaughter *et al.* (2015) are located within the CRC. The disaggregation method worked well, achieving natural Nash-Sutcliffe Efficiency (NSE) values ranging from 0.50–0.86. The parameter values obtained by Slaughter *et al.* (2015) were assigned to the CRC WQSAM model setup, because calibrating near perfect flows would provide the most accurate representation of the disaggregation parameters. Model nodes without flow data were assigned the same parameters as nodes with data where the catchments had similar characteristics in terms of climate and physical catchment properties (Chapter 3; Figure 3.7, Figure 3.10).

### **4.6.2. Temperature sub-model parameters**

The water temperature sub-model parameters were determined using the best visual fit to observed data. Observed water temperature does not exist for every water quality node therefore, calibrated parameters and average monthly water temperature values were assigned to nodes that fall within the same annual temperature range (see Chapter 3; Figure 3.8) as Rivers-Moore *et al.* (2008) suggests that the most significant element influencing water temperature is air temperature.

### **4.6.3. Water quality loading parameters**

Chapter 2 described how the concentrations of water quality constituents related to different flow fractions (surface, interflow and groundwater) can have a significant effect on in-stream water quality. One of the greatest challenges for modelling in-stream water quality is the lack of observed data for these various flow components. Therefore, a number of methods/approaches were used to assign water quality signatures to the flow components. Surface and interflow signatures were assigned based on ranges described in the literature in combination with land use maps (e.g. Table 4.3. and see Chapter 3; Figure 3.10). Observed borehole water quality data were used to assign ground water quality signatures (see Appendix B, Tables 5B to 8B). If no borehole water quality were available, a groundwater signature was assigned based on signatures described in literature or from nodes with data that share the same geological origin (see Chapter 3; Figure 3.4). Return flow concentrations were assigned based on ranges determined using WWTW discharge data (see Appendix B, Tables B1 to B4).



Table 4.3 Surface water quality signature ranges for irrigated agriculture based on literature

WQ	Min	Max	Source
PO <sub>4</sub> -P	0.01	2.72	Bondurant, 1971; Peterjohn & Correl, 1984; Shrestha & Kazama, 2007
NH <sub>4</sub> -N	0.250	3.63	Peterjohn & Correl, 1984; Shrestha & Kazama, 2007
NO <sub>3</sub> - N	0.01	10.5	Peterjohn & Correl, 1984; Shrestha & Kazama, 2007
TDS	10	1980	Shrestha & Kazama, 2007; Bauder and Brock, 2001

#### 4.6.4. Parameters representing in-stream water quality processes

In-stream water quality processes are not routinely measured, and intensive specialised laboratory work is required to determine values for some of these parameters, while others would probably have to be inferred from expert knowledge. These in-stream processes comprise of rates and constants e.g. POM decay rate and Theta for ammonia nitrification rate respectively. Some of these have been investigated and parameter ranges for water quality modelling have been specified (e.g. Bowie *et al.*, 1985; Sullivan *et al.*, 2011 and Neilson *et al.*, 2012). This study utilised parameter ranges specified in the literature (see Table 4.4) to guide calibration. The final calibrated parameters are presented in Appendix E with model equations and descriptors available at <http://www.ru.ac.za/iwr/software/waterqualitymodelling.php>.

Table 4.4 Maximum and minimum parameter values representing in-stream water quality processes based on the literature

Type of node	Range		Source
	Min	Max	
<b>River</b>			
NH <sub>4</sub> Nitrification Rate (d <sup>-1</sup> )	0.05	0.5	Bowie <i>et al.</i> 1985
Theta for ammonia nitrification rate	1.02	1.047	Bowie <i>et al.</i> 1985
POM decay rate(day <sup>-1</sup> ) at 20 °C	-	0.101	Sullivan <i>et al.</i> 2011
DOM decay rate (day <sup>-1</sup> )	-	0.121	Sullivan <i>et al.</i> 2011
<b>Reservoir</b>			
Algal Ammonia preference factor	0	0.9	Slaughter and Hughes (2013)
Partition coefficient for algal mortality	0	0.5	Slaughter and Hughes (2013)
Algal mortality rate (day <sup>-1</sup> )	0	0.8	Bowie <i>et al.</i> 1985
Algal excretion rate (day <sup>-1</sup> )	0	0.5	Neilson <i>et al.</i> 2012
Algal growth rate at T <sub>opt</sub> (day <sup>-1</sup> )	0.5	2.53	Bowie <i>et al.</i> 1985
Algal dark respiration rate at T <sub>opt</sub> (day <sup>-1</sup> )	0	0.05	Slaughter and Hughes (2013)

Table 4 .4 continued. Maximum and minimum parameter values representing in-stream water quality processes based on the literature

Type of node	Range		Source
	Min	Max	
<b>Reservoir</b>			
Algal settling proportion (day <sup>-1</sup> )	0	30	Bowie <i>et al.</i> (1985)
T <sub>min</sub> for algal growth and respiration (°C)	10	14	Bowie <i>et al.</i> (1985)
T <sub>opt</sub> for algal growth and respiration (°C)	20	28	Bowie <i>et al.</i> (1985)
T <sub>max</sub> for algal growth and respiration (°C)	35	40	Bowie <i>et al.</i> (1985)
Inorganic sediment settling proportion (day <sup>-1</sup> )	0.1	2	Neilson <i>et al.</i> (2012)
Organic sediment decay rate (day <sup>-1</sup> )	0.15	0.9	Sullivan <i>et al.</i> (2011)
Organic sediment burial rate (day <sup>-1</sup> )	-	-	
Theta for organic matter decomposition	-	1.045	Slaughter and Hughes (2013)
Organic matter stoichiometric coefficient for N	-	0.059	Sullivan <i>et al.</i> (2011)
Organic matter stoichiometric coefficient for P	-	0.004	Sullivan <i>et al.</i> (2011)
POM settling proportion (day <sup>-1</sup> )	0	0.5	Neilson <i>et al.</i> (2012)

## **Chapter 5: Model results**

The results include examples of the hydrological modelling components (disaggregation sub-model and baseflow separation technique) and the water quality modelling components. Finally, both hydrological and water quality are combined and analysed in the form of water quality seasonal loads.

### **5.1. Disaggregation results**

As previously discussed in Chapter 4, Slaughter *et al.* (2015) tested the disaggregation method used by the WQSAM water quality model in two catchments of South Africa, namely the CRC (Mpumalanga) and the Buffalo River Catchment (Eastern Cape). Using near perfect flows (observed flows with missing data filled in with simulated flows), they achieved acceptable NSE values (see Table 5.1, Column B) for seven catchments in the CRC. To determine the success of utilising these parameters, NSE values were calculated for disaggregated flows vs. observed flows at points where gauging stations exist. The efficiencies obtained were substantially lower than those achieved using near perfect flows, with the highest natural NSE value achieved at node X21F-2 of -0.027 (see Table 5.1, Column C).

Table 5.1 Nash-Sutcliffe Efficiencies for yield model flow monthly volumes vs. observed flow monthly volumes (A): near perfect daily disaggregations (taken from Slaughter *et al.*, 2015) (B) and yield model daily disaggregations (C).

Identifier	A		B		C	
	Yield model NSE		Near perfect NSE		Disaggregated NSE	
Catchment	Natural	Log	Natural	Log	Natural	Log
X21F (node X21F-2)	-0.042	-0.415	0.613	0.831	-0.027	0.323
X22A (node X22A-2)	-0.732	-3.289	0.862	0.939	-0.519	-2.502
X23A (node X23A-2)	-0.425	-0.769	0.637	0.842	-0.16	-0.3
X23C (node X23C-2)	-1.009	-0.611	0.539	0.851	-0.391	-0.281
X23D (node X23D-2)	-0.525	-0.791	0.494	0.858	-0.131	-0.448
X23E (node X23E-2)	-1.279	-0.108	0.632	0.902	-0.479	0.221
X24H (node X24H-1)	-1.191	-4.375	0.612	0.863	-0.69	-9.274

To identify why there is a substantial decrease in efficiencies of cumulative disaggregated flows, monthly volumes of cumulative flows were compared to monthly observed volumes. This was done as the disaggregation sub-model volume-corrects disaggregated daily flow volumes to the yield model monthly flow volumes, and a discrepancy between observed and yield model flow volumes could explain the poor disaggregation efficiencies shown in Table 5.1, Column C. The flow volumes simulated by the yield model achieved poor NSE values when compared to observed volumes (see Table 5.1, Column A). Figure 5.1 shows a short time series (approximately a year) of monthly observed flow volumes (DWS gauge X2H011) and cumulative yield model flow (at node X21F-2). The yield model flow volumes frequently deviate from the observed flow volumes (Figure 5.1). Figure 5.2 illustrates the disaggregation results for the same time period.

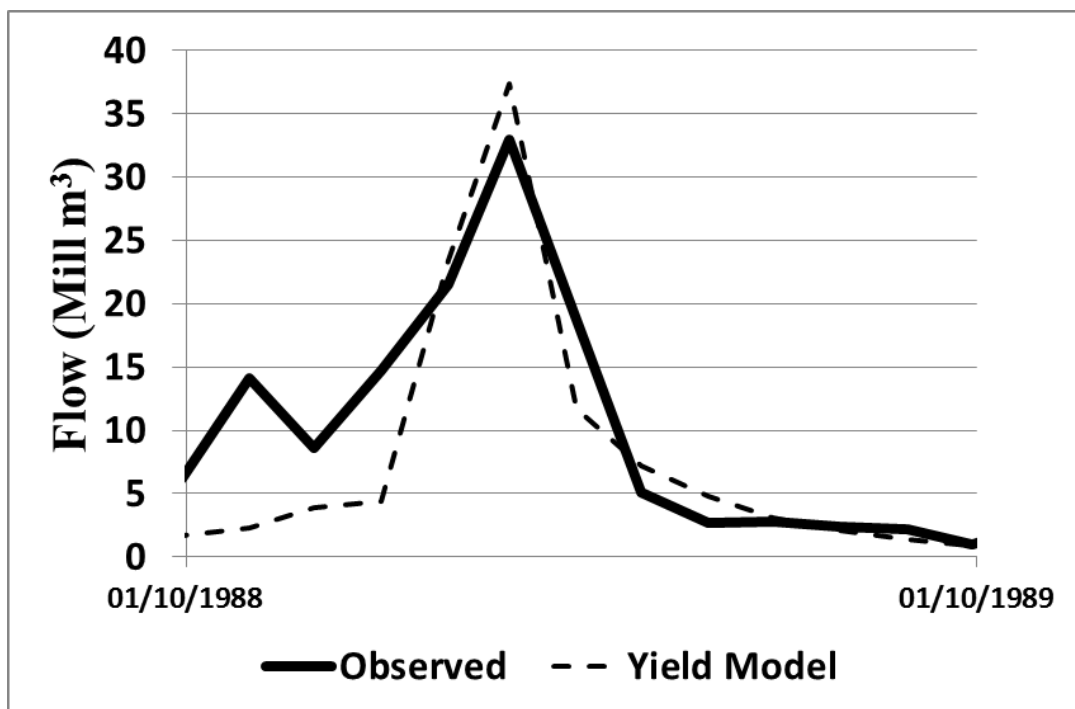


Figure 5.1 Monthly flow volumes (Mill m<sup>3</sup>) for the yield model (node X21F-2) vs. observed flow (DWS gauge X2H011).

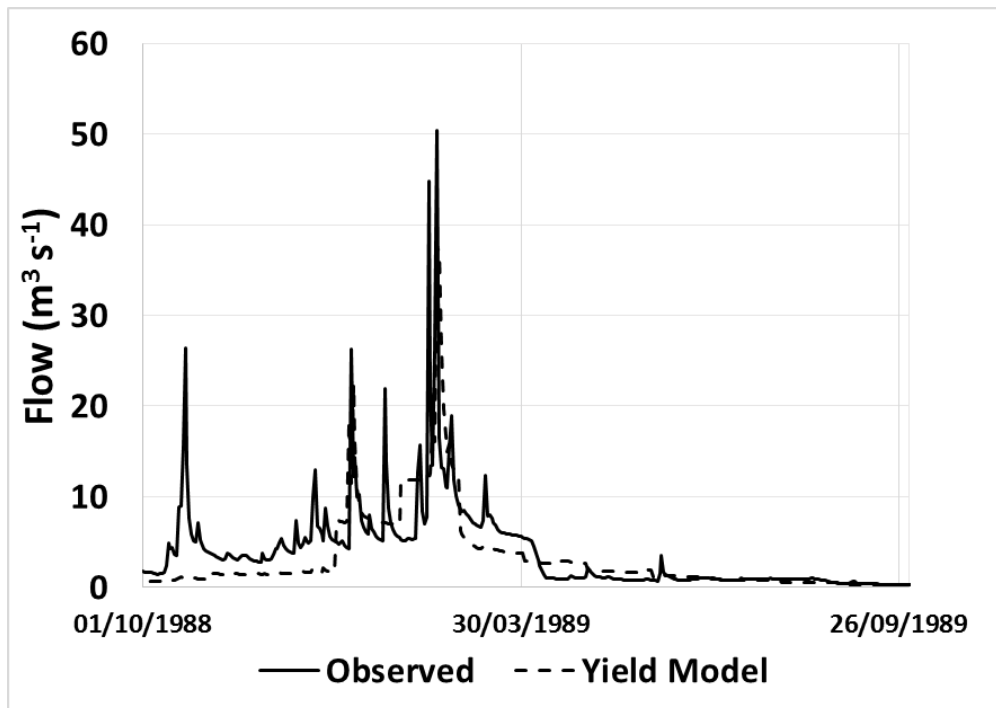


Figure 5.2 Cumulative disaggregated daily simulated flow based on yield model flows at node X21F-2 vs. observed daily flow at DWS gauge X2H011

Many of the observed flow gauging sites are located downstream of more than a single incremental flow node, and in this study, only simple accumulation of the incremental simulated daily flows was used to compare with the observed flows. However, attenuation effects within the channels and reservoirs could play a major role in affecting the time distribution of flow at downstream sites at a daily time scale, even if this not evident at monthly time scales. Figure 5.3 is a conceptual diagram which demonstrates the potential effect of attenuation. The version of WQSAM used in this study did not consider attenuation effects; therefore, some assessment of attenuation effects in the CRC is required to determine if this could account for some of the poor NSE statistics. The timing of flow was compared for upstream vs. downstream nodes using non-dimensional flow ( $\text{m}^3 \text{s}^{-1} \text{km}^{-2}$ ) hydrographs. Non-dimensional flows allow the user to compare very large flows to smaller flows on the same scale. Figure 5.4 represents non-dimensional hydrographs for observed upstream flows (at node X21F-2) and downstream flows (at node X22K-2), and there is no clear indication that attenuation is occurring on a daily scale within this part of the catchment. Similarly,

additional evaluations in other parts of the CRC did not reveal any evidence of attenuation that could account for the poor NSE statistics. The NSE monthly yield model flows vs. observed presented in Table 5.1, Column A, show that the cumulative yield model flows poorly represent observed flows. Figure 5.5 shows that some of the FDCs of yield model simulated flows fit corresponding observed FDC relatively well. Where FDC fits are very poor, such as X24H-1 where low flows are under simulated, the NSE disaggregated flow NSE is poor (see Table 4.1). It is important to note that where simulated monthly yield model flows achieved better NSE statistics, the same is seen in the disaggregation NSE statistics (see Table 4.1). Therefore, there is evidence that the poor NSE results achieved for disaggregations are linked to the representativeness of the cumulative yield model flows.

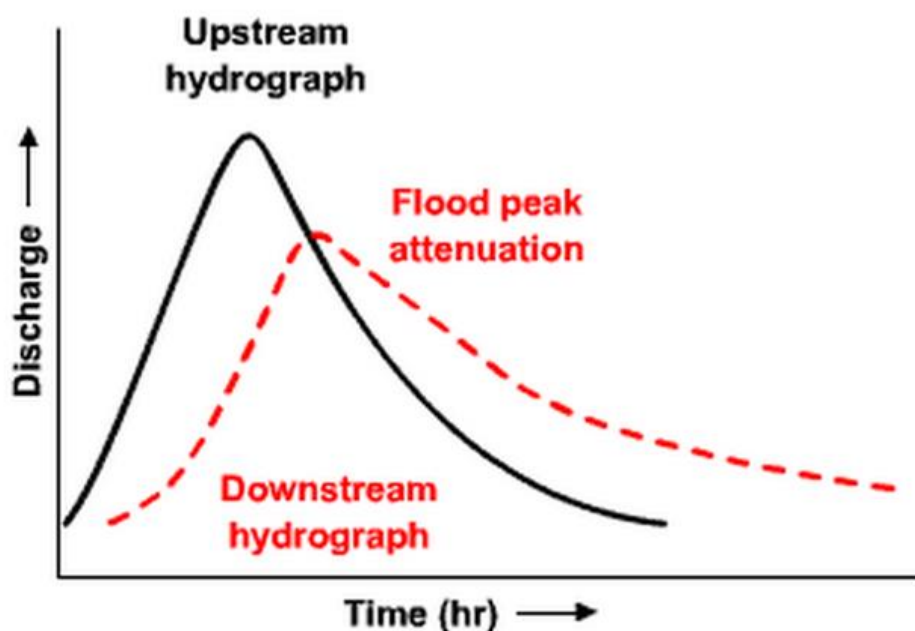


Figure 5.3 An example of a conceptual hydrograph demonstrating the influence of attenuation (taken from COMET, 2010).

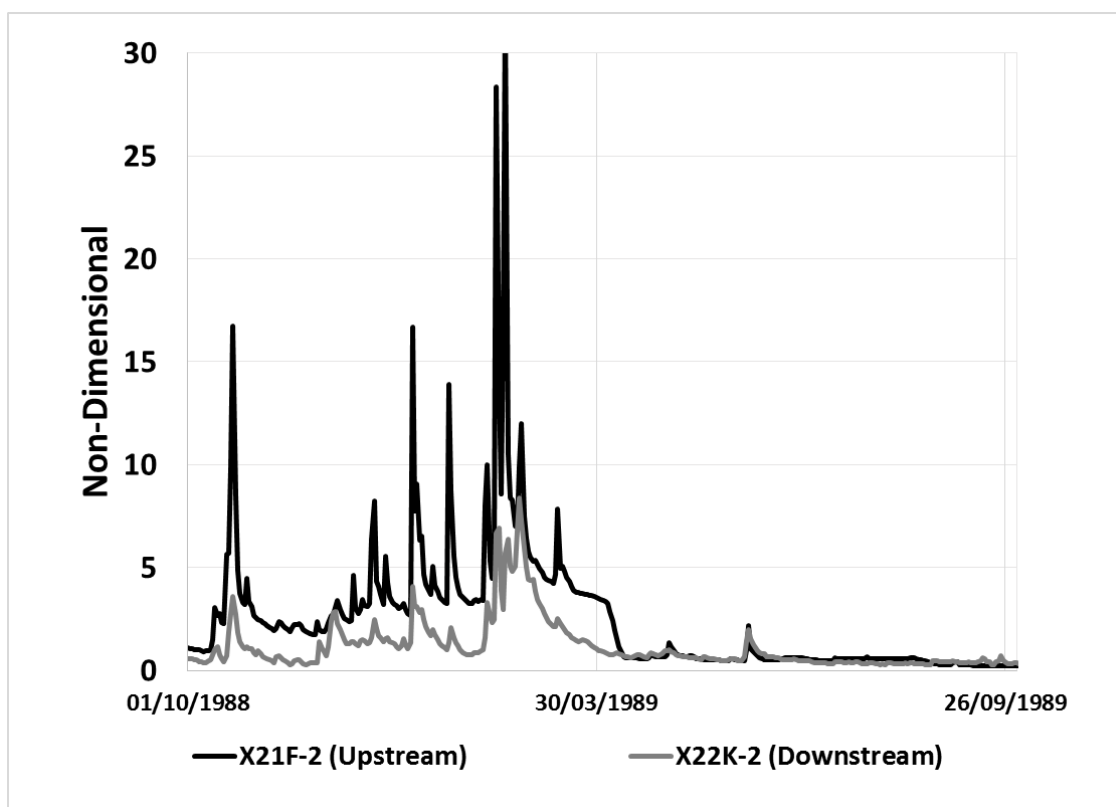


Figure 5.4 Non-dimensional hydrograph showing upstream (node X21F-2) and downstream (node X22K-2) non-dimensional observed flows

## 5.2. Baseflow separation results

The stacked area graphs shown in Figures 5.6 and 5.7 represent stream flow fractions of surface flow, groundwater flow and interflow, respectively, for an upstream node X22A-2 and a downstream node X24H-1. Figure 5.6 shows that for the upstream node X22A-2, groundwater flow has been simulated as the main contributor to total flow; contributing 71% to total flow (see Table 5.2). Groundwater contribution decreases for the downstream node X24H-1 to 41%, while surface flow and interflow contributions increase (see Table 5.2, Figure 5.7). Figures 5.6 and 5.7 also show that surface flow dominates high flows while groundwater flow dominates low flows. Surface flow responds fastest to rainfall, while interflow displays more gradual changes. Groundwater is the slowest to react, and shows the most sustained flow over changes in total flow and is present across all flow conditions (see Figure 5.8).

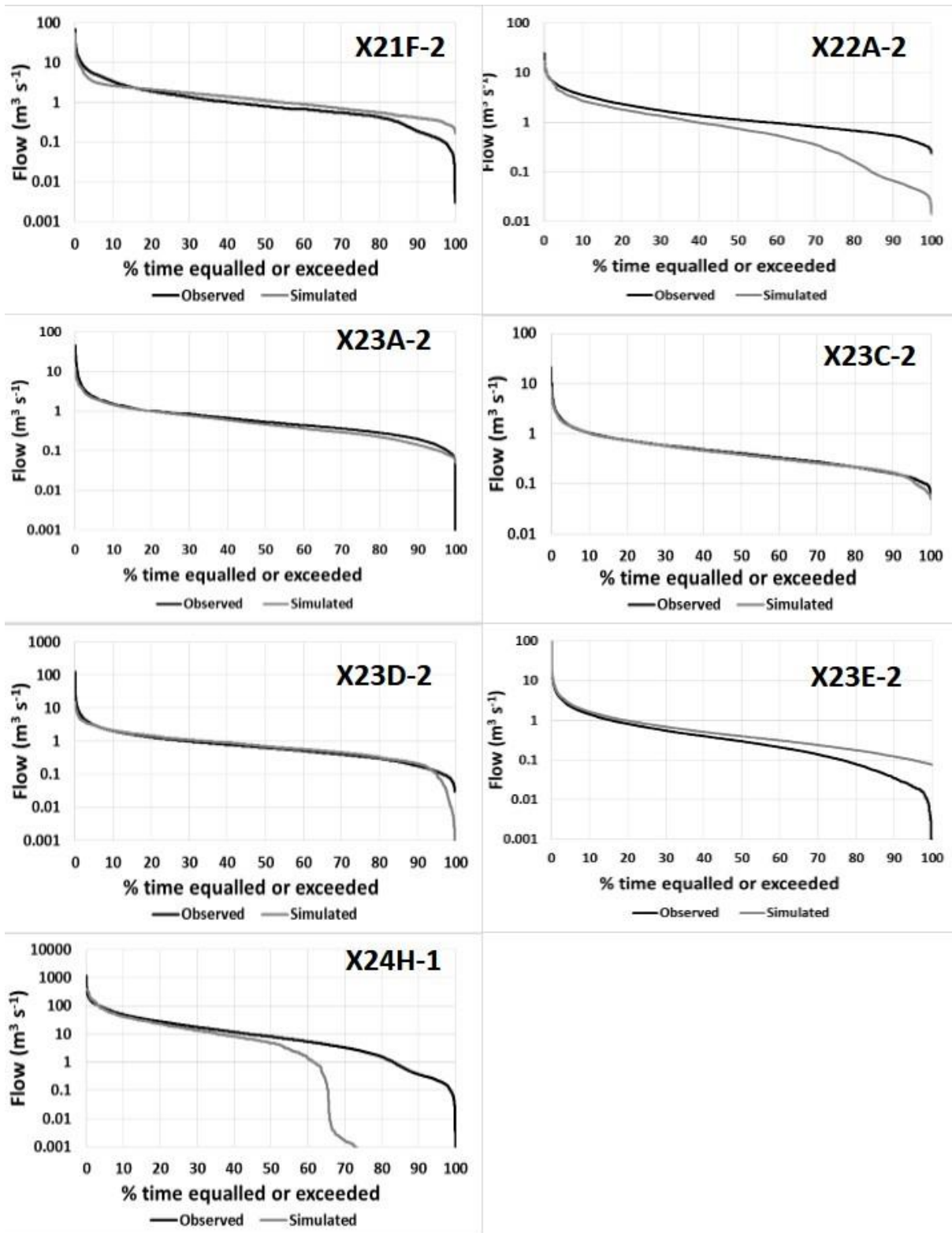


Figure 5.5 Daily flow duration curves for observed stream flow vs. cumulative disaggregated daily stream flow. Node names are presented in the top right hand corner of each graph



It is important to note that parameters for the baseflow separation sub-model were not determined through calibration, as there are no available observed data to calibrate against. Therefore, fixed parameters determined by Hughes *et al.* (2010) were used. Thus, simulated flow fraction contributions may be inaccurate. Hughes (2010) found that when modelling the Sabie catchment to the north of the CRC, the groundwater contributions varied seasonally, contributing up to 21% during wet periods and 43% during dry periods (Hughes, 2010). Therefore, contributions of 71% groundwater (see Table 5.2) may be too high, which can influence the water quality results. It may be necessary in a future study to calibrate baseflow separation parameters to ensure representative flow fraction contributions are achieved.

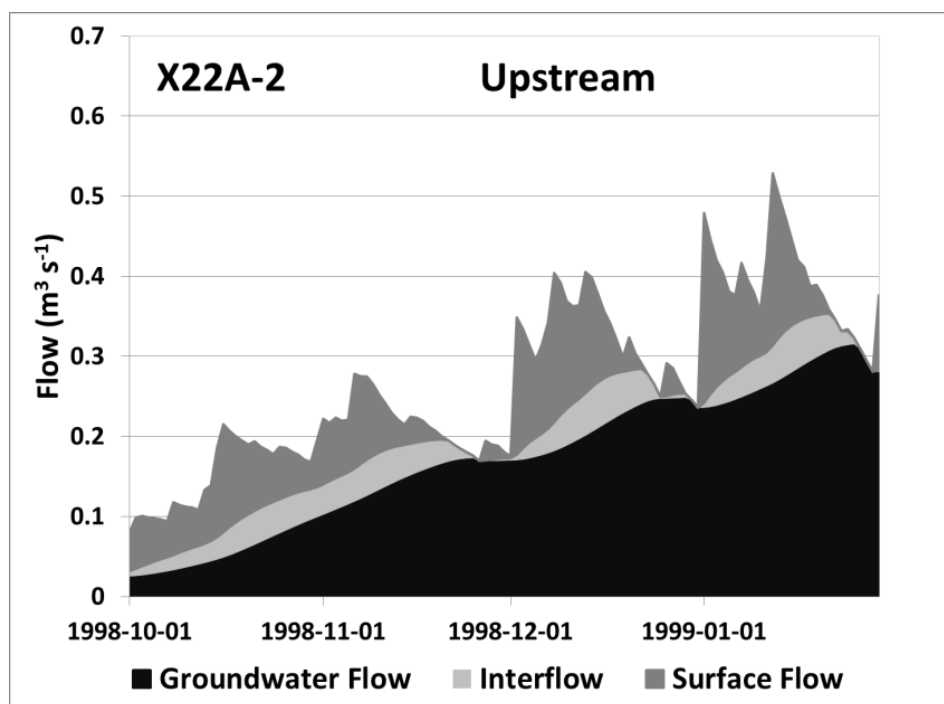


Figure 5.6 Separation of incremental stream flows coming into river node X22A-2 (upstream) on the Houtbosloop as a stacked area graph. A portion of the full simulation period is shown.

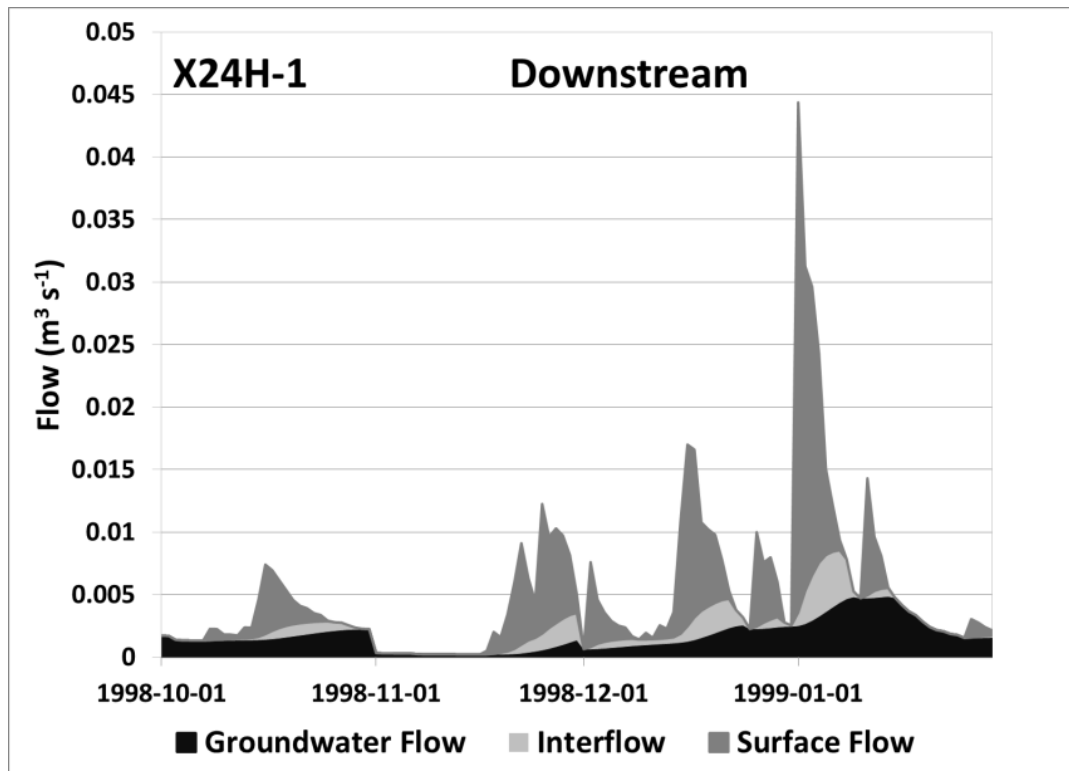


Figure 5.7 Separation of incremental stream flows coming into river node X24H-1 (downstream) on the Crocodile River as a stacked area graph. A portion of the full simulation period is shown.

Table 5.2 Percentage contribution by flow fractions to total stream flow for an upstream node (X22A-2) and a downstream node (X24H-1) for the period 1981–2004.

Node	Simulated Interflow	Simulated Groundwater Flow	Simulated Surface Flow
X22A-2 (Upstream)	8%	71%	21%
X24H-1 (Downstream)	13%	49%	38%

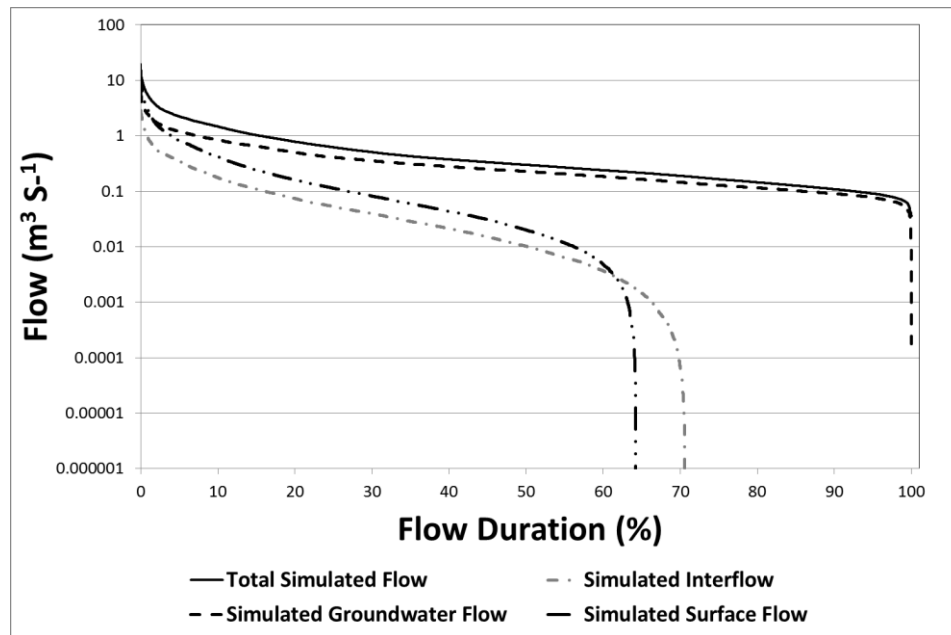


Figure 5.8 Example of baseflow separation results for node X22A-2 (upstream) showing simulated total stream flow and, surface, groundwater and interflow as flow duration curves.

### 5.3. Temperature sub-model results

As observed water temperature data are sparse within the CRC, at only a few nodes could the model be calibrated against observed water temperature data (see Figure 5.9). The model simulations are generally representative of observed water temperature, achieving NSE values ranging from 0.76 to 0.96 based on average monthly temperatures.

### 5.4. Water quality calibration results

The water quality model simulation period covered the full simulation period by the yield model (i.e. up to 2004), as the majority of the available water quality data sets covered the period 1981–2004 (see Chapter 4; Table 4.1). The modelling procedure comprised calibrating parameters for the first 10 years (period 1981–1991), and then validating those parameters for the period 1991–2004. The calibration/validation approach is a standard modelling procedure to validate/verify model parameters, although the approach has also been criticized (Oreskes *et al.*, 1994). However, in this study, the use of the calibration/validation approach was also used to determine if static water quality parameters could be used in WQSAM, especially when increasing trends in water quality concentrations are evident within some of the sub-catchments in the CRC. Calibration of all water quality constituents was guided by the NSE

statistic calculated for values at selected quantiles on the observed and simulated concentration frequency distributions (i.e. 1%, 10%, 20% etc.). This approach (rather than comparing individual time series values) was adopted for three reasons. Firstly, there are relatively few observed water quality data values. Secondly, this approach avoids the problems associated with poor correspondence between individual daily observed and simulated flow values. Thirdly, the main objective of the water quality model is to simulate the frequency characteristics of the different quality components. All results for calibration and validation are presented in Appendix C. Nodes that had more than 50 observed data samples for the calibration period (1981–1991) and validation period (1991–2004) were analysed (see Table 5.3). This section presents representative examples taken from all the results provided in Appendix C.

Table 5.4 presents the results for the calibration period 1981–1991 for all calibrated water quality constituents. Reasonable calibration results were achieved at most nodes with NSEs for TDS ranging from 0.8 to 0.98, nitrates + nitrites from 0.49 to 0.93, ammonium from 0.31 to 0.88 and phosphates 0.3 to 0.92 (see Figure 5.10). Klipkoppie Dam achieved reasonable simulations for TDS and phosphates (with NSEs of 0.72 and 0.83, respectively), with less representative simulations of nitrates + nitrites and phosphates achieving NSEs of 0.35 and 0.46, respectively.

The validation (period 1991–2004) results show highly variable NSEs (see Table 5.5) with some nodes achieving relatively sound NSEs for the validation, such as TDS at node X23HGauge and nitrates + nitrites at node X23E-2 (see Figure 5.11, A and B). However, the majority of the validation simulations showed a decrease in NSEs (e.g. TDS at node X21K-2 and nitrates + nitrites at node X22A-2; see Figure 5.11, C and D) relative to the calibration period. The large variations in NSEs for a number of the nodes may be as a result of either development impacts or issues related to the way in which the model represents processes. Therefore, nodes that achieved poor validation results were recalibrated for the period 1991–2004 starting with parameter values achieved in the calibration period (1981–1991), and only the loading parameters were changed keeping process parameters the same until an optimal fit was achieved. The results for the recalibration period 1991–2004 are presented in Table 5.6.

The simulated time series for the period (1981–1991) were concatenated with the time series for the period (1991–2004) to give a simulated time series for all water quality constituents

for the full period 1981–2004. The concatenated time series were used to calculate monthly simulated loads. The percentage deviations from the mean monthly observed loads versus mean monthly simulated loads were then determined (see Figure 5.12). A negative percentage deviation indicates that the observed load is smaller than the simulated load (and vice versa for positive percentage deviations). In some cases monthly loads were over-simulated (e.g. TDS and phosphates at node X21F-2, see Figure 5.13) and drastically under-simulated (e.g. ammonium and phosphates at node MontroseFalls, see Figure 5.13). The best seasonal fits for TDS were at node X23HGauge, nitrates + nitrites at node X21K-2, ammonium at node X23HGauge and phosphates at X24H-1 (see Figure 5.13.).

Water quality simulations that achieve poor fits for concentration frequency curves and/or seasonal fits may be caused by a number of factors that are interlinked. These include incorrect flow volumes from the yield model and/or inaccurate volumes of baseflow contribution. In addition, lack of observed data make fitting concentration curves difficult, as seen in Figure 5.10 where  $\text{NH}_4\text{-N}$  observed data are sparse, resulting in an incomplete observed concentration frequency curve with a detection limit of  $(0.02 \text{ mg } \ell^{-1})$ . Catchment activities such as, land use and management might be continuously changing which may influence in-stream water quality; these processes are not represented within WQSAM, as static signatures are assigned to parameters which would result in poor validation results. These results are discussed in further detail in the Chapter 6, with a discussion on why these results were achieved and how they relate to the use of WQSAM as a WQDSS aiding the IWQMP in the CRC.

## Chapter 5: Model results

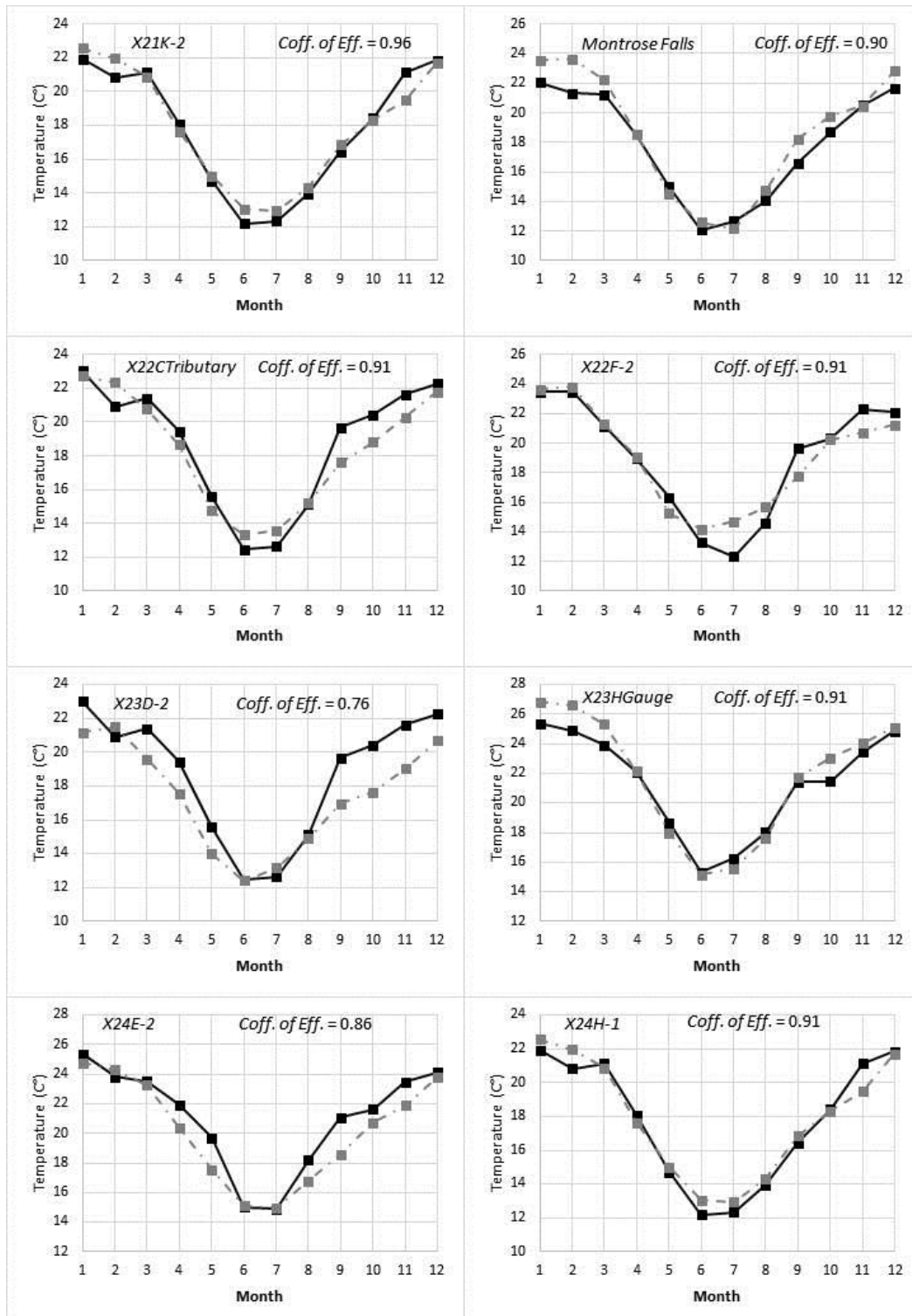


Figure 5.9 Examples of seasonal water temperature graphs showing simulated in grey and observed in black. Node name appears in the top left hand corner of each graph with the Nash-Sutcliffe coefficient of efficiency to its right

## Chapter 5: Model results

Table 5.3 Overview of data availability for all nodes linked to water quality gauging stations. Nodes highlighted in grey failed to meet the criteria of >50 samples with observed flow present.

Node	River Name	WQ Gauging Station	Flow Data Present	Number of observed records for periods	
				1981–1991	1991–2004
KlipkoppieDam	White River	X2R02	Dam	61	97
KwenaDam	Crocodile	X2R05	Dam	10	127
LongmereDam	White River	X2R01	Dam	37	101
MontroseFalls	Crocodile	X2H013	Yes	444	314
PrimkopDam	White River	X2R04	Dam	35	101
WitklipDam	Sand River	X2R03	Dam	28	75
X21D-2	Crocodile	X2H033	Yes	158	8
X21F-2	Elands	X2H011	Yes	72	310
X21K-2	Elands	X2H015	Yes	451	486
X22A-2	Houtbosloop	X2H014	Yes	157	135
X22CTributary	Rietspruit	X2H031	No	153	139
X22E-1	Kruisfonteinspruit	X2H035	Yes	6	6
X22F-2	Nels	X2H005	Yes	157	249
X22H-3	White River	X2H023	Yes	153	8
X22J-2	Crocodile	X2H006	Yes	99	215
X22K-2	Crocodile	X2H032	Yes	434	465
X23A-2	Noordkaap	X2H010	Yes	153	139
X23C-2	Suidkaap	X2H024	Yes	60	1
X23D-2	Suidkaap	X2H031	Yes	153	139
X23E-2	Queens	X2H008	Yes	152	135
X23HGuage	Kaap	X2H022	Yes	452	242
X24A-2	Nsikazi	X2H072	Yes	6	101
X24E-2	Crocodile	X2H017	Yes	444	329
X24H-1	Crocodile	X2H016	Yes	452	627

Table 5.4 Table of Nash-Sutcliffe model efficiency coefficients for simulated vs. observed data for the calibration period (1981–1991).

Node	Nash–Sutcliffe model efficiency coefficient for calibration period (1981–1991)			
	TDS	NO3-N + NO2-N	NH4-N	PO4-P
KlipkoppieDam	0.72	0.35	0.46	0.83
MontroseFalls	0.93	0.49	0.78	0.3
X21F-2	0.83	0.78	0.48	0.51
X21K-2	0.91	0.85	0.26	0.91
X22A-2	0.8	0.83	0.88	0.85
X22F-2	0.84	0.82	0.48	0.75
X22J-2	0.98	0.83	0.91	0.85
X22K-2	0.92	0.66	0.39	0.77
X23A-2	0.95	0.89	0.31	0.92
X23D-2	0.92	0.71	0.4	0.63
X23E-2	0.93	0.84	0.65	0.8
X23HGuage	0.95	0.88	0.79	0.87
X24E-2	0.91	0.75	0.64	0.75
X24H-1	0.95	0.93	0.72	0.62



Table 5.5 Table of Nash-Sutcliffe model efficiency coefficients for simulated vs observed data for the validation period (1991–2004).

Node	Nash–Sutcliffe model efficiency coefficient for validation period (1991–2004)			
	TDS	NO3-N + NO2-N	NH4-N	PO4-P
KlipkoppieDam	0.51	0.06	-0.04	0.5
MontroseFalls	0.86	0.69	0.4	-0.11
X21F-2	-0.71	0.02	0.26	-0.48
X21K-2	-1	0.34	0.58	0.11
X22A-2	0.61	-1.44	0.36	-0.11
X22F-2	0.69	0.25	0.71	-0.09
X22J-2	-0.11	-9.03	-1.43	-0.08
X22K-2	0.01	-2.73	0.84	-0.46
X23A-2	0.49	0.35	0.73	0.7
X23D-2	0.88	-0.42	0.67	0.13
X23E-2	0.81	0.92	0.91	0.1
X23HGuage	0.97	0.63	0.56	0.41
X24E-2	0.73	-0.86	0.04	-0.12
X24H-1	0.63	0.69	0.96	0.06

Table 5.6 Table of Nash-Sutcliffe model efficiency coefficients for simulated vs observed water quality data for the re-calibration period (1991–2004).

Node	Nash–Sutcliffe model efficiency coefficient for re-calibration period (1991–2004)			
	TDS	NO3-N + NO2-N	NH4-N	PO4-P
KlipkoppieDam	0.45	0.49	0.56	0.79
MontroseFalls	0.86	0.89	0.65	0.89
X21F-2	0.83	0.84	0.91	0.83
X21K-2	0.92	0.79	0.77	0.8
X22A-2	0.61	0.76	0.66	0.94
X22F-2	0.74	0.86	0.71	0.97
X22J-2	0.83	0.94	0.82	0.82
X22K-2	0.62	0.73	0.87	0.75
X23A-2	0.87	0.79	0.79	0.7
X23D-2	0.88	0.96	0.86	0.87
X23E-2	0.81	0.92	0.81	0.79
X23HGuage	0.97	0.91	0.94	0.74
X24E-2	0.84	0.95	0.79	0.95
X24H-1	0.77	0.92	0.89	0.8

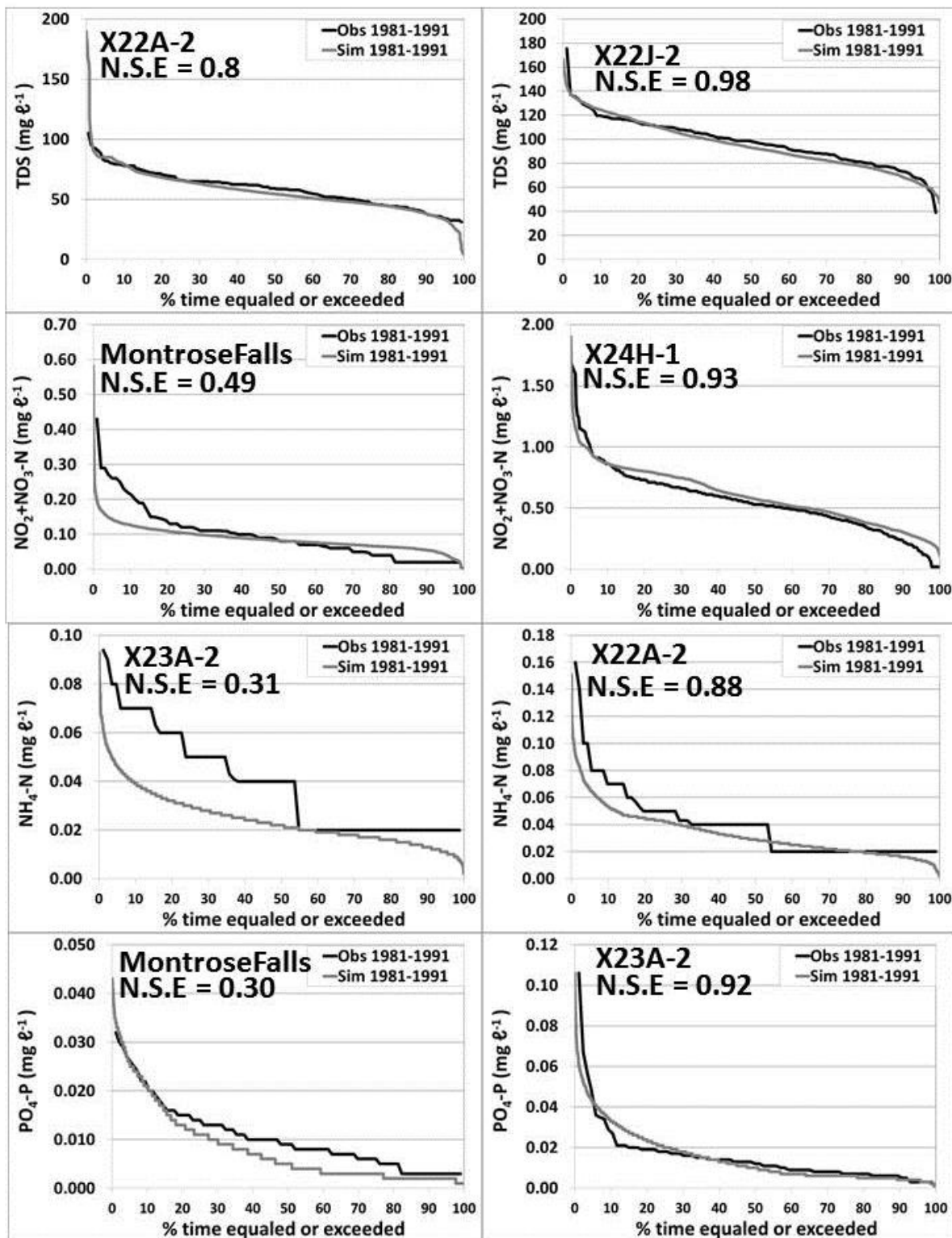


Figure 5.10 Frequency distribution graphs showing examples of calibration results (for period 1991–2004). Worst fits are depicted on the left vs. best fits on the right for TDS,  $\text{NO}_2 + \text{NO}_3$ ,  $\text{NH}_4$  and  $\text{PO}_4$ . Node name is represented in the top left hand corner of each graph with the Nash-Sutcliff coefficient of efficiency (NSE) below it.

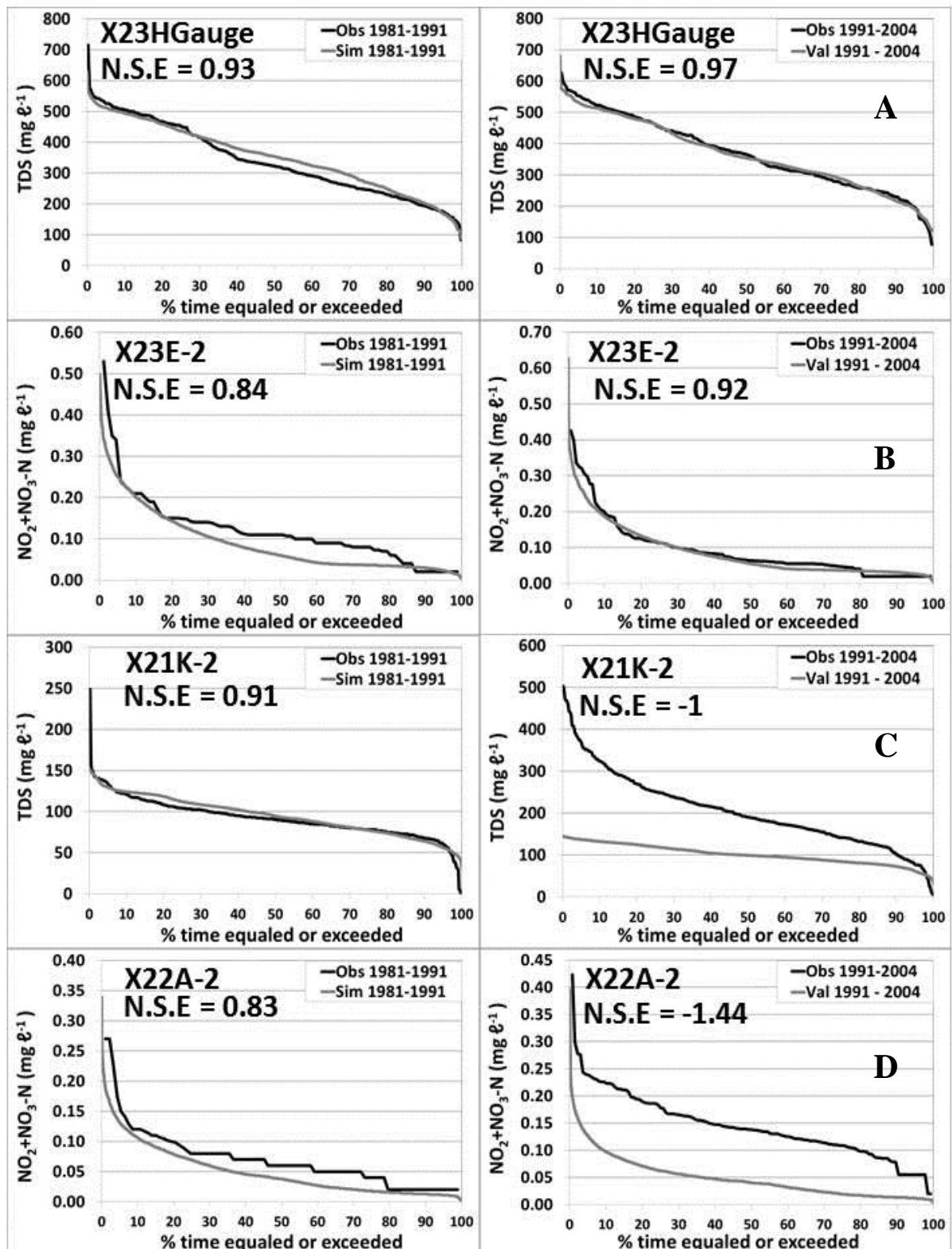


Figure 5.11 Frequency distribution graphs showing examples of validation results exhibiting little change (A and B) and major changes (C and D) in efficiencies. Node name is represented in the top left hand corner of each graph with the Nash-Sutcliffe Coefficient of efficiency (NSE) below it.

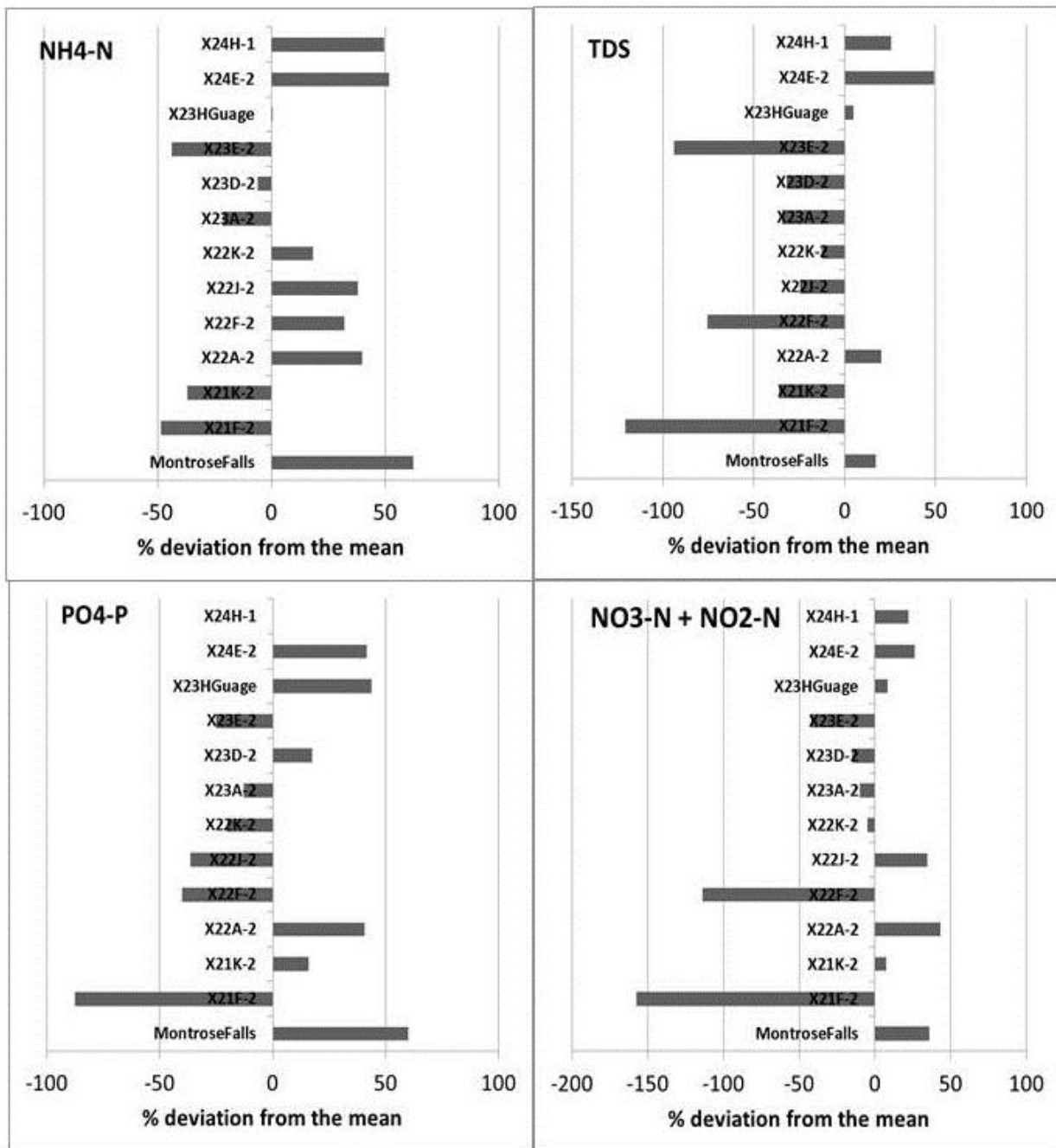


Figure 5.12 Deviation from the mean percentages for simulated vs observed monthly loads for NH<sub>4</sub>-N, TDS, PO<sub>4</sub>-P and NO<sub>3</sub>-N + NO<sub>2</sub>-N for the entire simulation period (1981–2004).

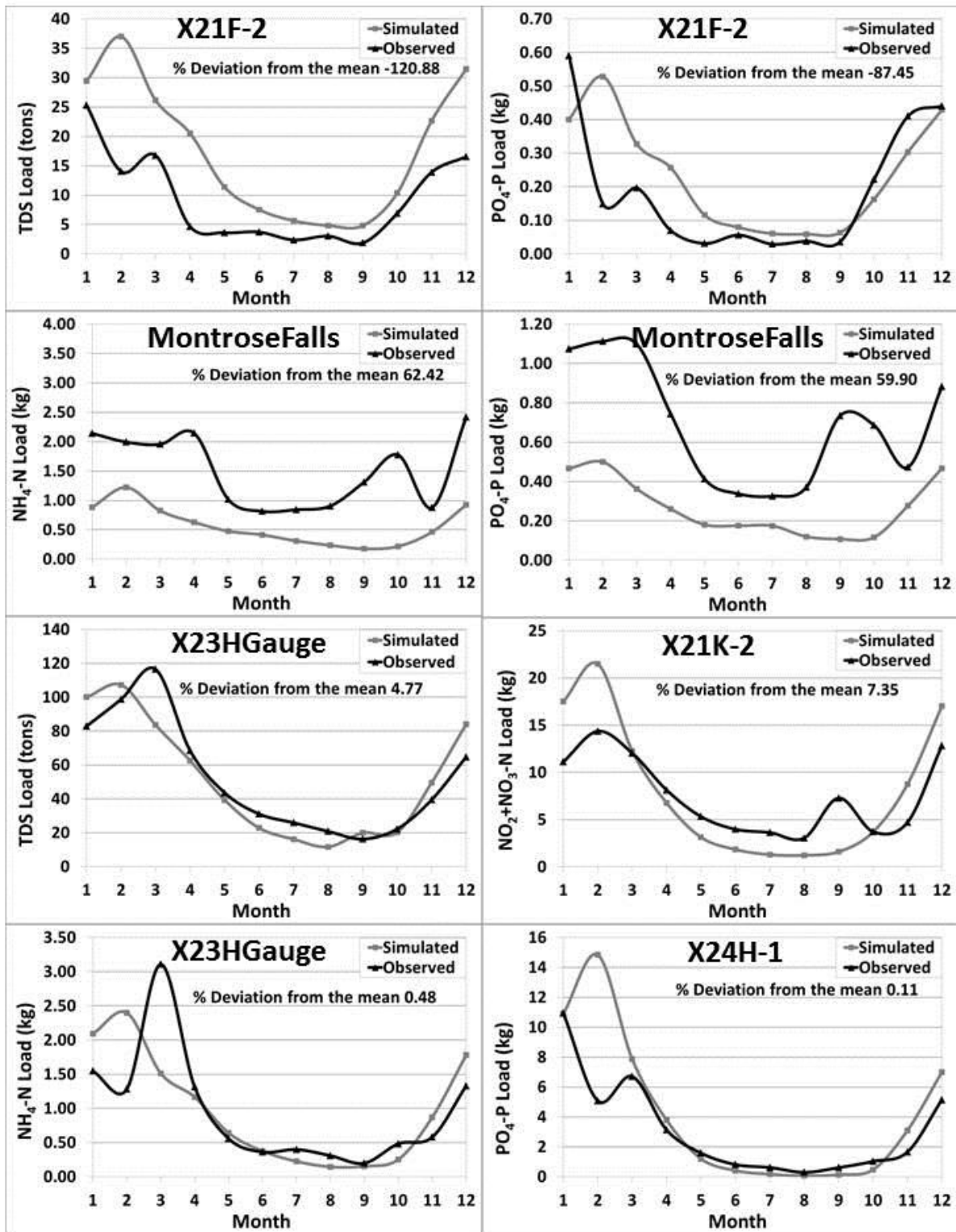


Figure 5.13 Seasonal load graphs showing mean monthly observed and simulated loads. Node name is represented in the center of each graph with the percentage deviation from the mean below it.

## **Chapter 6: Discussion and conclusions**

The applicability of water quality modelling for water management is affected by many factors. Huang and Xia (2001) discussed three of these factors. Firstly, water quality management processes are complex in nature, with many inter-relationships that cannot be expressed by mathematical formulas, while non-linearity that exists in these systems are often difficult to effectively simulate. Secondly, the lack of information to accurately assign parameter values requires the modeller to assign values based on implicit knowledge. Therefore, the model may only be useful for part of a decision support system and should be viewed as one of several tools providing the information necessary to make management decisions. Thirdly, the uncertainty related to water quality models is difficult to quantify, which might deter resource managers from utilising such models for management. The following sections address the two overarching questions raised in Chapter 1 which were: 1) can WQSAM generate simulations of water quality that are appropriate for management requirements and; 2) can the outputs be used for future scenario analysis to facilitate water quality management planning within the CRC?

### **6.1. WQSAM model data requirements**

Marsili-Libelli and Giusti (2008) state that one of the major challenges of modelling is the availability of data required to run and calibrate models. Even in developed countries, complex models often require additional sampling additional to what is already available. For this reason, Halfon (1983) and Beck (1987) advocate the use of simpler models, with the model structures being designed to derive crucial information from available data. The data constraints associated with modelling can almost always be linked to the scale at which a modeller is working, and the complexity of the model being applied (Borah and Bera, 2003). While WQSAM's governing development paradigm was to maintain a level of requisite simplicity, it was designed to be used at the catchment scale (rather than a single river reach) and therefore, will inherently require a large extent of data to be collated. In addition, the development process for WQSAM recognised the importance of functioning on a daily time step due to transient event influences on water quality. Therefore, the added complexity and data requirements for disaggregating monthly yield model flows to daily flows cannot be avoided, as simulating at a monthly time step would not capture sufficient temporal variation in water quality. Averaging water quality over monthly time steps would not provide sufficient information about the likely extremes of the frequency distributions of water

## Chapter 6: Discussion and conclusions

quality that managers would need to identify thresholds of potential concern. All the minimum data needed to set up WQSAM were successfully acquired and Table 6.1 lists the data availability in the CRC in relation to the minimum data requirements of WQSAM.

Table 6.1 Overview of the temporal and spatial availability of data in the CRC required by WQSAM.

Data Required	Availability	Temporal Resolution	Spatial Resolution	Notes
TDS	Always	Monthly	> Quaternary	Calculated from Electrical Conductivity which is the most commonly measured water quality constituent
NH <sub>4</sub> -N	Occasionally	Monthly	> Quaternary	Not commonly measured with far fewer samples than TDS. Large number of samples with the value of the detection limit
NO <sub>3</sub> -N + NO <sub>2</sub> -N	Occasionally	Monthly	> Quaternary	
PO <sub>4</sub> -P	Occasionally	Monthly	> Quaternary	
Daily Rainfall	Always	Daily	Sub-Quaternary	Ground based rainfall is available on daily resolution however, there are large temporal gaps in the available datasets.
Daily Flow	Always	Daily	> Quaternary	
Water Temperature	Seldom	Monthly	> Quaternary	While water temperature is the least expensive to measure, there are large temporal gaps in the datasets, especially in regards to monitoring reservoirs
Air Temperature	Always	Daily	Sub-Quaternary	Database available is currently out of date, only covering up until year 2000.

Difficulties encountered with data collection for the CRC model setup included some large temporal gaps in water quality data sets, data format differences and the sheer extent of data



needed. The SAWS rainfall data have many missing values, and therefore, the Lynch (2004) rainfall database was used. This reduced the extent of effort required to collate the required rainfall data. However, the missing data in the original weather station data of the SAWS has been ‘infilled’ from that of neighbouring weather stations, so the rainfall data from the Lynch database may not always capture the spatial and temporal variability in rainfall. Ndomba *et al.* (2008) applied the SWAT model in a data scarce catchment in Tanzania, and found that reliable rainfall data had a major influence on the model simulation accuracy. When calibrating the model, the more observed data WQSAM has access to, the more representative the simulations will be, as the observed data represents a greater span of events. However, the model can use relatively small amounts of data with an associated increase in uncertainty. Since the model is designed to simulate only the most critical processes affecting water quality, the uncertainty associated with the lack of data is expected to be less than for a more data intensive and complex model, a similar result found by Marsili-Libelli and Giusti (2008).

## **6.2. The advantages and disadvantages of adding a water quality model to an existing monthly yield model**

Monthly yield models are the water resource management standard in South Africa and have been deemed adequate for simulating non-naturalised flows for water resource management and planning. Consequently, there are monthly yield model setups for most economically important catchments in South Africa, such as the CRC. Since these systems models are accepted and trusted within water resource management, it makes sense for a WQDSS to link to an existing yield model, rather than try and re-create the water quantity simulations (an approach supported by Borah and Bera, 2003 and Wilby *et al.*, 2006). Using a yield systems model representation of a catchment has advantages for management as well, as management can link water quantity from any node of interest to the water quality simulations. By linking to an already existing yield model, the water quality modeller has access to the knowledge and experience of flow modelling. However, the water quality results are therefore also dependent on the uncertainties and errors that exist in the simulated flow volumes.

The structure of the WReMP yield model for the CRC was determined by a hydrologist as well as ecologists (e.g. creating environmental water requirement nodes) working with the Inkomati-Usuthu Catchment Management Agency (IUCMA). Basing the structure of the WQSAM model on an already integrated yield model is highly beneficial as the yield model

has been interrogated and accepted by stakeholders in the catchment. There will always be a reliance on reliably simulated hydrology, regardless of whether a water quality model is integrated with an existing yield model or whether the quality model simulates the hydrology of the catchment independently. WQSAM relies on sound hydrological simulations in order to representatively simulate water quality. Inevitably, uncertainty in the yield model simulations are carried through into the WQSAM water quality simulations. As WQSAM functions on a daily time step, monthly flows have to be disaggregated to daily, which has proved to be time consuming and sometimes challenging where there is a lack of available flow and rainfall data. However, it is important to note that if WQSAM were not integrated with the WReMP systems model, it would be required to generate its own daily systems flow information and systems structure, and would be faced with inevitable issues of flow and rainfall data uncertainty.

One key dilemma caused by linking the WQSAM model to a yield model is that the spatial representation and resolution that are relevant to water quantity management, might not be relevant for water quality management. This is evident from the way the WReMP model setup sometimes groups several return flows at one node (e.g. grouping all return flows from Nelspruit), which may be adequate for simulating water quantity, but may be problematic from a water quality point of view. This disadvantage would be more evident if one of the intended uses of WQSAM were to assist in assigning TMDL allocations. Therefore, it is crucial that water quality modellers using WQSAM should communicate with yield modellers to ensure the systems setup is adequate for both sets of objectives and methods.

In catchments that exhibit a great deal of flow attenuation, downstream disaggregated simulated flows would be too peaked, as the yield model does not need to account for daily attenuations due to its monthly time step. At the time of the study, the attenuation component of WQSAM was still under development and was not available for use in this project. However, comparison of observed flow hydrographs for the upstream and downstream nodes in the CRC did not show any evidence of attenuation at the daily scale, and therefore, the lack of an attenuation component in WQSAM is not expected to present a problem in this study. It is possible that attenuation does occur at the sub-daily time scale, but simulating such effects is beyond the resolution of WQSAM.

A more important issue affecting the success of the water quality simulations is the accuracy of the yield model monthly flow volume simulations. While the current version of the yield

model for the CRC has been accepted by the stakeholders, this study has demonstrated that for the purposes of water quality modelling, some aspects of the simulations require improvement. It is quite possible that the monthly volume simulations were assessed for their ability to estimate yields at different points in the system and found to be adequate. However, there are parts of the system where the yield model low flow simulations do not match the present day observed flow conditions in the river (see Figure 5.1). These poor monthly simulations have had an impact on the ability of WQSAM to simulate daily flows and consequently on the water quality simulations. While the daily flow simulations are therefore partly dependent on the available daily rainfall data and the WQSAM disaggregation parameters, they are also dependent on the reliability of the monthly flows simulated by the yield model.

### **6.3. Baseflow separation sub-model overview**

Chapter 2 outlined the importance of incorporating the various components of stream flow into a water quality model, as different sources of stream flow (surface, interflow and groundwater flow) carry different loads of water quality constituents that will contribute to the final in-stream water quality concentrations (Kebede, 2013). The WQSAM baseflow separation technique separates the disaggregated incremental flows into the three stream flow components, with the user having to enter two parameter values (Hughes *et al.*, 2003). The resulting separated stream flow components are used to simulate diffuse sources of water quality variable load inputs. For example, for urban areas the surface incremental flow should have elevated phosphate and nitrate signatures, and to a lesser extent the interflow and groundwater flow. Agricultural practices would suggest an elevated nitrate signature in surface flow and to a lesser extent interflow and groundwater flow (as noted during high flow events by Bowes *et al.*, 2008). Groundwater is strongly influenced by geological origin with higher TDS concentrations being associated with underlying geology of marine origin (as found by Day *et al.*, 1998).

The lack of reliable information on the relative contributions of the three stream flow components in various parts of the CRC precluded any attempts at calibrating the base flow separation parameters. Fixed baseflow parameters were therefore assigned to all nodes throughout the CRC, and these generated results which are consistent in some ways with expected variations in the relative contribution of the three stream flow components (Figure 5.6 and 5.7). In upstream nodes stream flows are groundwater dominated and

downstream nodes are dominated by a combination of surface and interflow (Cey *et al.*, 1998; Sear *et al.*, 1999). However, some of the upstream groundwater contributions are overestimated compared to values suggested by Hughes (2010) based on data from similar catchments in the Sabie River basin to the north. Variations in the contributions of the three components are caused by a number of factors (topography, geology, soil and vegetation cover). Improvements in the baseflow separation parameters could be achieved by targeted investigations in different parts of the catchment that could include hydrological modelling, hydrograph analysis of observed flows and water quality and isotope studies (Kapangzawiri *et al.*, 2011). However, these analyses were beyond the scope of this research.

#### **6.4. Temperature sub-model overview**

Rivers-Moore *et al.* (2008) applied four simple linear regression models to simulate water temperature in four major river systems across South Africa. The models varied in their number of parameters, one including all parameters thought to relate to processes influencing water temperature including air temperature, flow and relative humidity, while another only included parameters related to air temperature. They found that only air temperature had a significant influence on water temperature within these South African catchments, and this model was incorporated into WQSAM. It has been found that while river water temperature simulations are relatively accurate, reservoir water temperature simulations are not. The reason for this is that the water temperature model component within WQSAM does not take into account reservoir stratification, but if this were to be included, the complexity and data requirements of the model would drastically increase.

The temperature model achieved sound results for simulated river water temperature for the CRC (Figure 5.9). However, it is important to note that parameters were calibrated against incomplete water temperature datasets as temperature is not routinely measured and do not achieve the recommended minimum of one monthly sample. This may result in an incomplete or misrepresented seasonal temperature graph, with a maximum of 24 samples representing each calendar month of the simulation period (1981 to 2004) if once-monthly samples were available. Therefore, fitting seasonal curves during calibration can be difficult, as an observed average monthly temperature can be skewed by an abnormally high or low sample value. While the model achieved relatively good monthly averages, individual daily observations were not always well simulated.

### 6.5. Overview of simulated water quality

The WQSAM model achieved representative water quality concentration frequency distribution simulations for most water quality constituents for the majority of subcatchments where observed data were available (Figure 5.10). The best results were achieved for the conservative variable TDS, and the worse for the non-conservative nutrients. Being conservative, TDS remains chemically unchanged throughout its life span in a river and simulating TDS therefore only requires simple dilution and mass-balance modelling with few parameters (Slaughter, 2011a). However, nutrient chemical forms, are constantly changing under the influence of various interlinked processes; therefore, modelling non-conservative variables requires additional parameters, which introduces additional uncertainty associated with the simulations. The validation results indicate that there is very little consistency within the catchment with simulated water quality not achieving optimal fits to observed water quality for some of the nodes (see Table 5.5). While the validation exercise, as described by Oreskes *et al.* (1994) was conducted to test the model parameterisation, it can also be used to evaluate the water quality process representation in the model and the underlying assumptions made during the model setup. In this sense, the unsatisfactory outcomes for many of the validation results can be attributed to using static water quality loading parameters in a system that exhibits both stationarity and non-stationarity in water quality across a 24 year period (see Figure 6.1) Trend analyses for all the DWS gauges used can be found in Appendix D. The development of non-static water quality signatures to account for the non-stationarity of systems had not been developed yet at the time this research was conducted.

Where non-stationarity was present (Figure 6.1 A), WQSAM achieved poor NSE values for validation results (e.g. X21K-2 NSE = -1), while sound results (e.g. X23HGauge NSE = 0.97) were evident where stationarity was present (Figure 6.1 B). It is important to note that sound validation results were obtained for simulations that showed stationarity over a time period of  $\pm 10$  years. Cyclical trends are present within shorter time periods that may not be accurately captured by the model, as seen by the polynomial trends (e.g. Figure 6.1) for all DWS monitoring stations (see Appendix D). This is similar to what Jarvie *et al.* (2001) found when applying the INCA model to European catchments, with the model representing long term periods well but being less accurate for short term simulations.

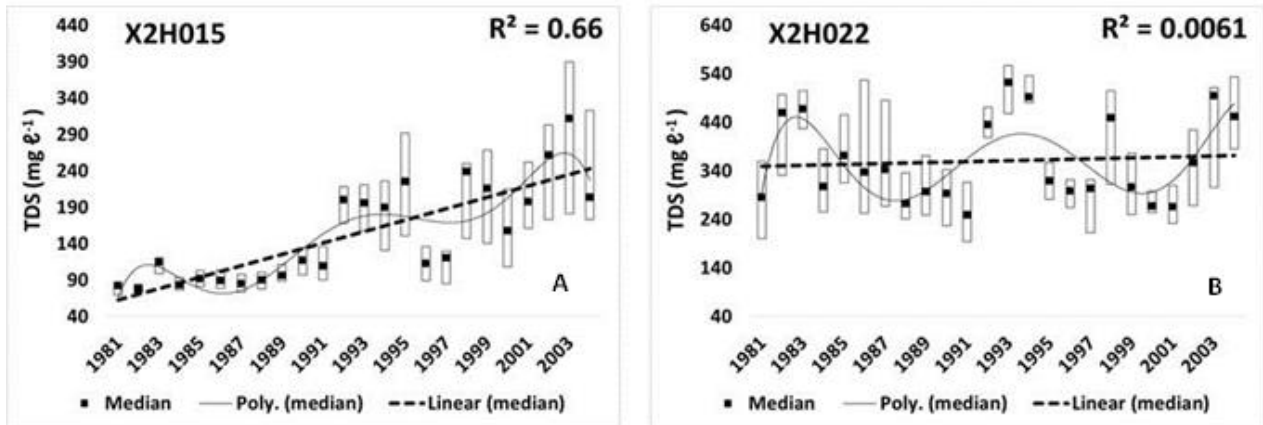


Figure 6.1 Observed water quality box plots showing polynomial and linear trends for DWS gauges X2H015 (linked node X21K-2) showing evidence of non-stationarity and X2H022 (linked to node X23HGauge) showing stationarity.

While using concentration frequency distribution curves for calibration and validation is useful, as a single assessment method, it is not entirely representative of simulation reliability. The water quantity component of WQSAM plays a critical role in simulating water quality, and these should not be considered independently. Some of the seasonal load distributions (Figure 5.13) showed that WQSAM can adequately capture the variability of relationships between water quantity and quality (Figure 5.12). However, there were nodes that achieved sound concentration frequency distribution fits but poor seasonal load fits (see Node X21F-2 Figure 5.13). There are a number of possible explanations for this result:

1. simulated water quantity discrepancies (inaccuracies in the yield model flow volumes and baseflow separations);
2. lack of observed data and detection limits and;
3. variable return flows in reality (while the model simulates fixed return flows).

Discrepancies in water quantity (Figure 6.2, Label A) result in poor water quality simulations (Figure 6.2, Label B) as seen at node X24H-1 where the yield model undersimulates the low flow conditions and therefore the loads at low flows.

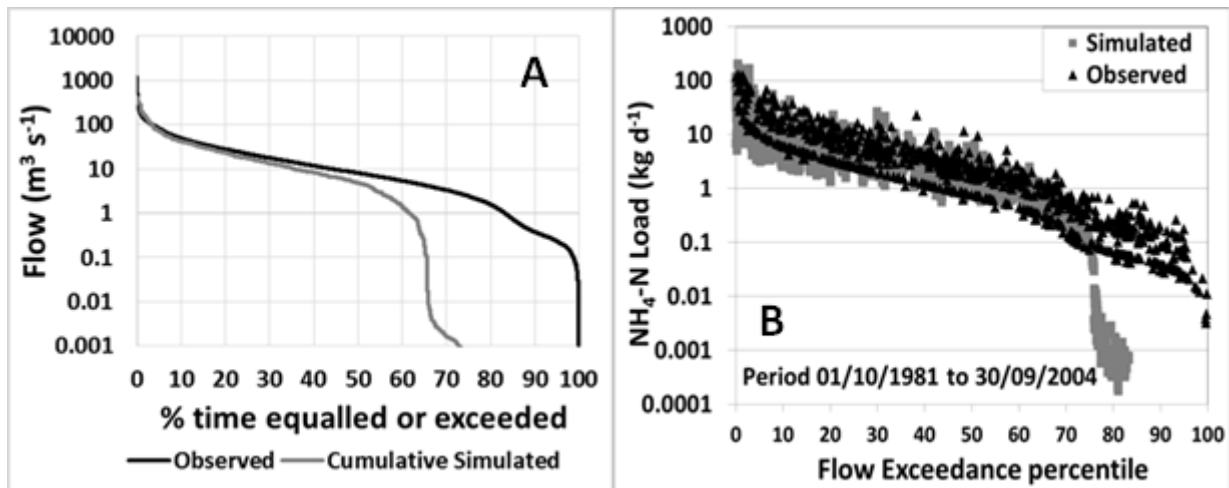


Figure 6.2 A) Daily flow duration curve showing observed vs. cumulative simulated flows for node X24H-1 (DWS gauge X2H016), B) Load duration curve showing observed vs. simulated  $\text{NH}_4\text{-N}$ .

The use of a range of analysis techniques may help identify incorrect parameterisation or inaccuracies in the underlying stream flows as shown in Figure 6.3 (Label B) where the primary contribution of  $\text{PO}_4\text{-P}$  according to the observed load distribution indicates non-point source surface contributions, as loads increase with flow (this was demonstrated by Bowes *et al.*, 2008). Based on user calibrated parameters, the simulated loads suggest that the primary contribution is groundwater or return flow in origin (see Figure 6.3, Label A). This discrepancy may indicate that the model was assigned either a groundwater or return flow concentration signature that is not representative of the observed data, resulting in the oversimulation of low flow loads (Figure 6.3, Label A). One other cause may be that the baseflow separation has produced an incorrect groundwater volume resulting in oversimulated loads of  $\text{PO}_4\text{-P}$  during low flow conditions. While water quality signatures may be easily recalibrated, there are no observed data available to calibrate the baseflow separation parameters. Therefore, it is vital for a water quality modeller to analyse results not only as concentrations, but to also include the stream flow component and analyse loads, which can drastically affect the conclusions reached about the success of the simulations.

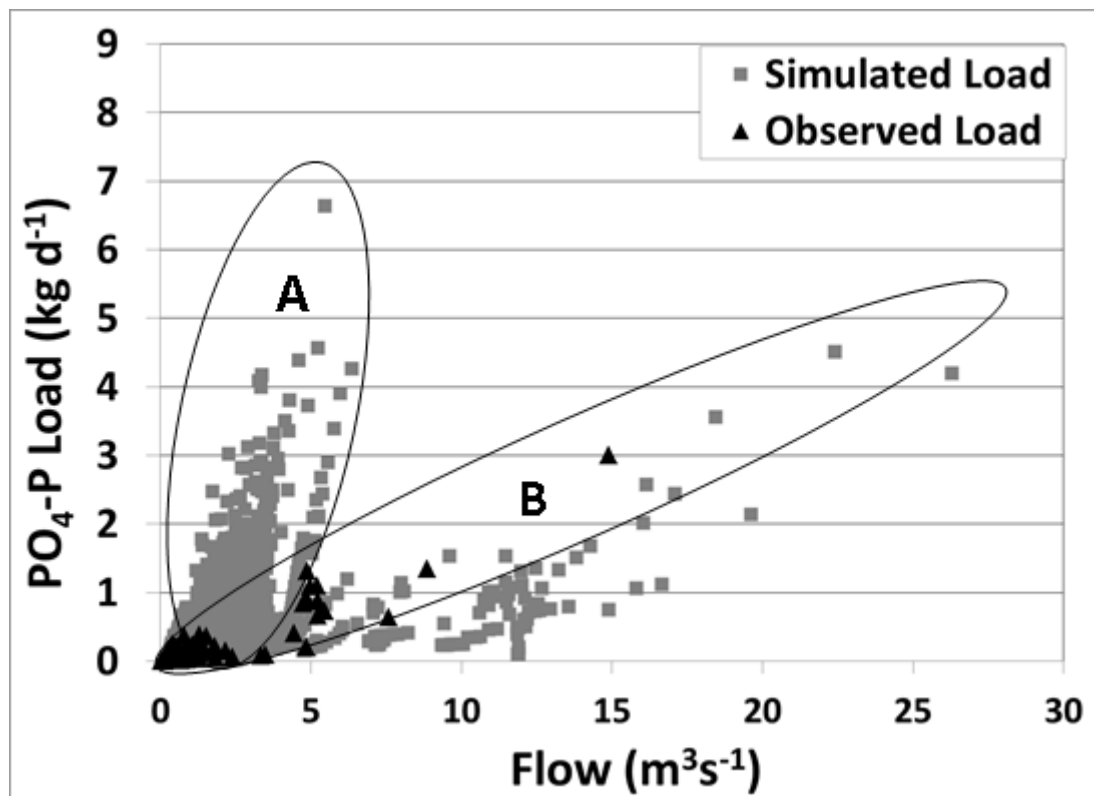


Figure 6.3 Graph showing PO<sub>4</sub>-P load (Observed and Simulated) vs. Flow (Observed and Cumulative Simulated). A) Groundwater and return flow source water quality, B) surface flow source water quality.

The LDCs of observed data presented in Chapter 3 (Figures 3.14 to 3.19) show that more water quality readings are captured during low flows than high flow conditions. This may result in under- or over-simulating of high flow water quality, as the model is typically calibrated to the observed concentration frequency curve. The simulated values for certain nodes in the CRC demonstrate poor seasonal fits to the observed data, primarily due to the variable return flow concentrations that result in inconsistent observed seasonal water quality distributions. An example is shown in Figure 6.4 for a node located below Nelspruit, where the observed data shows no distinct seasonal relationship. These observed patterns of variation in water quality are thought to be partly the result of processes that are not included in the model. An example is the possible variation in return flow volumes and concentrations from WWTWs (Slaughter and Hughes, 2013a) (the model assumes fixed values for both).



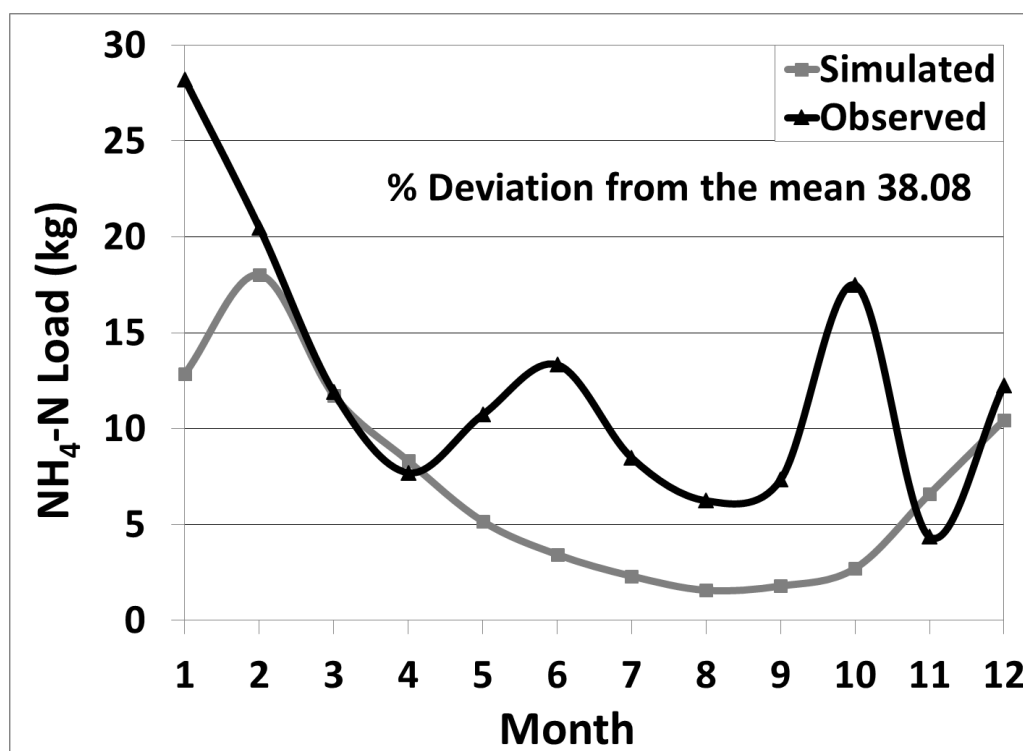


Figure 6.4 Seasonal distribution of observed vs. simulated average loads at node X22J-2. (The percentage deviation from the mean shows how far a simulation, on average, will deviate from the observed average (mean) with a positive percentage indicating an under-simulation)

### 6.6. Using WQSAM as a tool for management and the development of the IWQMP

The development of the Integrated Water Quality Management Process (IWQMP) consists of engagement with a number of water user stakeholders on a quarterly basis. In the early development phase of the IWQMP, the WQSAM model was proposed at a stakeholder meeting to address the overarching concerns raised during interviews in 2012 with regards to understanding water quantity and quality collectively to determine water quality compliance or non-compliance (JSM, 2013; Palmer *et al.*, 2013). The stakeholders were asked to propose which water quality variables should be simulated by the model. A number of variables were mentioned including nutrients, salts, manganese and pH (JSM, 2013). The model developer's aim was to maintain a requisite level of simplicity to retain the usefulness of the model in a South African management context. Therefore, due to data constraints and requisite simplicity, the model was proposed to simulate nutrients as  $\text{NH}_4$ ,  $\text{NH}_3 + \text{NO}_2$ ,  $\text{PO}_4$  and total dissolved solids (TDS) as indicative of salinity. It was also proposed that the model would be

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used where possible to address any of the eight principal issues which needed to be investigated for the development of the IWQMP as identified by the stakeholders:

1. the performance of waste water treatment works (WWTW).
2. disposal by irrigation of pulp and paper effluent.
3. nutrient enrichment (agriculture and WWTW).
4. accelerated sediment production (forestry).
5. dissolved manganese and iron (mining).
6. to identify and integrate diverse monitoring programmes and data.
7. to harmonise various water quality standards used by diverse industries.
8. to identify accredited analytical laboratories.

The likelihood of any water quality model including WQSAM simulating water quality constituents that are appropriate at all scales for all management contexts is low. This was demonstrated in the Core Stakeholder Meetings (CSM), with stakeholders highlighting the inability of WQSAM to model manganese and pH. With one stakeholder going as far as saying “a water quality model that does not simulate a key water quality variable within a catchment such as manganese for the sake of simplicity, defeats the purpose of a model in that context” (CSG, 2014b). That point was discussed in the meeting and the general recommendation reached was that a suite of different models be used to address the wide range of water quality variables of concern, such as specific salts (e.g. TEACHA model developed by Sebastian Jooste) or manganese.

It is not an uncommon practice for managers to use a suite of models, combining the use of a complex model such as the QUAL2K model for localised studies (covering a wide range of water quality variables) and a catchment scale model such as BASINS (covering a narrow range of water quality variables) commonly used in the TMDL process (Borah and Bera, 2003). It would be difficult to attempt to model a variable such as manganese in the CRC at this stage, as the DWS does not currently monitor manganese, and additional monitoring would be required to provide calibration data. WQSAM was developed to simulate water quality constituents that happen to be reasonably well represented in the observed monitoring data. Heath *et al.* (2010) describe the difficulties of setting up and maintaining effective

monitoring programmes in South Africa, as all sectors (agricultural, industry, domestic use and environmental requirements) are impacted by a wide range of different water quality variables, as is evident amongst the CRC stakeholders. However, running extensive and comprehensive monitoring programmes can be expensive and time consuming, therefore compromises are inevitably necessary.

To determine if WQSAM produced the simulated information that would be appropriate for the development of the IWQMP, we need to identify what the IUCMA is responsible for in the CRC as described in the Catchment Management Strategy (see summary CMS Table 6.3). In line with the CMS objectives, WQSAM could be used as a decision support system tool to address a number of the CMS sub strategy objectives (see Table 6.2).

Table 6.2 Summary of CMS sub-category objectives WQSAM may help to achieve.

<b>CMS Sub strategies</b>	<b>WQSAM possible capabilities</b>
<b>Resource Protection (RDM):</b>	Aid in determining compliance in relation to meeting Resource Quality Objectives (RQOs).
<b>Regulating water use (SDC):</b>	Aiding in the understanding of assimilation capacities of rivers for present and future scenarios, and to aid in discharge licensing.
<b>Information and Monitoring:</b>	Providing a collective database of all historical hydrological (flow and rainfall) and water quality data sets for the CRC.

Stakeholders see value in WQSAM not only as tool for simulating future water quality scenarios based on hydrological changes simulated by the WReMP model, but also as a decision support system (CSG, 2014a). As a WQDSS, WQSAM can provide reliable analyses of observed and simulated water quality in the form of concentration and load frequency curves, a process which would otherwise be time consuming. WQSAM could therefore provide stakeholders and the IUCMA with the capabilities of in-house analysis for effective compliance monitoring in accordance with the RQOs (see Figure 6.5 and 6.6). In addition, the issue of the current discharge licences being a fixed concentration limit regardless of seasonality (CSG, 2014a) was highlighted by the environmental control officer. The control environmental officer recommended that the WQSAM model could be used for

creating an understanding of assimilation capacities of rivers and assigning dynamic load targets to ensure RQOs are met, with an emphasis on controlling WWTW discharges (CSG, 2014a). This would be similar to the use of water quality models such as SWAT and BASINS, in the United States to investigate Best Management Practice (BMP) and aid in the development of TMDL standards.

### **6.7. Conclusion, limitations and recommendations**

The National Water Act recognises that protection of the quality of water resources is necessary to ensure sustainability of the nation's water resources in the interests of all water users, and aims to facilitate this protection through integrated management practices. The IWQMP aims to provide the IUCMA with the tools and knowledge to achieve integrated catchment management through a facilitated process with stakeholders. This research set out to explore the use of an integrated water quality and quantity model as a tool for integrated catchment management. WQSAM represents a relatively simplified approach to water quality modelling, developed to address management requirements for South African conditions, and was used to address the scientific requirements of the IWQMP. The specific research questions to be answered:

1. Is it acceptable to link existing water quantity models to WQSAM?
2. Are the water quality constituents modelled by WQSAM appropriate to water quality management requirements?
3. Does the available data in the CRC meet WQSAM's minimum data requirements?
4. Does WQSAM produce water quality information that is appropriate for the development of the IWQMP?

Table 6.3 Structured objectives and strategic actions of the Inkomati- Usuthu Catchment Management Agency (IUCMA) Catchment Management Strategy (CMS) (taken from IUCMA, 2010).

Red Text: Highest ICMA Priorities		OBJECTIVES					
		Practical IWRM to achieve equitable, sustainable, and efficient uses of Inkomati water resources which meet evolving stakeholder needs and legal obligations					
		A sustainable water resource		Collaborative and coordinated IWRM for wise socio-economic development		Secure financial arrangements for IWRM	
Sub Strategies Strategic Action Programmes	WRM Sub Strategies		Integration Sub Strategies	Facilitation Sub Strategies			
	Resource Protection (RDM)	Regulating Water Use (SDC)	Cooperative Governance & Institutions	Stakeholder Engagement	Information & Monitoring	Finance	
Achieving equity		<ul style="list-style-type: none"> <li>- Establish a viable, up to date and transparent system for water authorisation.</li> <li>- Develop a first Generation Water allocation plan</li> <li>- Implement Water Allocation Reform</li> </ul>	<ul style="list-style-type: none"> <li>- Coordinate activities to increase access to water for resource poor farmers</li> <li>- Facilitate innovative solutions to the water services backlog.</li> </ul>	<ul style="list-style-type: none"> <li>- Establish participatory IWRM decision-making process.</li> <li>- Facilitate empowerment programmes.</li> <li>- Establish Water User Associations.</li> </ul>		<ul style="list-style-type: none"> <li>- Develop and implement a realistic and cost effective process for processing water use licence applications.</li> </ul>	
Water Availability and Flow Management	<ul style="list-style-type: none"> <li>- Facilitate the progressive, and stakeholder centred implementation of the Reserve.</li> </ul>	<ul style="list-style-type: none"> <li>- Consolidate systems for integrated planning and operations of river systems</li> </ul>	<ul style="list-style-type: none"> <li>- Promote coordinated river operations.</li> <li>- Decrease water losses and increase water use efficiency</li> </ul>	<ul style="list-style-type: none"> <li>- Establish and maintain appropriate River Operations Committees.</li> <li>- Ensure Reserve processes are transparent and inclusive.</li> </ul>	<ul style="list-style-type: none"> <li>- Research systems, for integrated river operations.</li> <li>- Monitor progressive realisation of the Reserve and international obligations.</li> </ul>		
Managing water quality	<ul style="list-style-type: none"> <li>- Support DWA to classify the resource</li> </ul>	<ul style="list-style-type: none"> <li>- Consolidate and implement workable</li> </ul>	<ul style="list-style-type: none"> <li>- Institute a cooperative spatial/</li> </ul>	<ul style="list-style-type: none"> <li>- Ensure implementation of</li> </ul>	<ul style="list-style-type: none"> <li>- Implement accessible and</li> </ul>	<ul style="list-style-type: none"> <li>- Implement Waste Discharge system to</li> </ul>	

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Table 6.3 continued. Structured objectives and strategic actions of the Inkomati- Usuthu Catchment Management Agency (IUCMA) Catchment Management Strategy (CMS) (taken from IUCMA, 2010).

	and setting Resource Quality Objectives  - Implement the above	procedures to determine license conditions for wastewater disposal.	develop. planning for water sustainability  - Manage pollution incidents.  - Prevent further water quality degradation.	Resource Quality Objectives and Reserve are transparent and inclusive.	transparent water quality and ecosystem monitoring systems.	cover costs of managing quality of the water resource
<b>Generating and managing knowledge</b>			- Build knowledge sharing networks nationally and internationally.	- Embed systems of social co-learning / co-generation of knowledge into IWRM decision-making processes.	- Identify monitoring & information Institutions  - operationalise learning reflection and review system  - Participate in IWRM networks etc.  - Learning Strategy	
<b>Achieving compliance and enforcement</b>	- Ensure the necessary monitoring requirements for compliance are implemented	- Consolidate clear and realistic standards which different types of water use must be compliant  - Ensure appropriate Enforcement of the different water uses	- Investigate enforcement needs and methods  - Develop transparent system for dealing with transgressors.	- Awareness and education to help with mindset changes.	- Operationalise transparent and accessible systems for monitoring compliance, and actions against transgressors	- Ensure cost recovery from transgressors in terms of Sections 19 and 20 of National Water Act
<b>Generating revenue</b>					- Audit for transparent and directed use of IWRM funding.  - Operationalise payment monitoring	- Investigate and develop realistic mechanisms through which water use charges can be implemented.

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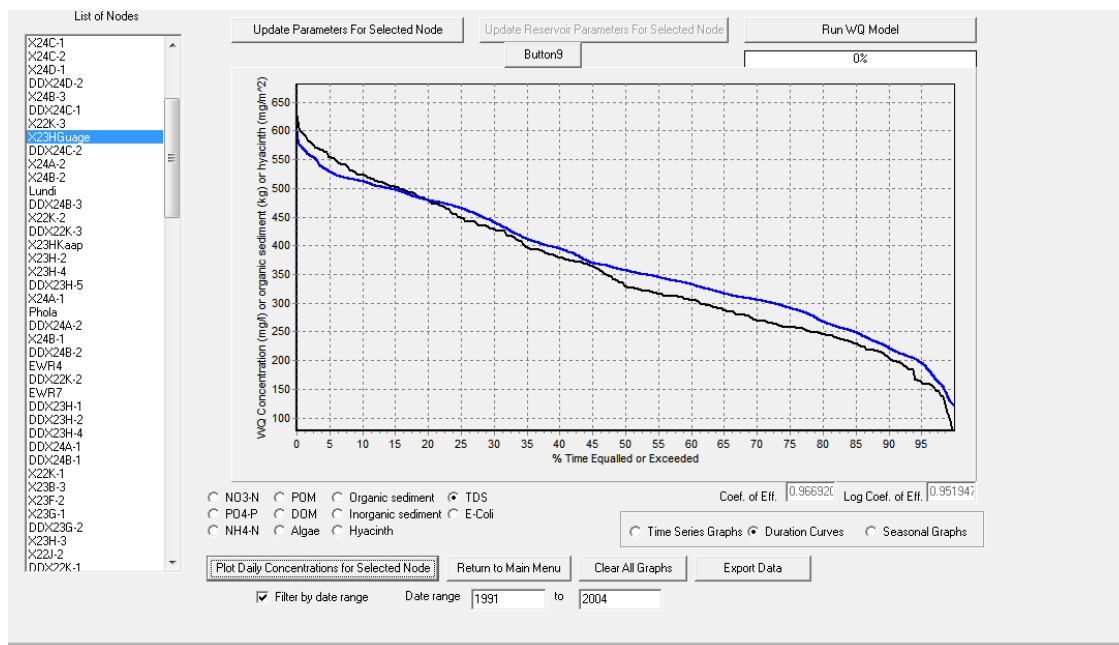


Figure 6.5 Screenshot of WQSAM user interface showing the Frequency Distribution utility. Black line represents observed water quality; blue line represents simulated water quality.

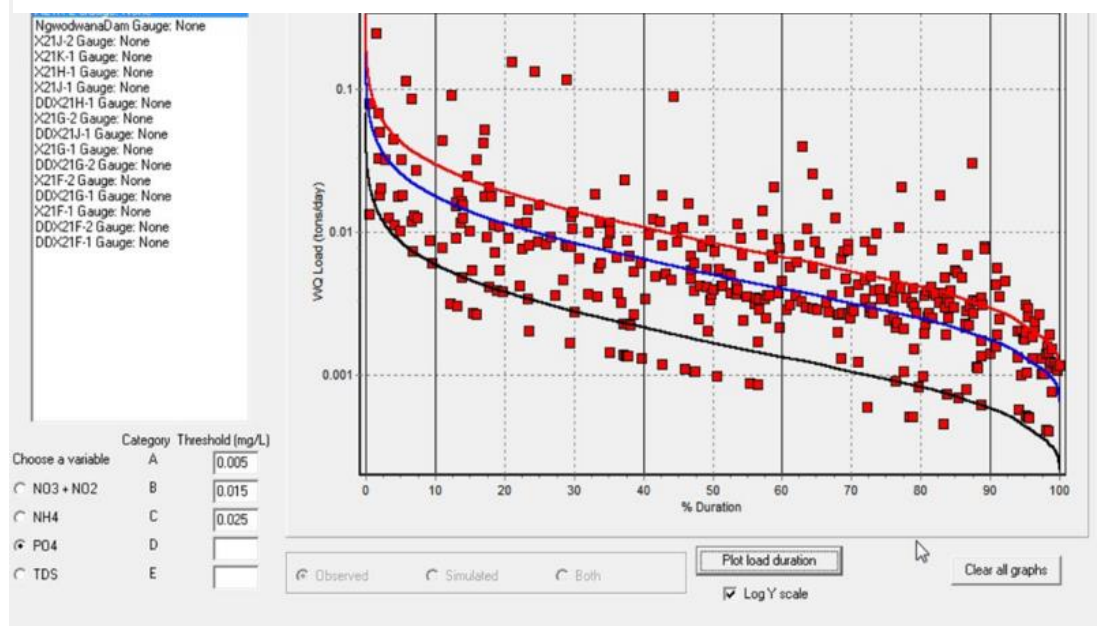


Figure 6.6 Screenshot of WQSAM user interface showing the automated Load Duration Curve (LDC) utility. Red squares represent observed loads, continuous lines (Black, Blue and Red) relate to Resource Quality Objectives input as concentration thresholds.

### **6.7.1. Answering research questions**

The minimum data requirements required to run WQSAM in the CRC were met, aided by the benefits of linking an existing water quantity model, fulfilling flow and structural system requirements. However, it is important to note that although the yield model simulations may be deemed adequate for quantity management, there were a number of issues related to its use in the CRC for water quality simulations. These included poor volume simulations which could be linked to non-stationarity as the yield model is calibrated for a specific time period (e.g. present day) even though its simulations spanned from 1920 to 2004. Secondly, the yield model lumps all return flows as a single return flow, which may be an issue for managers wanting to deal with specific return flows of concern. However, it is equally important to note that without the integration of the yield model, WQSAM would be required to simulate its own hydrology and create the required nodal structure. This would result in a large investment of time using the same uncertain data used to establish the yield model.

While the model only simulates a few water quality constituents and their critical processes, it was able to produce acceptable simulations for the time periods ( $\pm 10$  years) where the observed data are largely stationary and the underlying hydrology was sound. While the model at the time of the study did not simulate all the water quality constituents required for integrated water management, the constituents simulated were deemed important by stakeholders, especially with regard to managing WWTW discharges. Furthermore, value was seen in WQSAM as a WQDSS with not only the model simulations being useful, but the analysis it provides for both observed and simulated data as well. In addition how they can be used to help monitor compliance with RQOs once they had been established for the CRC. It is important to note that water quality modelling is a simplification of highly complex systems and therefore, cannot be seen as a comprehensive representation of a water resource system. Nevertheless, WQSAM was able to provide increased understanding of complex interactions, such as between water quality and quantity, which is required for IWQMP to be successful, and identified as a critical information gap in the CRC.

### **6.7.2. Limitations and recommendations**

A number of limitations were identified. The first identified limitation was that it can be time consuming to manually collate WQSAM's extensive inputs, a process exacerbated by differing data formats and database errors. There is a need for a pre-processing program to



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help effectively and efficiently process all data requirements for setting up and maintenance of the model.

The use of fixed water quality signatures fails to capture water quality changes, where non-stationarity in land use and return flows result in trends over time. Therefore, it is highly recommended that a method be developed to assign dynamic water quality signatures, to take account of non-stationarity. Similarly, short term variations in return flow volumes and concentrations need to be better accounted for in the model. The accuracy of WQSAM's water quality simulations are reliant on accurate yield model hydrological and structural inputs. It is recommended that the integration of the use of the two models be improved such that any problems in the quantity simulations that affect the quality simulations are identified and corrected (where possible) through re-calibration and/or re-structuring of the yield model. Similarly, it may be necessary to modify the node structure used in the yield model to account for specific water quality issues of concern (i.e. more detailed representation of return flows).

Future studies could focus on attempting to identify and quantify where possible the uncertainties involved with simulating water quality using WQSAM. In addition, a number of stakeholders requested that additional water quality constituents be included, and this could be further investigated to determine if it is feasible for the CRC. As the model was accepted by the IUCMA and addresses some of the many management requirements of IUCMA, the yield model future scenarios should be run to determine water quality outcomes.

In conclusion, WQSAM was able to simulate water quality constituents reasonably well and was able to adequately capture the predominant relationships between water quantity and quality as well as their variability across spatial and temporal scales, generating information that is relevant to the IWQMP within the CRC. While a number of limitations were identified in this study, many could be dealt with in future studies or model updates with relative ease. For example, implementing an attenuation model component or adding dynamic return flow and flow component concentrations to account for catchment non-stationarity would increase the simulated water quality reliability. Issues with the yield model flow volumes have already been dealt with in an updated WReMP model setup for the CRC, which includes more nodes and updated return flows. Unfortunately, the updated WReMP setup was only completed near the end of 2014, and was out of the time range of this Master's thesis to be implemented. The updated WReMP model will be used in the final product to be operationalised by the IUCMA

in 2015. WQSAM shows much potential as a WQDSS to be used as a tool for the IWQMP in the CRC which can be used along with many other tools such as Strategic Adaptive Management (SAM) and Cultural–Historical Activity Theory (CHAT), to form a better understanding of a complex social ecological system to support water resource management decisions. In addition, the integration of WQSAM with an existing yield model makes it possible for WQSAM to simulate water quality for a number of water quantity scenarios. This would allow water resource managers to assess the outcome of management scenarios on both water quantity and quality. For example, one of the yield model scenarios for the updated WReMP model simulates the effect on water quantity of building a proposed dam. WQSAM will be used to give some indication of the effect the reservoir will have on downstream water quality.

According to Huang and Xia (2001) research outputs seldom produce information that is directly useful for decision makers. This hinders the transition of many tools developed by researchers to the operationalised stage. The development of WQSAM attempted to avoid this problem as it was envisaged and developed specifically for the needs of water quality management within a South African context. WQSAM is constantly being updated to meet the needs of stakeholders and decision makers while maintaining a level of requisite simplicity. This has proven to be a successful governing paradigm, as the WQSAM model was accepted by the IUCMA, and will be operationalised and tested in 2015, with continual support from the Institute for Water Research at Rhodes University.

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Appendix A

Table A1. The table below represents the generic resource water quality objectives at a national level for South Africa (taken from DWA, 2012)

Variable	Units	Bound	Ideal	Sensitive user	Acceptable	Sensitive user	Tolerable	Sensitive user
Alkalinity (CaCO <sub>3</sub> )	mg/l	Upper	20	AAq	97.5	AAq	175	AAq
*Ammonia (NH <sub>3</sub> -N)	mg/l	Upper	0.015	Ecological	0.044	Ecological	0.073	Ecological
Calcium (Ca)	mg/l	Upper	10	Dom	80	BHN	80	BHN
*Chloride (Cl)	mg/l	Upper	40	In2	120	In2	175	In2
*EC	mS/m	Upper	30	In2	50	In2	85	Ecological
Fluoride (F)	mg/l	Upper	0.7	Dom	1	Dom	1.5	Dom
Magnesium (Mg)	mg/l	Upper	70	Dom	100	Dom	100	Dom
NO <sub>3</sub> (NO <sub>3</sub> -N)	mg/l	Upper	6	Alr	10	Alr	20	Alr
*pH	units	Upper	≤ 8	In2	<8.4	In2		
		Lower	≥6.5	Alr AAq In2	>8.0	Alr AAq In2		
Potassium (K)	mg/l	Upper	25	Dom	50	Dom	100	Dom
*PO <sub>4</sub> -P	mg/l	Upper	0.005	Ecological	0.015	Ecological	0.025	Ecological
SAR	mmol/l	Upper	2	Alr	8	Alr	15	Alr
Sodium (Na)	mg/l	Upper	70	Alr	92.5	Alr	115	Alr
*SO <sub>4</sub>	mg/l	Upper	80	In2	165	In2	250	In2
TDS	mg/l	Upper	200	In2	350	In2	800	In2
Si	mg/l	Upper	10	In2	25	In2	40	In2

Basic Human Needs

BHN

Agriculture - Aquaculture

AAq

Domestic use

Dom

Industrial - Category 2

In2

Agriculture - Irrigation

Alr

\*Selected water quality variables used for the water quality status planning review

Table A2 to A27 are statistical summaries of ammonium, nitrites + nitrites, TIN, and orthophosphates for all the water quality gauging sites in the CRC. The DWS gauge is given in the first column of each table. The structures of the tables are based on methods described in Malan and Day (2005).

Table A2

<b>X2H005</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	555	557	551	553
	mean	0.041	0.162	0.205	0.018
	median	0.02	0.15	0.180	0.014
	standard deviation	0.052	0.194	0.211	0.03
	mean - 3SD	-0.11	-0.42	-0.43	-0.08
	mean + 3SD	0.197	0.743	0.836	0.112
	min	0.015	0.02	0.04	0.003
	max	0.78	2.81	2.864	0.647
		N02 + NO3	TIN		PO <sub>4</sub>
	%> 0.12	57.6	68.2	%>0.018	3.6
Data Period	07 November 1962	16 August 2012			

Table A3

<b>X2H006</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	502	506	502	502
	mean	0.087	0.640	0.729	0.041
	median	0.06	0.57	0.649	0.0285
	standard deviation	0.108	0.492	0.523	0.04
	mean - 3SD	-0.24	-0.83	-0.84	-0.08
	mean + 3SD	0.410	2.115	2.297	0.166
	min	0.015	0.02	0.04	0.003
	max	1.024	4.46	4.48	0.32
		N02 + NO3	TIN		PO <sub>4</sub>
	%> 0.12	89.9	92.6	%>0.018	2.8
Data Period	05 March 1962	17 August 2012			

Table A4

<b>X2H008</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	403	405	401	402
	mean	0.041	0.092	0.134	0.021
	median	0.02	0.06	0.111	0.014
	standard deviation	0.030	0.097	0.100	0.07
	mean - 3SD	-0.05	-0.20	-0.17	-0.17
	mean + 3SD	0.132	0.382	0.433	0.217
	min	0.015	0.01	0.03	0.003
	max	0.175	0.88	0.903	1.264
	<b>N02 + NO3</b>	<b>TIN</b>		<b>PO<sub>4</sub></b>	
%> 0.12	21.7	44.6	%>0.018	4.0	
Data Period	26 November 1969	28 June 2012			

Table A5

<b>X2H010</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	367	368	364	365
	mean	0.035	0.050	0.085	0.019
	median	0.02	0.04	0.070	0.015
	standard deviation	0.031	0.048	0.059	0.02
	mean - 3SD	-0.06	-0.09	-0.09	-0.04
	mean + 3SD	0.127	0.195	0.263	0.074
	min	0.015	0.01	0.03	0.003
	max	0.327	0.48	0.522	0.15
	<b>N02 + NO3</b>	<b>TIN</b>		<b>PO<sub>4</sub></b>	
%> 0.12	6.3	15.4	%>0.018	4.4	
Data Period	11 October 1963	16 August 2012			

Table A6

<b>X2H011</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	500	502	499	499
	mean	0.043	0.162	0.206	0.031
	median	0.02	0.12	0.169	0.018
	standard deviation	0.042	0.192	0.206	0.06
	mean - 3SD	-0.08	-0.42	-0.41	-0.15
	mean + 3SD	0.169	0.739	0.824	0.209
	min	0.015	0.02	0.04	0.003
	max	0.333	1.93	2.083	1.002
	<b>N02 + NO3</b>	<b>TIN</b>		<b>PO<sub>4</sub></b>	
%> 0.12	48.4	63.3	%>0.018	5.2	
Data Period	23 March 1972	02 March 2009			

Table A7

<b>X2H012</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	275	275	272	275
	mean	0.049	0.187	0.233	0.043
	median	0.025	0.09	0.138	0.0175
	standard deviation	0.052	0.273	0.295	0.07
	mean - 3SD	-0.11	-0.63	-0.65	-0.16
	mean + 3SD	0.204	1.006	1.119	0.245
	min	0.015	0.02	0.04	0.003
	max	0.414	2.31	2.622	0.39
	<b>N02 + NO3</b>	<b>TIN</b>		<b>PO<sub>4</sub></b>	
%> 0.12	43.3	56.3	%>0.018	4.4	
Data Period	23 March 1972	14 August 2012			



Table A8

<b>X2H013</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	587	601	581	607
	mean	0.050	0.141	0.177	0.028
	median	0.025	0.09	0.130	0.014
	standard deviation	0.068	0.280	0.276	0.08
	mean - 3SD	-0.15	-0.70	-0.65	-0.23
	mean + 3SD	0.252	0.980	1.005	0.282
	min	0.015	0.01	0.03	0.003
	max	0.86	3.32	3.363	1.4
		N02 + NO3	TIN		PO <sub>4</sub>
	%> 0.12	35.3	53.2	%>0.018	2.5
Data Period	24 April 1966	27 September 2012			

Table A9

<b>X2H014</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	401	400	397	401
	mean	0.040	0.088	0.129	0.014
	median	0.02	0.08	0.120	0.011
	standard deviation	0.054	0.068	0.081	0.03
	mean - 3SD	-0.12	-0.12	-0.11	-0.07
	mean + 3SD	0.203	0.292	0.373	0.093
	min	0.015	0.01	0.038	0.003
	max	0.78	0.42	0.8	0.474
		N02 + NO3	TIN		PO <sub>4</sub>
	%> 0.12	27.3	47.9	%>0.018	3.7
Data Period	02 August 1966	15 August 2012			

Table A10

<b>X2H015</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	807	798	796	807
	mean	0.048	0.155	0.200	0.023
	median	0.02	0.13	0.168	0.016
	standard deviation	0.133	0.184	0.225	0.04
	mean - 3SD	-0.35	-0.40	-0.48	-0.10
	mean + 3SD	0.448	0.705	0.877	0.146
	min	0.015	0.02	0.04	0.003
	max	3.418	3.00	3.497	0.9
		<b>N02 + NO3</b>	<b>TIN</b>		<b>PO<sub>4</sub></b>
%> 0.12	52.4	64.6	%>0.018	2.9	
Data Period	23 March 1972	15 August 2012			

Table A11

<b>X2H016</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	1164	1166	1163	1165
	mean	0.054	0.480	0.533	0.023
	median	0.046	0.44	0.496	0.02
	standard deviation	0.060	0.442	0.449	0.02
	mean - 3SD	-0.13	-0.85	-0.81	-0.03
	mean + 3SD	0.234	1.806	1.879	0.077
	min	0.015	0.02	0.04	0.003
	max	1.42	9.07	9.09	0.231
		<b>N02 + NO3</b>	<b>TIN</b>		<b>PO<sub>4</sub></b>
%> 0.12	83.8	89.0	%>0.018	3.6	
Data Period	20 February 1970	25 June 2012			

Table A12

<b>X2H017</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	905	911	904	906
	mean	0.064	0.549	0.615	0.028
	median	0.05	0.56	0.622	0.022
	standard deviation	0.268	0.344	0.428	0.02
	mean - 3SD	-0.74	-0.48	-0.67	-0.04
	mean + 3SD	0.867	1.582	1.898	0.100
	min	0.015	0.01	0.03	0.003
	max	7.981	3.13	8.001	0.3
	N02 + NO3	TIN		PO <sub>4</sub>	
%> 0.12	84.4	88.6	%>0.018	3.8	
Data Period	27 November 1969	08 June 2009			

Table A13

<b>X2H022</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	519	521	517	519
	mean	0.058	0.574	0.633	0.027
	median	0.047	0.51	0.580	0.022
	standard deviation	0.058	0.483	0.489	0.02
	mean - 3SD	-0.12	-0.88	-0.83	-0.04
	mean + 3SD	0.231	2.024	2.098	0.096
	min	0.015	0.02	0.04	0.003
	max	0.66	6.73	6.75	0.18
	N02 + NO3	TIN		PO <sub>4</sub>	
%> 0.12	89.3	92.5	%>0.018	3.1	
Data Period	20 June 1962	14 May 2012			

Table A14

<b>X2H032</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	722	724	722	722
	mean	0.047	0.694	0.742	0.060
	median	0.036	0.58	0.639	0.041
	standard deviation	0.039	0.564	0.566	0.08
	mean - 3SD	-0.07	-1.00	-0.96	-0.18
	mean + 3SD	0.165	2.386	2.440	0.302
	min	0.015	0.01	0.03	0.003
	max	0.384	8.80	8.825	1.594
	<b>N02 + NO3</b>	<b>TIN</b>		<b>PO<sub>4</sub></b>	
%> 0.12	90.6	92.5	%>0.018	2.5	
Data Period	26 March 1972	14 May 2012			

Table A15

<b>X2H035</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	54	53	53	54
	mean	0.036	0.081	0.117	0.013
	median	0.025	0.05	0.083	0.01
	standard deviation	0.022	0.121	0.133	0.01
	mean - 3SD	-0.03	-0.28	-0.28	-0.02
	mean + 3SD	0.101	0.446	0.518	0.043
	min	0.015	0.01	0.03	0.003
	max	0.103	0.85	0.956	0.055
	<b>N02 + NO3</b>	<b>TIN</b>		<b>PO<sub>4</sub></b>	
%> 0.12	15.1	30.2	%>0.018	1.9	
Data Period	29 May 1984	11 August 2011			

Table A16

<b>X2H036</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	630	631	629	630
	mean	0.056	0.390	0.446	0.027
	median	0.047	0.38	0.427	0.022
	standard deviation	0.057	0.277	0.282	0.03
	mean - 3SD	-0.11	-0.44	-0.40	-0.07
	mean + 3SD	0.227	1.221	1.292	0.120
	min	0.015	0.02	0.04	0.003
	max	0.9	2.38	2.423	0.433
		N02 + NO3	TIN		PO <sub>4</sub>
	%> 0.12	79.9	86.5	%>0.018	2.7
Data Period	07 October 1982	22 June 2012			

Table A17

<b>X2H046</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	619	620	619	620
	mean	0.048	0.555	0.603	0.060
	median	0.04	0.57	0.618	0.031
	standard deviation	0.041	0.313	0.321	0.59
	mean - 3SD	-0.08	-0.38	-0.36	-1.70
	mean + 3SD	0.172	1.494	1.565	1.817
	min	0.015	0.01	0.03	0.005
	max	0.476	1.68	1.743	14.6
		N02 + NO3	TIN		PO <sub>4</sub>
	%> 0.12	87.4	89.7	%>0.018	1.8
Data Period	01 October 1986	20 June 2012			

Table A18

<b>X2H048</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	271	275	261	287
	mean	0.101	0.667	0.746	0.091
	median	0.041	0.59	0.616	0.024
	standard deviation	0.328	0.867	1.106	0.43
	mean - 3SD	-0.88	-1.94	-2.57	-1.21
	mean + 3SD	1.083	3.268	4.063	1.389
	min	0.015	0.01	0.03	0.003
	max	3.8	11.30	15.1	5.4
		N02 + NO3	TIN		PO <sub>4</sub>
	%> 0.12	81.1	84.3	%>0.018	2.4
Data Period	17 October 1983	26 September 2012			

Table A19

<b>X2H049</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	158	158	158	158
	mean	0.051	0.547	0.597	0.021
	median	0.05	0.54	0.584	0.0175
	standard deviation	0.028	0.277	0.284	0.01
	mean - 3SD	-0.03	-0.28	-0.25	-0.02
	mean + 3SD	0.135	1.376	1.448	0.064
	min	0.015	0.02	0.04	0.003
	max	0.243	1.41	1.45	0.084
		N02 + NO3	TIN		PO <sub>4</sub>
	%> 0.12	92.4	93.0	%>0.018	3.2
Data Period	17 October 1983	31 January 2004			

Table A20

X2H050		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	176	176	176	176
	mean	0.053	0.453	0.507	0.019
	median	0.05	0.48	0.525	0.015
	standard deviation	0.050	0.285	0.280	0.01
	mean - 3SD	-0.10	-0.40	-0.33	-0.02
	mean + 3SD	0.204	1.309	1.347	0.057
	min	0.015	0.02	0.04	0.003
	max	0.402	1.41	1.43	0.0775
	N02 + NO3	TIN		PO <sub>4</sub>	
%> 0.12	81.3	90.9	%>0.018	2.8	
Data Period	17 October 1983	18 February 2005			

Table A21

X2H070		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	280	267	267	278
	mean	0.058	0.170	0.229	0.022
	median	0.02	0.15	0.200	0.015
	standard deviation	0.165	0.124	0.202	0.04
	mean - 3SD	-0.44	-0.20	-0.38	-0.10
	mean + 3SD	0.554	0.540	0.835	0.144
	min	0.015	0.01	0.03	0.003
	max	1.867	1.13	1.996	0.447
	N02 + NO3	TIN		PO <sub>4</sub>	
%> 0.12	64.8	81.6	%>0.018	1.8	
Data Period	24 October 1983	15 August 2012			

Table A22

X2H072		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>	
	n	102	102	102	102	
	mean	0.050	0.310	0.359	0.043	
	median	0.03775	0.10	0.141	0.019	
	standard deviation	0.081	0.485	0.488	0.14	
	mean - 3SD	-0.19	-1.14	-1.11	-0.39	
	mean + 3SD	0.293	1.764	1.824	0.476	
	min	0.02	0.02	0.04	0.003	
	max	0.802	2.77	2.786	1.411	
			N02 + NO3	TIN		PO <sub>4</sub>
	%> 0.12	45.1	52.9	%>0.018	1.0	
Data Period	06 April 1990	28 August 2001				

Table A23

X2R001		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>	
	n	219	229	219	220	
	mean	0.081	0.055	0.134	0.019	
	median	0.049	0.03	0.092	0.013	
	standard deviation	0.130	0.093	0.157	0.03	
	mean - 3SD	-0.31	-0.23	-0.34	-0.08	
	mean + 3SD	0.470	0.335	0.604	0.119	
	min	0.015	0.01	0.03	0.003	
	max	1.154	0.87	1.174	0.419	
			N02 + NO3	TIN		PO <sub>4</sub>
	%> 0.12	6.1	32.4	%>0.018	2.3	
Data Period	20 March 1968	01 July 2011				



Table A24

<b>X2R002</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	222	221	221	221
	mean	0.066	0.050	0.116	0.017
	median	0.046	0.04	0.089	0.013
	standard deviation	0.076	0.074	0.106	0.02
	mean - 3SD	-0.16	-0.17	-0.20	-0.03
	mean + 3SD	0.293	0.273	0.433	0.065
	min	0.015	0.01	0.03	0.003
	max	0.622	0.60	0.662	0.157
		<b>N02 + N03</b>	<b>TIN</b>		<b>PO<sub>4</sub></b>
	%> 0.12	5.9	24.4	%>0.018	2.7
Data Period	16 March 1975	09 April 2012			

Table A25

<b>X2R003</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	224	224	220	226
	mean	0.072	0.051	0.123	0.039
	median	0.05	0.04	0.095	0.012
	standard deviation	0.079	0.073	0.106	0.37
	mean - 3SD	-0.16	-0.17	-0.19	-1.08
	mean + 3SD	0.308	0.269	0.440	1.154
	min	0.015	0.01	0.03	0.003
	max	0.609	0.71	0.775	5.595
		<b>N02 + N03</b>	<b>TIN</b>		<b>PO<sub>4</sub></b>
	%> 0.12	4.9	32.7	%>0.018	1.8
Data Period	16 March 1975	27 June 2012			

Table A26

<b>X2R004</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	246	248	244	246
	mean	0.056	0.112	0.165	0.022
	median	0.04	0.04	0.102	0.016
	standard deviation	0.065	0.158	0.167	0.02
	mean - 3SD	-0.14	-0.36	-0.34	-0.04
	mean + 3SD	0.252	0.584	0.666	0.084
	min	0.015	0.01	0.03	0.003
	max	0.546	1.02	1.06	0.144
	N02 + NO3	TIN		PO <sub>4</sub>	
%> 0.12	26.2	41.4	%>0.018	2.0	
Data Period	06 January 1972	29 June 2012			

Table A27

<b>X2R005</b>		<b>NH<sub>4</sub></b>	<b>NO<sub>2</sub> + NO<sub>3</sub></b>	<b>TIN</b>	<b>PO<sub>4</sub></b>
	n	187	189	187	186
	mean	0.041	0.145	0.186	0.019
	median	0.02	0.12	0.150	0.015
	standard deviation	0.040	0.156	0.161	0.02
	mean - 3SD	-0.08	-0.32	-0.30	-0.03
	mean + 3SD	0.160	0.614	0.669	0.071
	min	0.015	0.01	0.03	0.003
	max	0.312	1.40	1.417	0.164
	N02 + NO3	TIN		PO <sub>4</sub>	
%> 0.12	48.7	65.8	%>0.018	3.2	
Data Period	30 October 1984	15 August 2012			

## Appendix B

Table B1. Summary statistics for TDS

WWTW Name	TDS		
	Mean	Minimum	Maximum
Matsulu WWTW	286.52	7.2	488.15
Kingstonvale WWTW	365.40	15.3	585.00
Emthonjeni WWTW	351.64	27.4	1053.00
Machadodorp WWTW	526.64	52.7	1027.00
Watervale Boven WWTW	251.17	2.2	1690.00
Millys WWTW	551.33	16.6	1183.00
White River WWTW	396.60	4.4	1222.00
Barberton WWTW	317.48	41.2	540.80

Table B2. Summary statistics for NH4-N

WWTW Name	NH4-N		
	Mean	Minimum	Maximum
Matsulu WWTW	0.58	0.03	10.40
Kingstonvale WWTW	4.08	0.03	18.39
Emthonjeni WWTW	15.06	0.03	39.30
Machadodorp WWTW	24.03	12.70	48.00
Watervale Boven WWTW	1.97	0.03	12.32
Millys WWTW	34.50	0.10	116.00
White River WWTW	18.80	0.03	41.40
Barberton WWTW	5.26	0.03	35.83

Table B3. Summary statistics for NO3-NO2-N

WWTW Name	NO3 + NO2-N		
	Mean	Minimum	Maximum
Matsulu WWTW	5.24	0.80	11.00
Kingstonvale WWTW	5.77	0.03	13.64
Emthonjeni WWTW	8.22	0.03	49.96
Machadodorp WWTW	2.16	0.10	6.10
Watervale Boven WWTW	8.28	0.03	140.00
Millys WWTW	26.22	0.10	79.82
White River WWTW	3.54	0.03	24.65
Barberton WWTW	16.09	0.70	63.00

Table B4. Summary Statistics for PO4-P

WWTW Name	PO4-P		
	Mean	Minimum	Maximum
Matsulu WWTW	3.40	0.05	6.10
Kingstonvale WWTW	3.93	0.10	10.67
Emthonjeni WWTW	5.76	0.20	23.21
Machadodorp WWTW	5.52	0.20	8.70
Watervale Boven WWTW	1.76	0.05	8.30
Millys WWTW	11.27	0.30	19.20
White River WWTW	5.51	0.05	20.60
Barberton WWTW	5.27	0.05	12.80

Table B5. Borehole TDS data

<b>Sub-quaternary</b>	<b>Mean</b>	<b>Minimum</b>	<b>Maximum</b>	<b>Borehole gauge ID</b>
X21A-1	83.200	83.200	83.200	172679
X21D-1	225.550	225.550	225.550	172681
X21E-1	38.350	38.350	38.350	172583
X21F-1	136.175	49.400	222.950	173926
X21F-2	413.373	57.850	2236.000	90091
X21J-1	442.325	262.600	622.050	172507
X21J-2	705.033	347.750	1384.500	174138
X22A-2	114.400	114.400	114.400	173927
X22C-1	198.250	198.250	198.250	172509
X22C-2	1150.500	1150.500	1150.500	172578
X22D-2	32.500	31.850	33.150	173911
X22D-3	113.100	83.850	142.350	173913
X22E-3	196.950	196.950	196.950	163707
X22H-2	195.325	79.300	311.350	172581
X22H-3	295.100	295.100	295.100	173914
X22J-2	175.500	175.500	175.500	172519
X22K-1	261.625	252.200	271.050	161350
X22K-2	295.100	295.100	295.100	161349
X22K-3	343.850	236.600	445.250	172523
X23A-2	250.250	250.250	250.250	173916
X23B-1	582.400	582.400	582.400	172579
X23B-2	107.250	87.100	127.400	172508
X23B-3	429.000	429.000	429.000	172516
X23D-2	184.167	124.800	401.050	161352
X23F-2	610.350	610.350	610.350	172524
X23G-2	373.750	326.300	421.200	172521
X23H-1	650.650	650.650	650.650	172520
X23H-2	305.221	131.950	625.950	161793
X23H-4	576.550	576.550	576.550	169177
X23H-5	558.350	404.950	890.500	169168
X24A-1	187.850	134.550	241.150	1000012700
X24A-2	621.725	518.700	724.750	168486
X24B-2	100.750	100.750	100.750	172582
X24B-3	949.384	104.000	6370.000	1000012810
X24C-1	448.630	361.400	528.450	168611
X24D-2	485.195	139.750	1326.000	90107
X24E-1	653.250	630.500	676.000	168518
X24E-2	627.055	458.250	743.600	168608
X24F-1	658.450	253.500	823.550	172576
X24G-1	579.687	208.650	1202.500	168513
X24H-1	1243.214	141.050	2873.000	175811
X24H-2	933.400	56.550	8489.000	90051

Table B6. Borehole Nitrates + Nitrites data

<b>Sub-</b>	<b>Mean</b>	<b>Minimum</b>	<b>Maximum</b>	<b>Borehole gauge ID</b>
X21A-1	2.92000	2.92000	2.92000	172679
X21D-1	0.09600	0.09600	0.09600	172681
X21E-1	0.12200	0.12200	0.12200	172583
X21F-1	0.39650	0.22700	0.56600	173926
X21F-2	0.06779	0.00000	0.58300	90091
X21J-1	1.13350	0.61700	1.65000	172507
X21J-2	0.53150	0.13700	1.06700	174138
X22A-2	0.61900	0.61900	0.61900	173927
X22C-1	3.65800	3.65800	3.65800	172509
X22C-2	7.87000	7.87000	7.87000	172578
X22D-2	0.22900	0.22800	0.23000	173911
X22D-3	2.94500	0.02000	5.87000	173913
X22E-3	0.02000	0.02000	0.02000	163707
X22H-2	2.58550	2.48000	2.69100	172581
X22H-3	0.02000	0.02000	0.02000	173914
X22J-2	1.38800	1.38800	1.38800	172519
X22K-1	0.24100	0.13200	0.35000	161350
X22K-2	4.37000	4.37000	4.37000	161349
X22K-3	4.17900	0.10000	10.93800	172523
X23A-2	0.07900	0.07900	0.07900	173916
X23B-1	10.95300	10.95300	10.95300	172579
X23B-2	0.52550	0.23600	0.81500	172508
X23B-3	0.02000	0.02000	0.02000	172516
X23D-2	2.56783	0.98000	4.66000	161352
X23F-2	2.44300	2.44300	2.44300	172524
X23G-2	4.65300	4.36200	4.94400	172521
X23H-1	4.97700	4.97700	4.97700	172520
X23H-2	2.66157	0.02000	10.24200	161793
X23H-4	0.11200	0.11200	0.11200	169177
X23H-5	3.03125	0.21400	9.15600	169168
X24A-1	3.17600	0.74500	5.60700	1000012700
X24A-2	0.77400	0.08800	1.46000	168486
X24B-2	5.99300	5.99300	5.99300	172582
X24B-3	4.74841	0.00000	13.89200	1000012810
X24C-1	1.88460	0.02000	5.92000	168611
X24D-2	2.68573	0.02000	6.40500	90107
X24E-1	0.02000	0.02000	0.02000	168518
X24E-2	0.13420	0.02000	0.70300	168608
X24F-1	0.92500	0.61900	1.43500	172576
X24G-1	0.25691	0.00000	3.69600	168513
X24H-1	4.42182	0.02000	19.74600	175811
X24H-2	2.19818	0.00000	9.66300	90051

Table B7. Borehole Orthophosphates data

<b>Sub-quaternary</b>	<b>PO4 Mean</b>	<b>PO4 Minimum</b>	<b>PO4 Maximum</b>	<b>Borehole gauge ID</b>
X21A-1	0.028000	0.028000	0.028000	172679
X21D-1	0.023000	0.023000	0.023000	172681
X21E-1	0.011000	0.011000	0.011000	172583
X21F-1	4.528500	0.057000	9.000000	173926
X21F-2	1.843333	0.000000	9.000000	90091
X21J-1	0.017500	0.013000	0.022000	172507
X21J-2	0.022000	0.010000	0.037000	174138
X22A-2	0.025000	0.025000	0.025000	173927
X22C-1	7.000000	7.000000	7.000000	172509
X22C-2	0.012000	0.012000	0.012000	172578
X22D-2	3.000000	3.000000	3.000000	173911
X22D-3	1.500000	0.000000	3.000000	173913
X22E-3	0.014000	0.014000	0.014000	163707
X22H-2	0.013500	0.000000	0.027000	172581
X22H-3	0.020000	0.020000	0.020000	173914
X22J-2	0.050000	0.050000	0.050000	172519
X22K-1	3.505000	0.010000	7.000000	161350
X22K-2	3.000000	3.000000	3.000000	161349
X22K-3	6.006000	0.018000	9.000000	172523
X23A-2	0.018000	0.018000	0.018000	173916
X23B-1	0.024000	0.024000	0.024000	172579
X23B-2	0.072500	0.067000	0.078000	172508
X23B-3	0.011000	0.011000	0.011000	172516
X23D-2	1.015167	0.011000	6.000000	161352
X23F-2	9.000000	9.000000	9.000000	172524
X23G-2	0.017000	0.015000	0.019000	172521
X23H-1	0.100000	0.100000	0.100000	172520
X23H-2	3.575714	0.014000	7.000000	161793
X23H-4	0.015000	0.015000	0.015000	169177
X23H-5	2.017500	0.018000	8.000000	169168
X24A-1	0.014500	0.014000	0.015000	1000012700
X24A-2	6.500000	5.000000	8.000000	168486
X24B-2	0.026000	0.026000	0.026000	172582
X24B-3	0.037500	0.000000	0.169000	1000012810
X24C-1	0.034000	0.015000	0.054000	168611
X24D-2	0.847182	0.012000	9.000000	90107
X24E-1	0.027000	0.026000	0.028000	168518
X24E-2	0.029000	0.022000	0.035000	168608
X24F-1	2.262500	0.011000	9.000000	172576
X24G-1	0.024087	0.000000	0.048000	168513
X24H-1	3.011182	0.011000	8.000000	175811
X24H-2	0.371529	0.000000	6.000000	90051

Table B8. Borehole Ammonia data

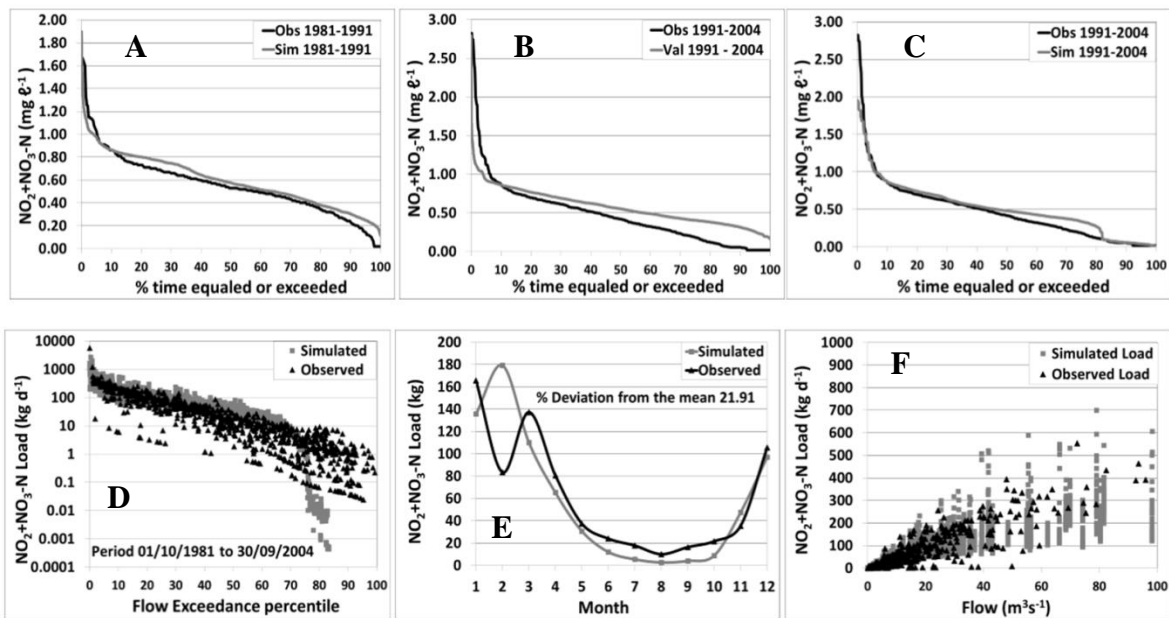
<b>Sub-quaternary</b>	<b>NH4 Mean</b>	<b>NH4 Minimum</b>	<b>NH4 Maximum</b>	<b>Borehole gauge ID</b>
X21A-1	0.043000	0.043000	0.043000	172679
X21D-1	0.050000	0.050000	0.050000	172681
X21E-1	0.020000	0.020000	0.020000	172583
X21F-1	0.037000	0.020000	0.054000	173926
X21F-2	0.065667	0.000000	0.415000	90091
X21J-1	0.030500	0.020000	0.041000	172507
X21J-2	0.020000	0.020000	0.020000	174138
X22A-2	0.020000	0.020000	0.020000	173927
X22C-1	0.020000	0.020000	0.020000	172509
X22C-2	0.052000	0.052000	0.052000	172578
X22D-2	0.020000	0.020000	0.020000	173911
X22D-3	0.010000	0.000000	0.020000	173913
X22E-3	0.020000	0.020000	0.020000	163707
X22H-2	0.010000	0.000000	0.020000	172581
X22H-3	0.020000	0.020000	0.020000	173914
X22J-2	0.020000	0.020000	0.020000	172519
X22K-1	0.020000	0.020000	0.020000	161350
X22K-2	0.020000	0.020000	0.020000	161349
X22K-3	0.020000	0.020000	0.020000	172523
X23A-2	0.020000	0.020000	0.020000	173916
X23B-1	0.052000	0.052000	0.052000	172579
X23B-2	0.031500	0.020000	0.043000	172508
X23B-3	0.020000	0.020000	0.020000	172516
X23D-2	0.035000	0.020000	0.080000	161352
X23F-2	0.020000	0.020000	0.020000	172524
X23G-2	0.020000	0.020000	0.020000	172521
X23H-1	0.020000	0.020000	0.020000	172520
X23H-2	0.035429	0.020000	0.128000	161793
X23H-4	0.020000	0.020000	0.020000	169177
X23H-5	0.066000	0.020000	0.204000	169168
X24A-1	0.143500	0.020000	0.267000	1000012700
X24A-2	0.020000	0.020000	0.020000	168486
X24B-2	0.020000	0.020000	0.020000	172582
X24B-3	0.029000	0.000000	0.122000	1000012810
X24C-1	0.203400	0.020000	0.937000	168611
X24D-2	0.034818	0.020000	0.082000	90107
X24E-1	0.037000	0.020000	0.054000	168518
X24E-2	0.035700	0.020000	0.053000	168608
X24F-1	0.044500	0.020000	0.060000	172576
X24G-1	0.037391	0.000000	0.238000	168513
X24H-1	0.214636	0.020000	0.836000	175811
X24H-2	0.031118	0.000000	0.071000	90051



## Appendix C

The figures presented in this appendix with an example depicted in the figure below are structured as follows:

- A. calibration concentration frequency distribution curve
- B. validation concentration frequency distribution curve
- C. recalibrated frequency concentration distribution curve
- D. load Duration Curve
- E. seasonal Load Graphs (Month 1 is January)
- F. simulated and observed loads plotted against simulated and observed flow.



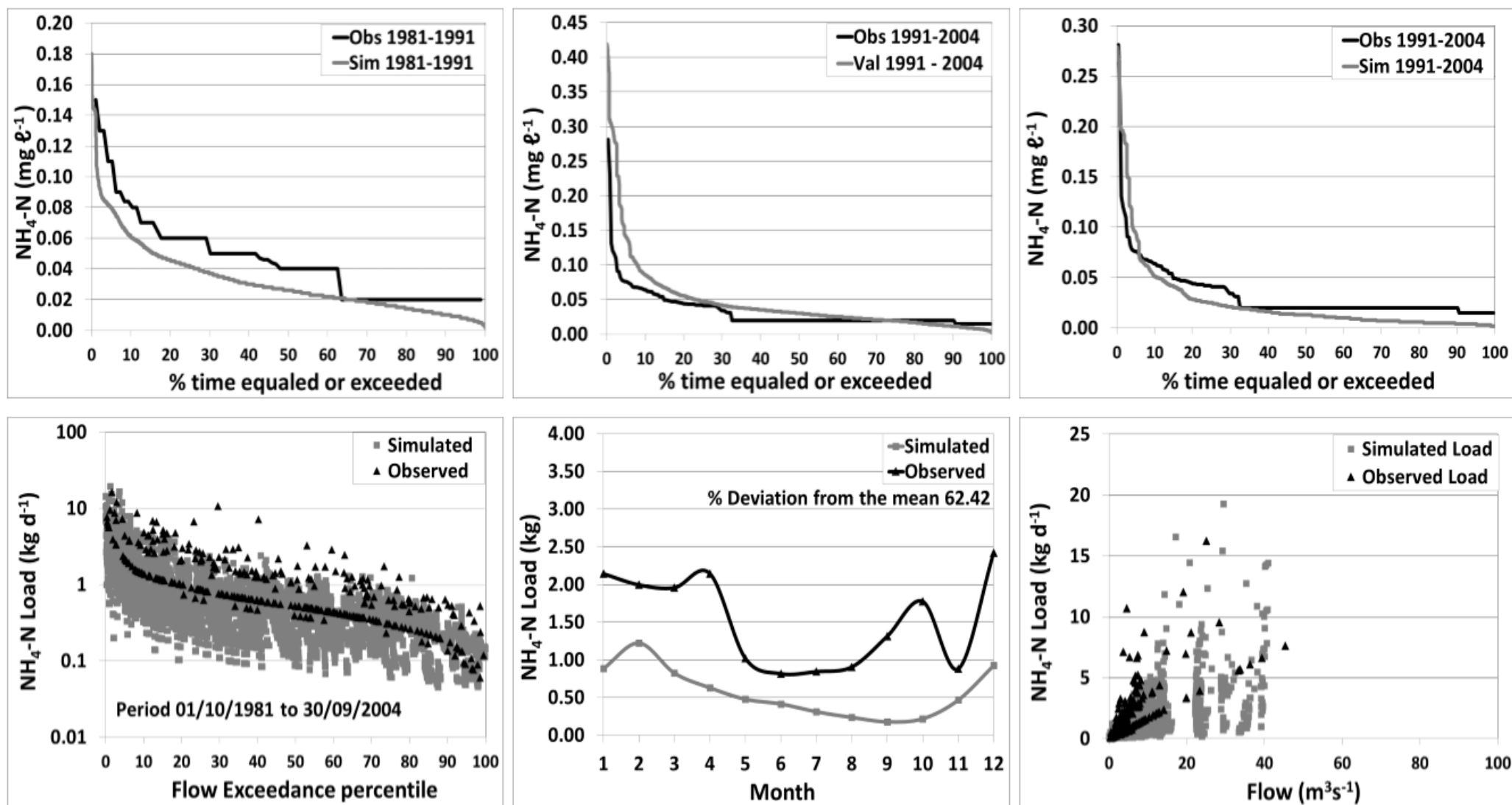


Figure C1. Simulated vs. observed results for  $\text{NH}_4\text{-N}$  at node MontroseFalls (gauging station X2H013) along the Crocodile River.

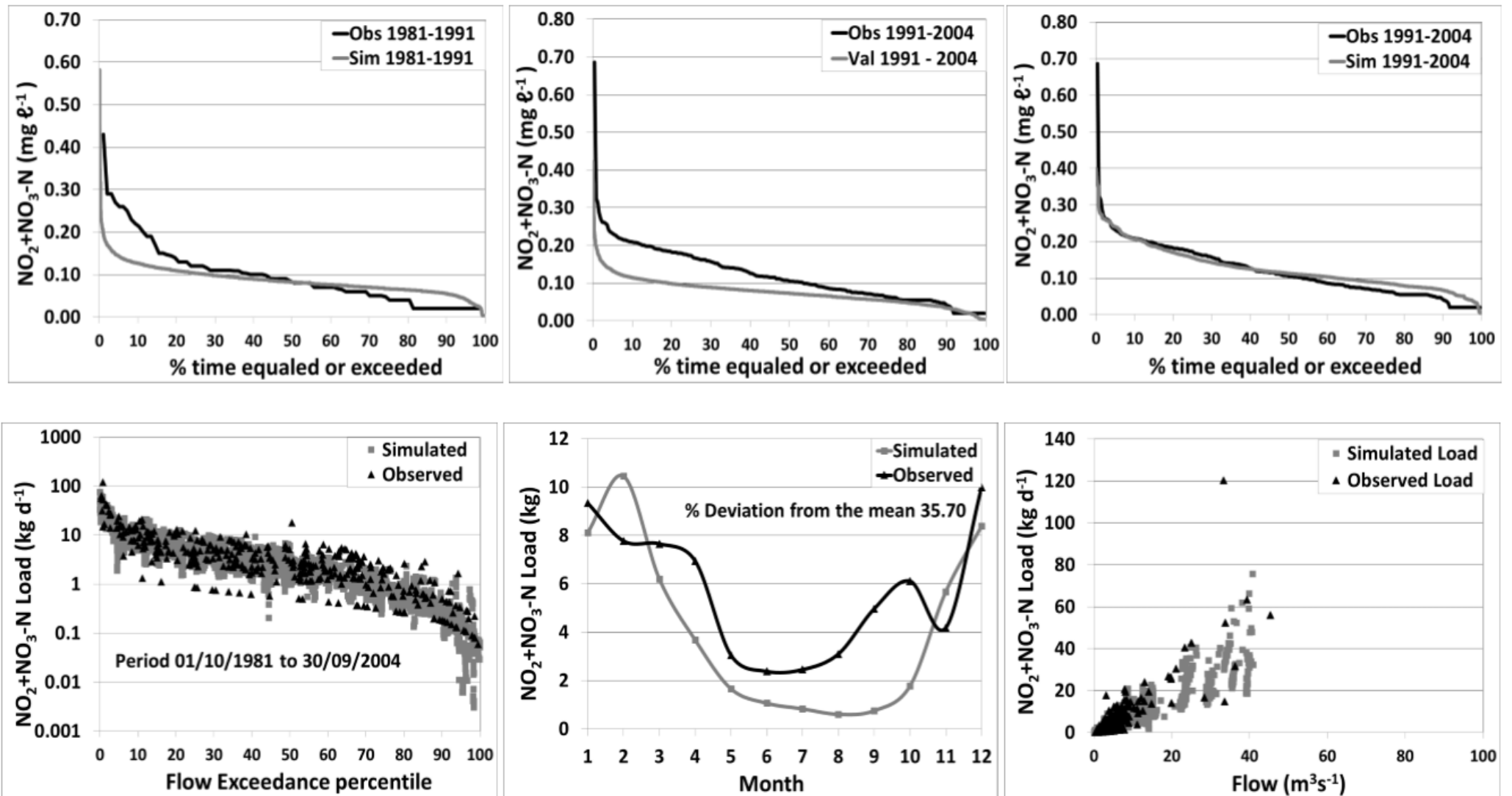


Figure C2. Simulated vs observed results for NO<sub>2</sub> + NO<sub>3</sub>-N at node MontroseFalls (gauging station X2H013) along the Crocodile River.

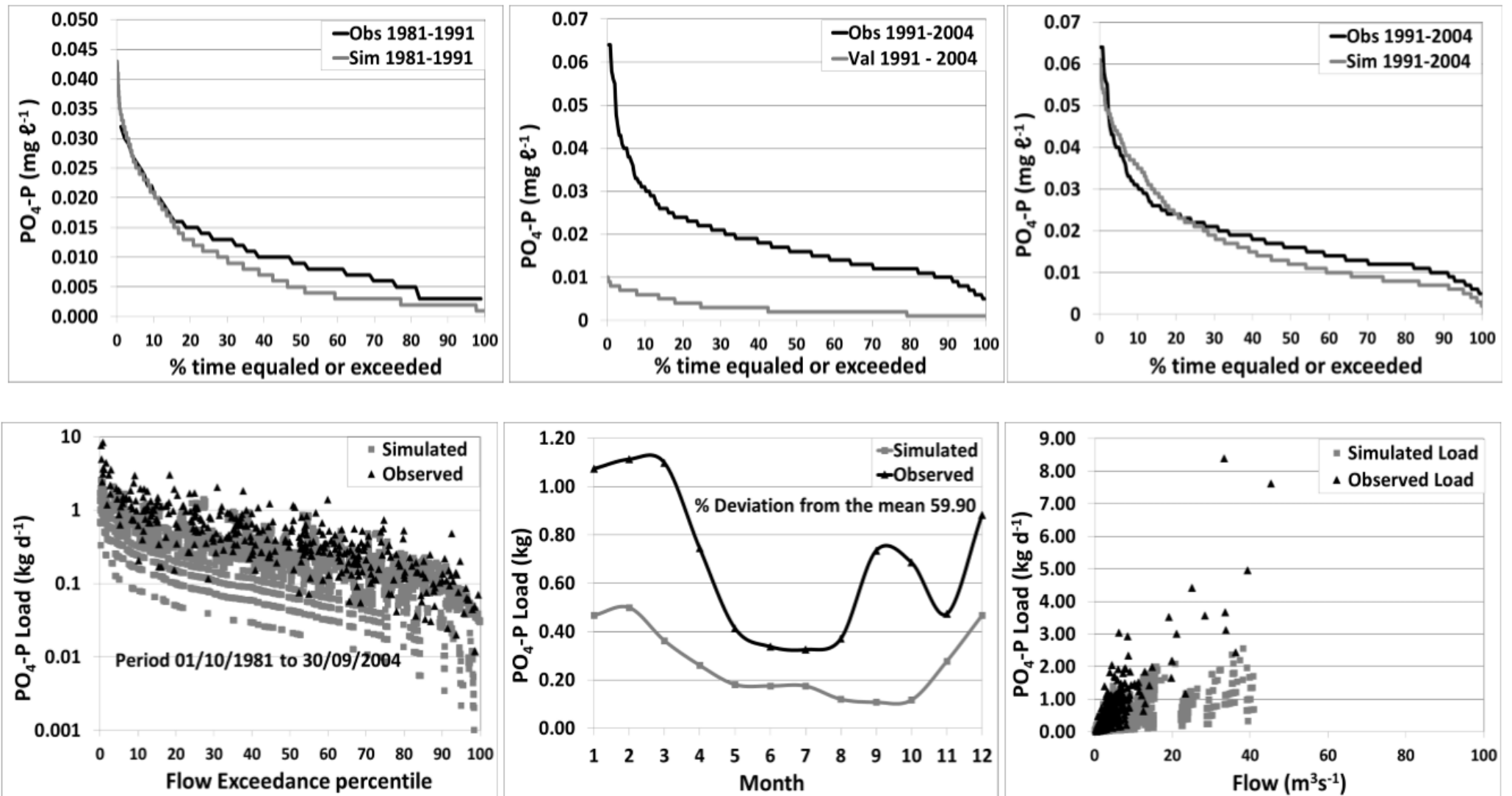


Figure C3. Simulated vs observed results for PO<sub>4</sub>-P at node MontroseFalls (gauging station X2H013) along the Crocodile River.

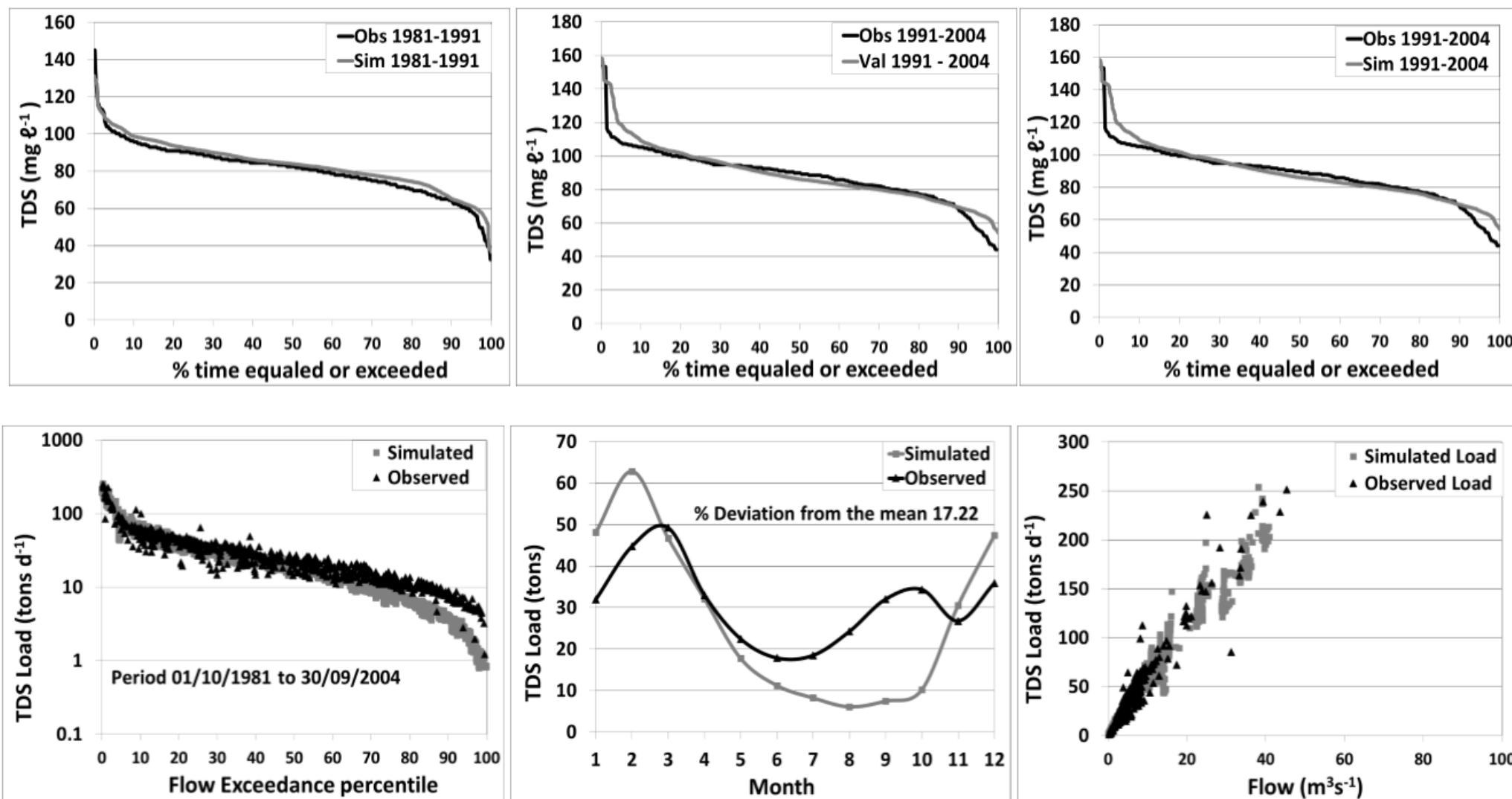


Figure C4. Simulated vs observed results for TDS at node MontroseFalls (gauging station X2H013) along the Crocodile River.

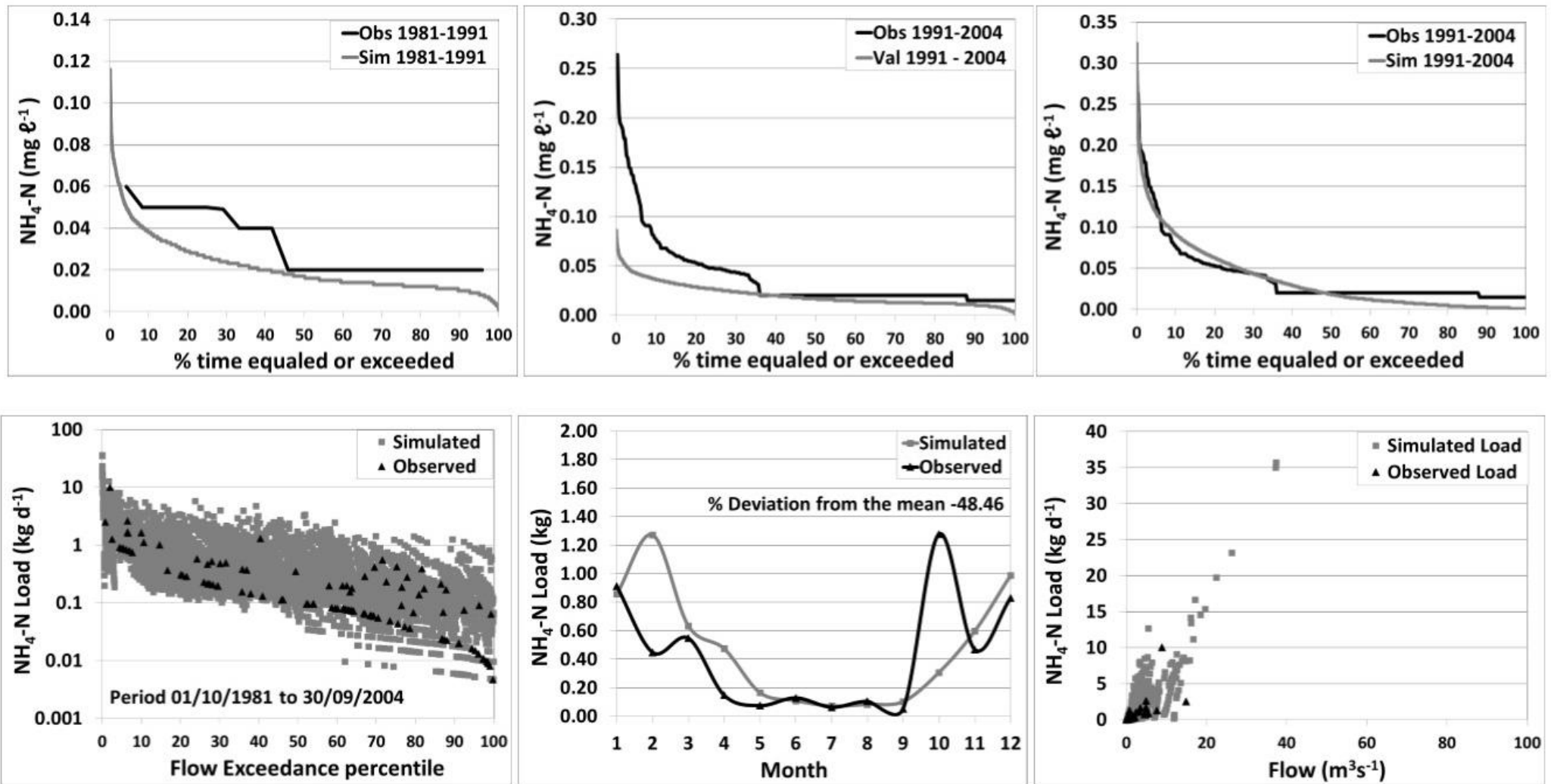


Figure C5. Simulated vs observed results for  $\text{NH}_4\text{-N}$  at node X21F-2 (gauging station X2H011) along the Elands River.

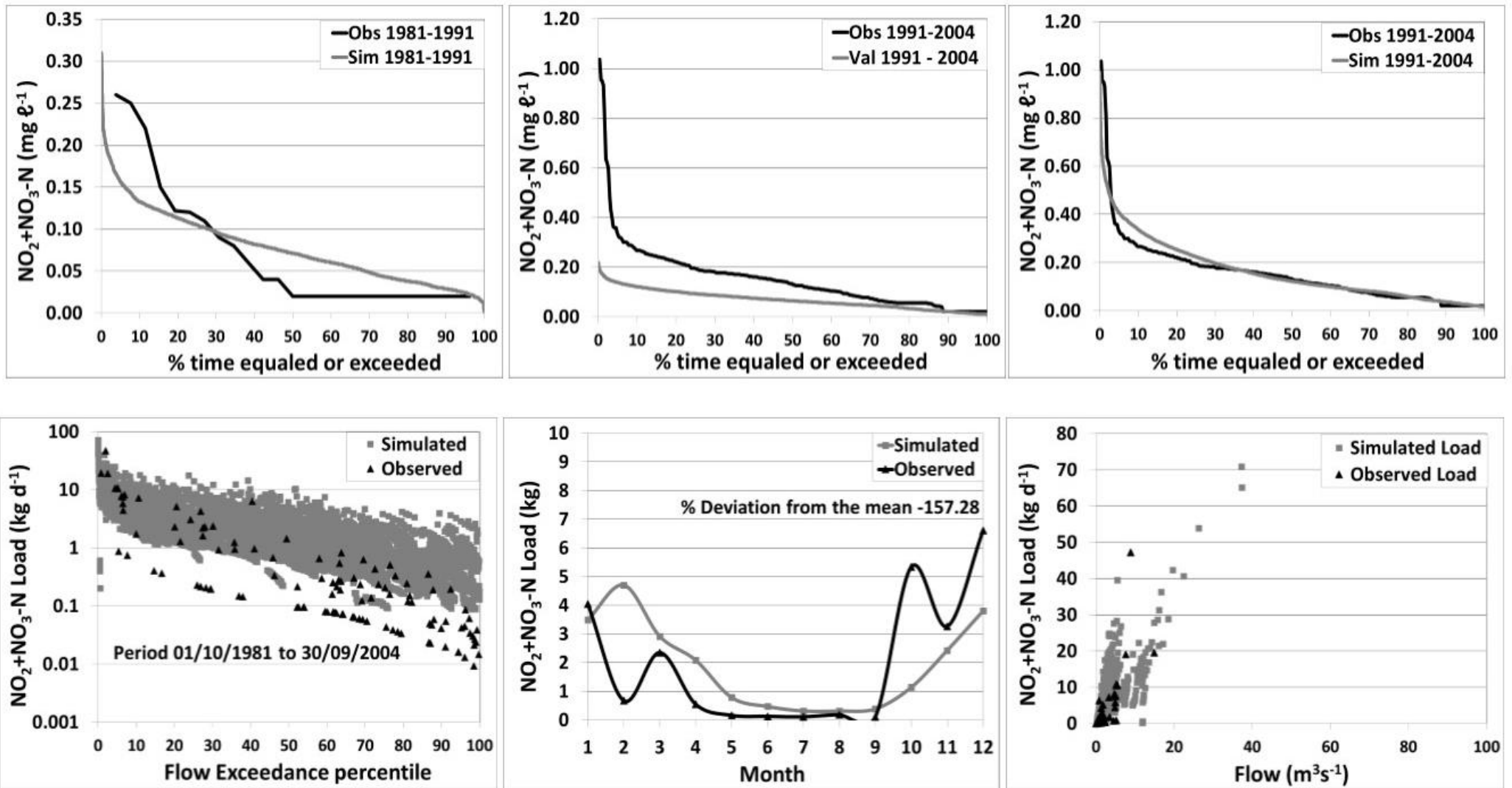


Figure C6. Simulated vs observed results for  $\text{NO}_2 + \text{NO}_3\text{-N}$  at node X21F-2 (gauging station X2H011) along the Elands River.

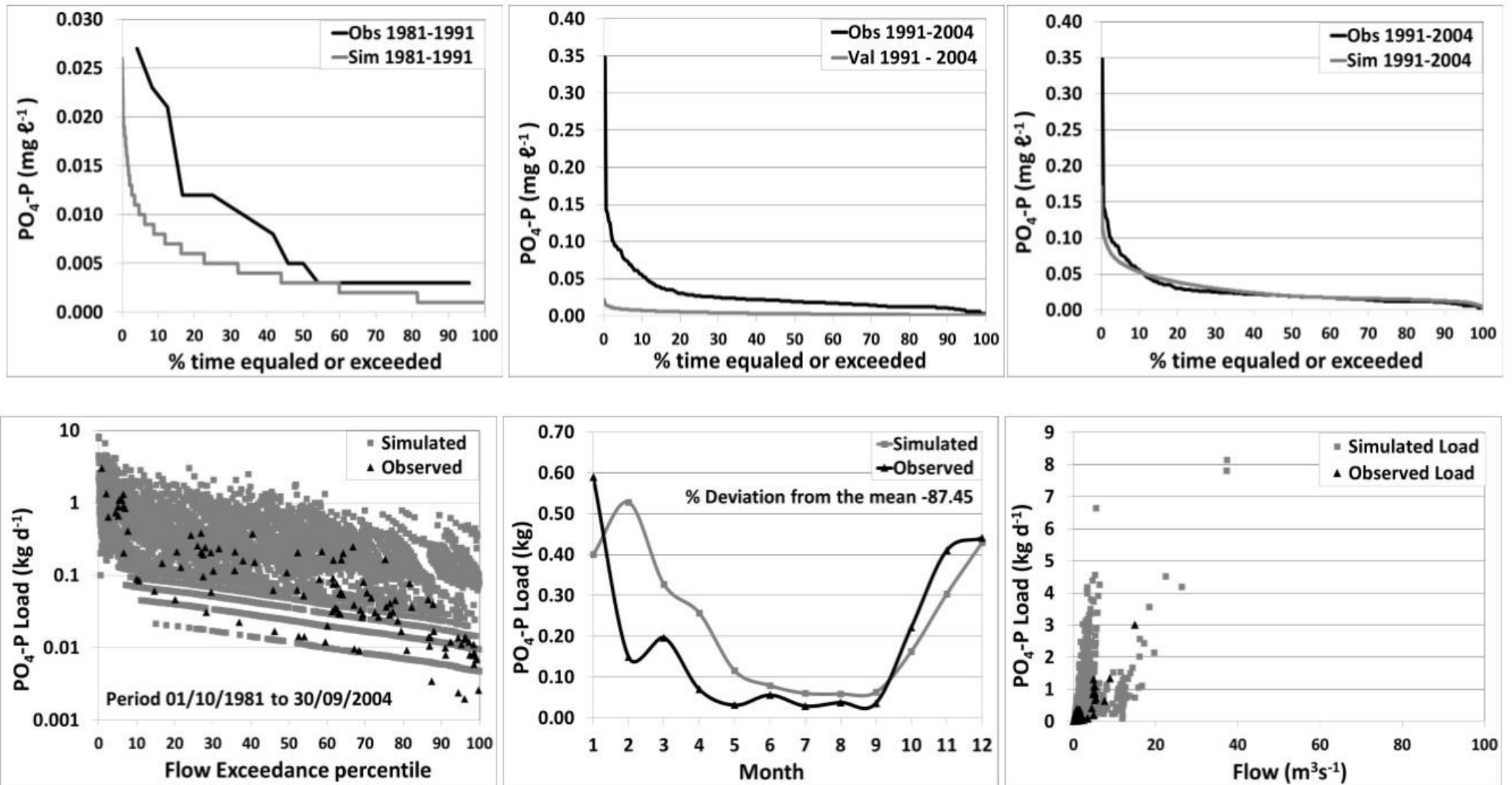


Figure C7. Simulated vs observed results for PO<sub>4</sub>-P at node X21F-2 (gauging station X2H011) along the Elands River.



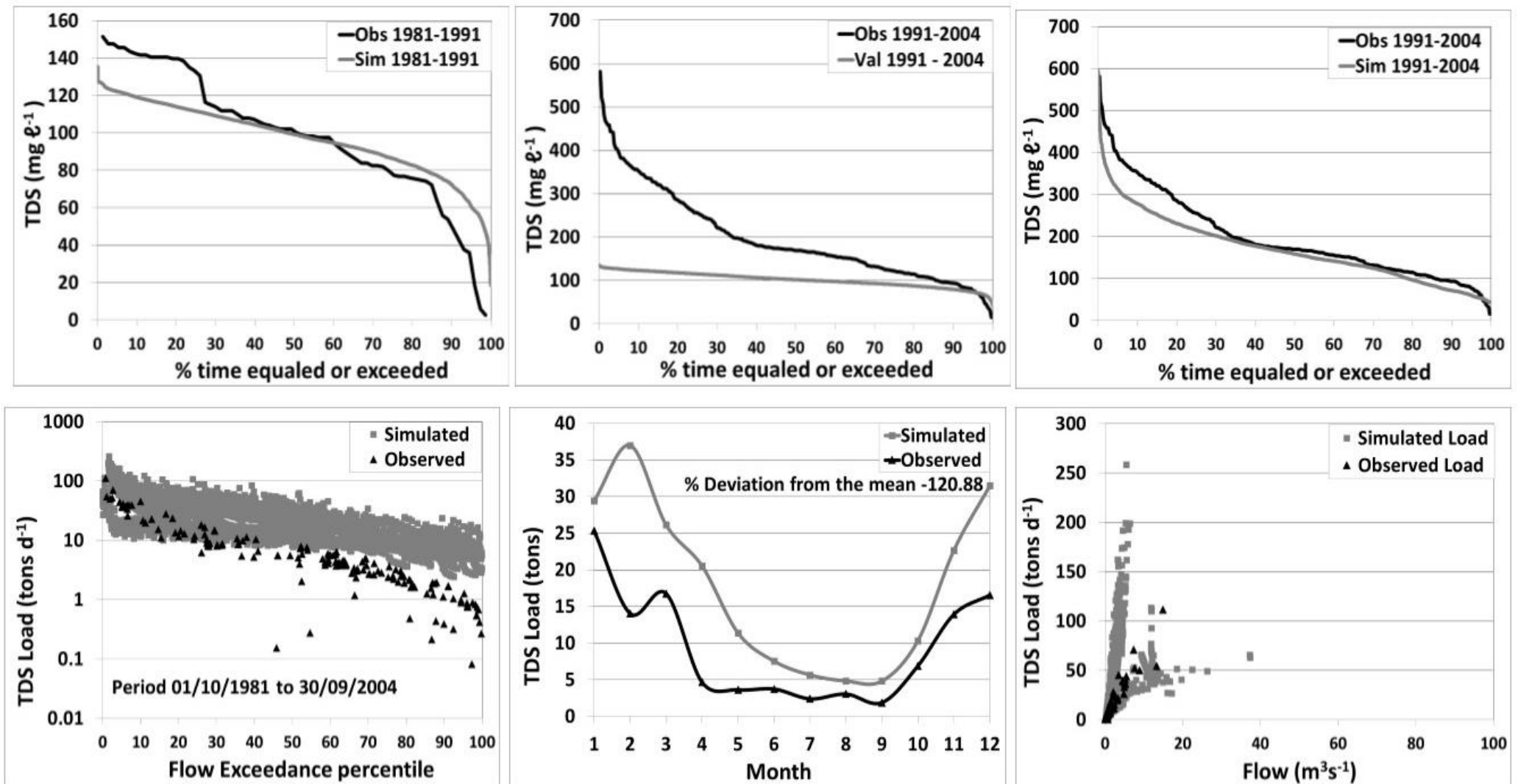


Figure C8. Simulated vs observed results for TDS at node X21F-2 (gauging station X2H011) along the Elands River.

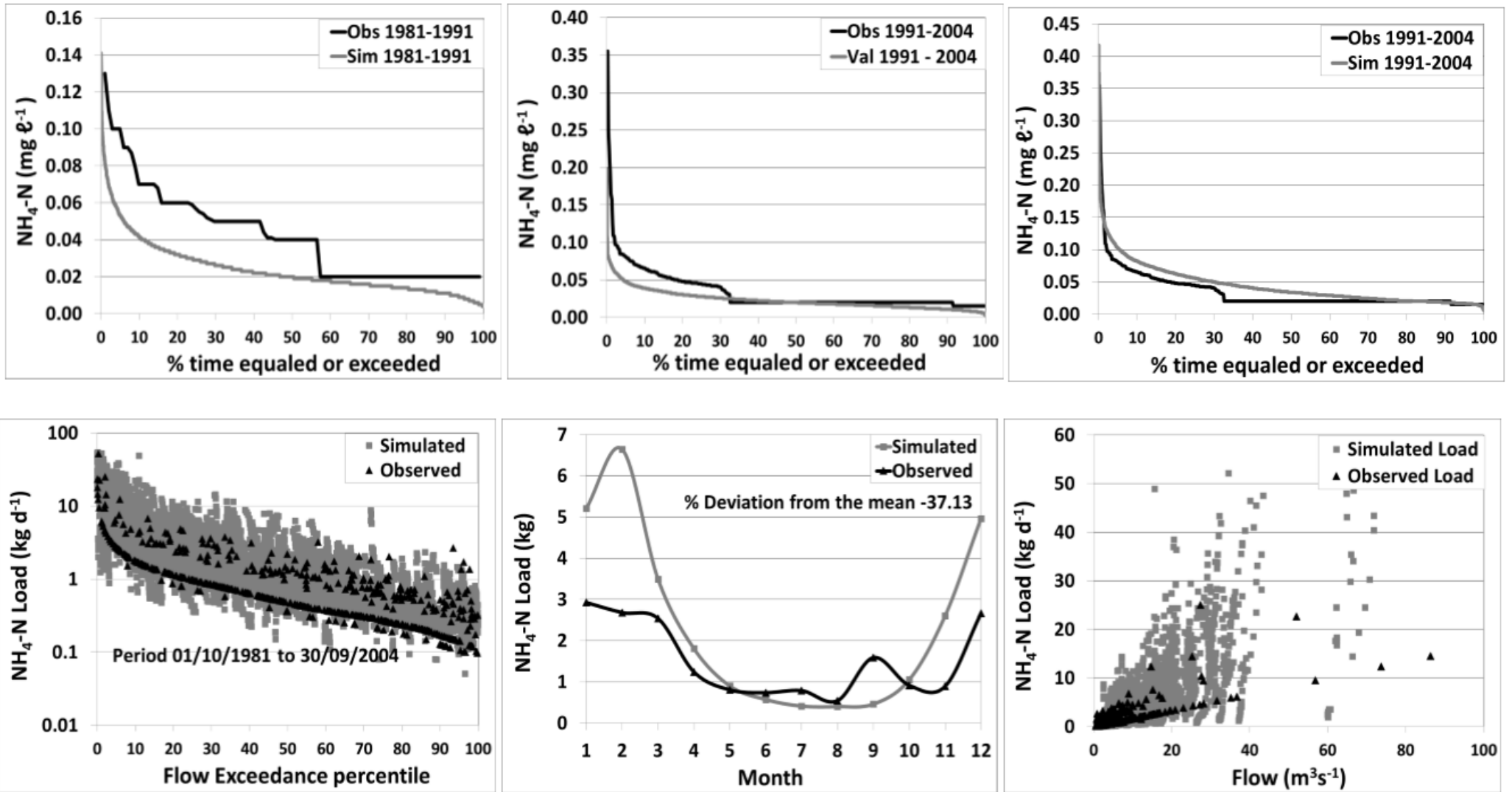


Figure C9. Simulated vs observed results for NH<sub>4</sub>-N at node X21K-2 (gauging station X2H015) along the Elands River.

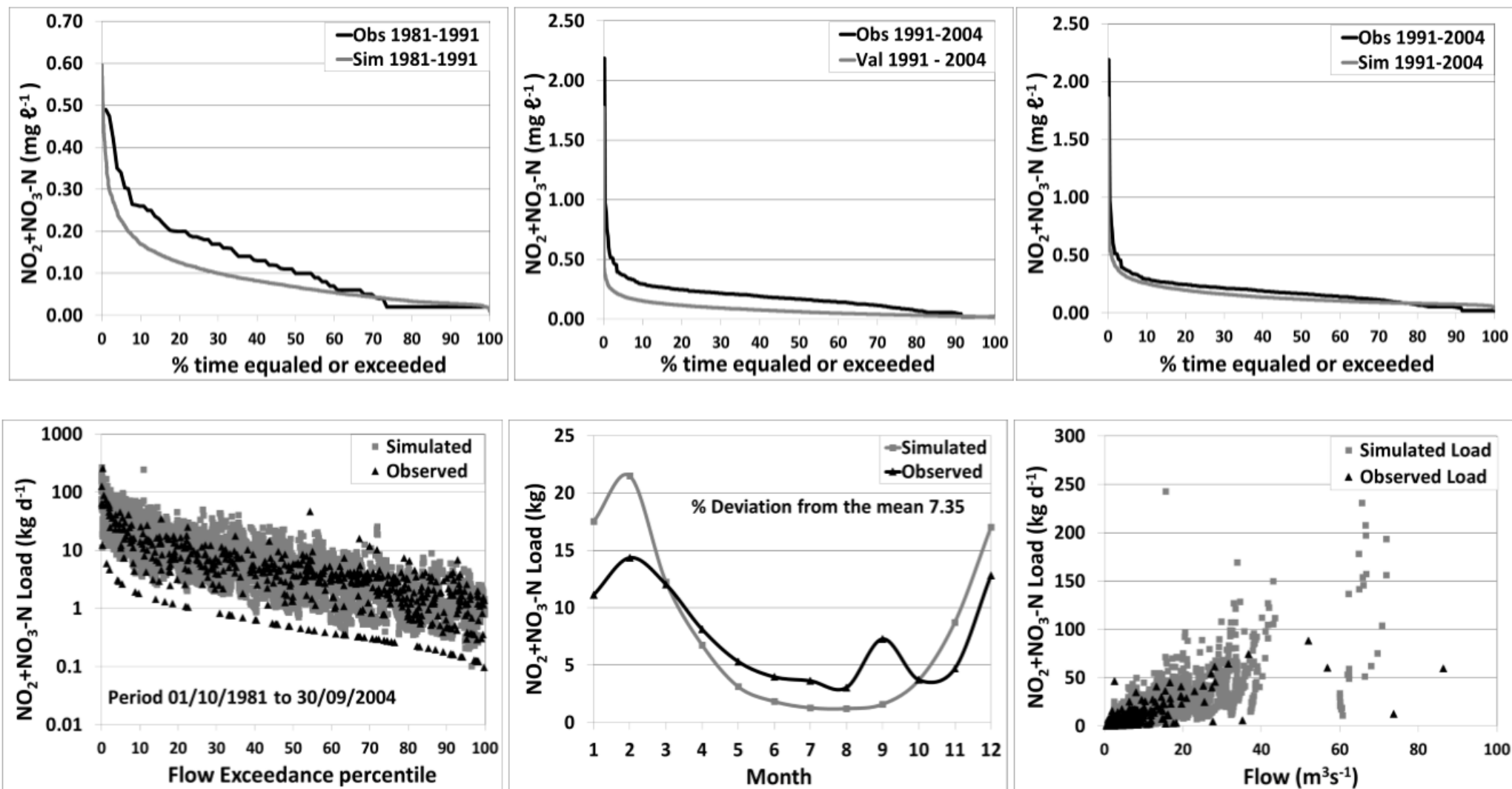


Figure C10. Simulated vs observed results for  $\text{NO}_2 + \text{NO}_3\text{-N}$  at node X21K-2 (gauging station X2H015) along the Elands River.

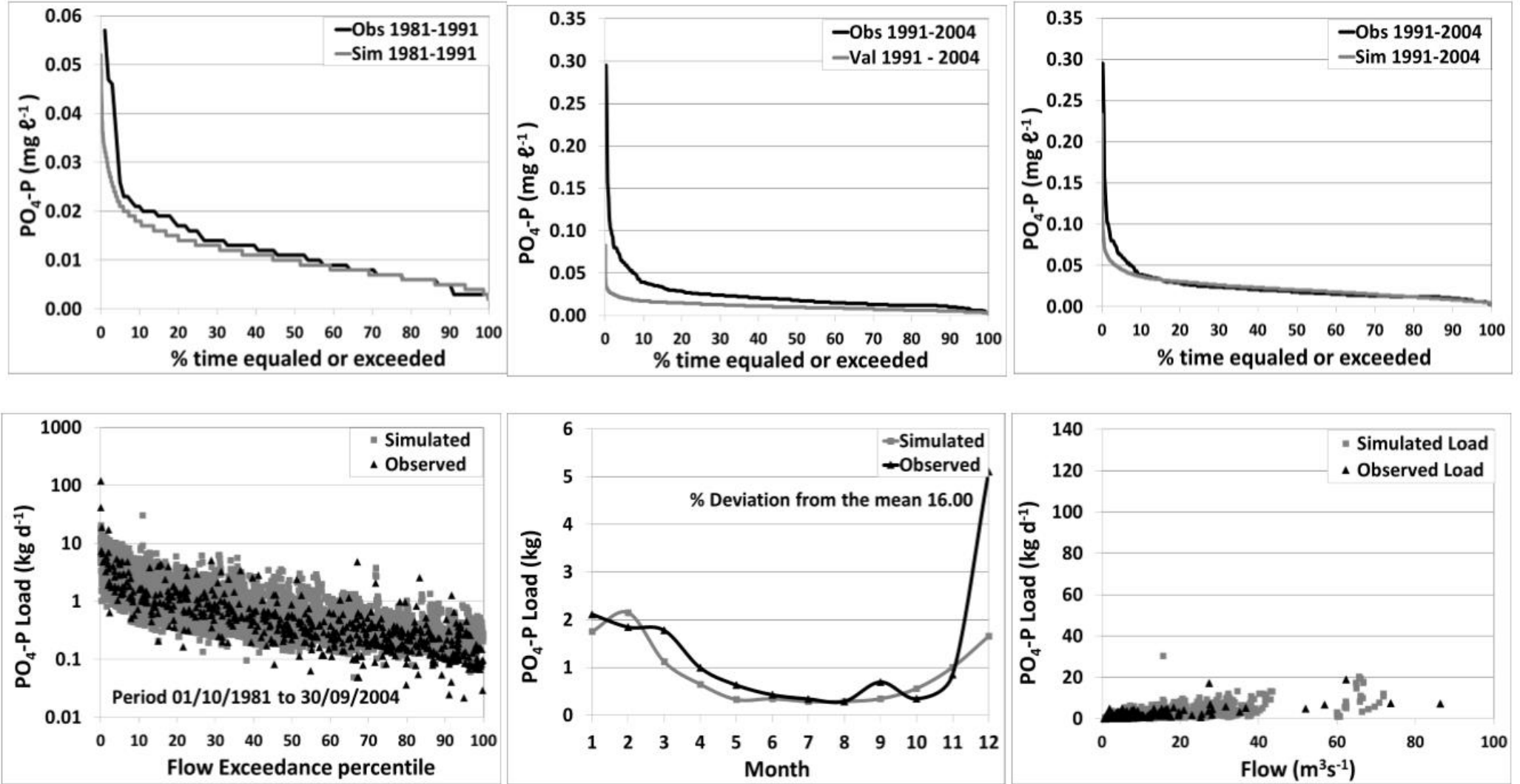


Figure C11. Simulated vs observed results for PO<sub>4</sub>-P at node X21K-2 (gauging station X2H015) along the Elands River.

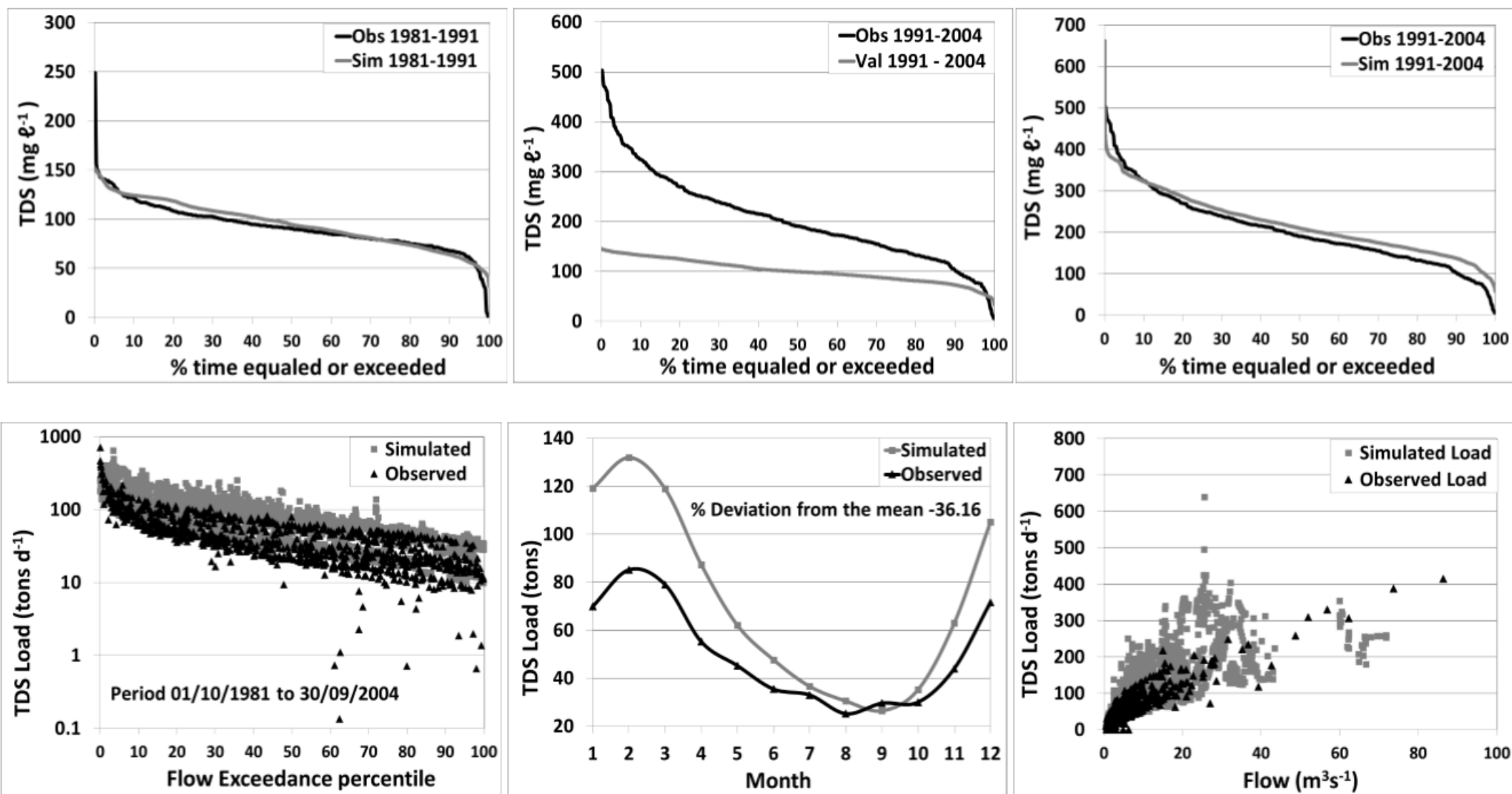


Figure C12. Simulated vs observed results for TDS at node X21K-2 (gauging station X2H015) along the Elands River.

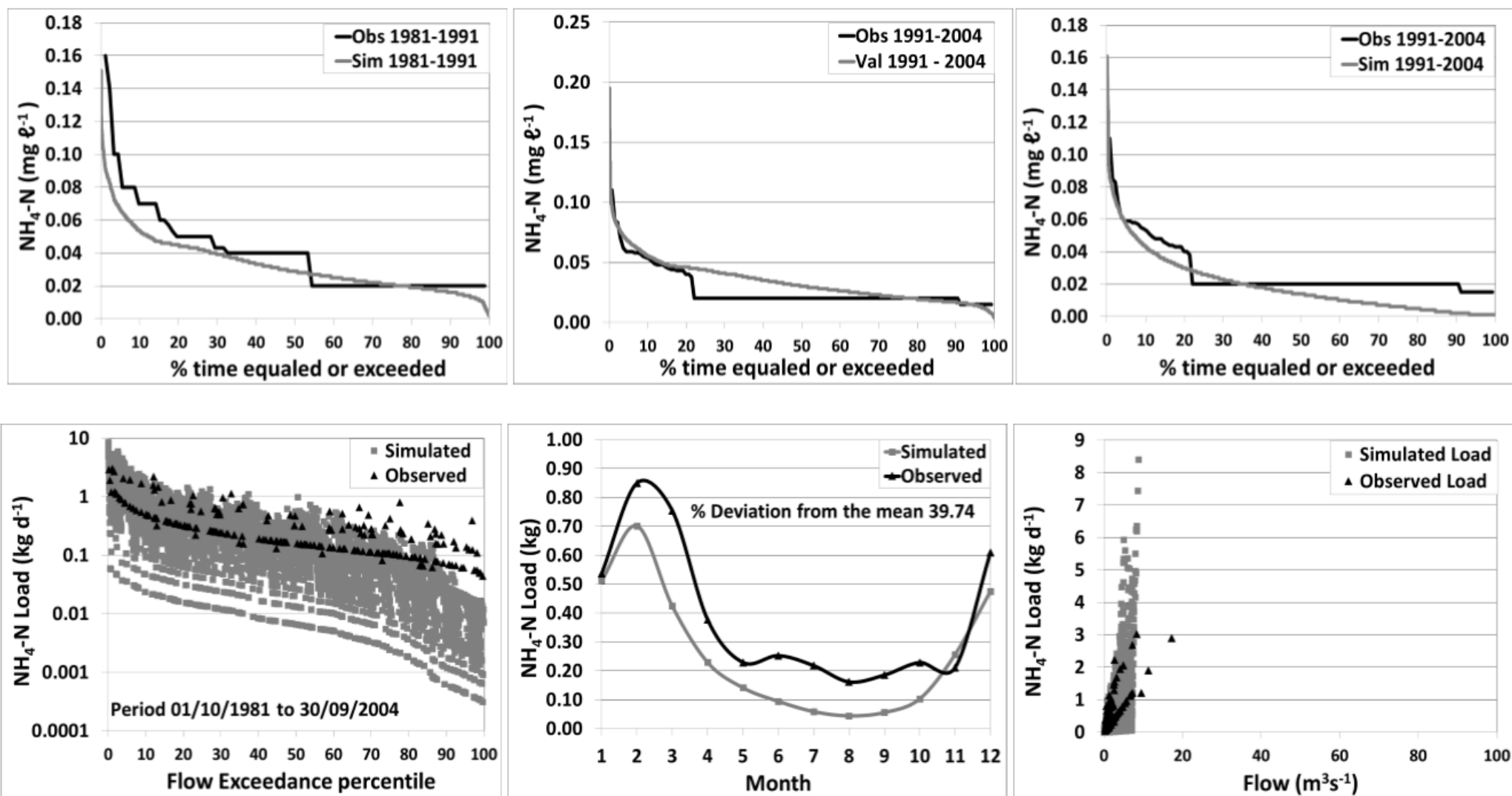


Figure C13. Simulated vs observed results for NH<sub>4</sub>-N at node X22A-2 (gauging station X2H014) along the Houtbosloop River.

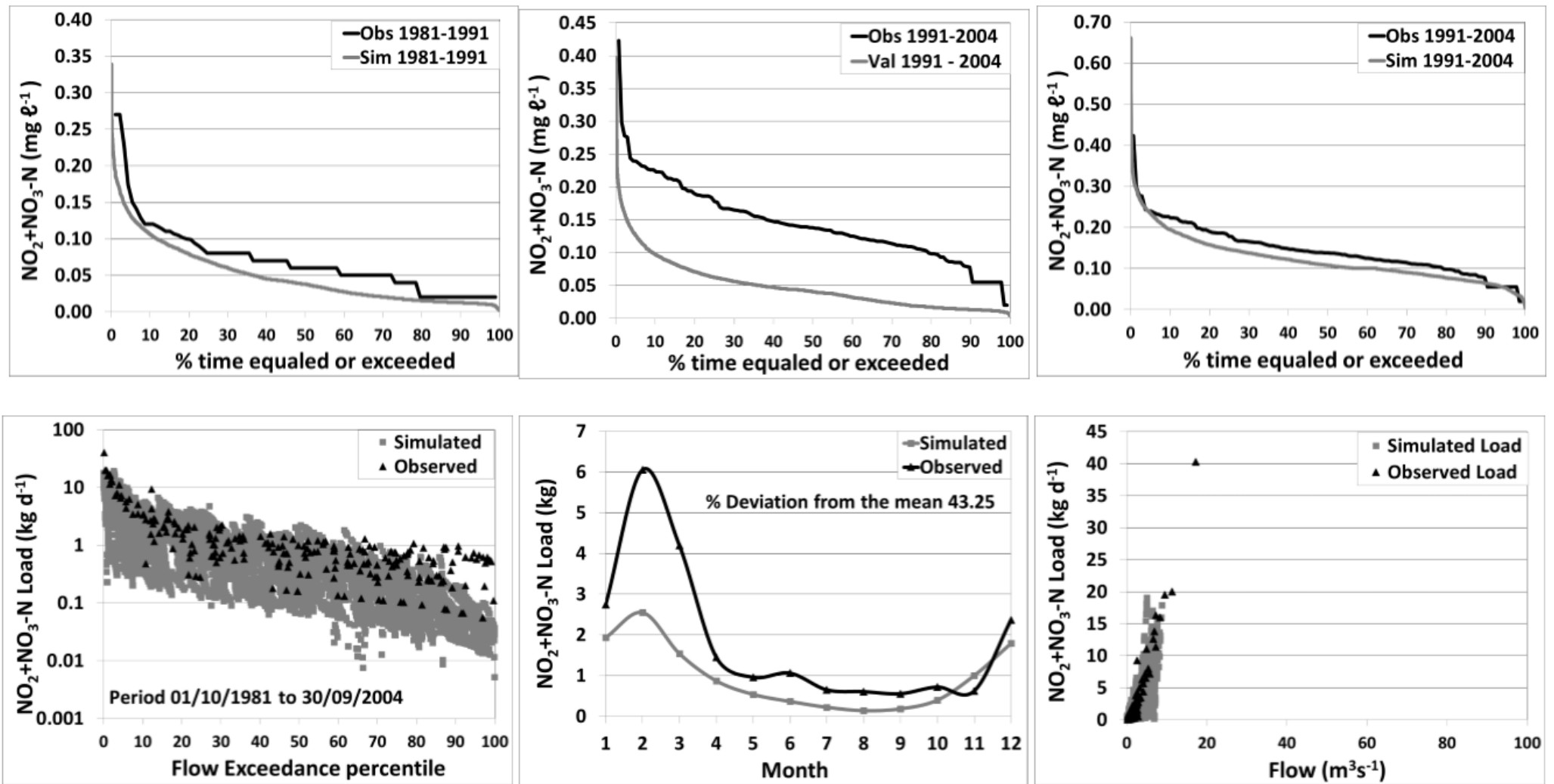


Figure C14. Simulated vs observed results for  $\text{NO}_2 + \text{NO}_3\text{-N}$  at node X22A-2 (gauging station X2H014) along the Houtbosloop River.

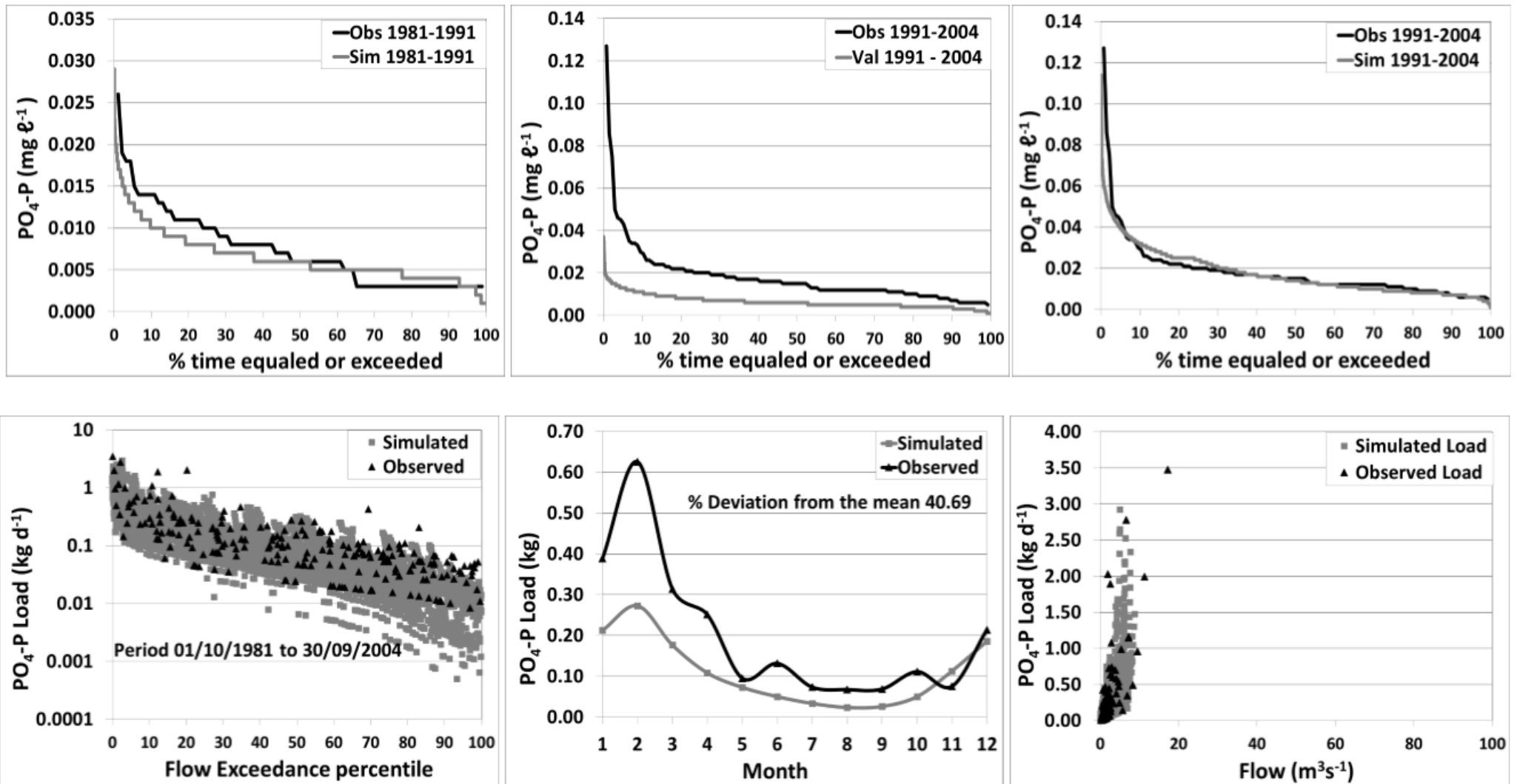


Figure C15. Simulated vs observed results for PO<sub>4</sub>-P at node X22A-2 (gauging station X2H014) along the Houtbosloop River.



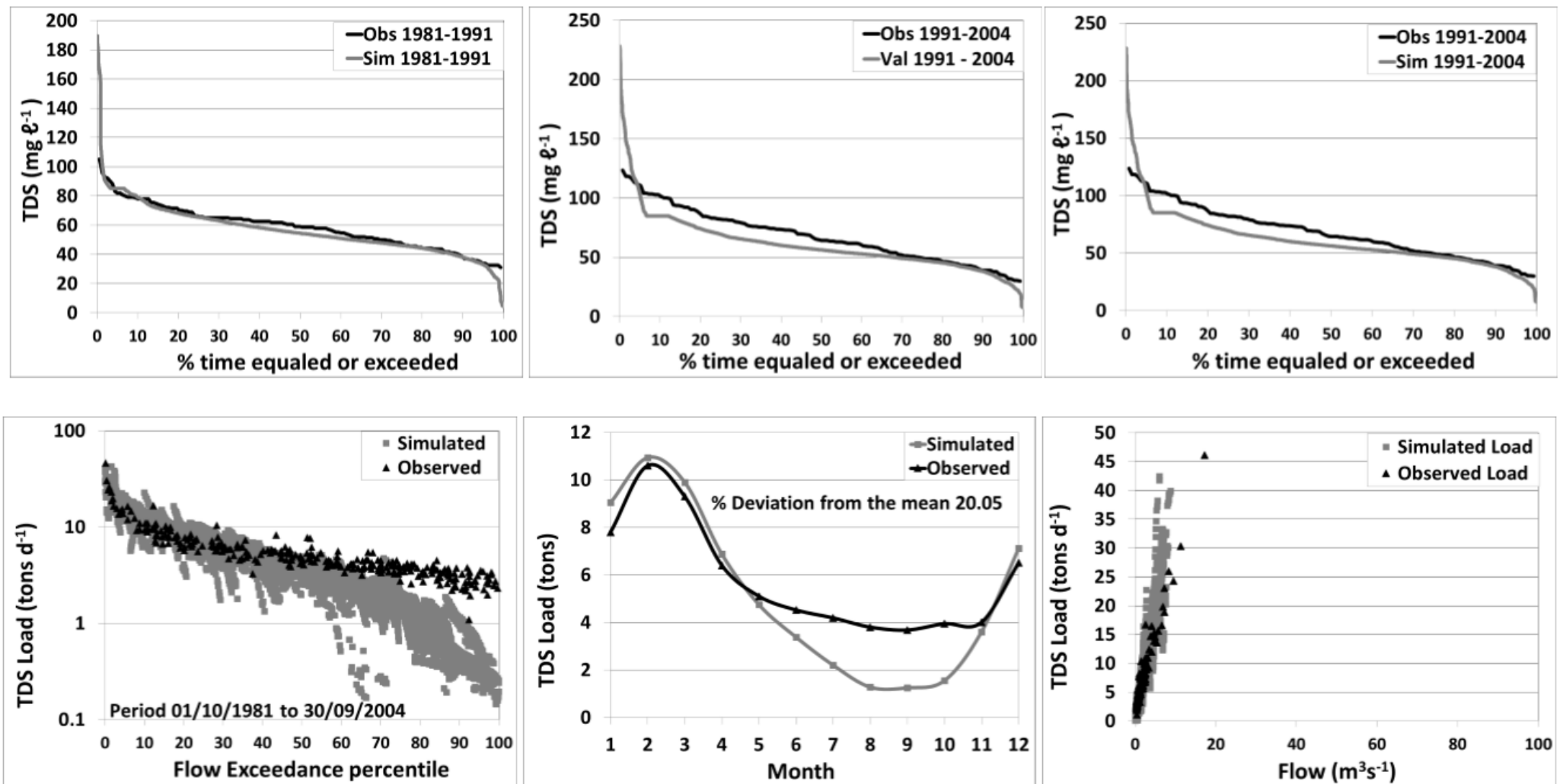


Figure C16. Simulated vs observed results for TDS at node X22A-2 (gauging station X2H014) along the Houtbosloop River.

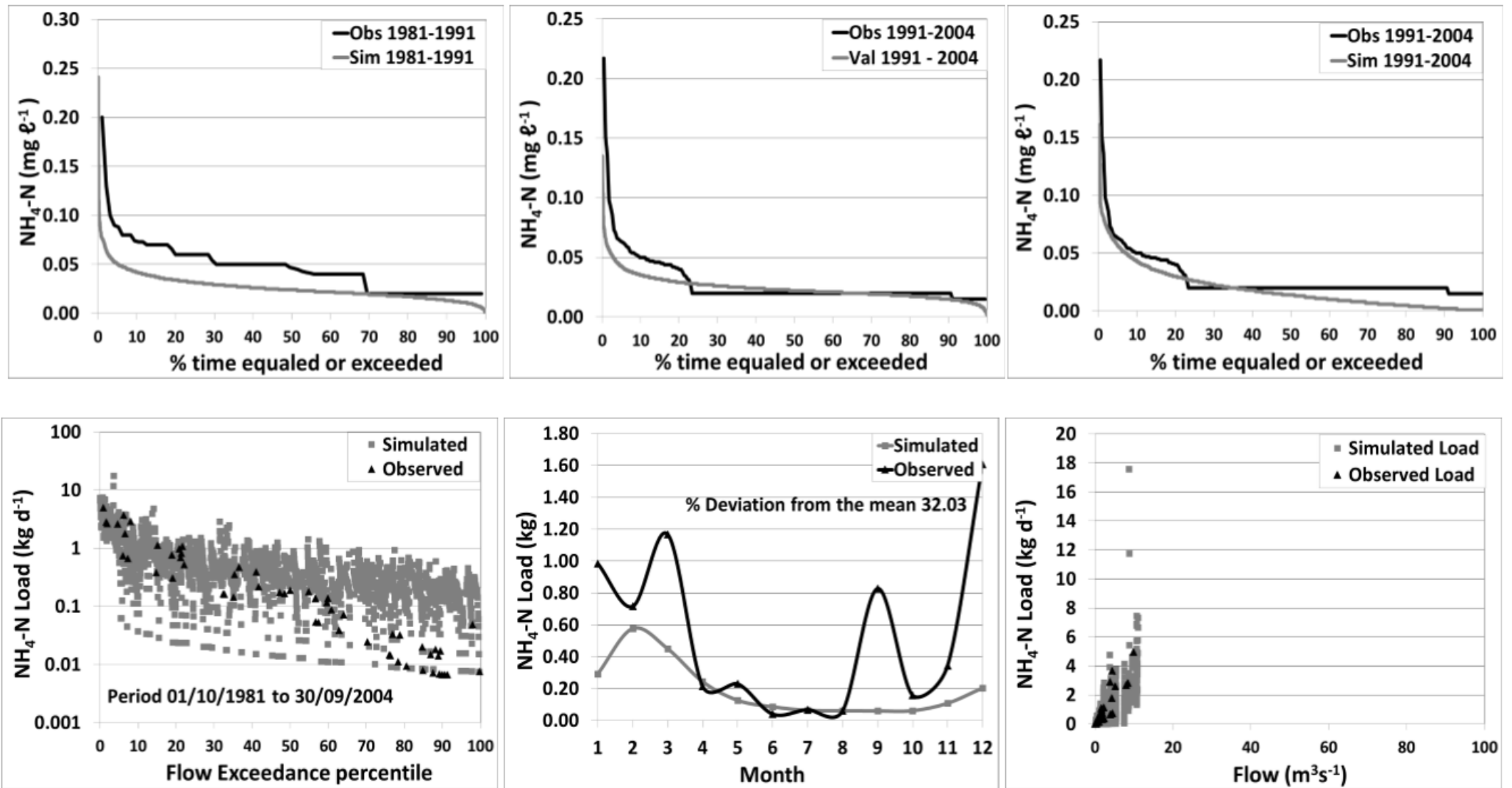


Figure C17. Simulated vs observed results for  $\text{NH}_4\text{-N}$  at node X22F-2 (gauging station X2H005) along the Nels River.

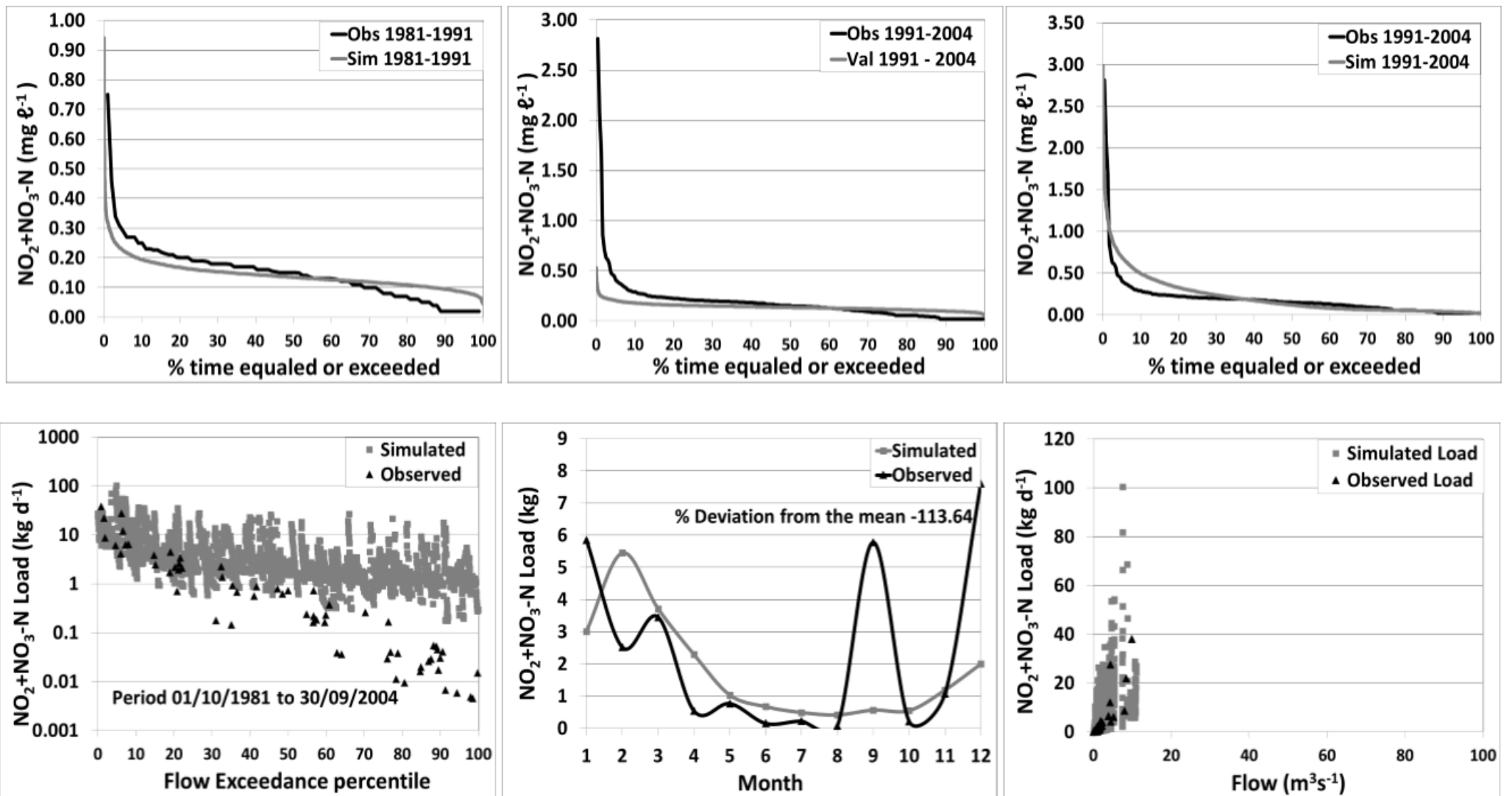


Figure C18. Simulated vs observed results for  $\text{NO}_2 + \text{NO}_3\text{-N}$  at node X22F-2 (gauging station X2H005) along the Nels River.

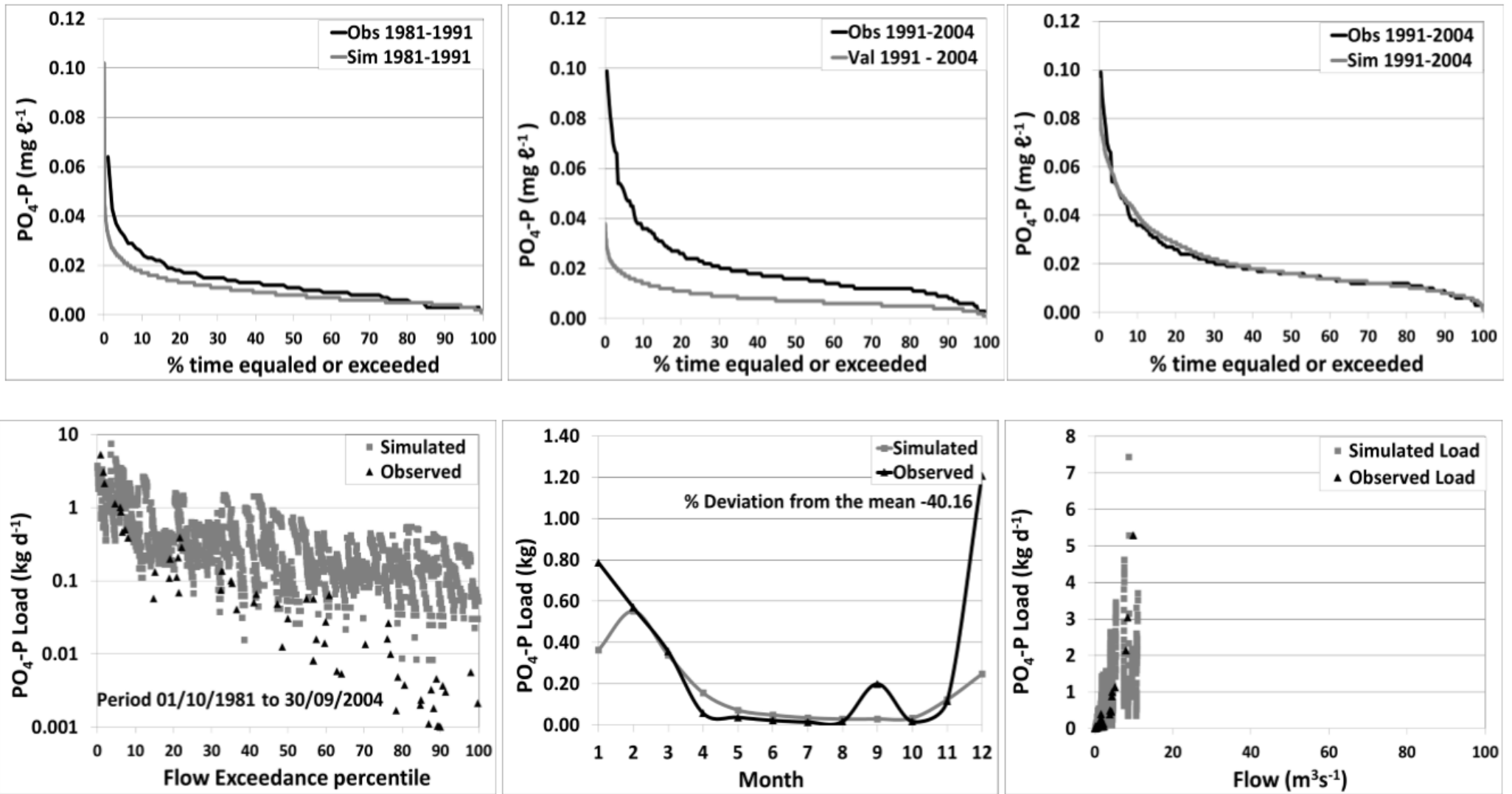


Figure C19. Simulated vs observed results for PO<sub>4</sub>-P at node X22F-2 (gauging station X2H005) along the Nels River.

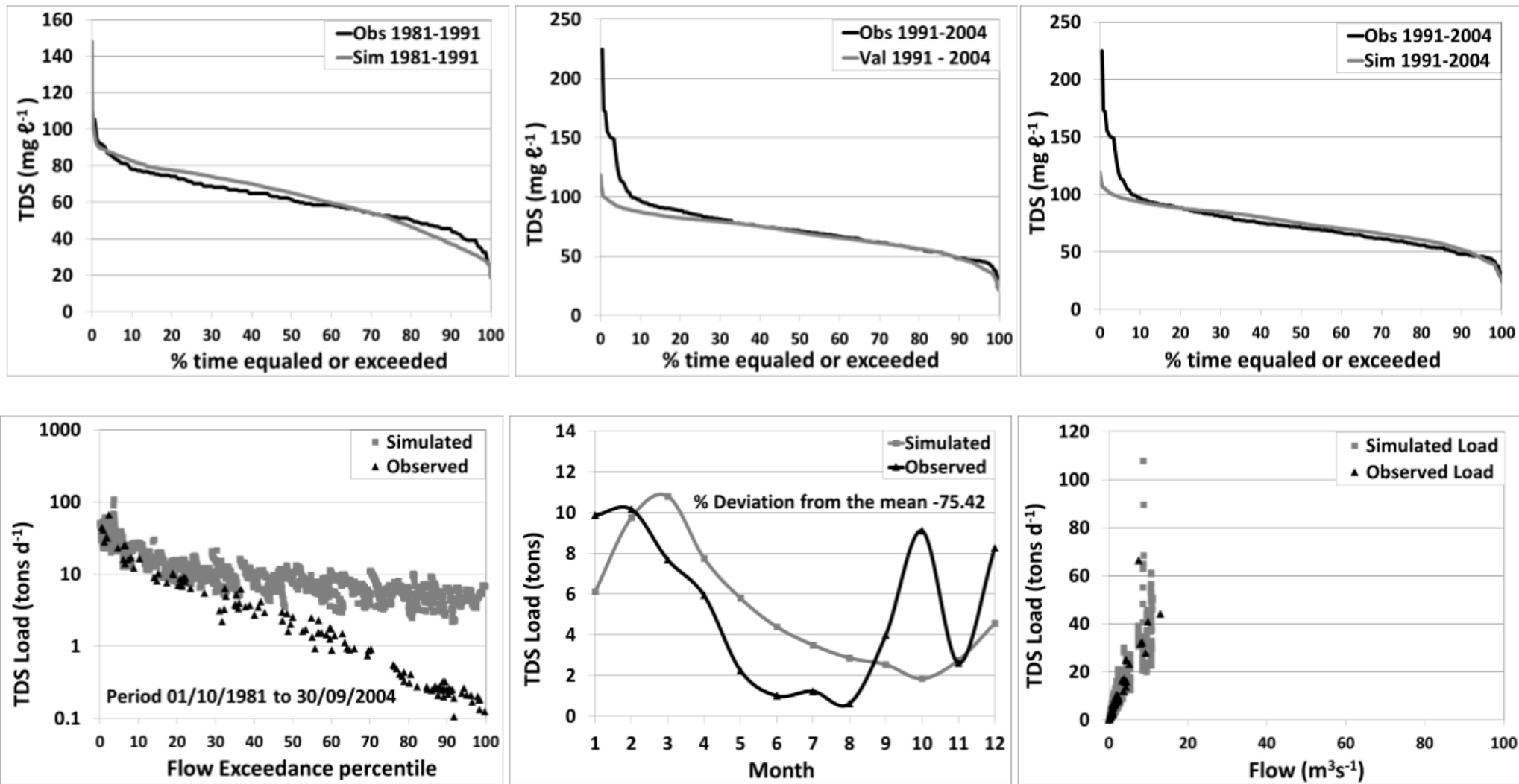


Figure C20. Simulated vs observed results for TDS at node X22F-2 (gauging station X2H005) along the Nels River.

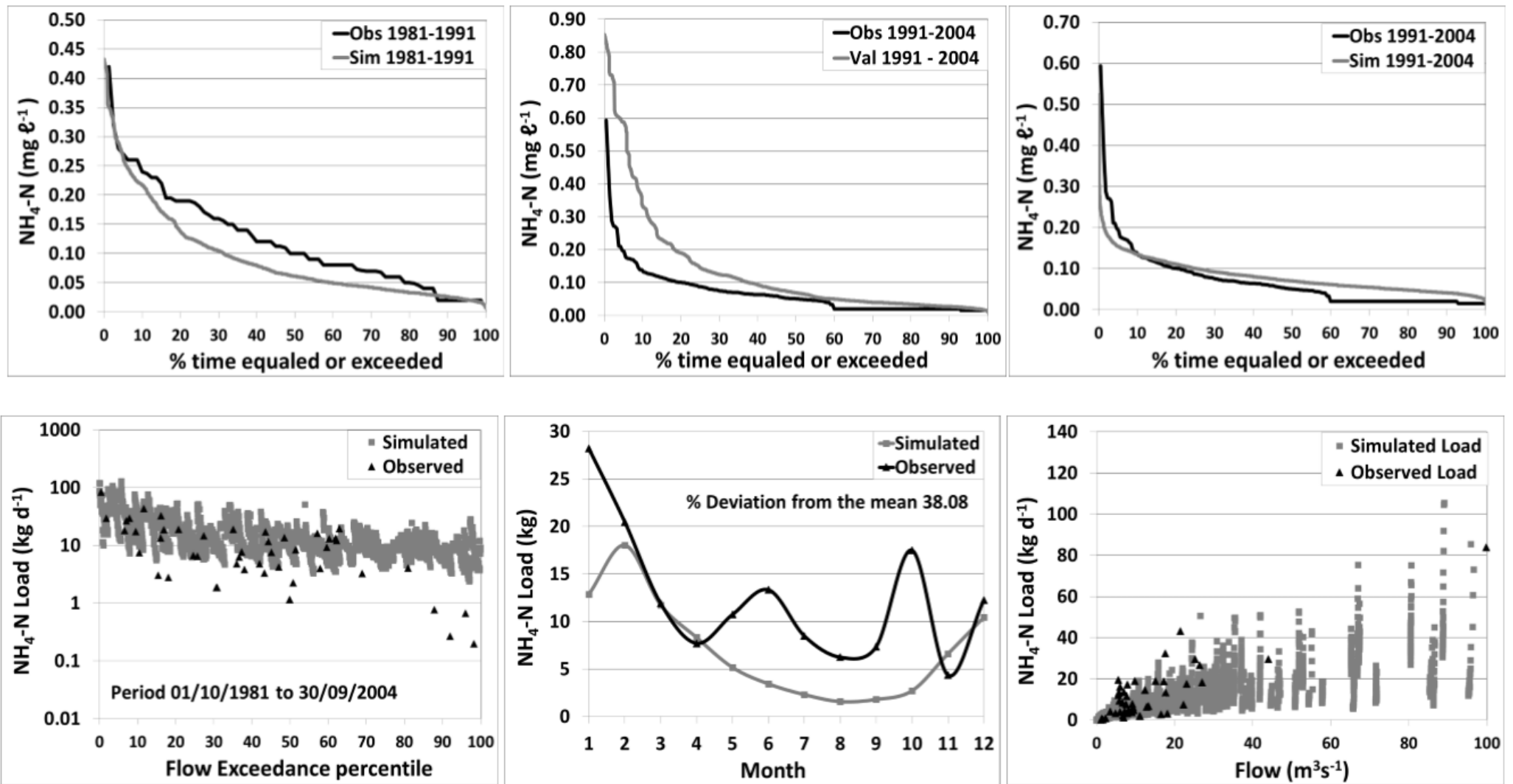


Figure C21. Simulated vs observed results for  $\text{NH}_4\text{-N}$  at node X22J-2 (gauging station X2H006) along the Crocodile River.

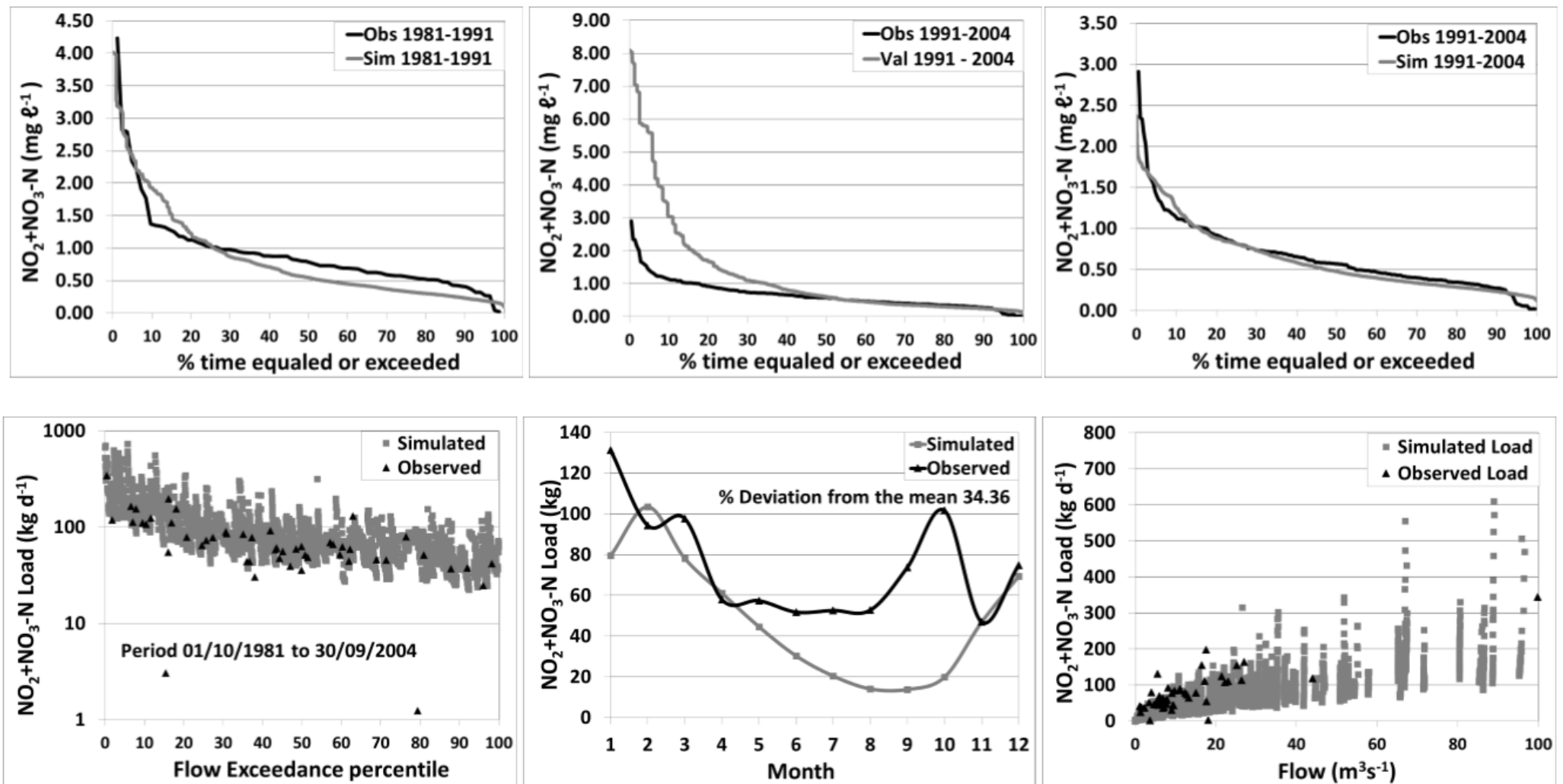


Figure C22. Simulated vs observed results for  $\text{NO}_2 + \text{NO}_3\text{-N}$  at node X22J-2 (gauging station X2H006) along the Crocodile River.

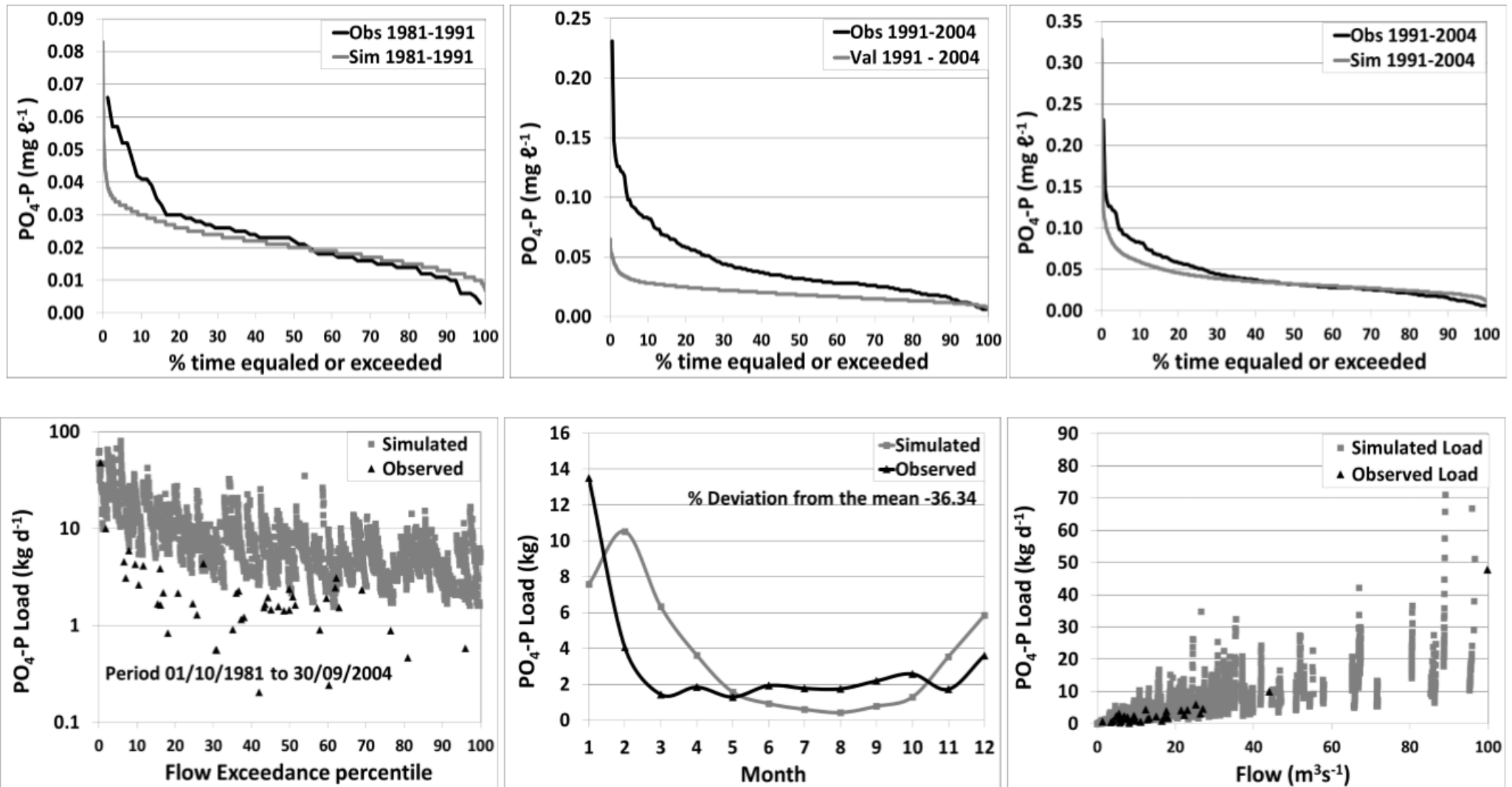


Figure C23. Simulated vs observed results for PO<sub>4</sub>-P at node X22J-2 (gauging station X2H006) along the Crocodile River.



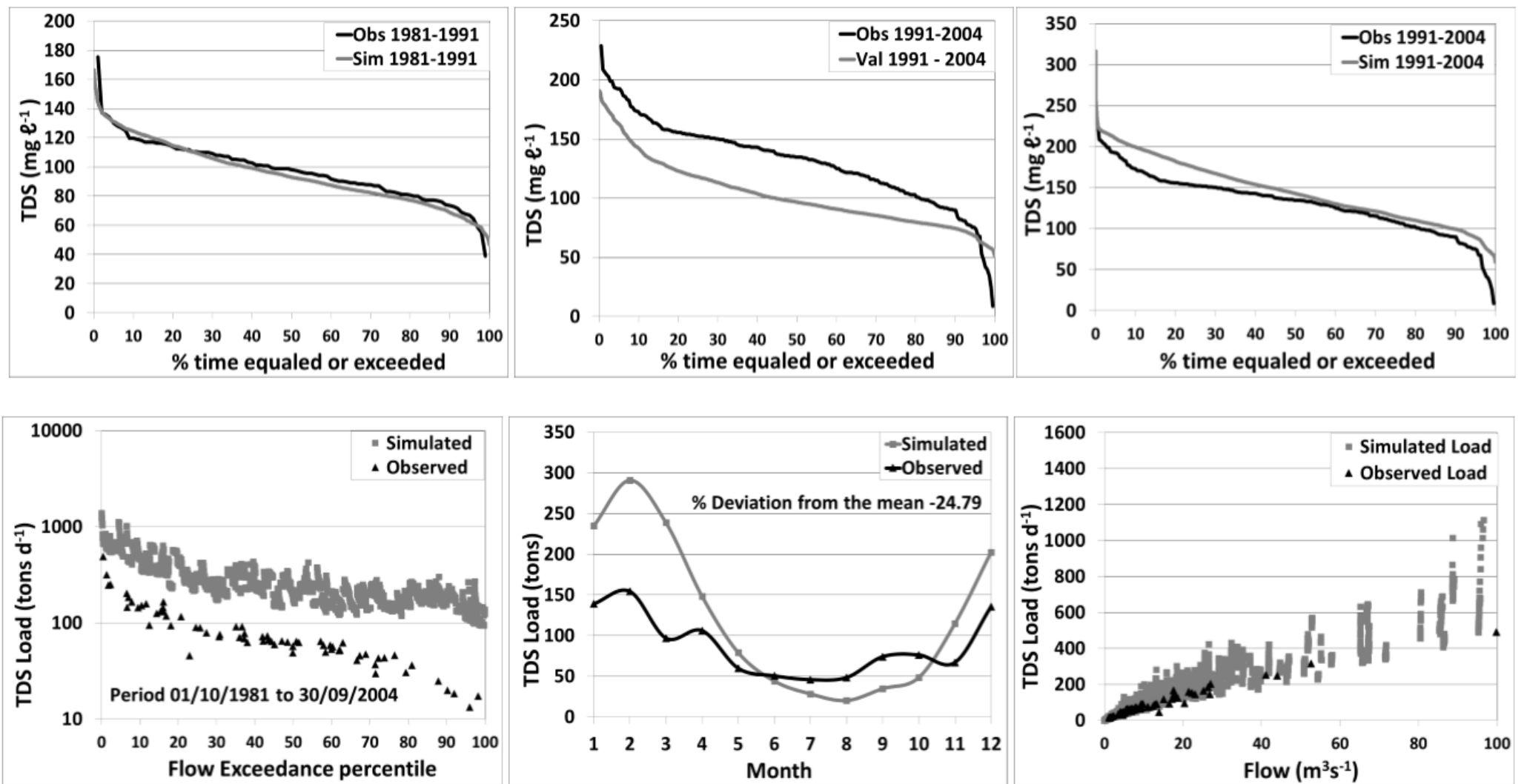


Figure C24. Simulated vs observed results for TDS at node X22J-2 (gauging station X2H006) along the Crocodile River.

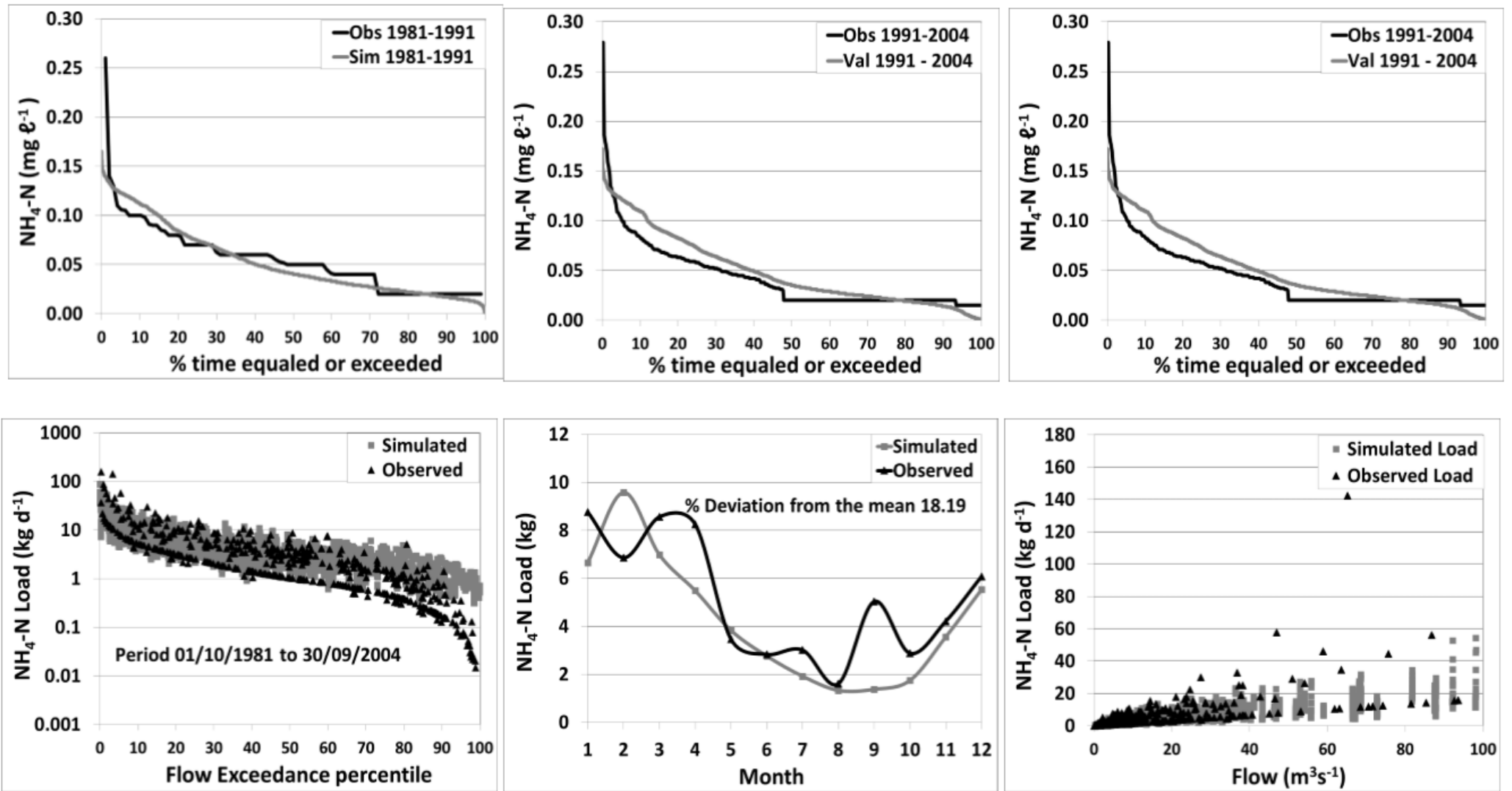


Figure C25. Simulated vs observed results for  $\text{NH}_4\text{-N}$  at node X22K-2 (gauging station X2H032) along the Crocodile River.

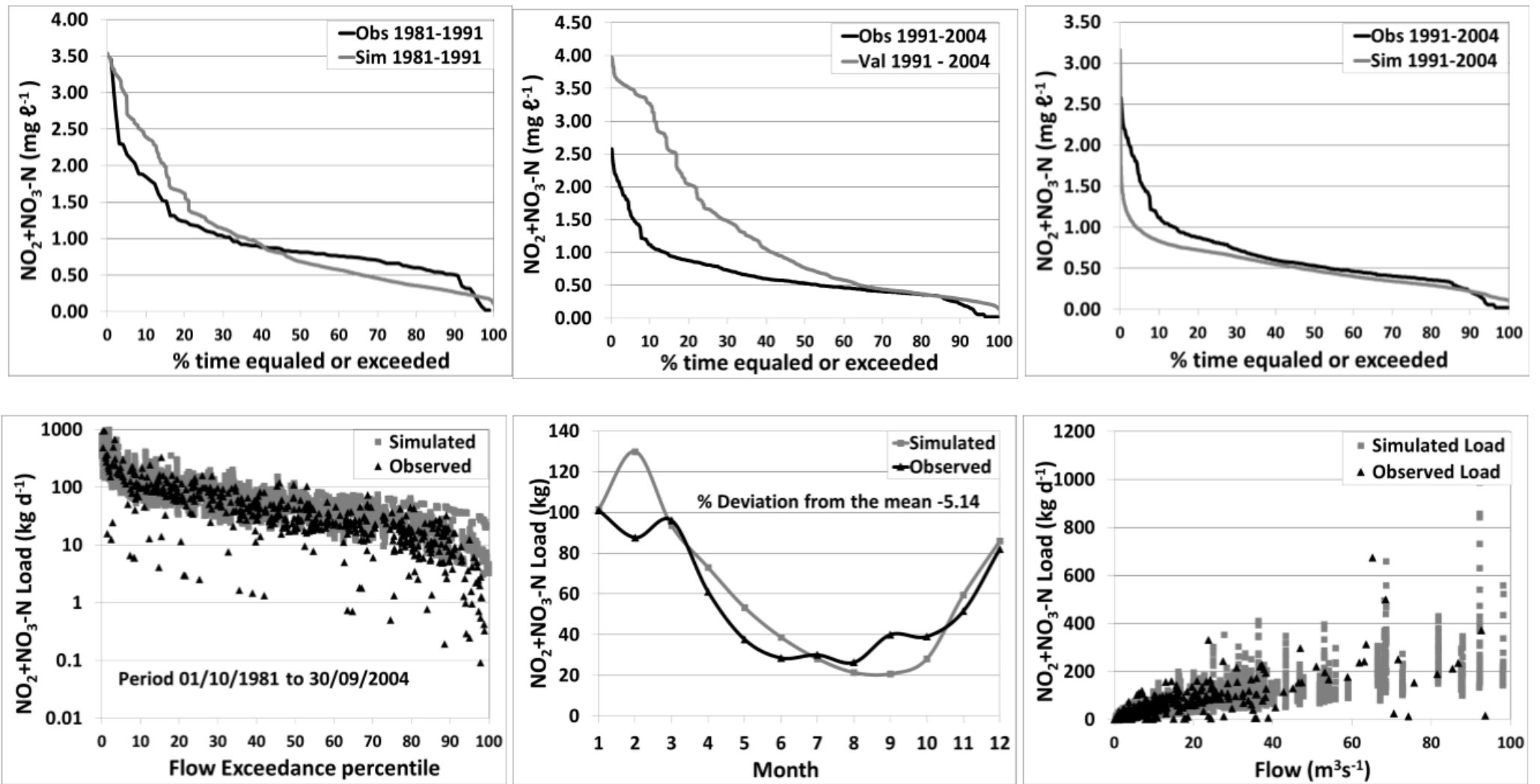


Figure C26. Simulated vs observed results for  $\text{NO}_2 + \text{NO}_3\text{-N}$  at node X22K-2 (gauging station X2H032) along the Crocodile River.

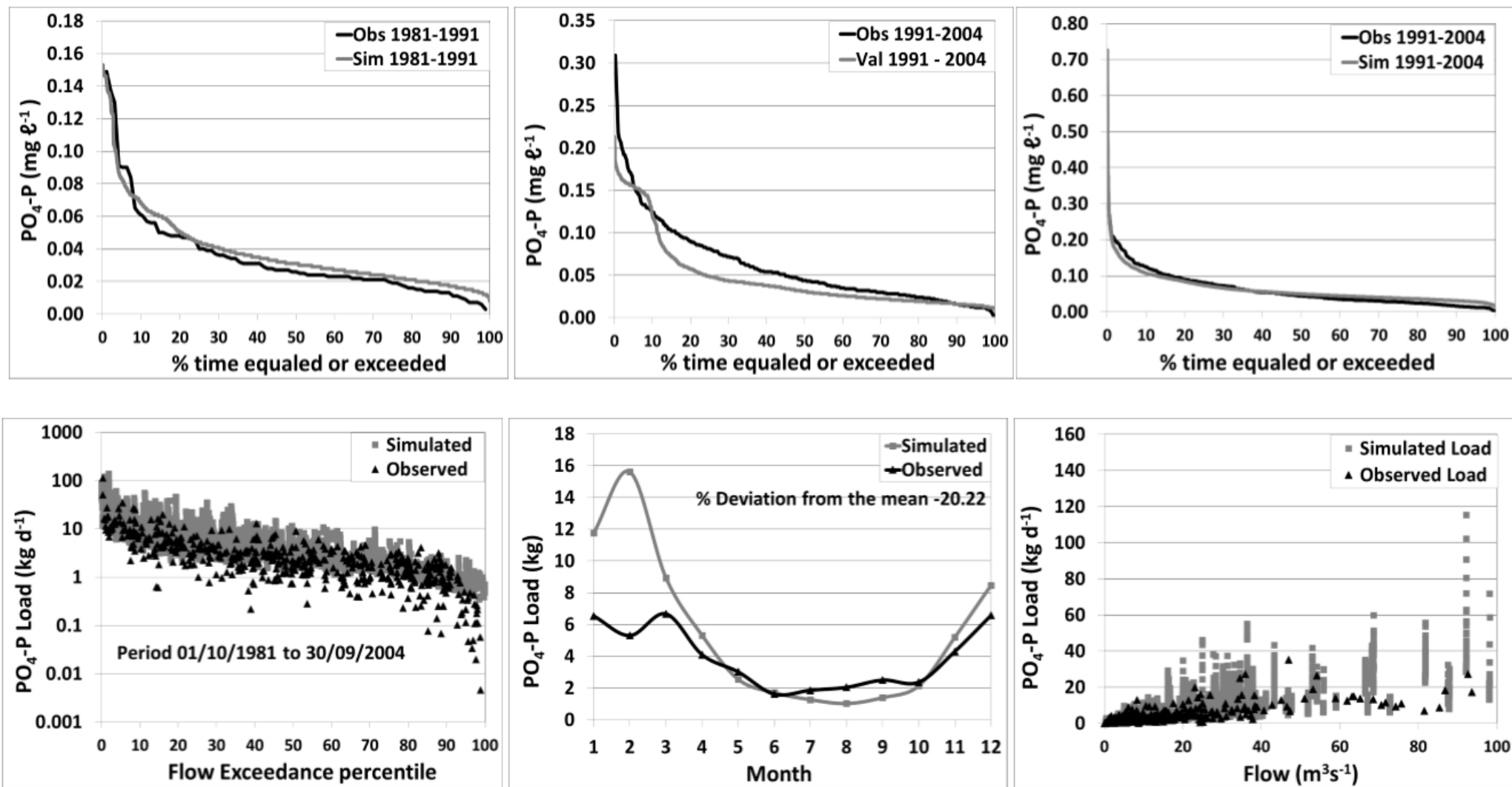


Figure C27. Simulated vs observed results for PO<sub>4</sub>-P at node X22K-2 (gauging station X2H032) along the Crocodile River.

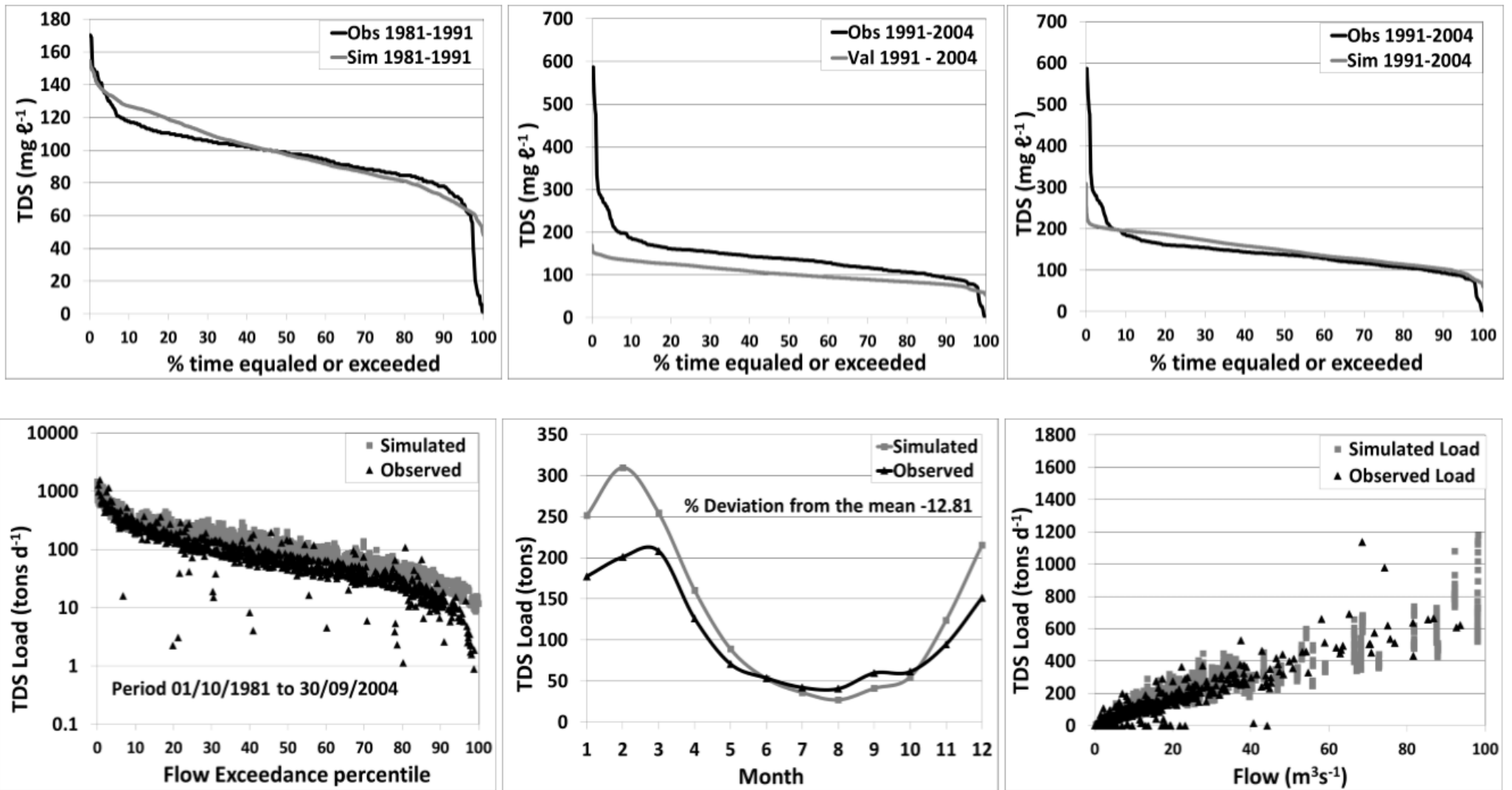


Figure C28. Simulated vs observed results for TDS at node X22K-2 (gauging station X2H032) along the Crocodile River.

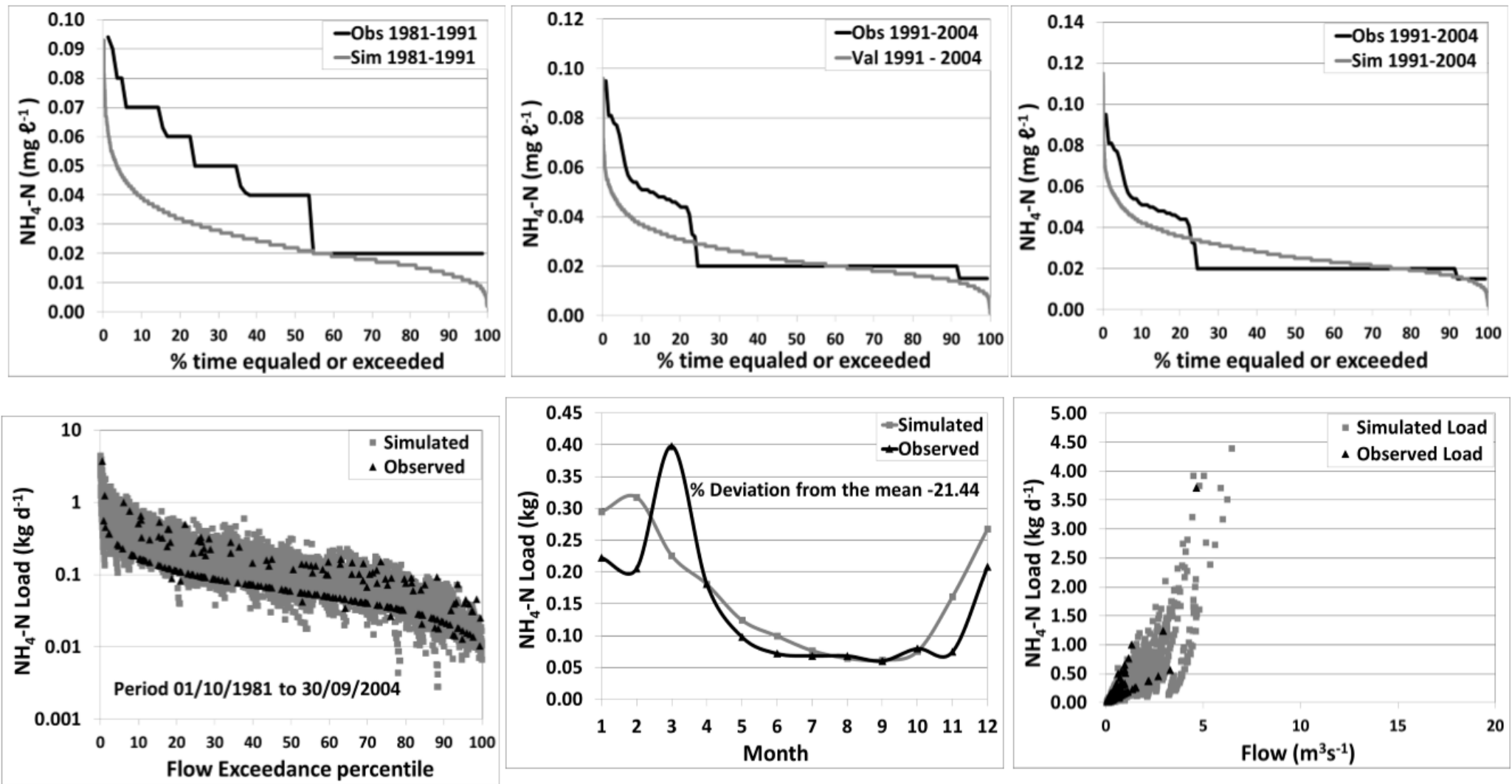


Figure C29. Simulated vs observed results for  $\text{NH}_4\text{-N}$  at node X23A-2 (gauging station X2H010) along the Noordkaap River.

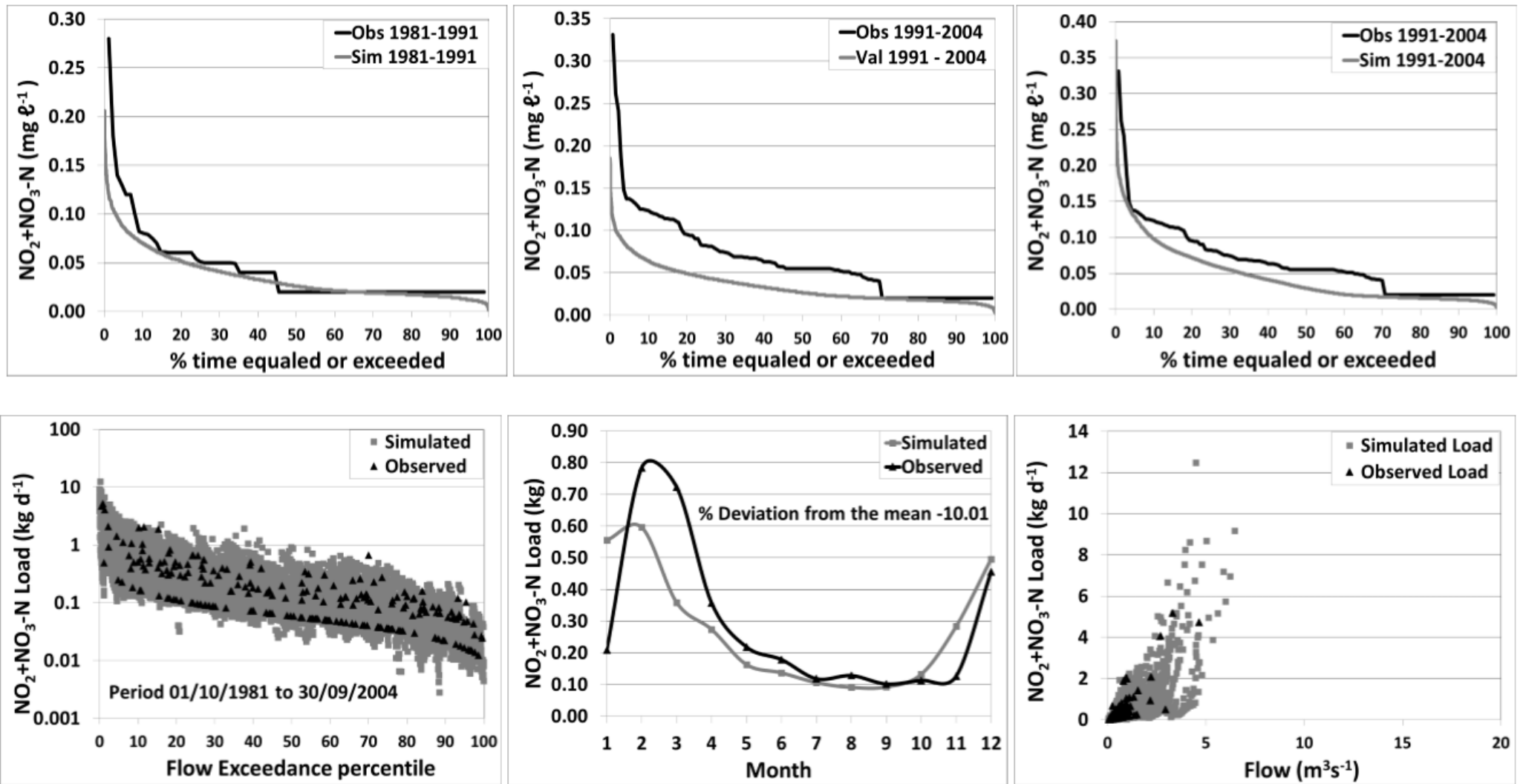


Figure C30. Simulated vs observed results for NO<sub>2</sub> + NO<sub>3</sub>-N at node X23A-2 (gauging station X2H010) along the Noordkaap River.

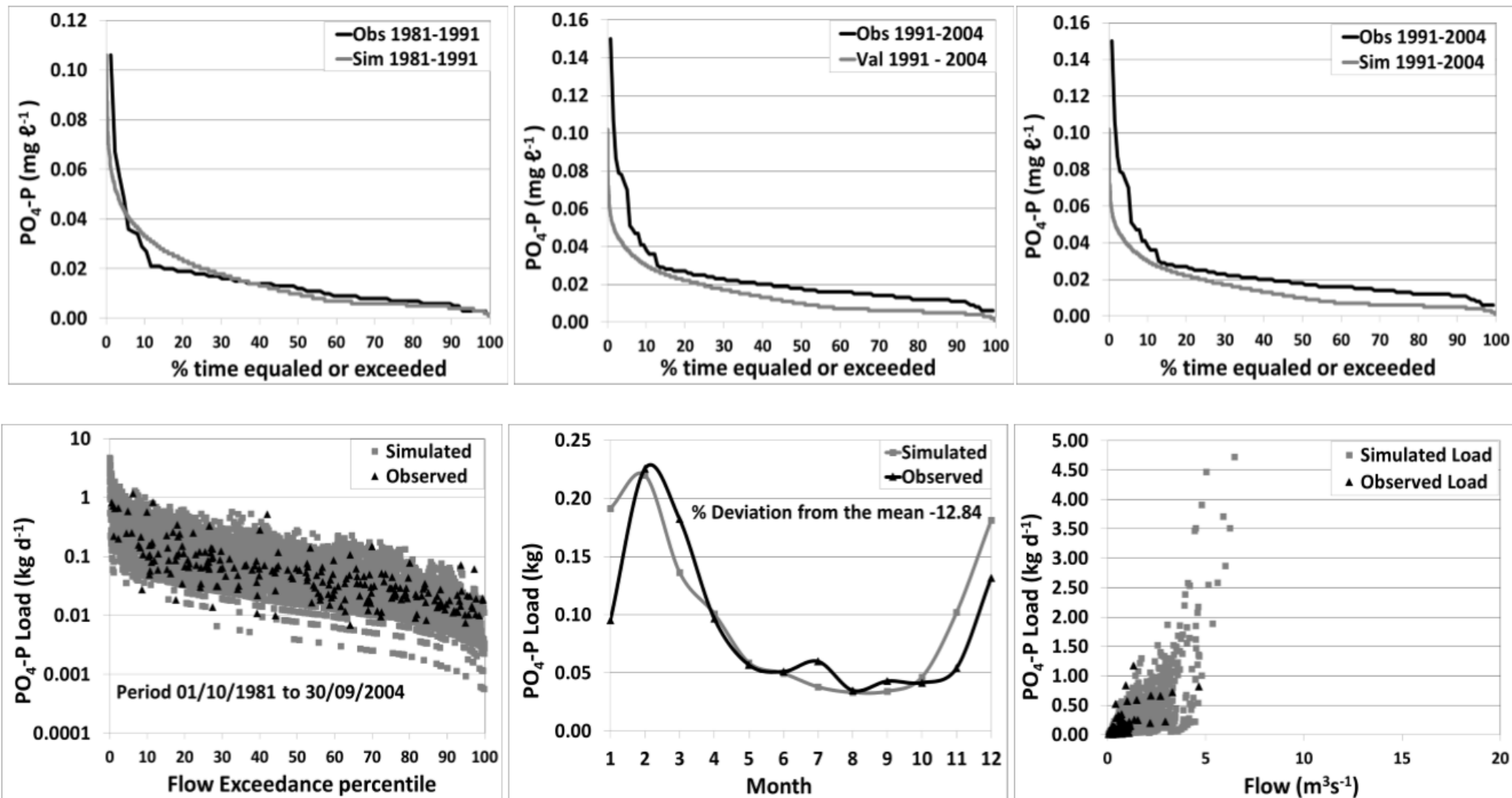


Figure C31. Simulated vs observed results for PO<sub>4</sub>-P at node X23A-2 (gauging station X2H010) along the Noordkaap River.



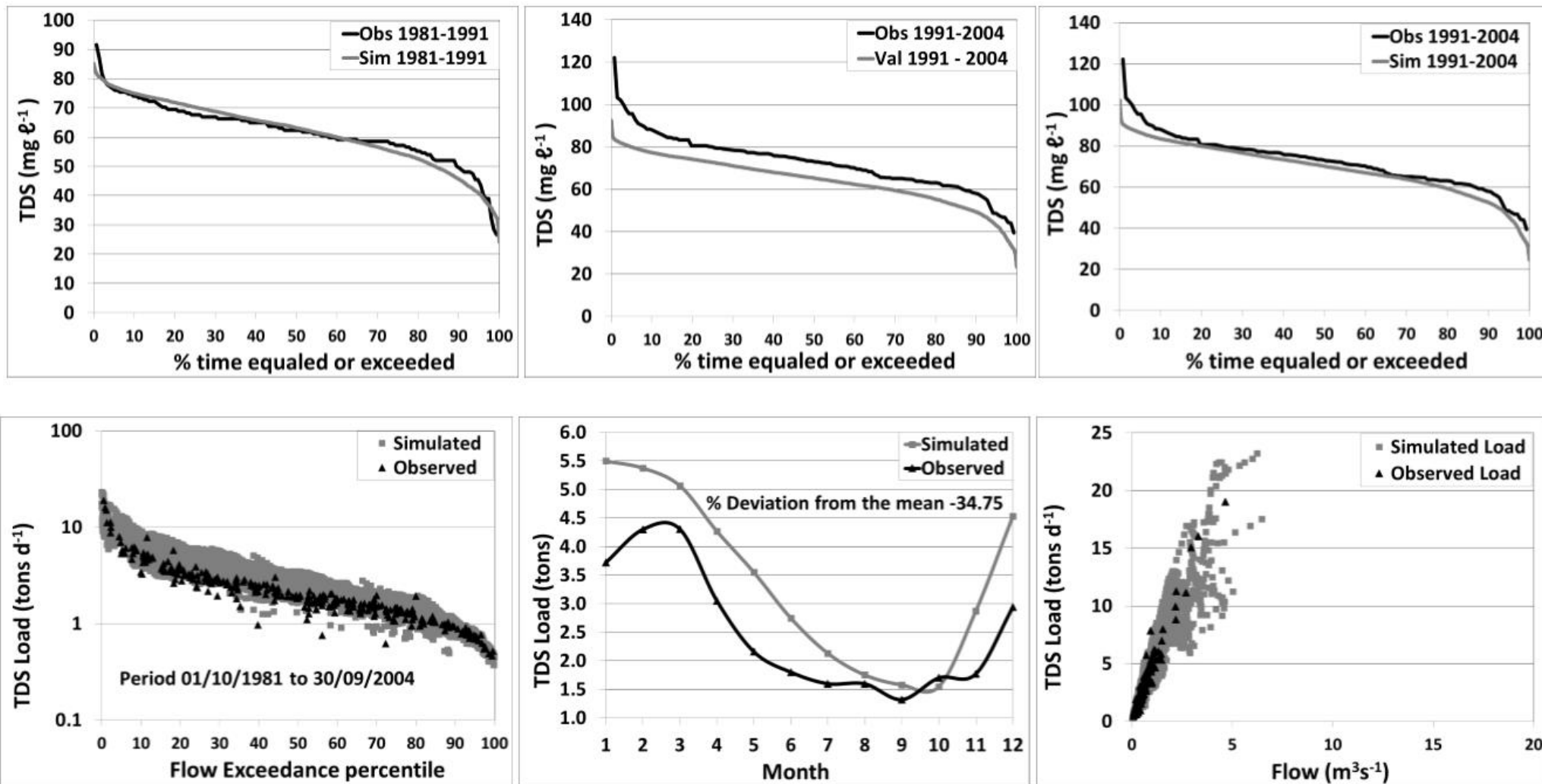


Figure C32. Simulated vs observed results for TDS at node X23A-2 (gauging station X2H010) along the Noordkaap River.

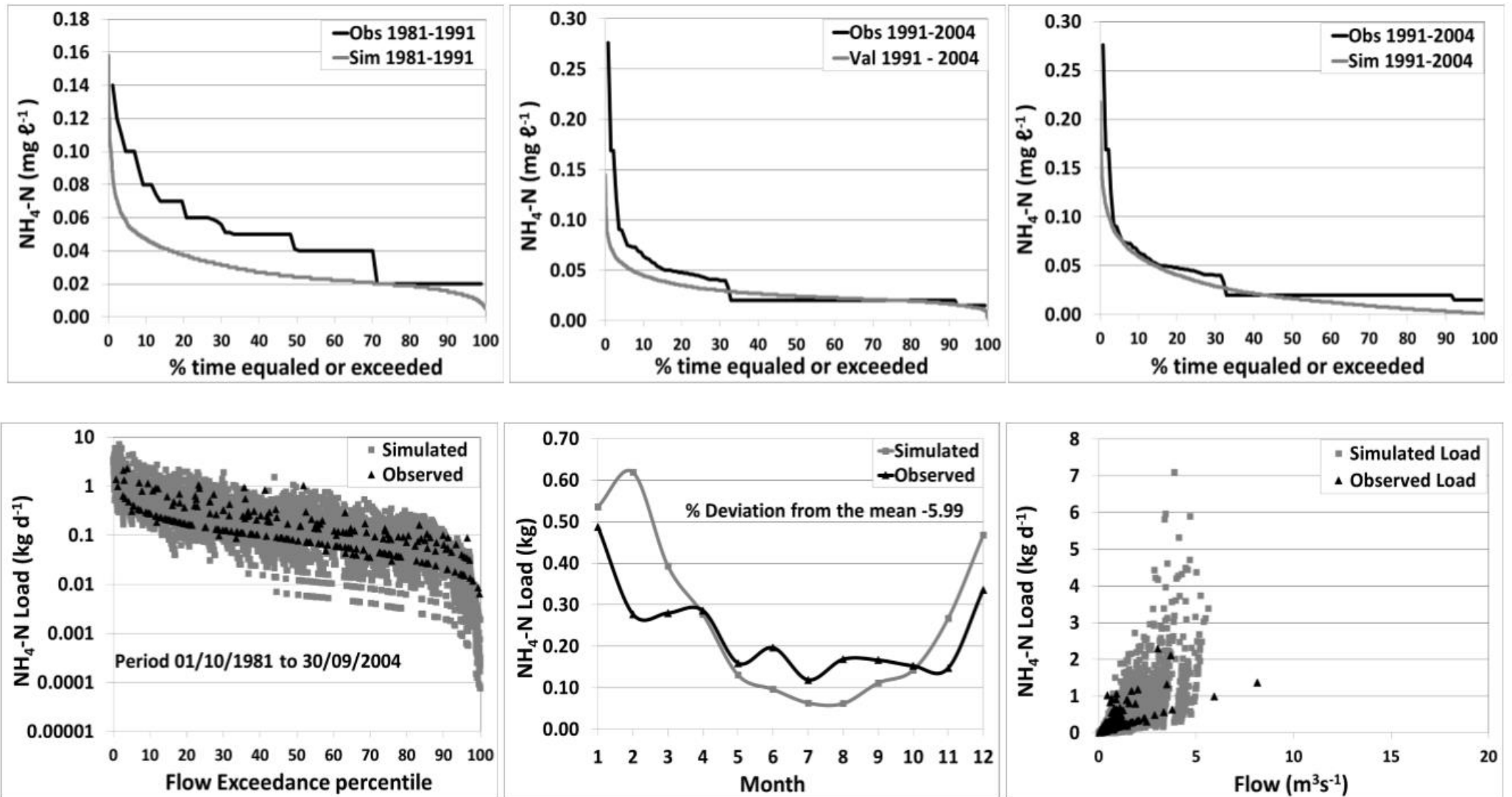


Figure C33. Simulated vs observed results for  $\text{NH}_4\text{-N}$  at node X23D-2 (gauging station X2H031) along the Suidkaap River.

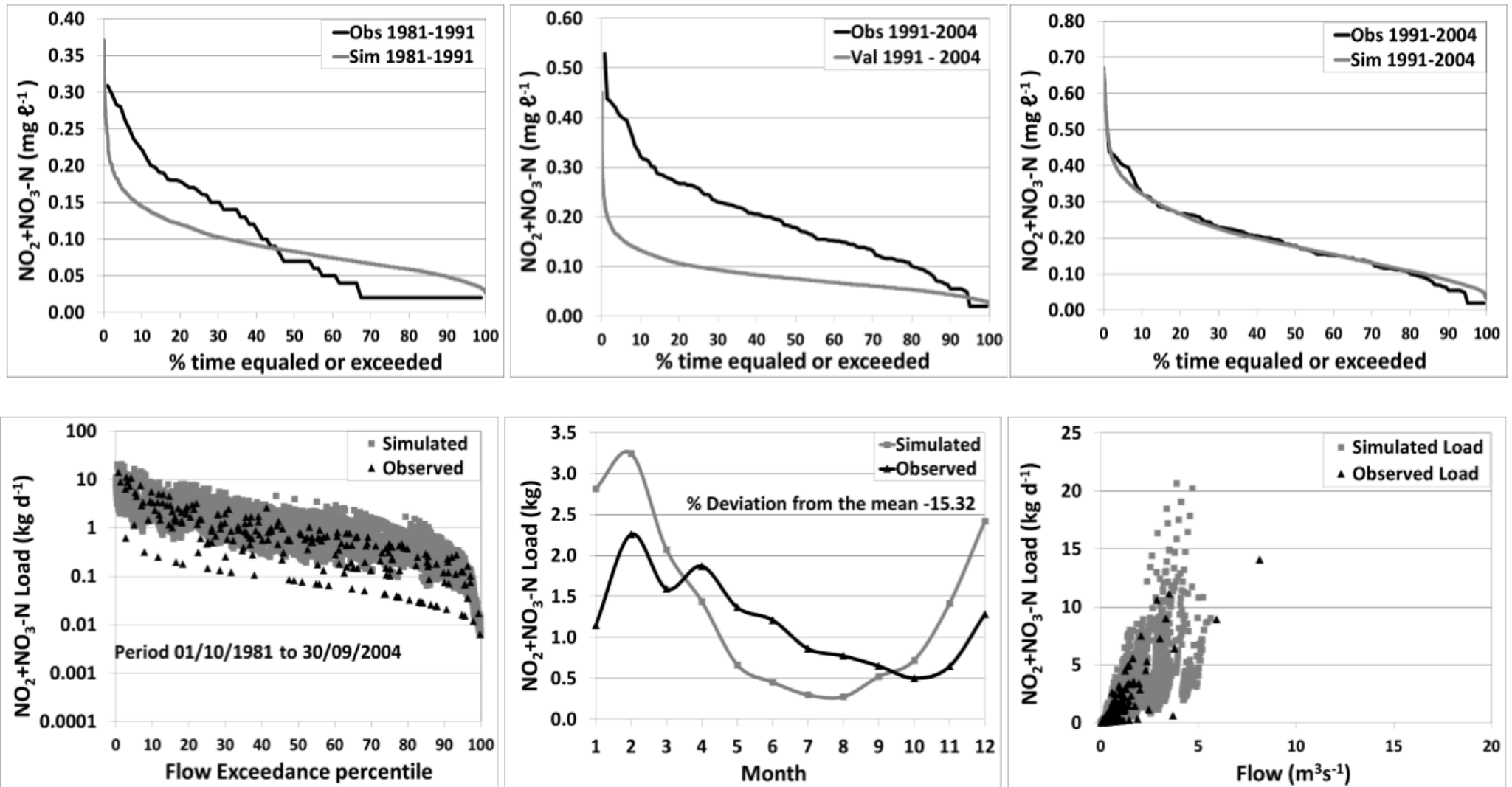


Figure C34. Simulated vs observed results for NO<sub>2</sub> + NO<sub>3</sub>-N at node X23D-2 (gauging station X2H031) along the Suidkaap River.

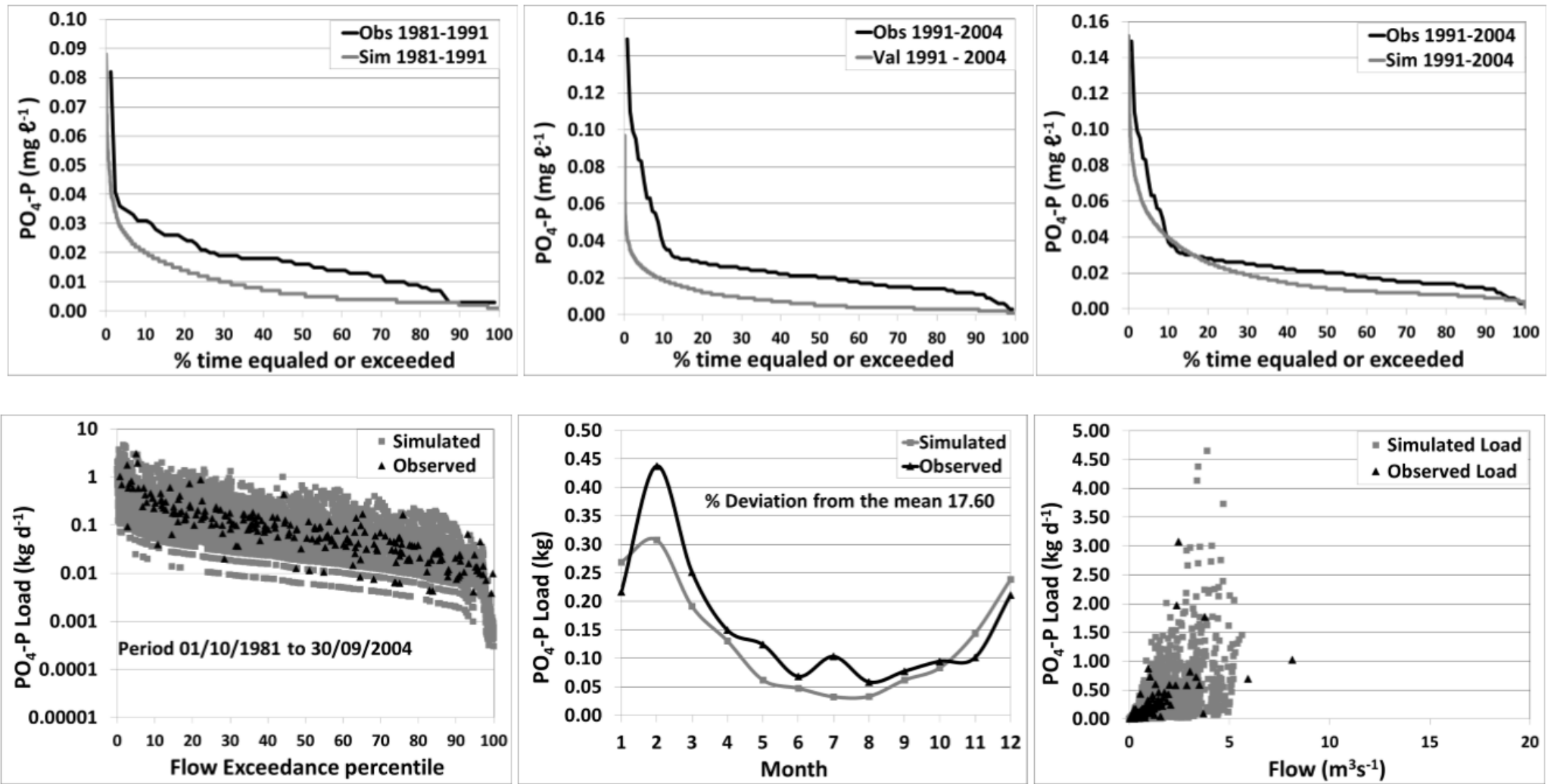


Figure C35. Simulated vs observed results for PO<sub>4</sub>-P at node X23D-2 (gauging station X2H031) along the Suidkaap River.

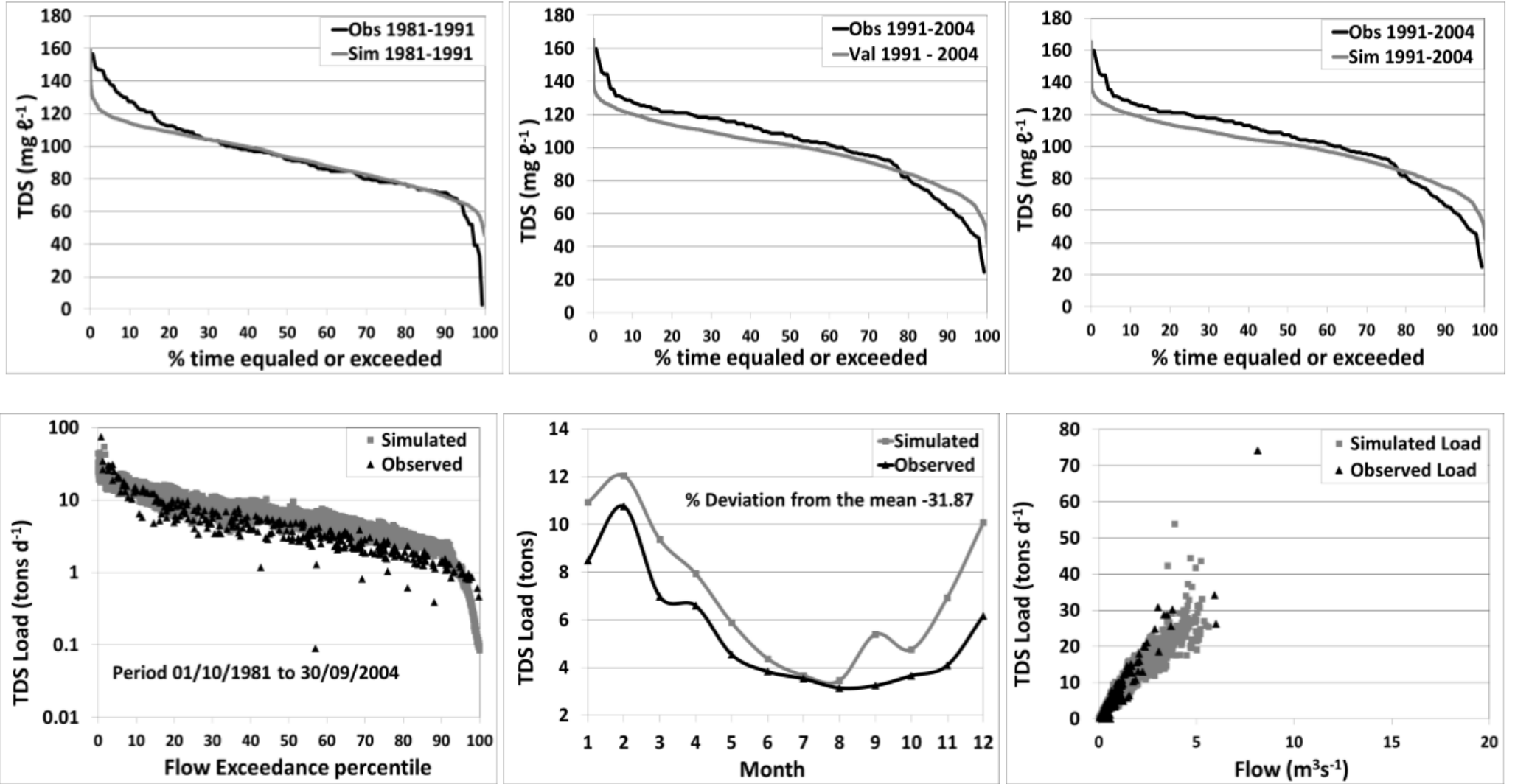


Figure C36. Simulated vs observed results for TDS at node X23D-2 (gauging station X2H031) along the Suidkaap River.

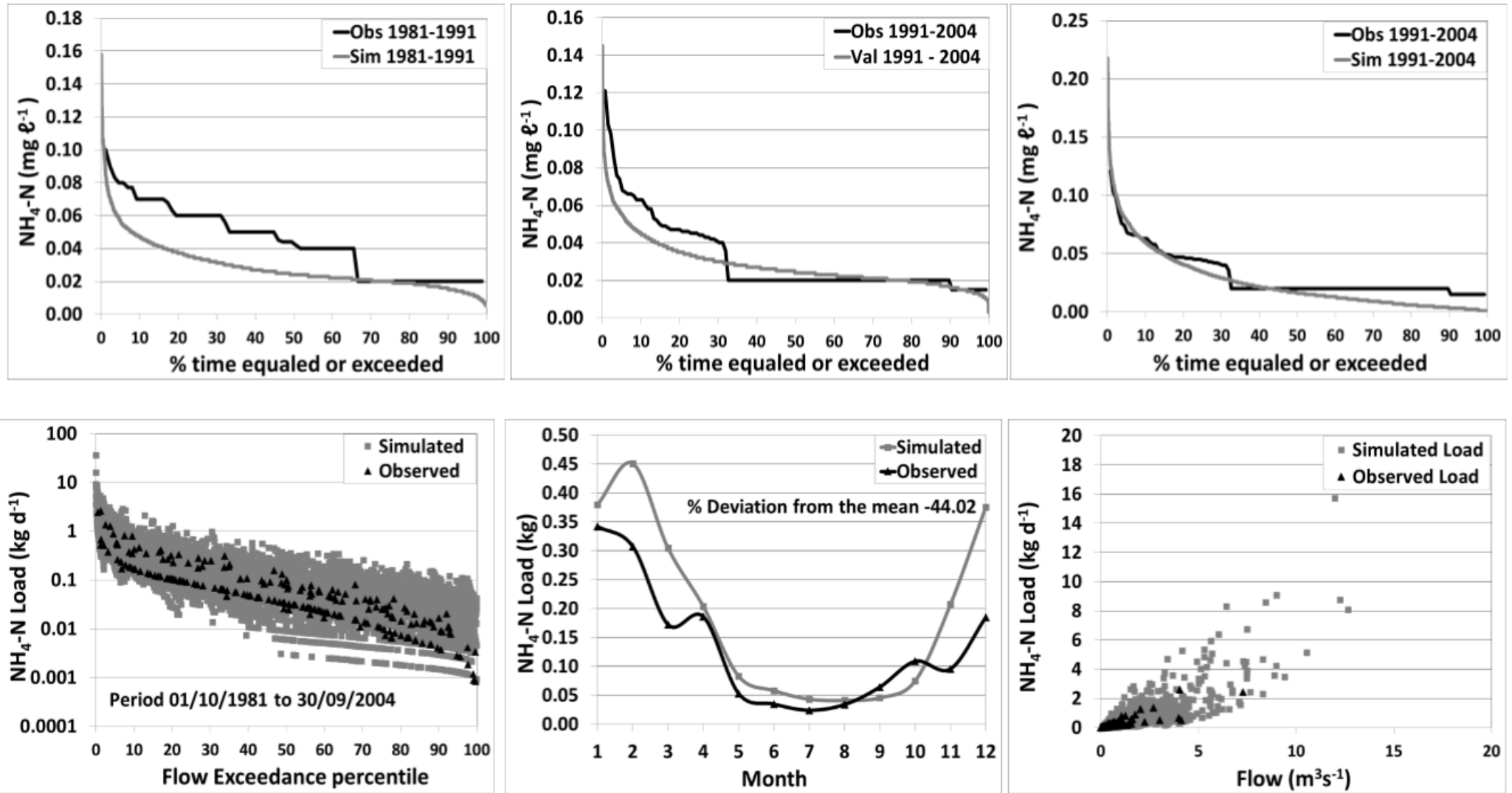


Figure C37. Simulated vs observed results for  $\text{NH}_4\text{-N}$  at node X23E-2 (gauging station X2H008) along the Queens River.

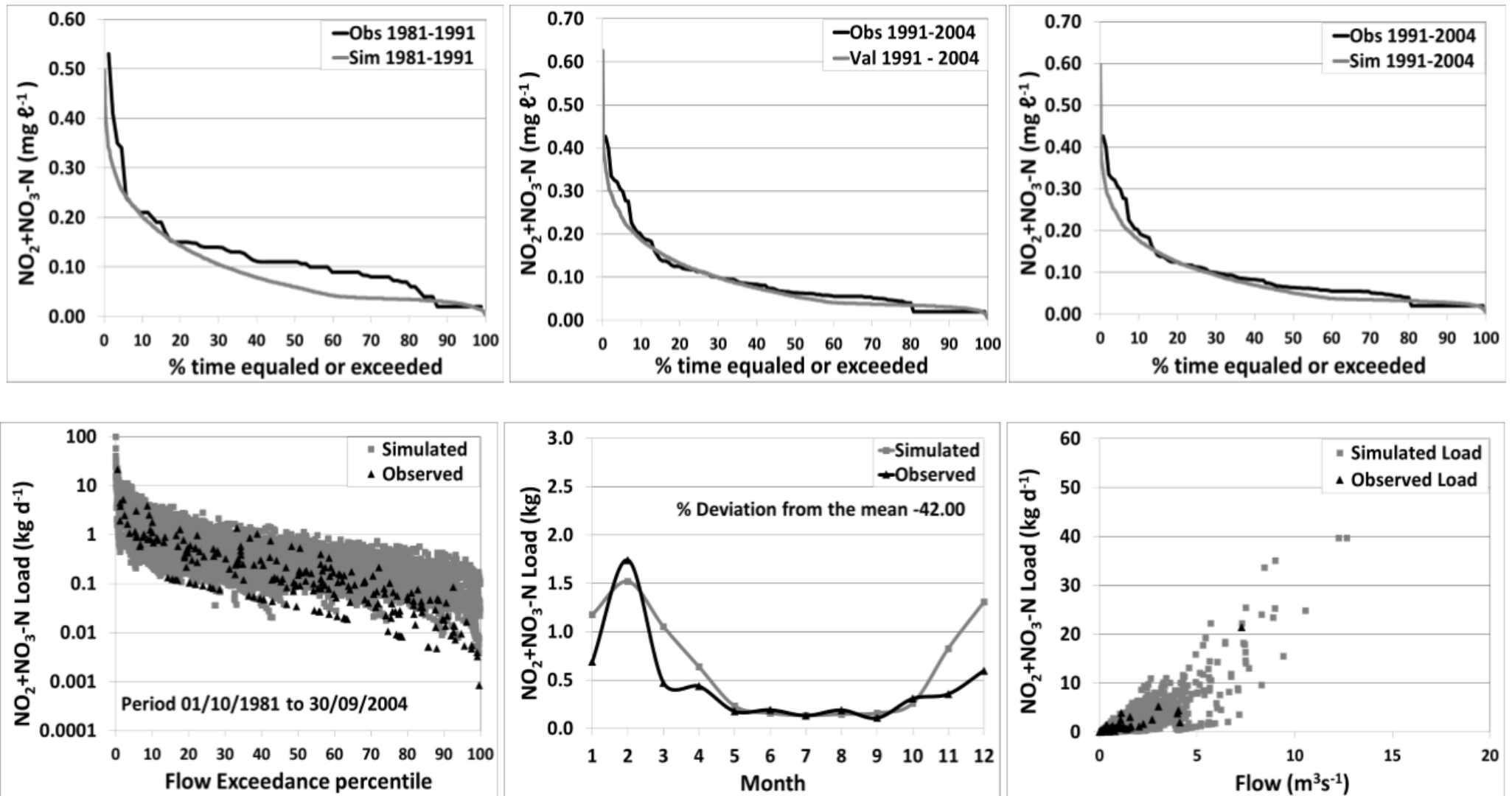


Figure C38. Simulated vs observed results for NO<sub>2</sub> + NO<sub>3</sub>-N at node X23E-2 (gauging station X2H008) along the Queens River.

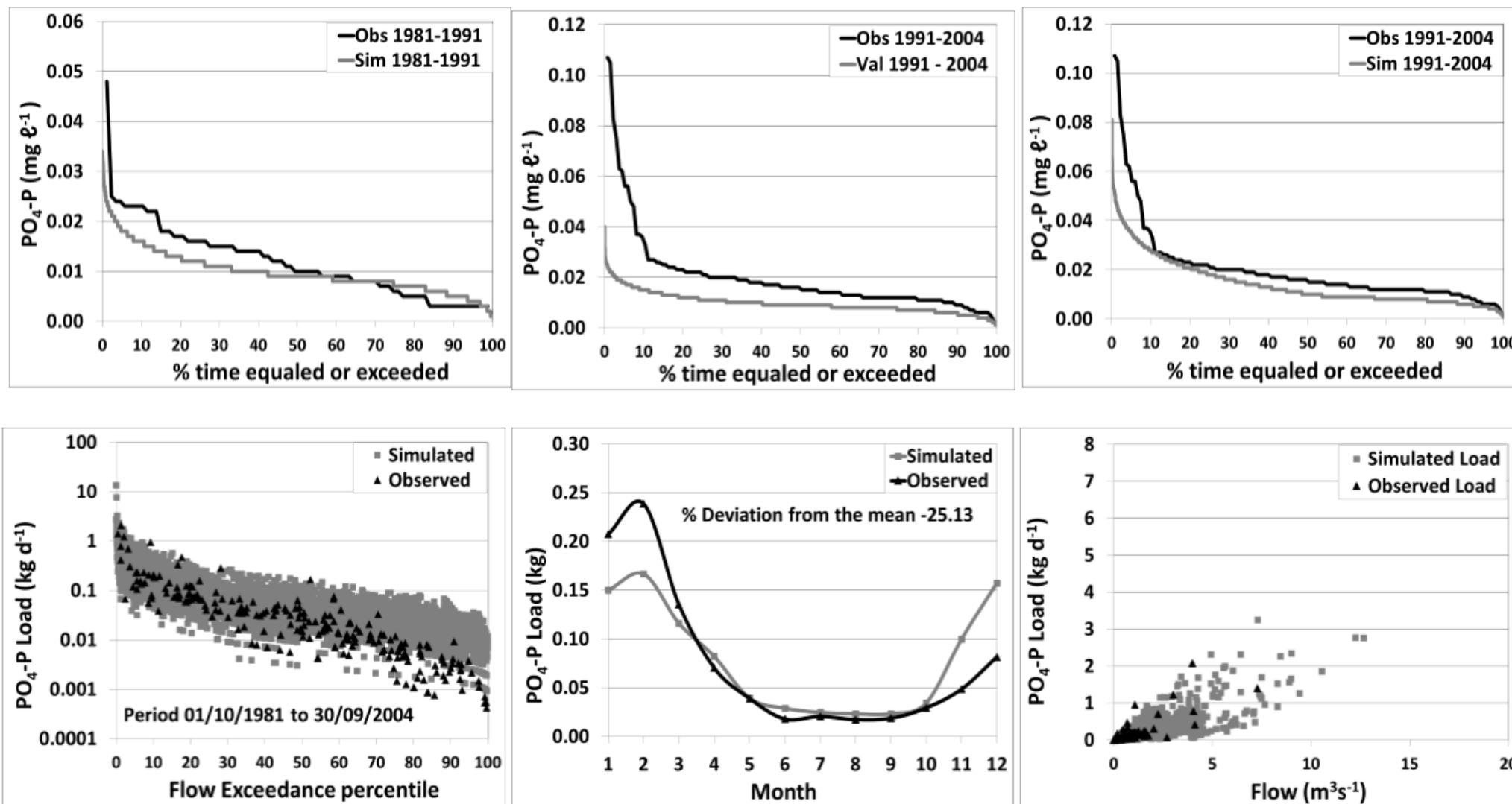


Figure C39. Simulated vs observed results for PO<sub>4</sub>-P at node X23E-2 (gauging station X2H008) along the Queens River.



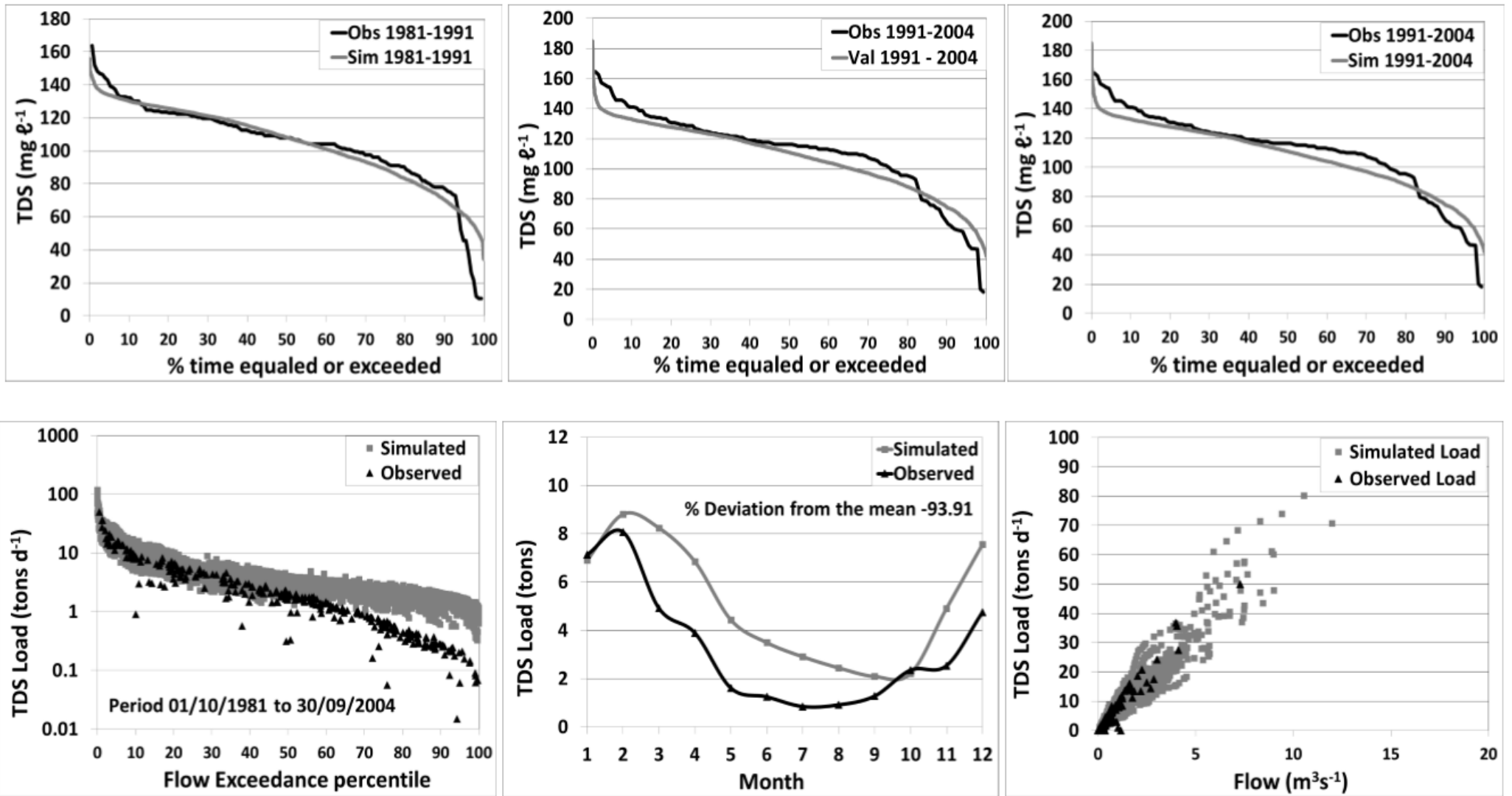


Figure C40. Simulated vs observed results for TDS at node X23E-2 (gauging station X2H008) along the Queens River.

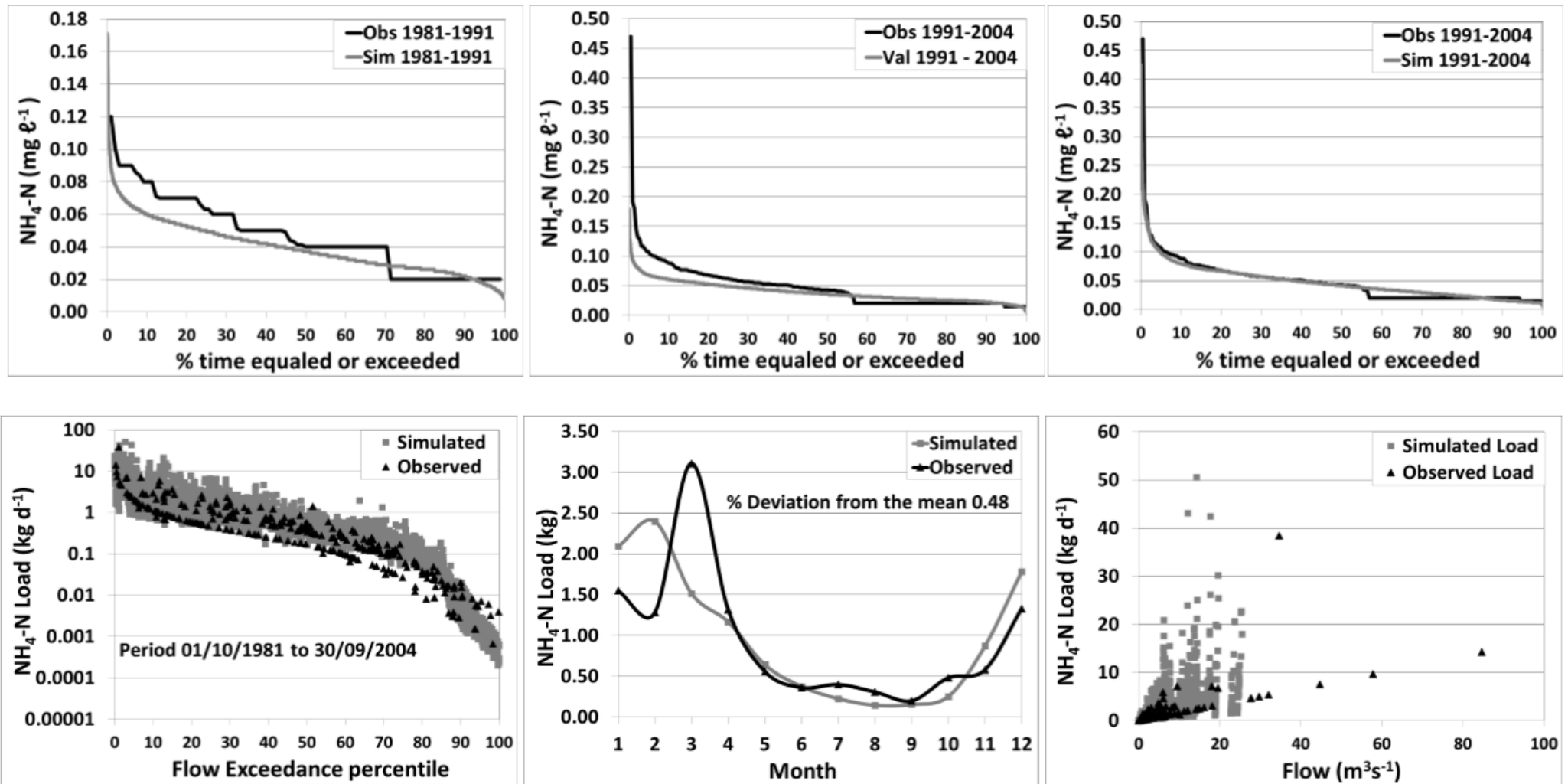


Figure C41. Simulated vs observed results for  $\text{NH}_4\text{-N}$  at node X23HGauge (gauging station X2H022) along the Kaap River.

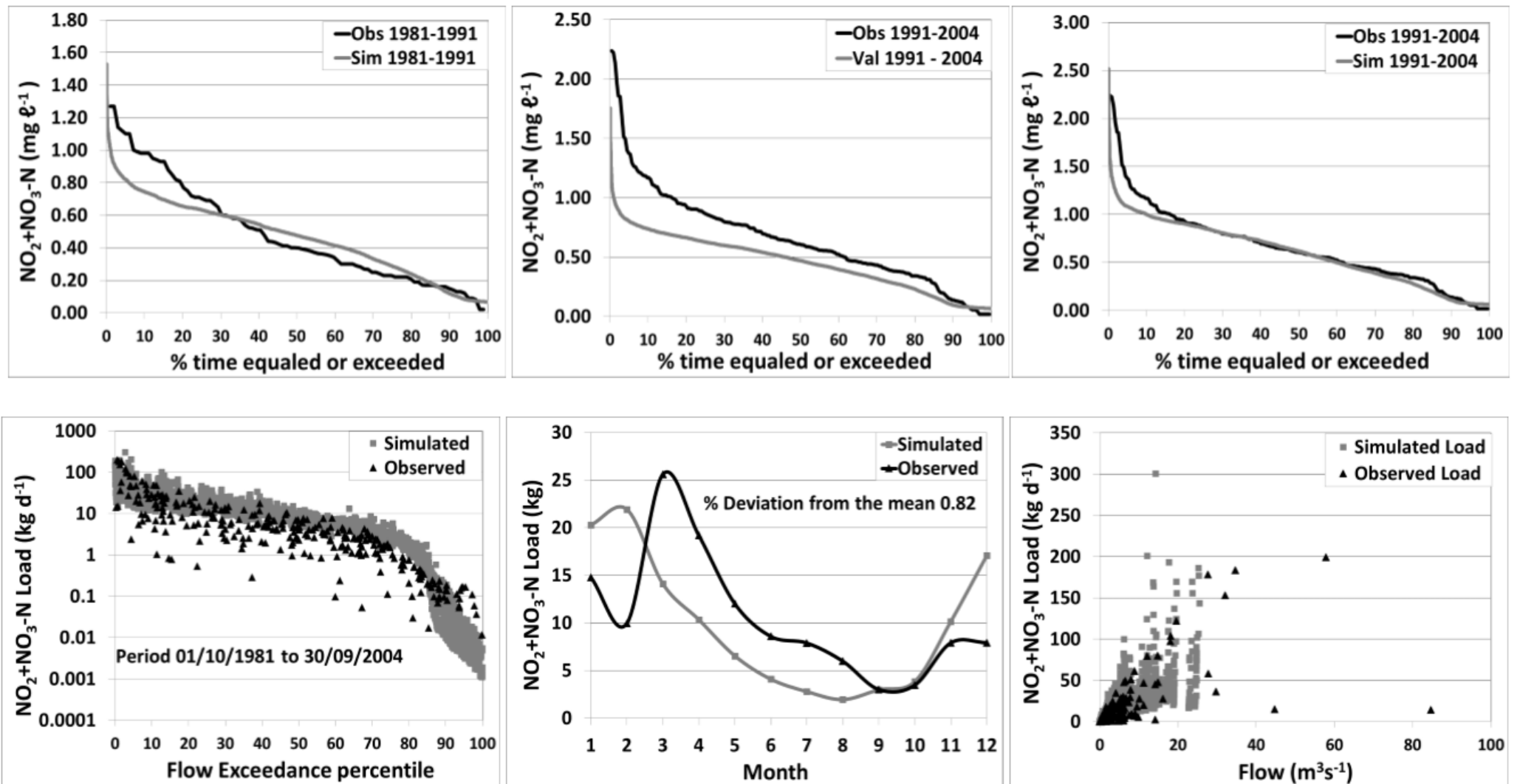


Figure C42. Simulated vs observed results for NO<sub>2</sub> + NO<sub>3</sub>-N at node X23HGauge (gauging station X2H022) along the Kaap River.

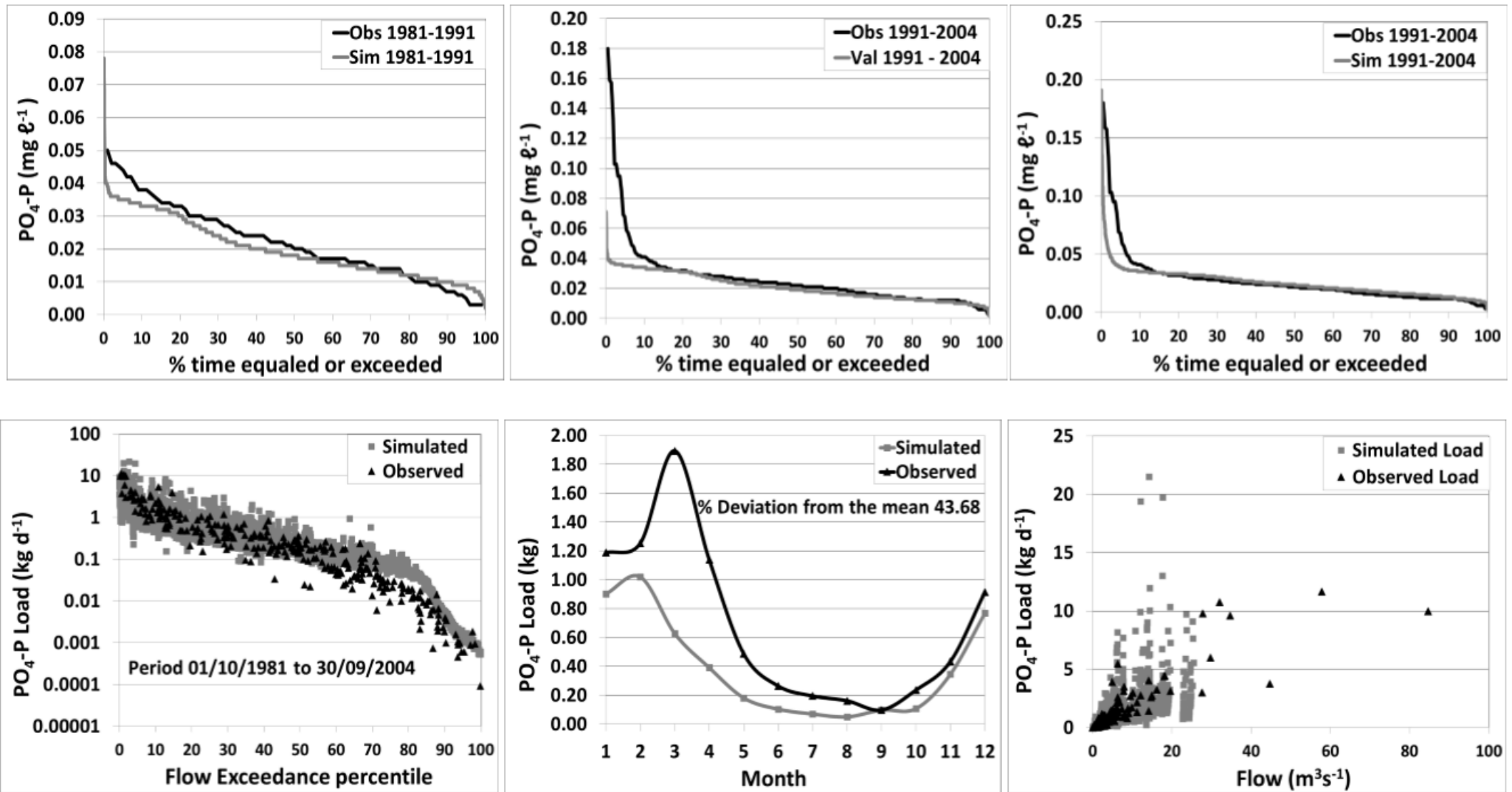


Figure C43. Simulated vs observed results for PO<sub>4</sub>-P at node X23HGauge (gauging station X2H022) along the Kaap River.

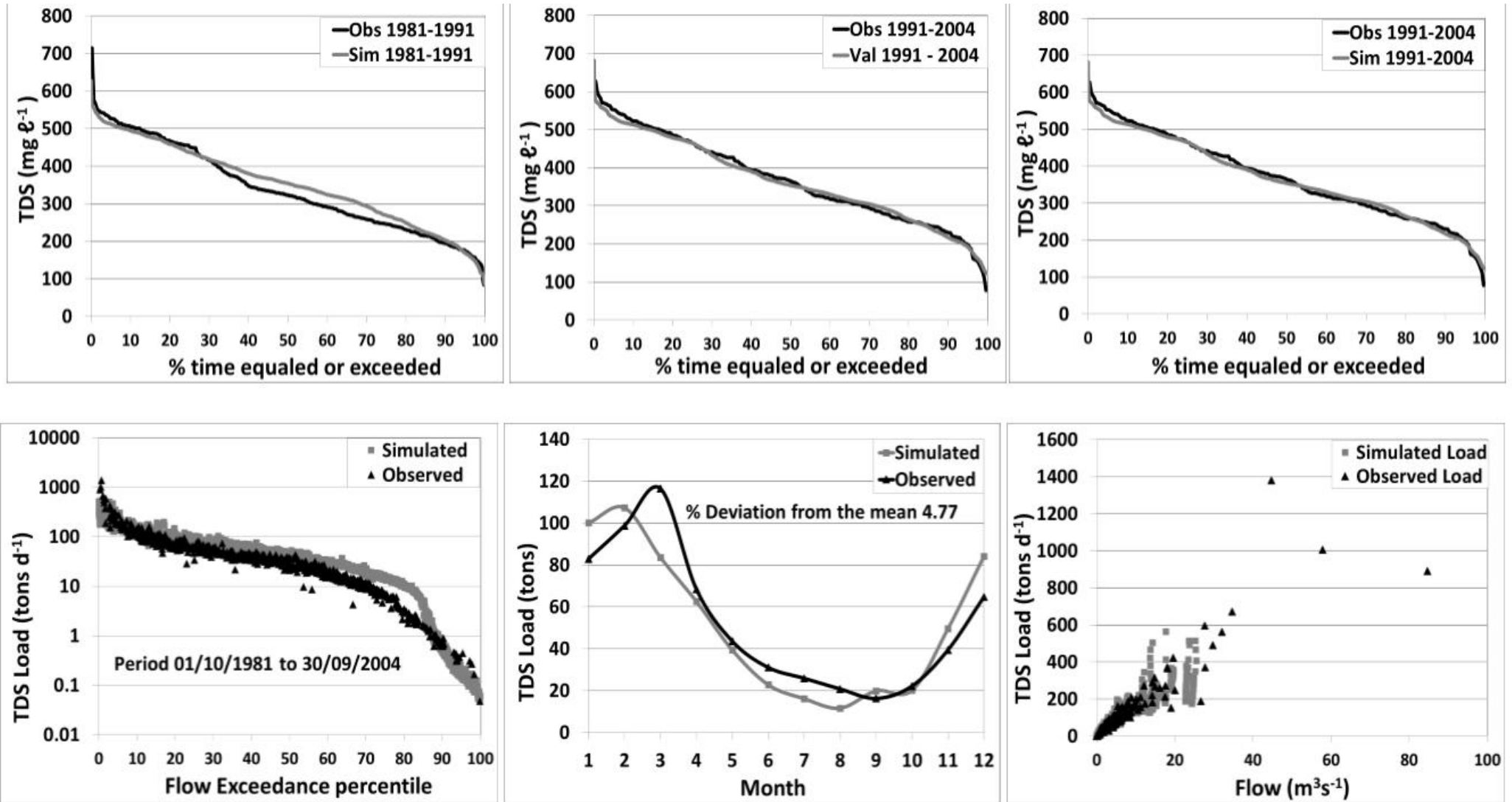


Figure C44. Simulated vs observed results for TDS at node X23HGauge (gauging station X2H022) along the Kaap River.

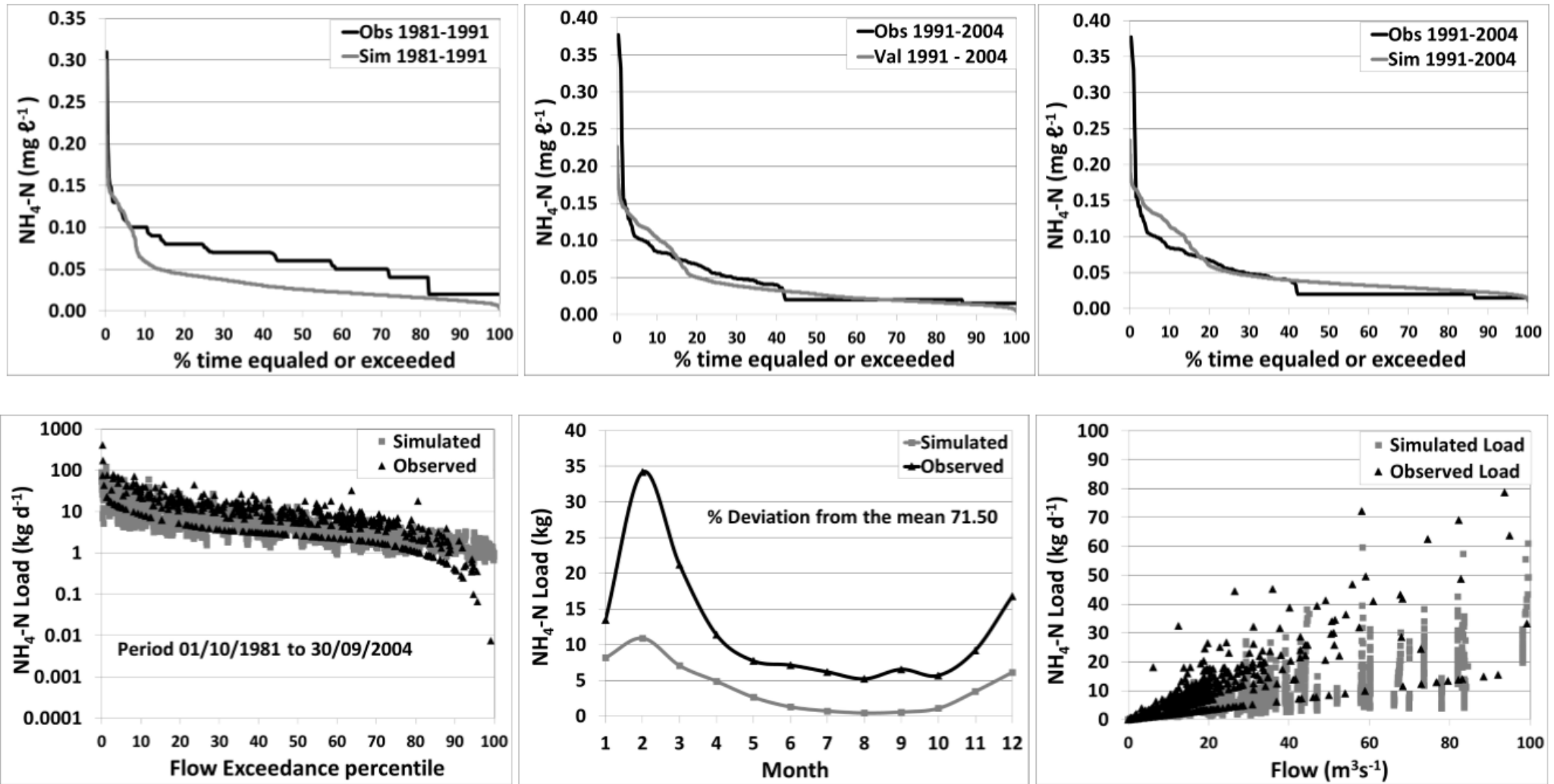


Figure C45. Simulated vs observed results for NH<sub>4</sub>-N at node X24E-2 (gauging station X2H017) along the Crocodile River.

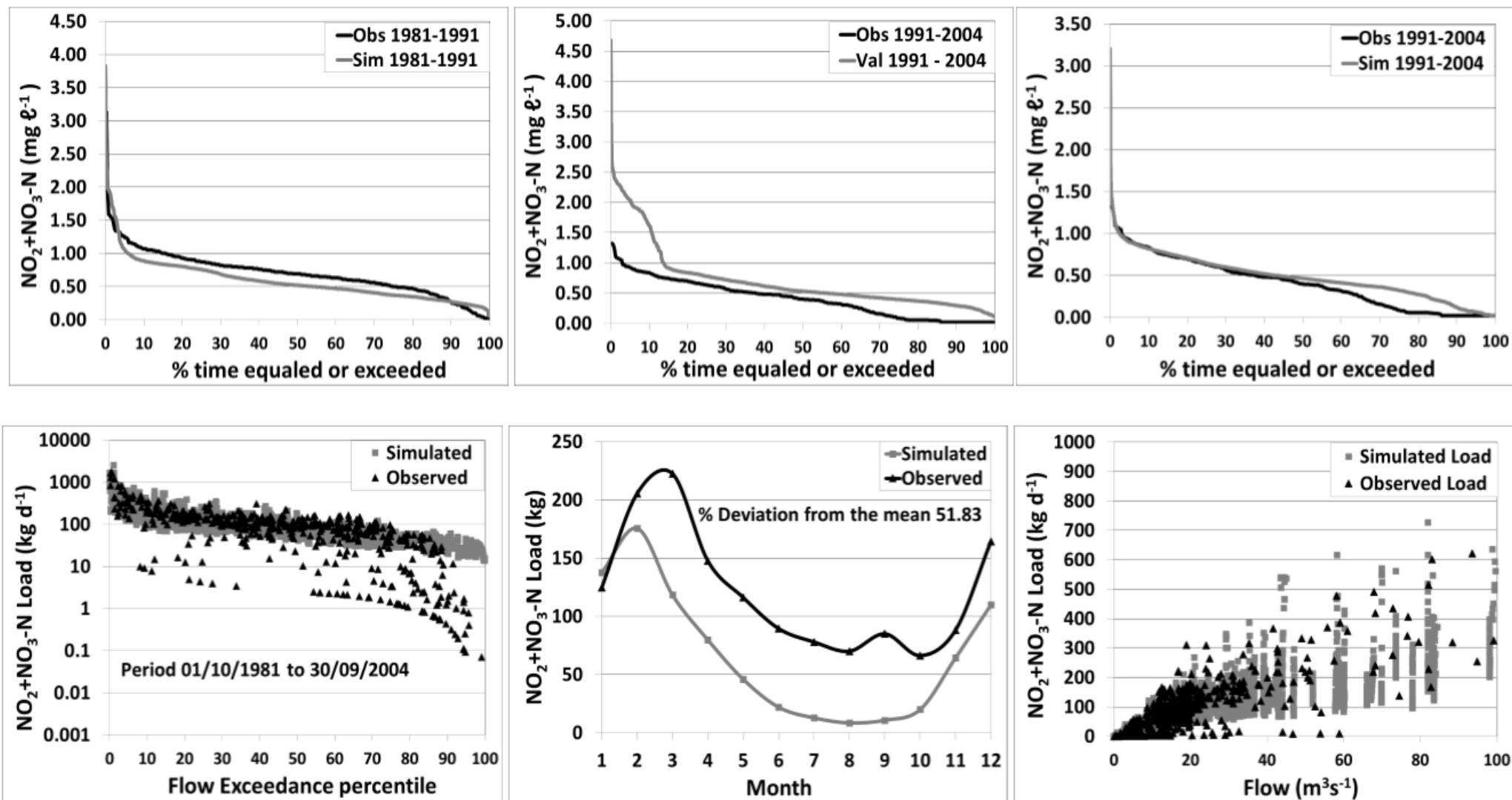


Figure C46. Simulated vs observed results for  $\text{NO}_2 + \text{NO}_3\text{-N}$  at node X24E-2 (gauging station X2H017) along the Crocodile River.

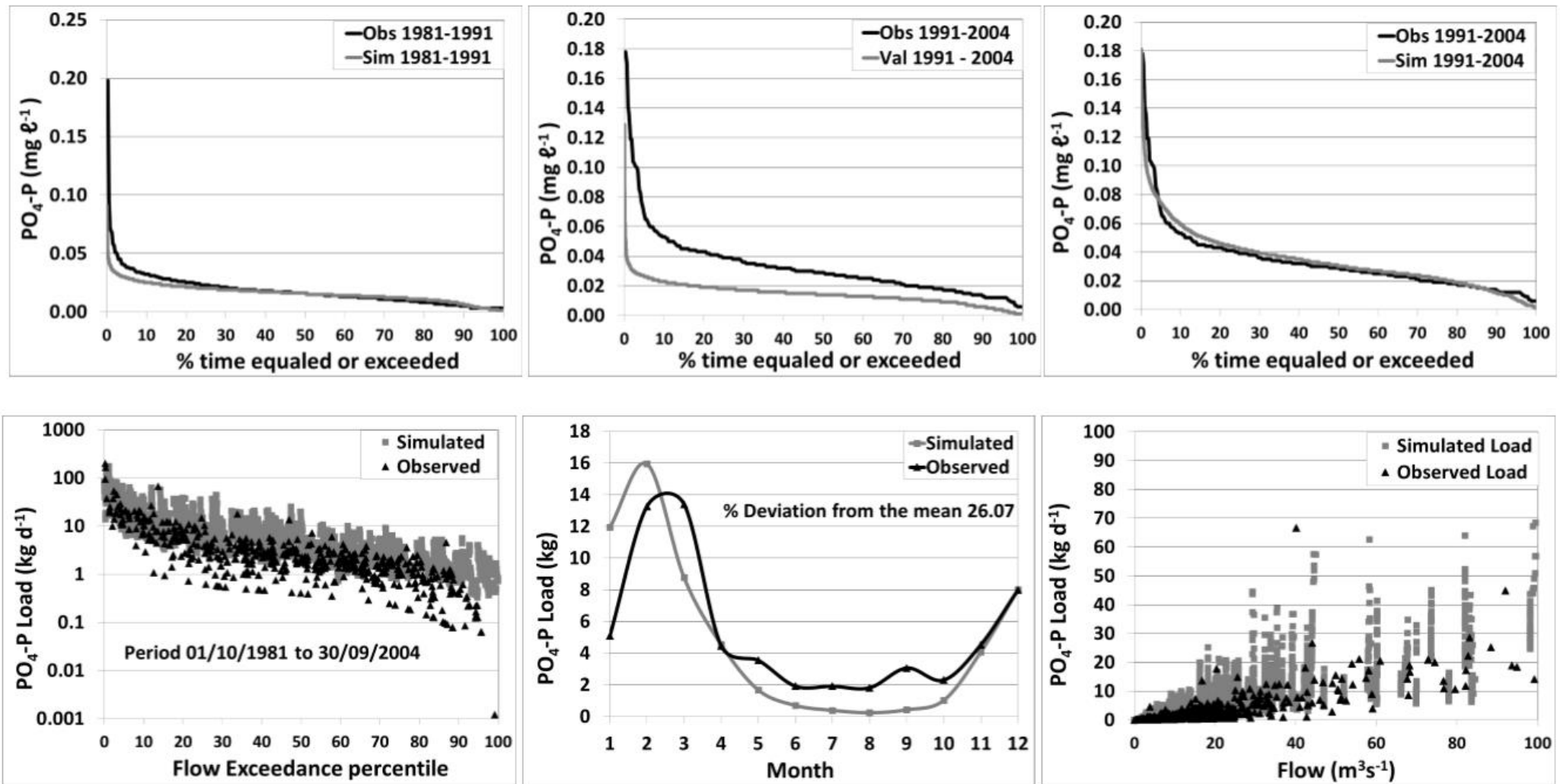


Figure C47. Simulated vs observed results for PO<sub>4</sub>-P at node X24E-2 (gauging station X2H017) along the Crocodile River.



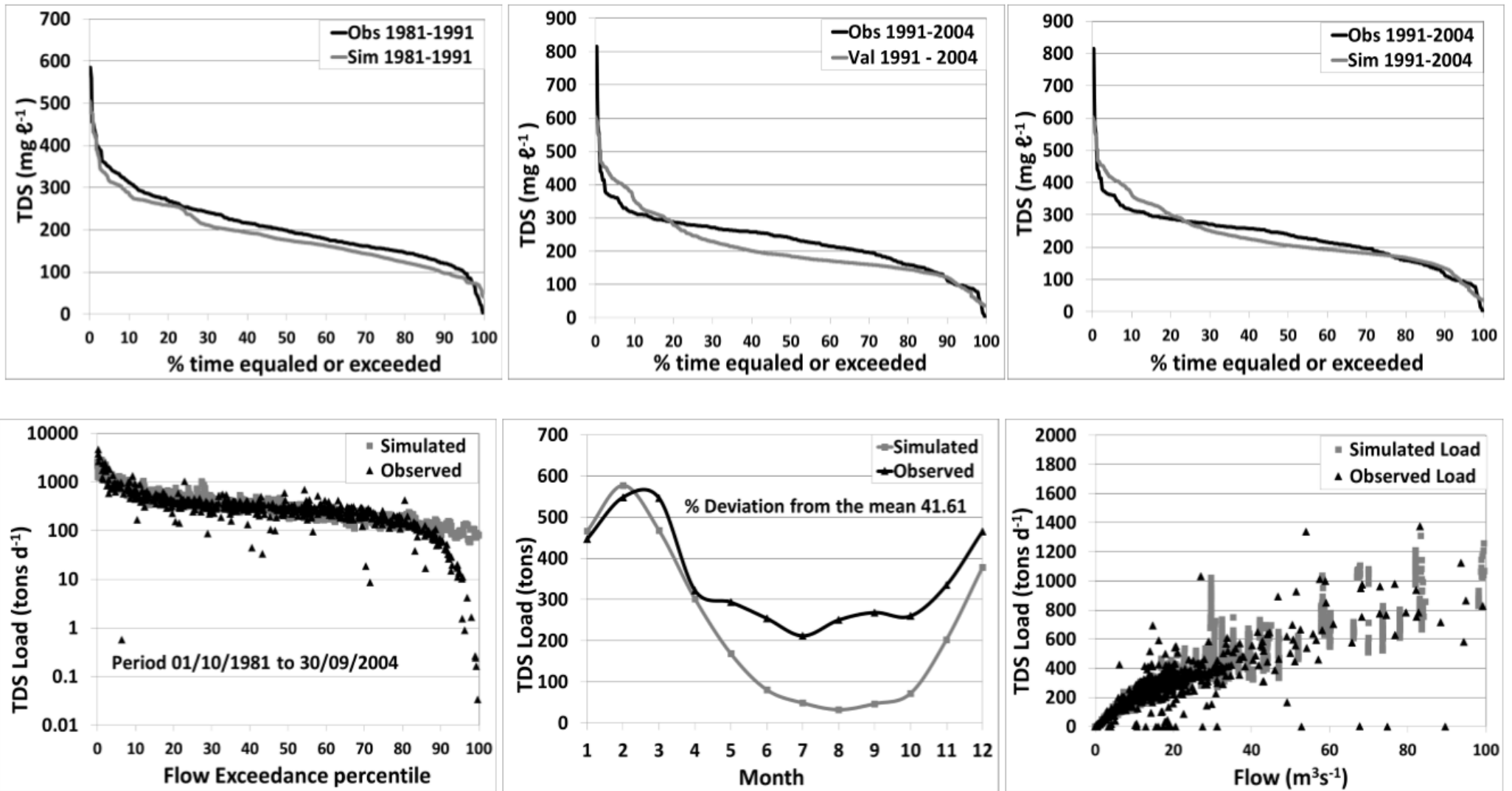


Figure C48. Simulated vs observed results for TDS at node X24E-2 (gauging station X2H017) along the Crocodile River.

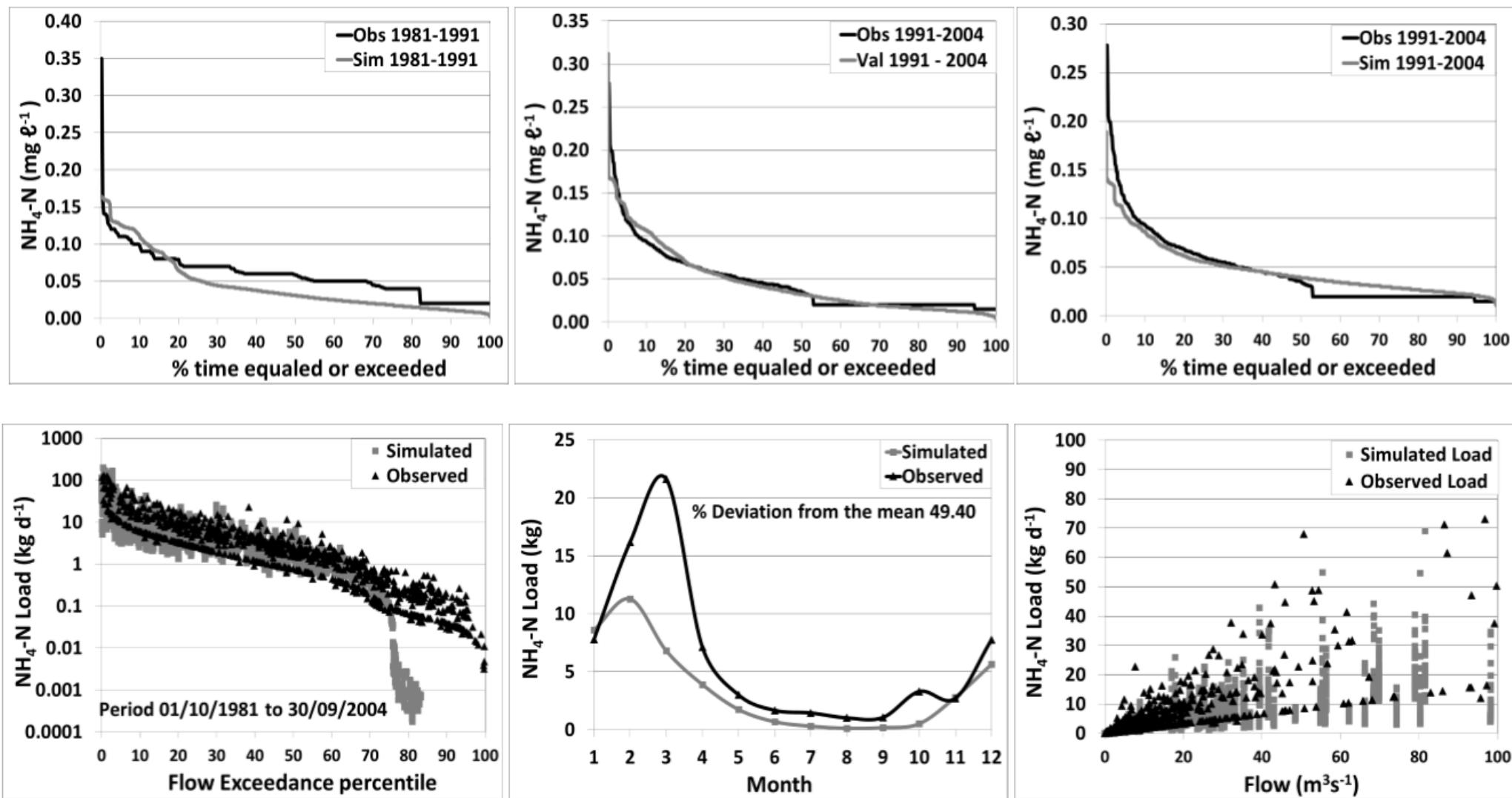


Figure C49. Simulated vs observed results for  $\text{NH}_4\text{-N}$  at node X24H-2 (gauging station X2H016) along the Crocodile River.

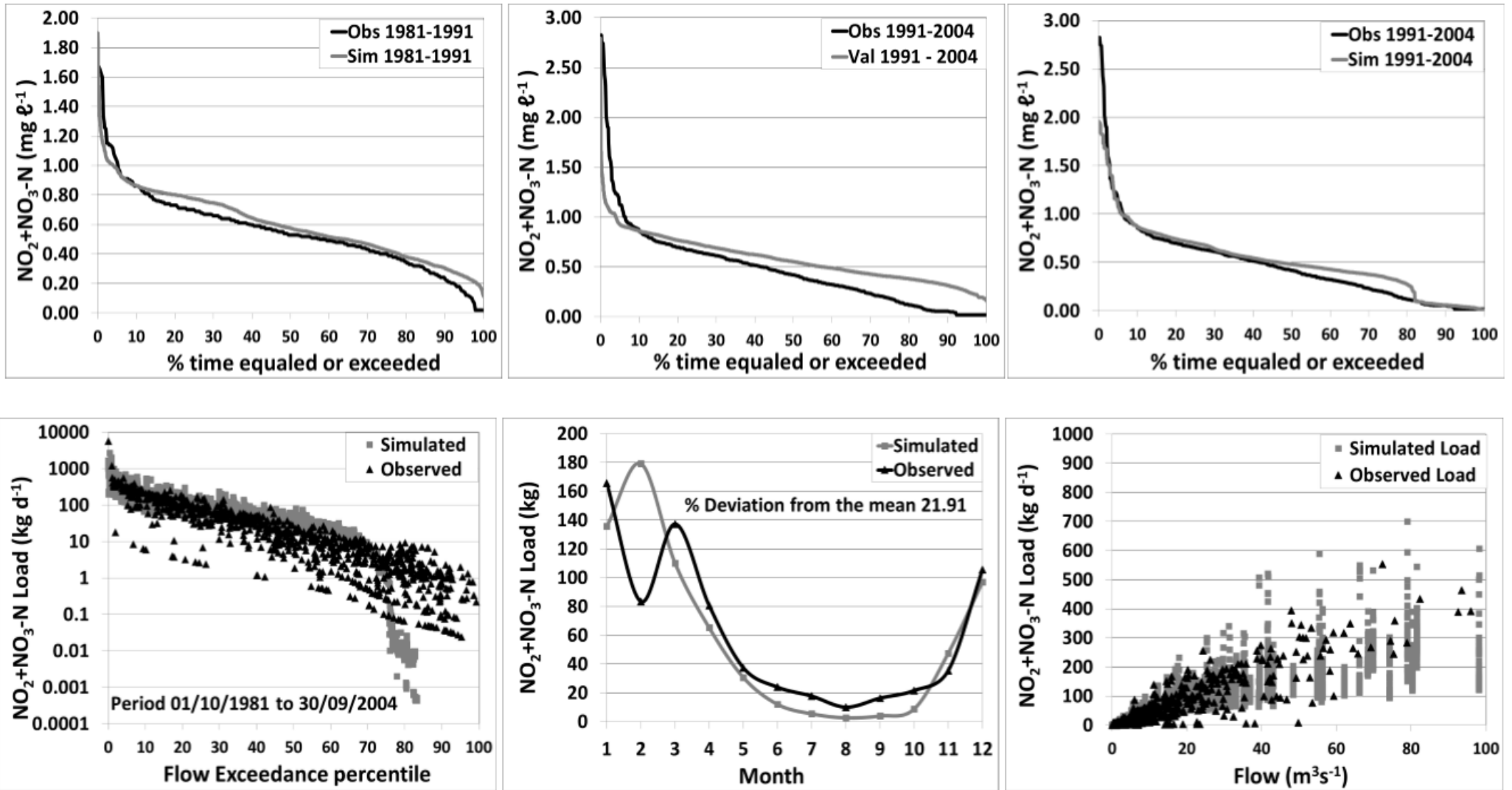


Figure C50. Simulated vs observed results for  $\text{NO}_2 + \text{NO}_3\text{-N}$  at node X24H-2 (gauging station X2H016) along the Crocodile River.

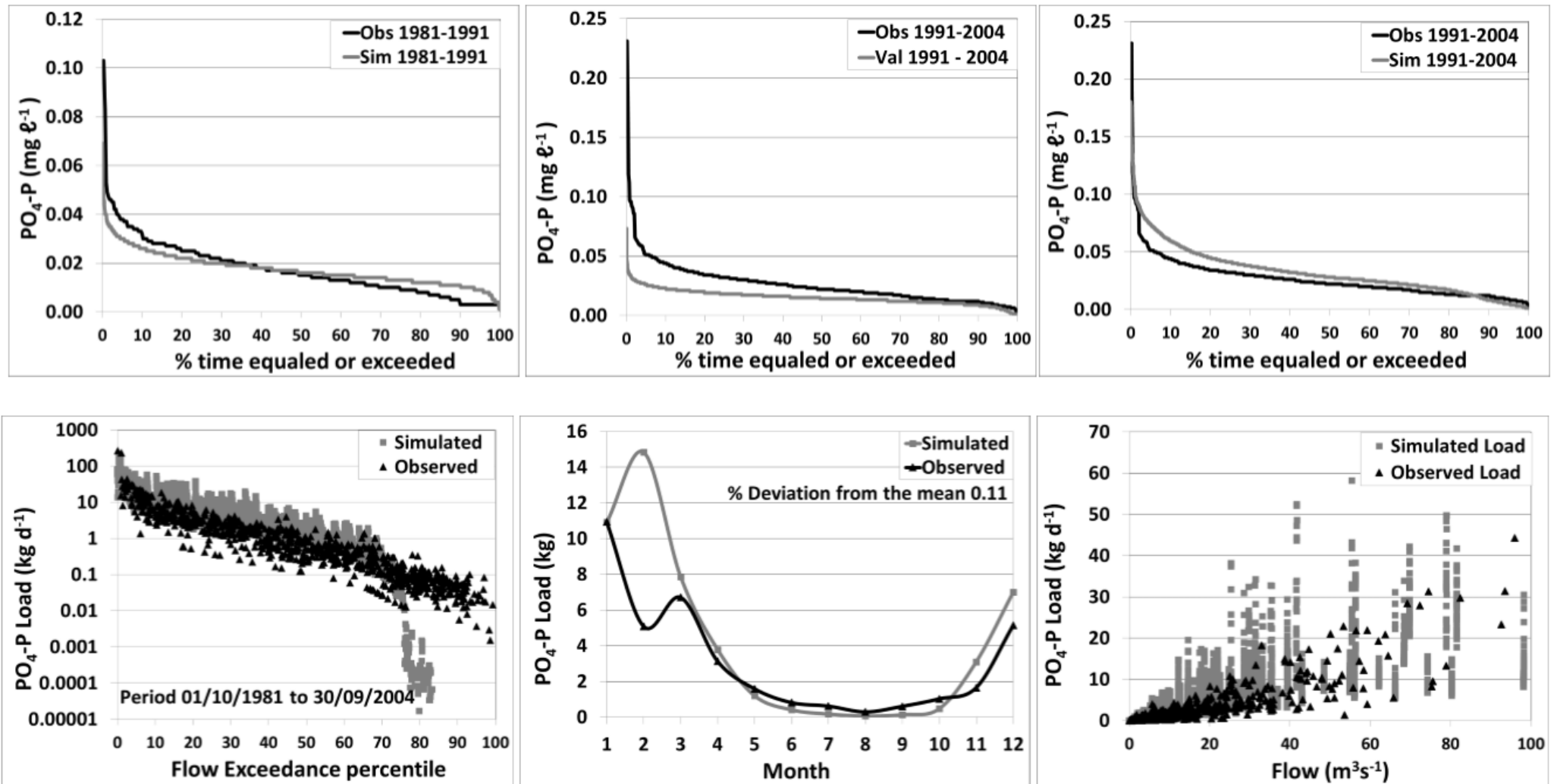


Figure C51. Simulated vs observed results for PO<sub>4</sub>-P at node X24H-2 (gauging station X2H016) along the Crocodile River.

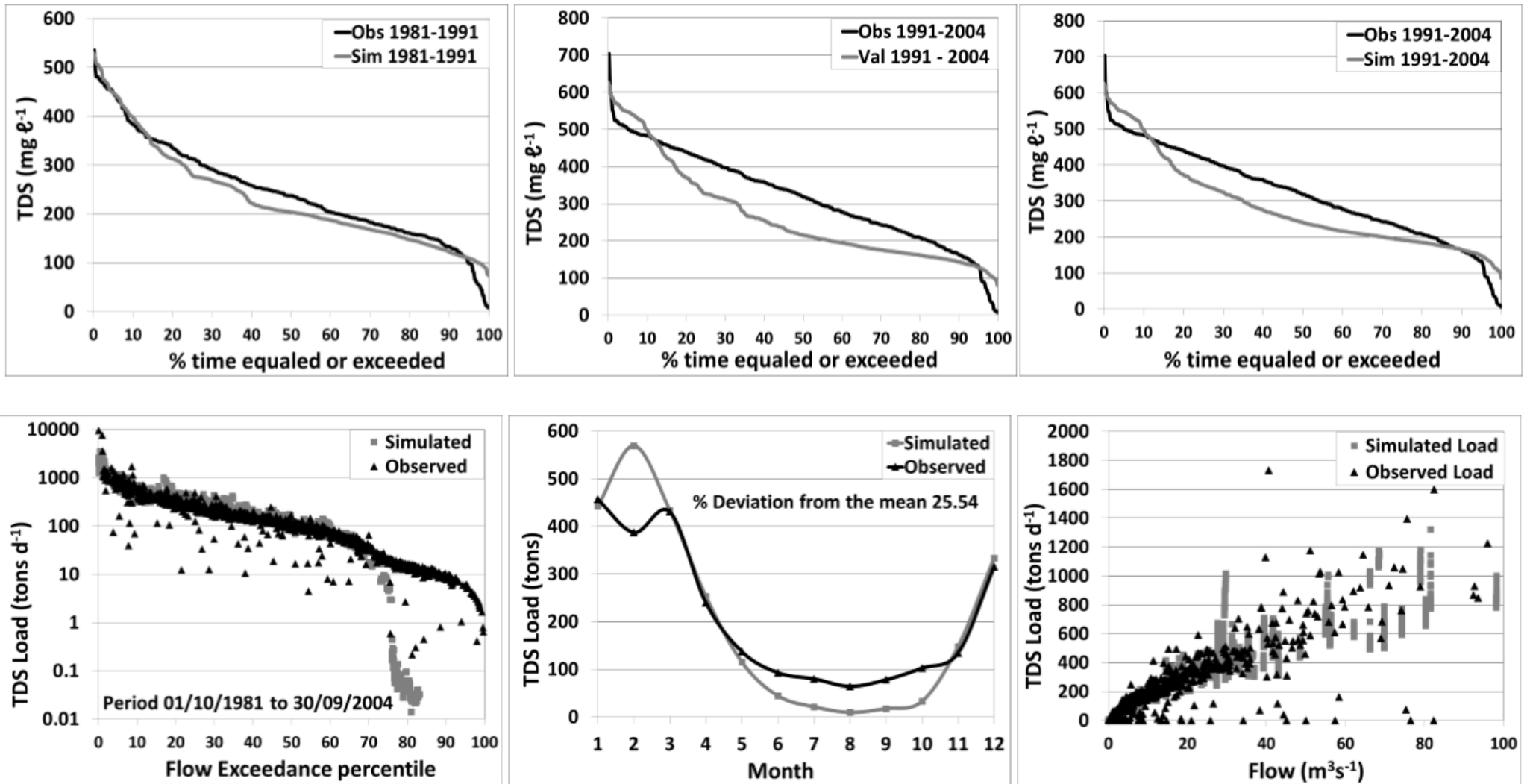


Figure C52. Simulated vs observed results for TDS at node X24H-2 (gauging station X2H016) along the Crocodile River.

Appendix D

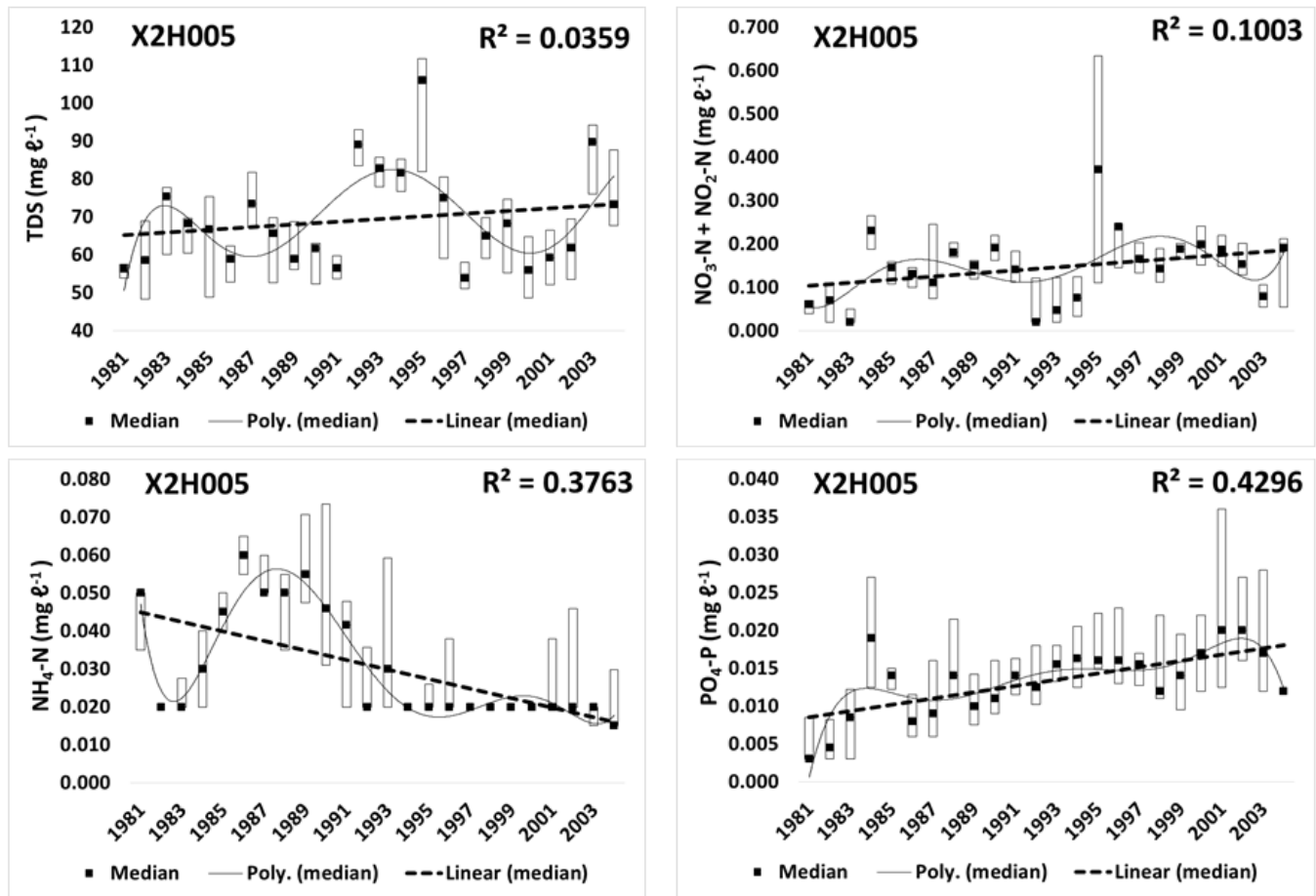


Figure D1. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H005 for the period 1981-2004.

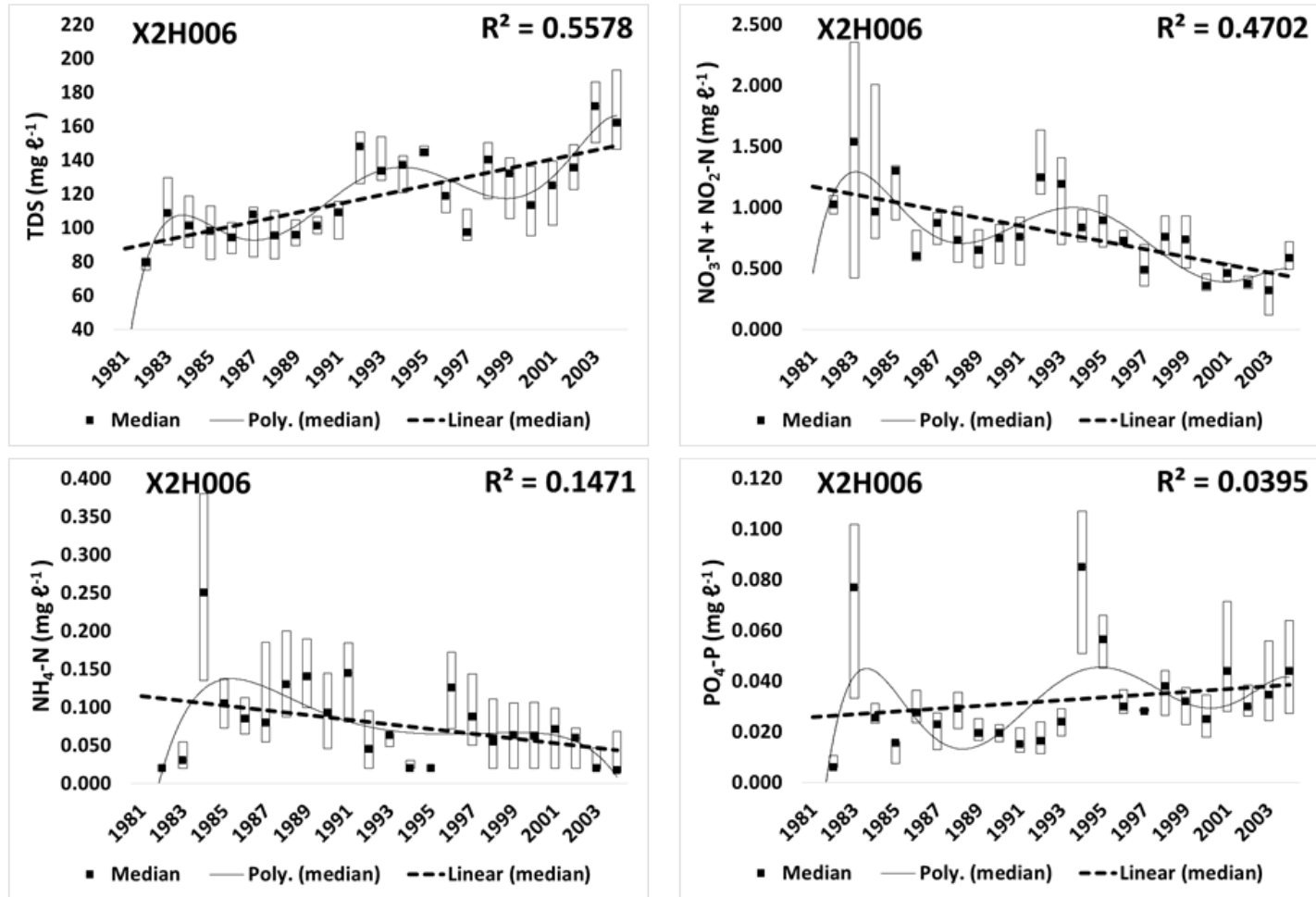


Figure D2. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H006 for the period 1981-2004.

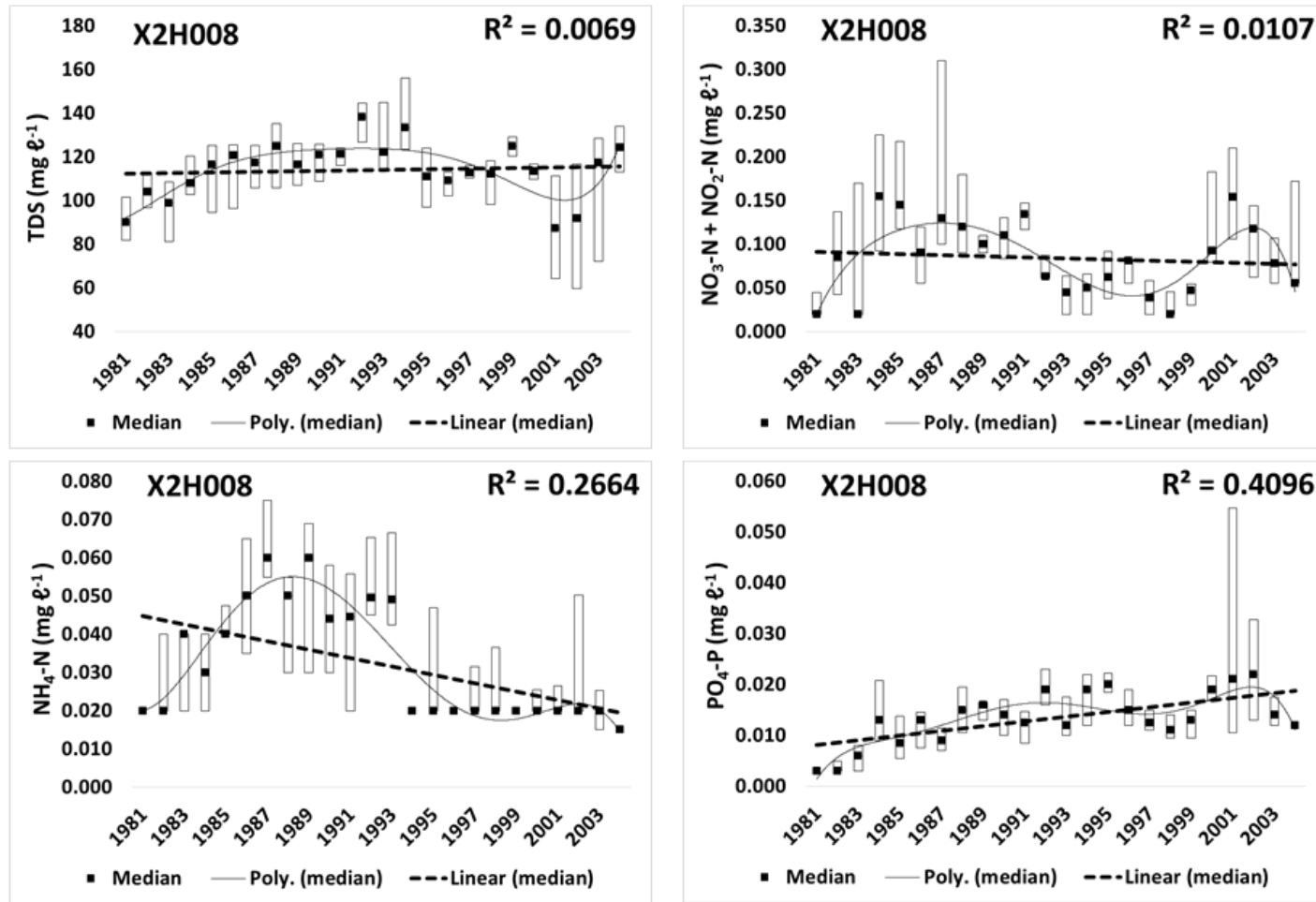


Figure D3. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H008 for the period 1981-2004.



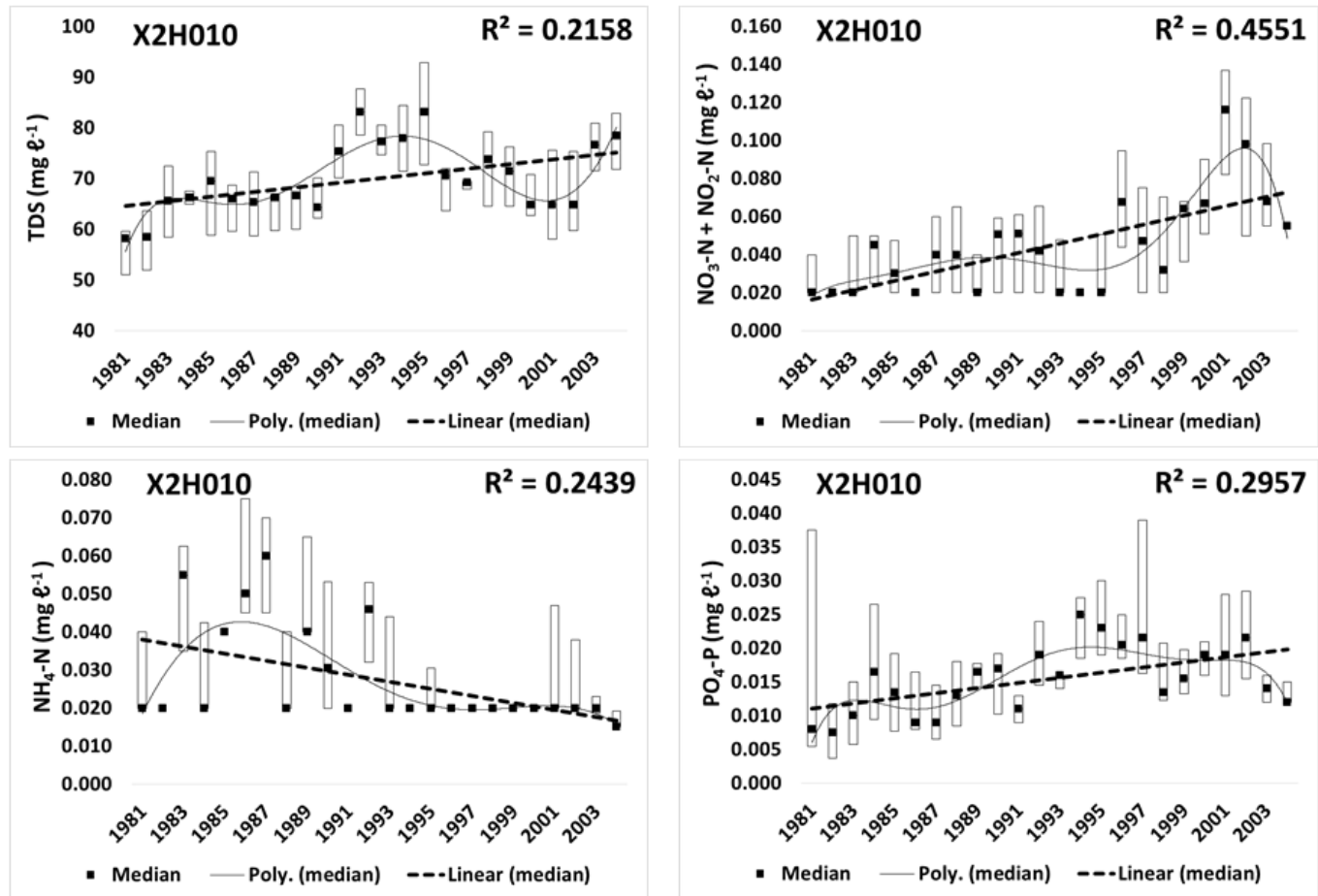


Figure D4. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H010 for the period 1981-2004.

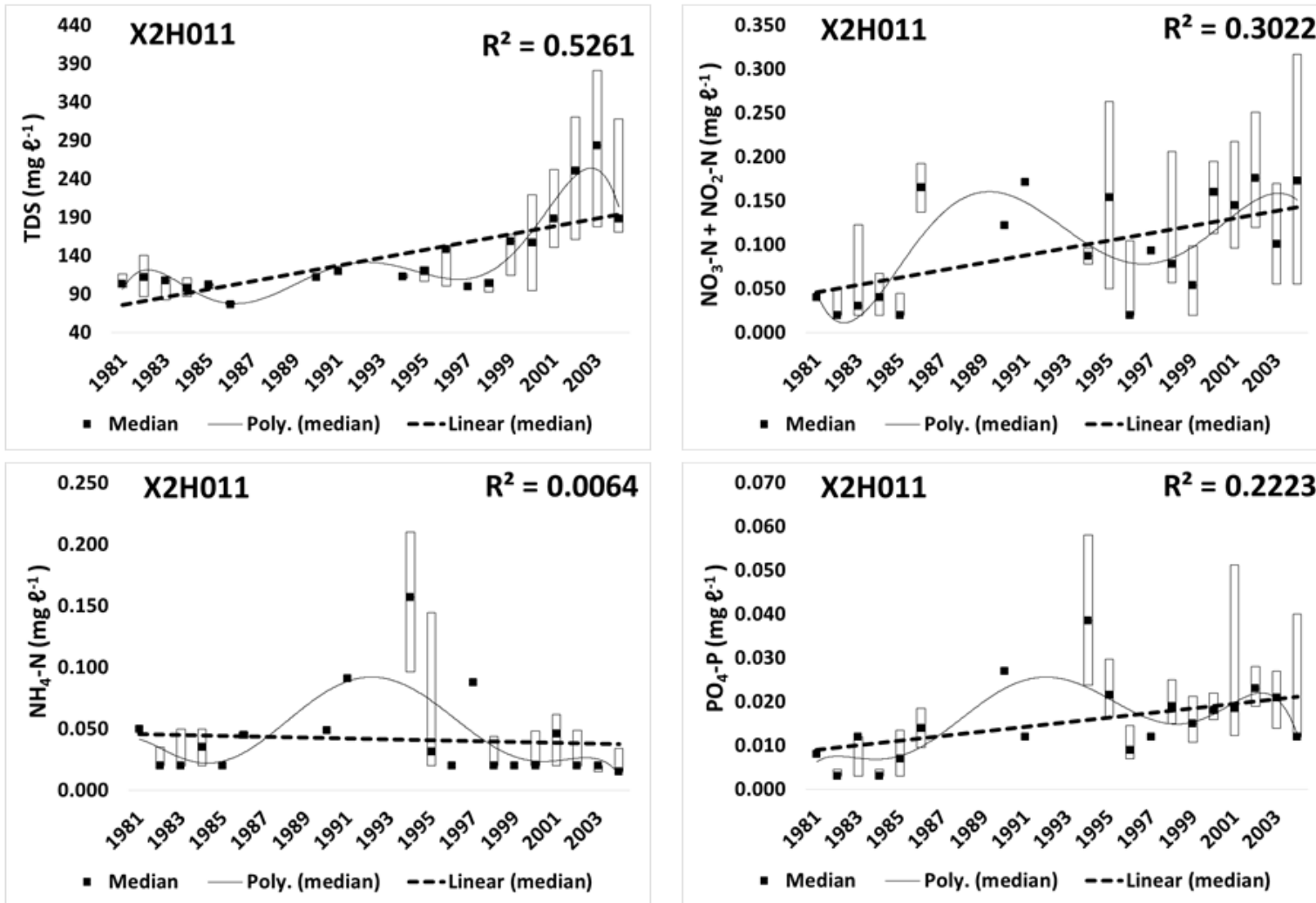


Figure D5. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H011 for the period 1981-2004.

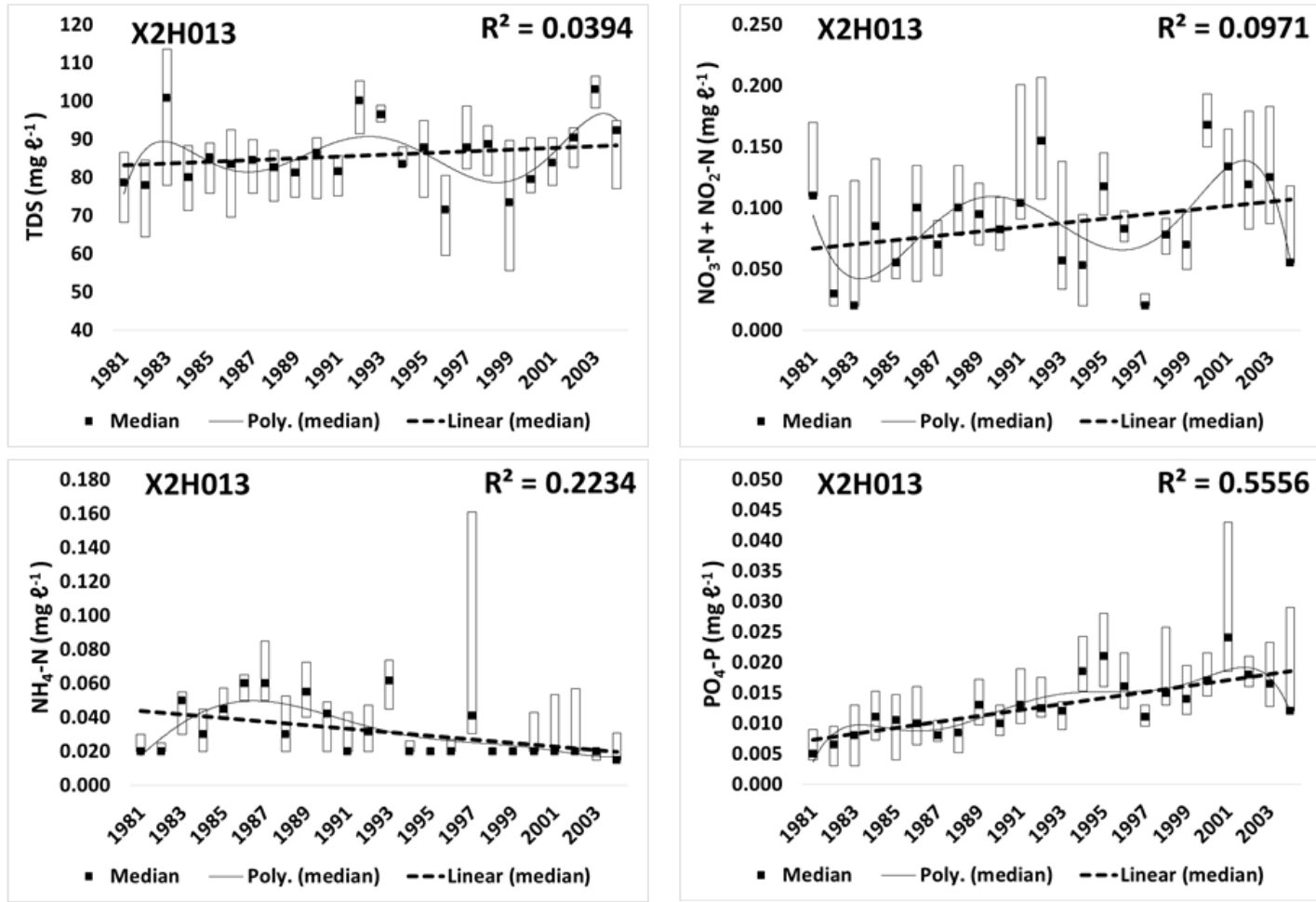


Figure D6. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H013 for the period 1981-2004.

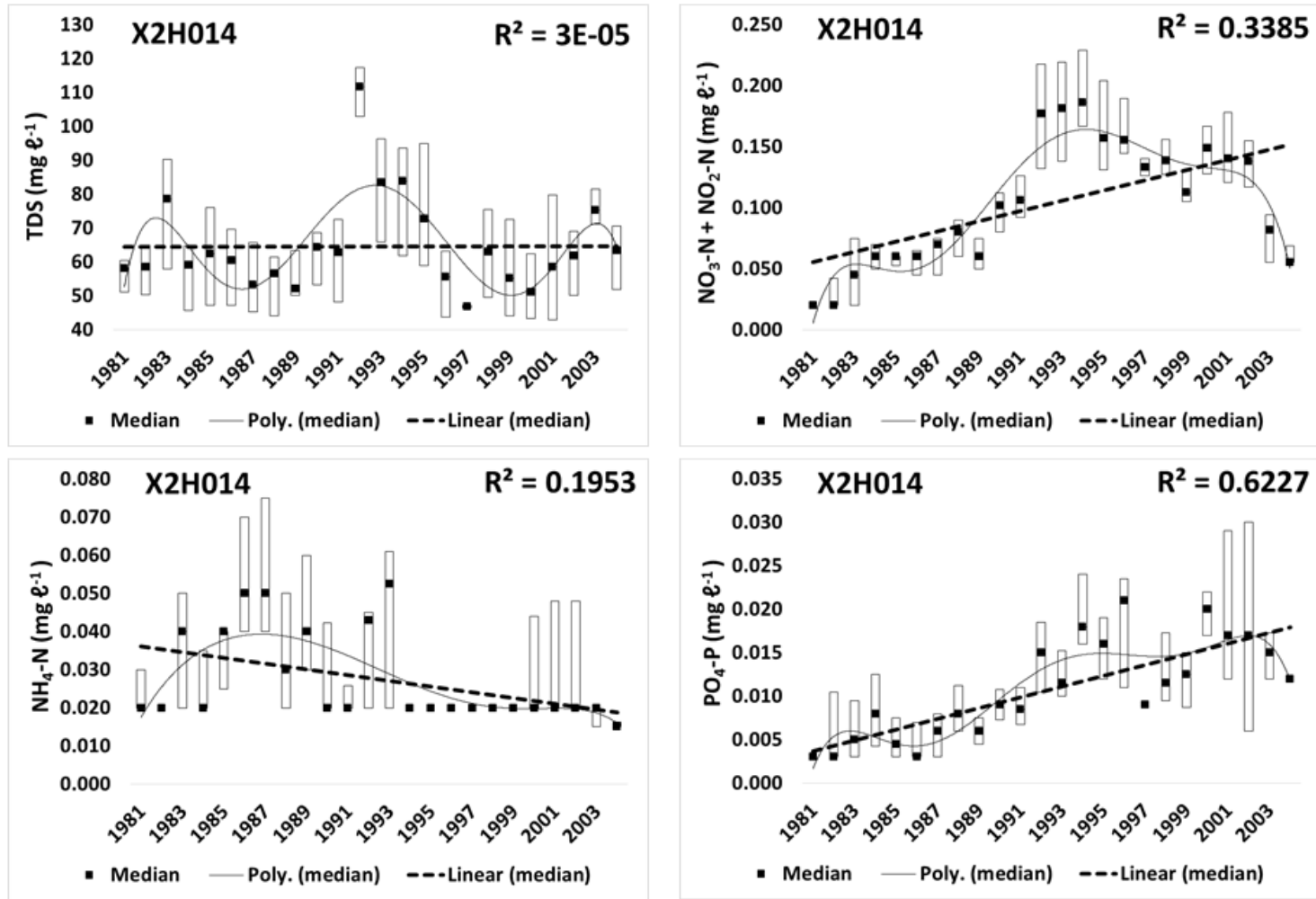


Figure D7. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H014 for the period 1981-2004.

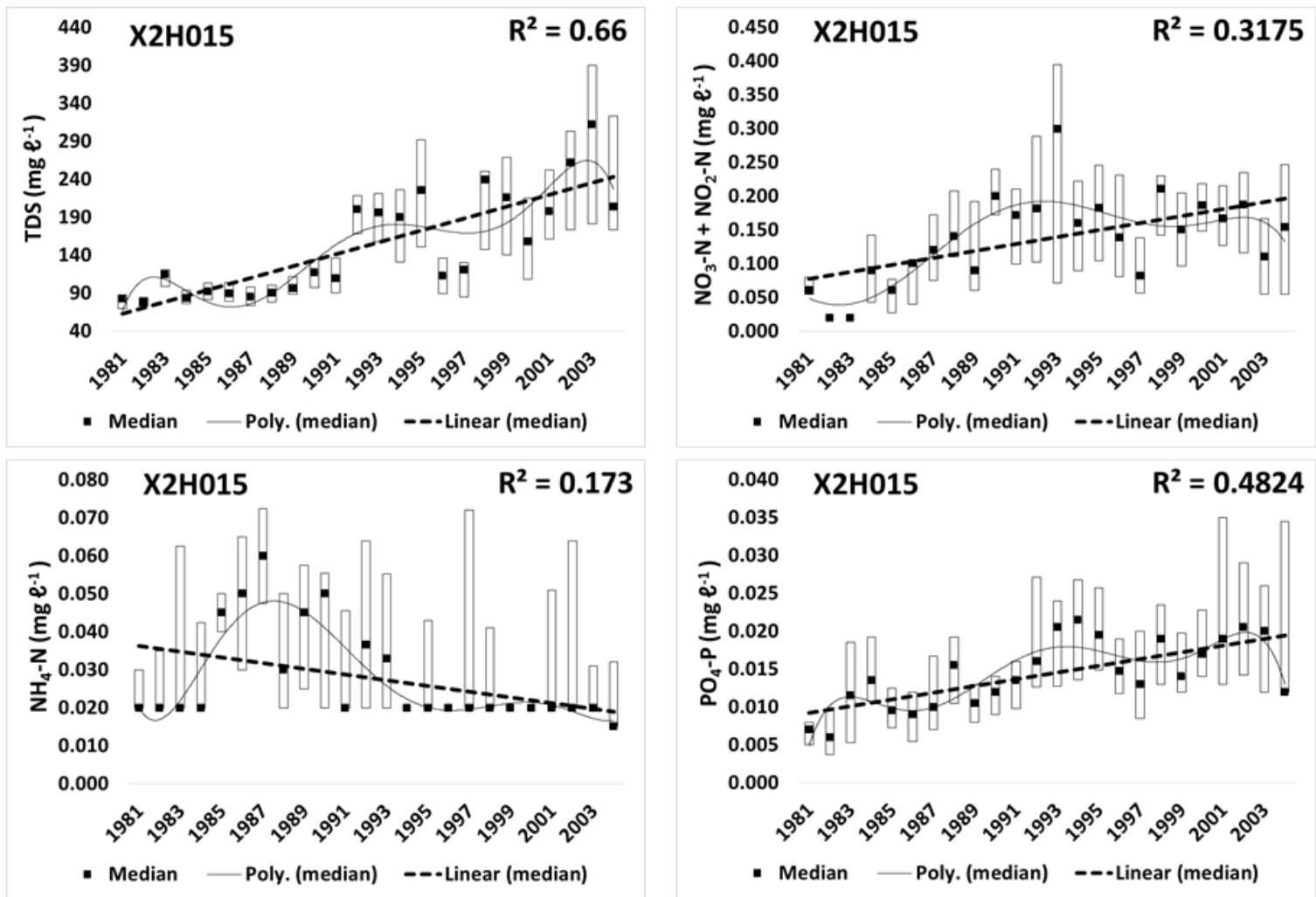


Figure D8. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H015 for the period 1981-2004.

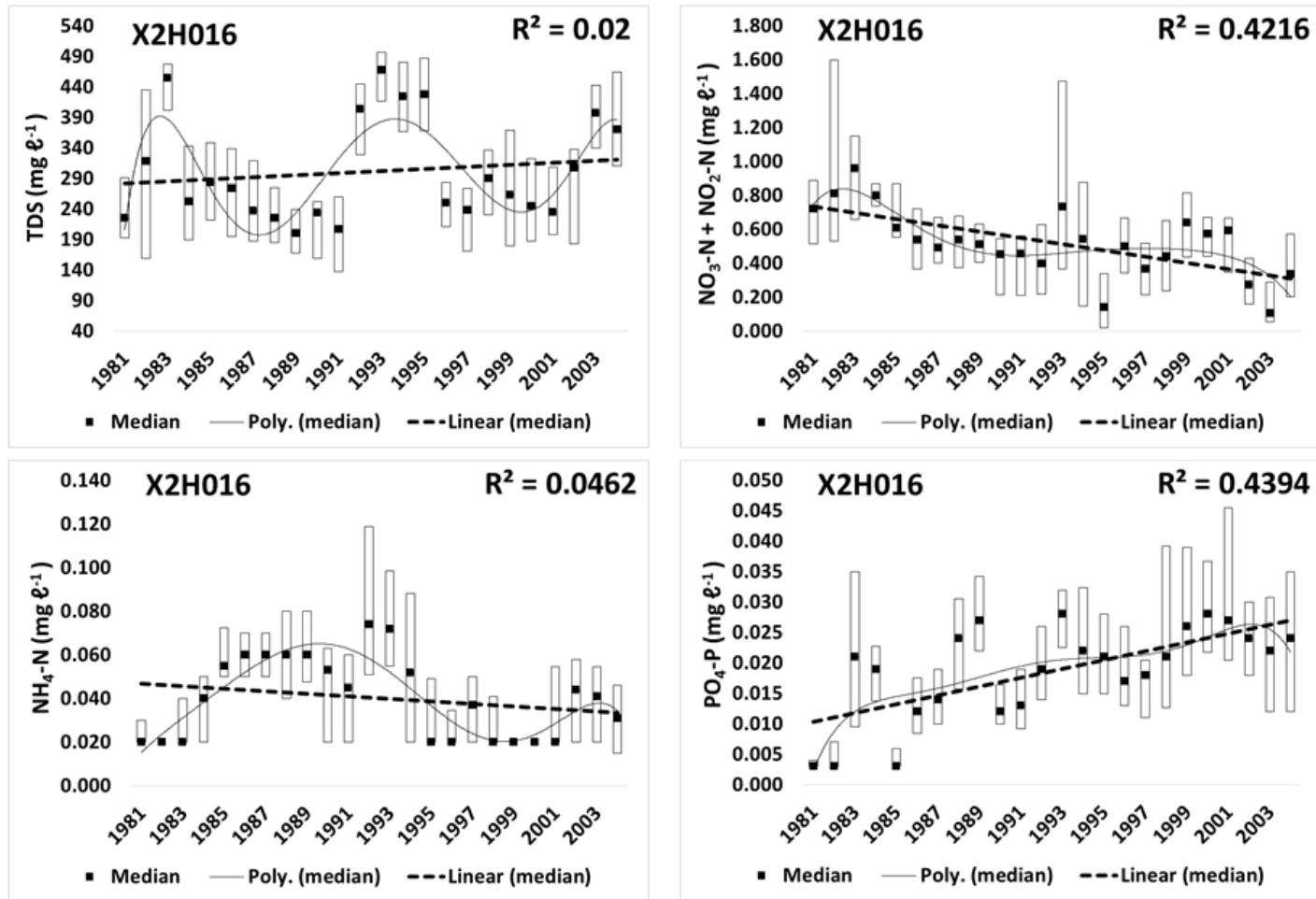


Figure D9. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H016 for the period 1981-2004.

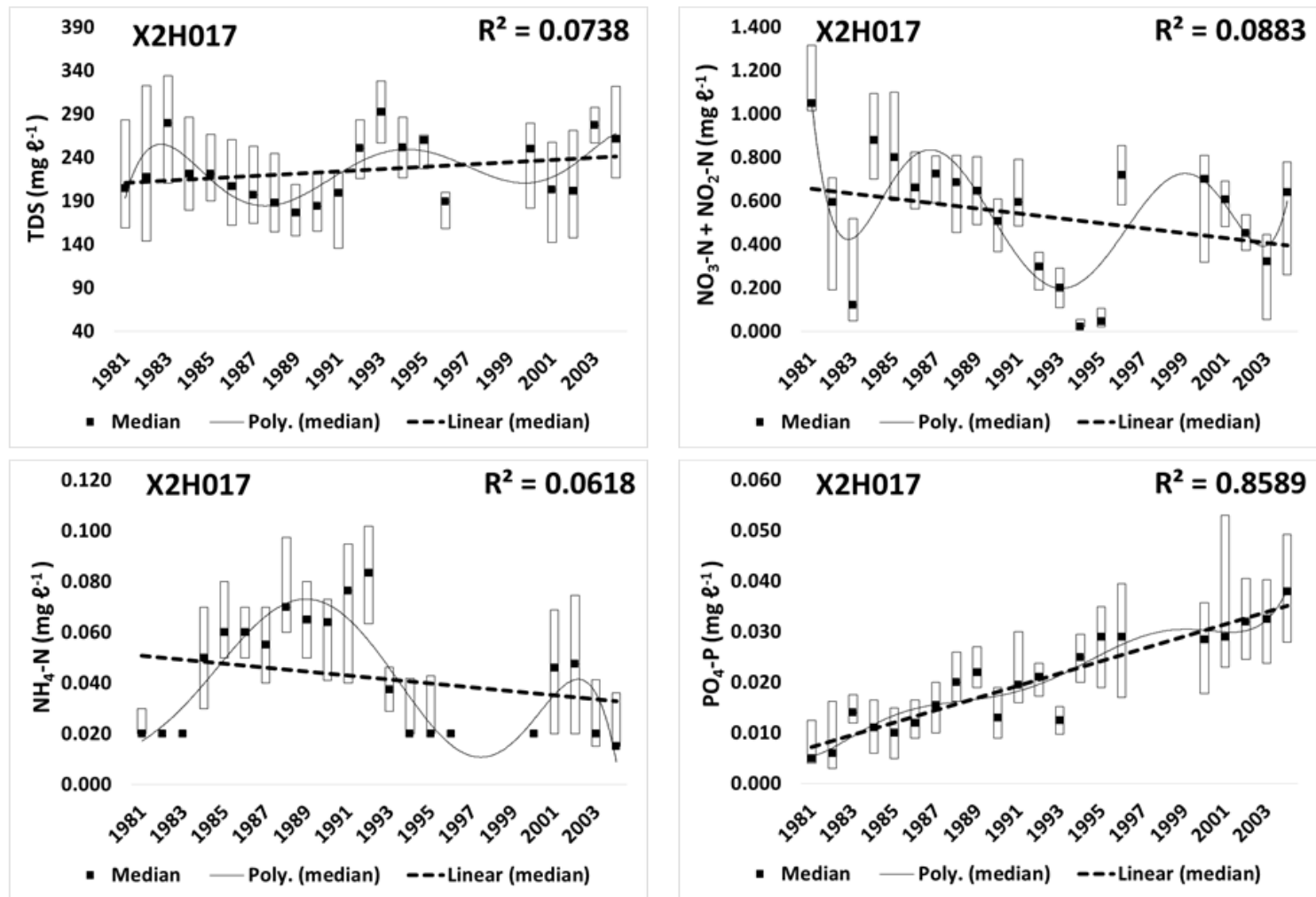


Figure D10. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H017 for the period 1981-2004.

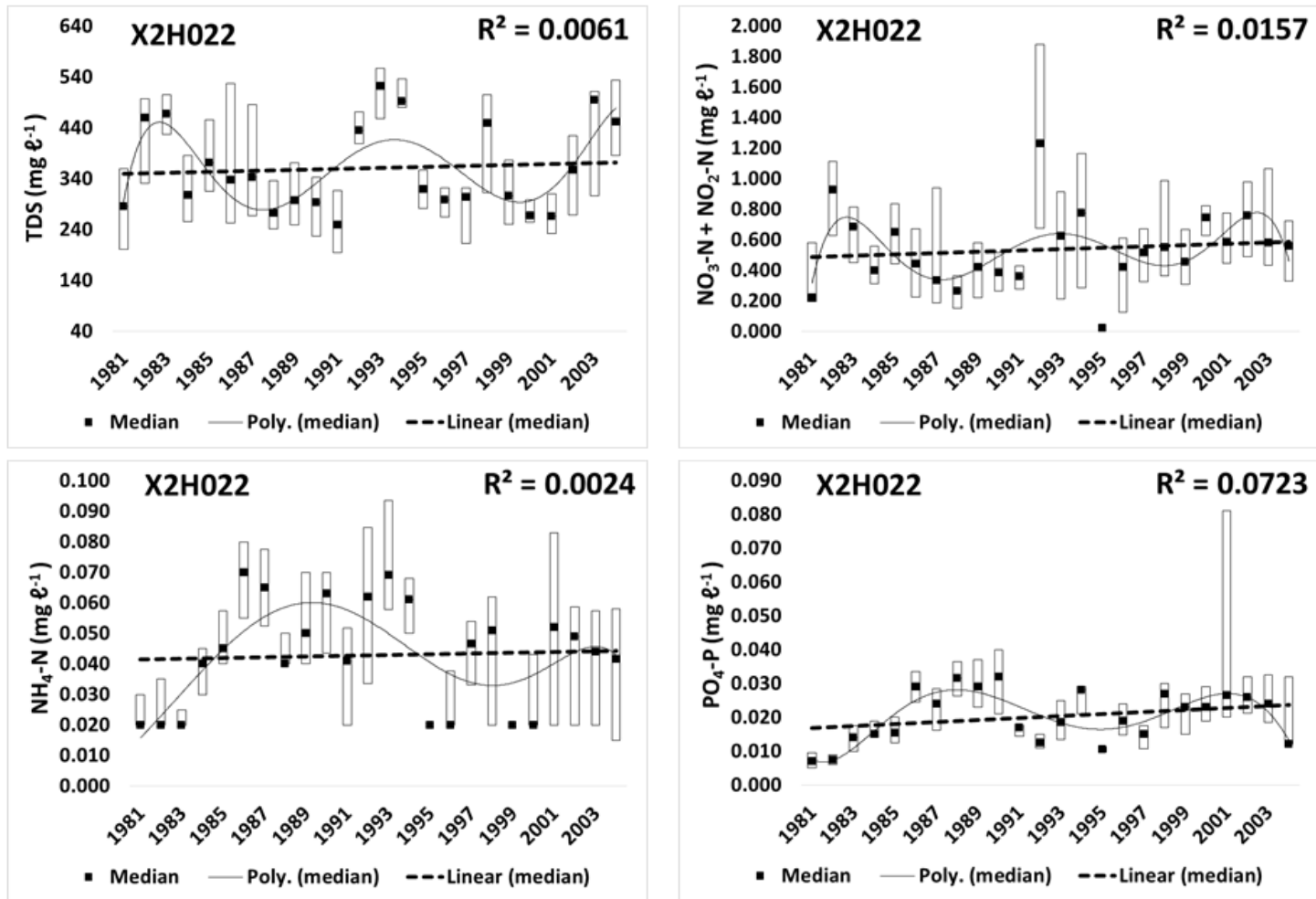


Figure D11. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H022 for the period 1981-2004.



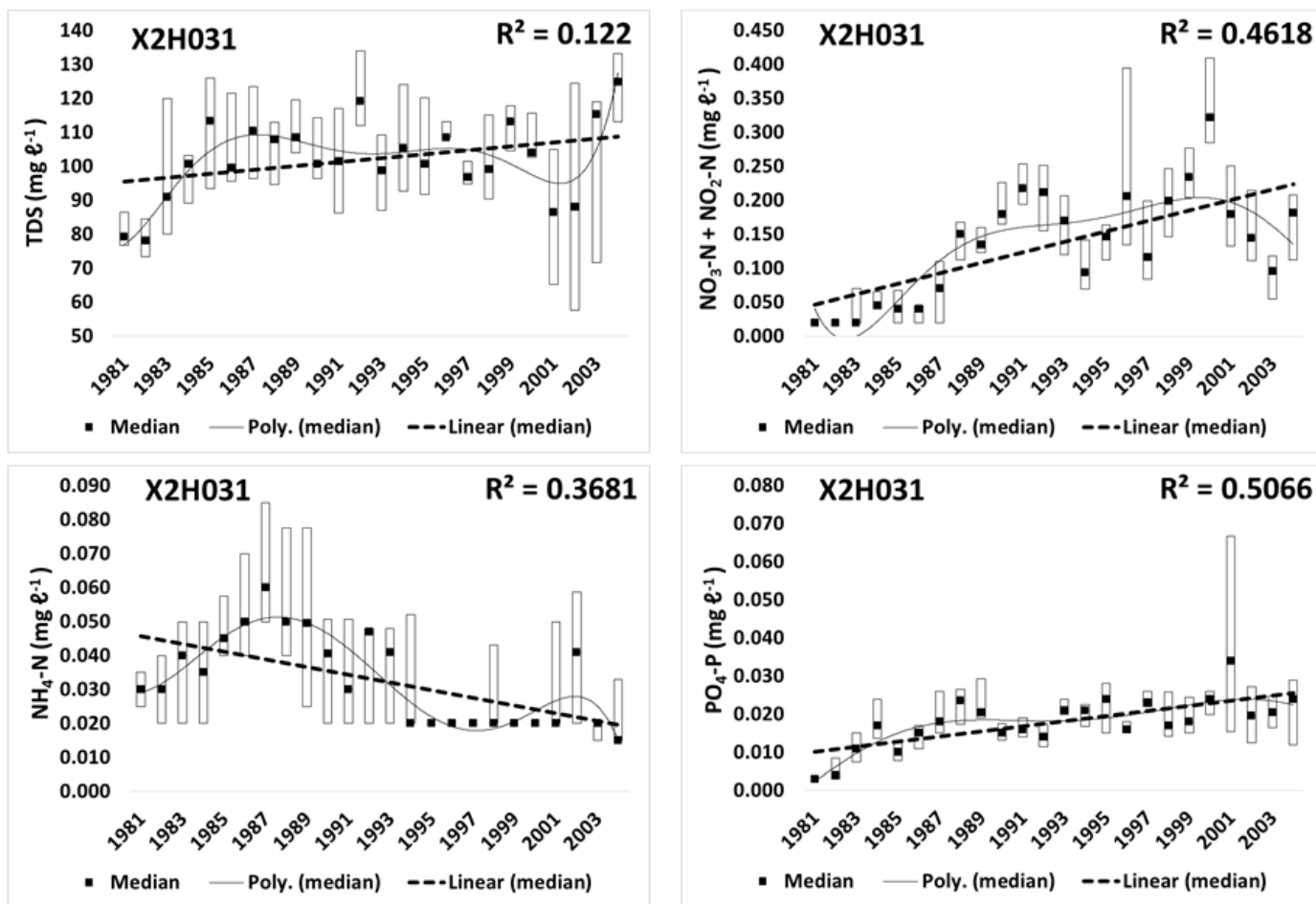


Figure D12. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H031 for the period 1981-2004.

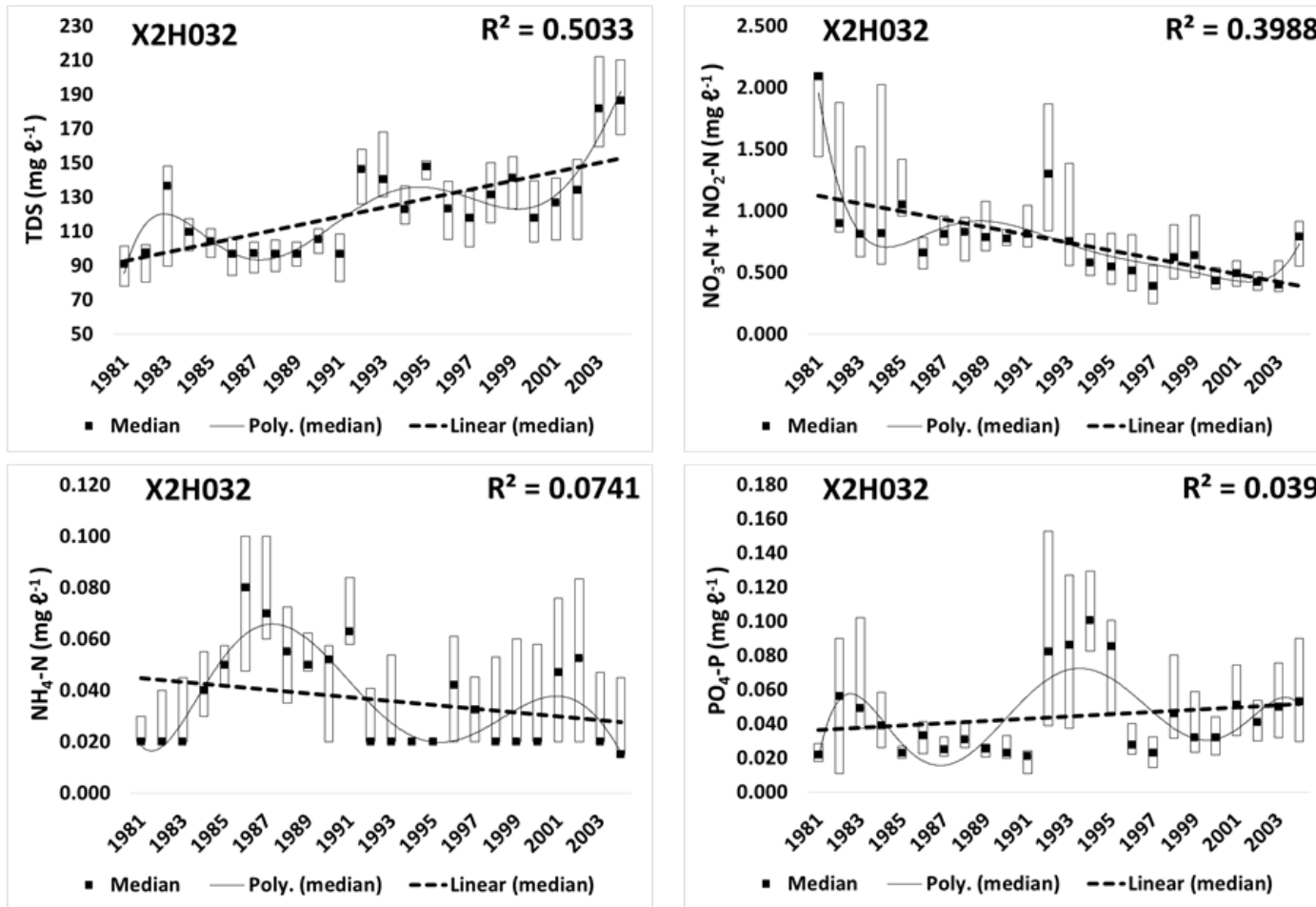


Figure D13. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2H032 for the period 1981-2004.

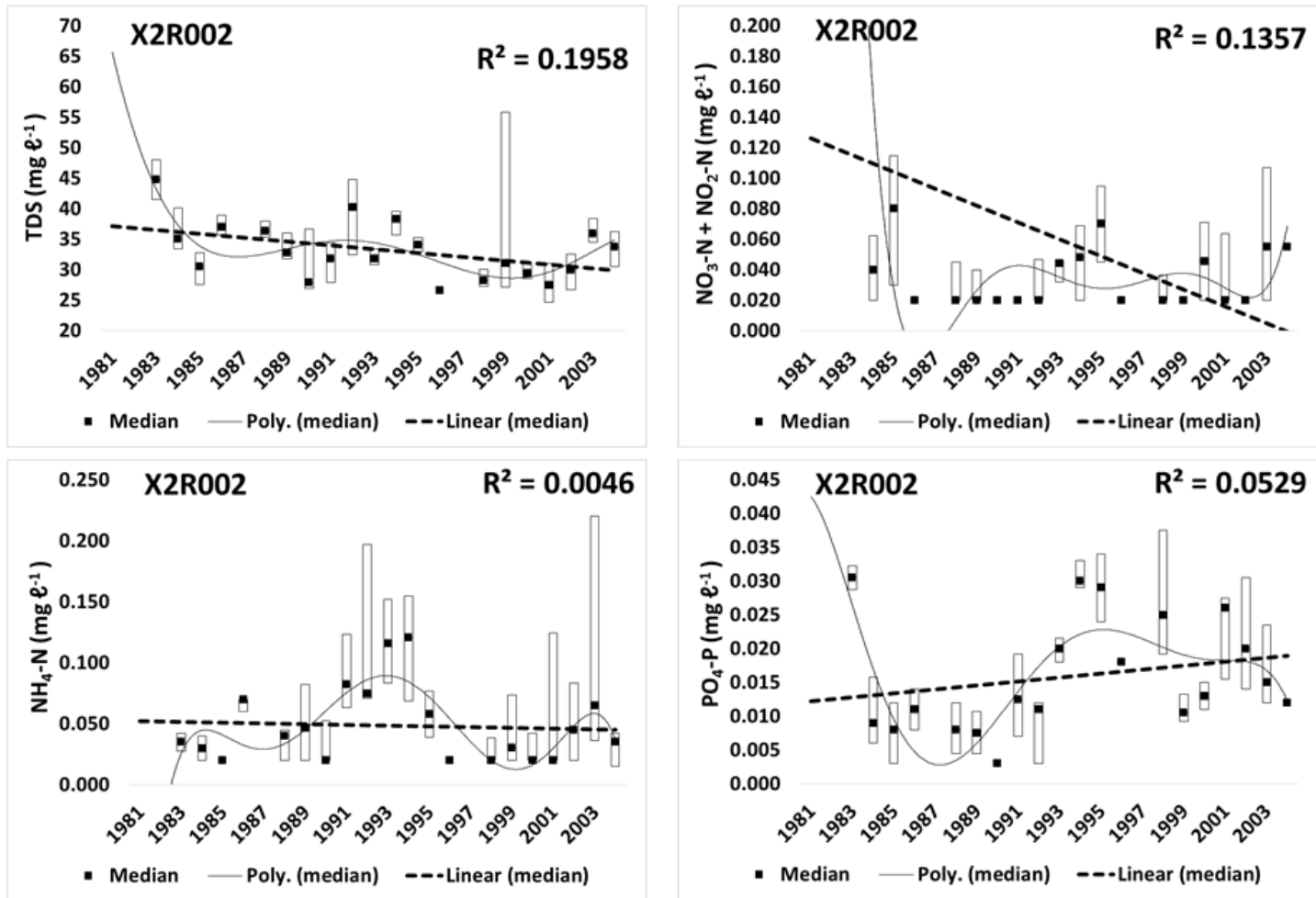


Figure D14. Water quality trends for TDS, Nitrates + Nitrites, Ammonium and Orthophosphates at DWS monitoring gauge X2R002 for the period 1981-2004.

## Appendix E

Table E1. River node water quality parameter values

Node	TDS Surface Water Conc. (mg/l)	TDS Interflow Water Conc. (mg/l)	TDS GW Water Conc. (mg/l)	TDS Return Flow Conc. (mg/l)	NH4 Surface Water Conc. (mg/l)	NH4 Interflow Water Conc. (mg/l)	NH4 GW Water Conc. (mg/l)	NH4 Return Flow Conc. (mg/l)	NH4 Nitrification Rate (d <sup>-1</sup> )	NO3 Surface Water Conc. (mg/l)	NO3 Interflow Water Conc. (mg/l)	NO3 GW Water Conc. (mg/l)	NO3 Return Flow Conc. (mg/l)	PO4 Surface Water Conc. (mg/l)	PO4 Interflow Water Conc. (mg/l)	PO4 GW Water Conc. (mg/l)	PO4 Return Flow Conc. (mg/l)
X21F-1	10	20	250	0	0.5	0.25	0	0	0.01	1.2	0.8	0	0	0.3	0.15	0.05	0
X21F-2	1200	35	400	0	0.4	0.2	0	0	0.01	1.2	0.8	0	0	0.2	0.1	0.05	0
X21G-1	10	20	85	5000	0.1	0.05	0.025	0.7	0.01	0.5	0.3	0.2	0.05	0.1	0	0	8
X21G-2	10	20	85	0	0.1	0.05	0	0	0.01	0.6	0.5	0.3	0	0.05	0.05	0.002	0
X21H-1	5	10	190	0	0.1	0.05	0	0	0.01	0.15	0.05	0	0	0.025	0	0.002	0
X21J-1	10	20	400	2500	0.4	0.2	0.025	0.6	0.01	0.8	0.2	0.1	0.4	0.075	0	0.005	0.2
X21J-2	10	20	350	0	0.2	0.1	0.025	0	0.01	0.9	0.2	0.1	0	0.05	0	0.005	0
X21K-1	10	20	85	0	0.1	0.05	0	0	0.01	0.1	0.05	0	0	0.025	0	0.002	0
X21K-2	10	20	400	5000	0.1	0.1	0.025	0.4	0.01	0.4	0.2	0.1	0.4	0.05	0.025	0	0.2
X21K-3	10	20	150	0	0.2	0.1	0	0	0.01	0.8	0	0	0	0.025	0	0.002	0
EWR1	10	20	195	0	0.01	0	0	0	0.01	0.1	0	0	0	0.01	0	0.028	0
X21A-1	10	20	195	200	0.2	0.1	0	0.5	0.01	0.8	0	0	0.5	0.025	0	0	0.005
X21A-2	5	10	195	0	0.01	0	0	0	0.01	0.1	0.05	0	0	0.01	0	0	0
X21B-1	10	20	65	0	0.2	0	0	0	0.01	0.1	0.05	0	0	0.01	0	0.028	0
X21B-2	10	20	195	0	0.01	0	0	0	0.01	0.1	0.05	0	0	0.025	0.015	0	0
EWR2	10	20	65	0	0.025	0	0	0	0.01	0.01	0	0	0	0.025	0.05	0	0
X21B-3	10	25	65	0	0.2	0.1	0	0	0.01	0.8	0.1	0	0	0.05	0	0	0

X21C-1	10	25	100	0	0.025	0	0	0	0.01	0.1	0	0	0	0.05	0.025	0	0
X21C-2	50	10	100	200	0.4	0.2	0	0.2	0.01	0.15	0.1	0	10	0.05	0	0	0.05
X21C-3	50	10	100	0	0.05	0	0	0	0.01	0.8	0	0	0	0.05	0	0.02	0
X21D-1	10	20	225	400	0	0	0	0	0.01	0	0	0	5	0	0	0.1	0.2
X21D-2	10	20	150	0	0	0	0	0	0.01	0	0	0	0	0	0	0.1	0
X21E-1	10	20	35	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
EWR3	10	20	30	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
X21E-2	10	20	195	0	0.4	0	0	0	0.8	0	0	0	0	0.025	0	0.1	0
MontroseFalls	10	20	65	200	0.2	0	0	0.4	0.01	0.4	0.2	0	0.1	0	0	0.1	0.05
X22A-1	20	40	65	0	0.08	0	0	0	0.01	0.2	0.4	0.1	0	0.025	0.001	0.005	0
X22A-2	10	20	85	0	0.1	0.025	0	0	0.01	0.2	0.1	0.1	0	0.12	0.001	0.025	0
X22BTributary	0	0	0	0	0.2	0.1	0	0	0.01	0.8	0	0	0	0.025	0	0.002	0
X22B-2	5	10	75	100	0.2	0.1	0	3	0.01	10	0	0	40	0.005	0	0	0
X22CTributary	10	20	175	1500	0.15	0.075	0.05	0.2	0.01	0.8	0.4	0	1.5	0.5	0	0.004	0.2
X22C-3	200	400	250	100	0.2	0.1	0	3	0.01	10	5	0	30	0.5	0	0	0.8
X22D-1	10	20	32.5	0	0.05	0.025	0	0	0.01	0.1	0.05	0.1	0	0.005	0.002	0	0
X22D-2	10	20	32.5	0	0.3	0	0	0	0.01	0.5	0.2	0.1	0	0.2	0	0	0
X22D-3	10	20	100	0	0.09	0.025	0	0	0.01	0.8	0.6	0	0	0.012	0.01	0.005	0
X22E-1	10	20	35	0	0.005	0	0	0	0.01	0.3	0	0	0	0.05	0	0.1	0
X22E-3	10	20	195	0	0.3	0	0	0	0.01	0.5	0.2	0.1	0	0.2	0	0	0
Spare	5	10	35	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
X22F-1	10	20	195	0	0.3	0	0	0	0.01	0.5	0.2	0.1	0	0.2	0	0	0
X22F-2	10	20	200	0	0.05	0.025	0	0	0.01	2	0.6	0.15	0	0.15	0.075	0.005	0
X22H-3	10	20	320	400	0.05	0	0.005	0	0.01	20	10	0.05	10	0.005	0	0	0
X22J-1	10	20	220	500	8	0.015	0	0.8	0.01	8	0.6	0	8	2.75	0	0	0.005
X22J-2	400	2000	300	0	0.05	0	0	0	0.1	3	5	0.1	0	2.75	0	0	0
X22K-1	100	100	300	150	0.6	0	0	0.25	0.01	0.1	0	0	0.05	2.75	0	0	0.05

EWR4	100	200	300	0	0.01	0	0	0	0.01	20	0	0	0	2.75	0	0	0
X22K-2	150	100	300	0	0	0	0	0	0.5	0.05	0	0	0	2.75	0	0	0
X22K-3	100	200	450	0	0.075	0.025	0.005	0	0.01	0.05	0	0	0	0.005	0	0	0
X23A-1	10	20	105	0	0.075	0.05	0.05	0	0.01	0.3	0.01	0.02	0	0.075	0.005	0.005	0
X23A-2	10	20	85	0	0.075	0.05	0.025	0	0.01	0.18	0.02	0.04	0	0.075	0.005	0.018	0
X23B-1	100	50	582	0	0.075	0.05	0.025	0	0.01	0.18	0.02	0.04	0	0.075	0.005	0.005	0
X23B-2	100	50	120	150	0.075	0.05	0.025	0	0.01	0.18	0.02	0.04	0	0.005	0	0	0.005
X23B-3	50	25	430	0	0.2	0.05	0	0	0.01	0.4	0.02	0.04	0	0.005	0	0	0
X23C-1	50	20	55	0	0.05	0.005	0	0	0.01	0.1	0.05	0	0	0.03	0	0.005	0
X23C-2	10	20	55	0	0.04	0.005	0	0	0.01	0.075	0.02	0	0	0.015	0	0.005	0
X23D-1	15	5	180	0	0.26	0.075	0	0	0.01	0.6	2	0	0	0.075	0.01	0.005	0
X23D-2	15	5	180	0	0.26	0.1	0	0	0.04	0.4	2	0.2	0	0.3	0.005	0.05	0
X23E-1	100	50	120	0	0.1	0.075	0.025	0	0.01	0.35	0.02	0.04	0	0.015	0	0.01	0
X23E-2	100	50	120	0	0.1	0.075	0.025	0	0.01	0.3	0.02	0.04	0	0.08	0	0.01	0
Barbeton	200	100	400	500	1.8	0.1	0	0	0.01	2	0.2	0	0	0.9	0	0.1	0
X23F-2	500	100	350	2500	0.2	0.1	0	6	0.01	5	0.02	0.04	15	0.005	0.005	0.005	0.005
X23G-1	100	50	250	0	0.2	0.1	0	0	0.01	0.18	0.02	0.04	0	0.025	0.005	0.005	0
EWR7	25	50	300	3500	0.2	0.1	0	0.2	0.01	5	0.02	0.04	10	0.005	0.002	0	0.05
X23Hkaap	100	50	250	3000	0.2	0.1	0	0.1	0.01	2	1	0.2	10	0.005	0.005	0.005	0.075
X23H-2	25	50	132	0	0.2	0.1	0	0	0.01	2	0.02	0.04	0	0	0	0.05	0
X23H-3	100	50	132	0	0.075	0.05	0.025	0	0.01	0.18	0.02	0.04	0	0.005	0	0	0
X23H-4	25	50	250	0	0.1	0.05	0	0	0.01	2	0.02	0.04	0	0	0	0.1	0
X23HGuage	25	50	300	1650	0.2	0.1	0	0.1	0.01	0.8	0.02	0.04	0.3	0.005	0	0	0.075
X24A-1	100	50	135	0	0.2	0.1	0.05	0	0.01	4	0.5	0.025	0	0.05	0	0	0
Phola	100	50	520	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
X24A-2	100	50	518	0	0.2	0.1	0	0	0.01	2	0	0	0	0.4	0	0.05	0
X24B-1	100	50	1000	0	0.075	0.05	0.025	0	0.01	0.5	0	0	0	0.1	0	0.05	0

X24B-2	100	50	1000	0	0.2	0.1	0	0	0.01	0.5	0	0	0	0.1	0	0.026	0
Lundi	100	50	1300	0	0.075	0.025	0.005	0	0.01	0.18	0	0	0	0.005	0	0	0
X24B-3	100	50	1100	0	0.2	0.1	0.005	0	0.01	0.05	0	0	0	0.1	0	0.038	0
X24C-1	100	50	550	0	0.2	0.1	0	0	0.01	0	0	0	0	0.005	0	0.005	0
X24C-2	10000	1000	3500	17500	0.2	0.1	0.005	0.6	0.01	0	0	0.05	50	0.005	0	0.005	0.05
X24D-1	100	50	450	0	0.075	0.05	0.025	0	0.01	0	0	0	0	0.005	0	0	0
EWR5	200	100	2000	1000	0.2	0.1	0.005	0.1	0.01	0.05	0	1	0.8	0.05	0	0	0.005
X24D-2 [Extra]	200	100	1400	100	0.2	0.1	0.005	0.2	0.01	10	5	1.2	0	0.4	0	0.1	0.001
X24E-1	200	100	850	0	0.8	0.1	0.05	0	0.01	0	0	0.02	0	0.005	0	0.1	0
X24E-2	100	50	740	0	0.2	0.1	0.005	0	0.04	0.005	0	0.2	0	0	0	0.15	0
X24F	10	20	600	300	0.2	0.1	0.005	0.1	0.01	0.1	0	0	0.1	0	0	0.085	0
X24G	10	20	600	0	0	0	0	0	0.01	0.1	0	0	0	0	0	0	0
X24H-1	10	20	650	300	0.2	0.1	0.005	0.15	0.01	0.1	0.05	0	0.1	0	0	0.05	0
EWR6	10	20	450	400	0	0	0	0	0.01	0	0	0	0	0	0	0	0
Mozambique2	10	20	450	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
End	0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX21F-1	10	15	132	1	0.05	0.025	0	1	0.01	0.4	0.2	0	1	0.005	0	0	1
DDX21F-2	10	15	145	0	0.1	0.05	0	0	0.01	0.4	0.2	0	0	0.025	0	0	0
DDX21G-1	10	20	150	200	0.2	0.1	0	0	0.01	0.05	0.025	0	0	0.025	0	0	0
DDX21G-2	100	10	200	0	0.1	0.05	0	0	0.01	0.025	0	0	0	0.025	0	0	0
DDX21H-1	1	1	1	0	0.1	0.05	0	0	0.01	0.025	0.002	0	0	0.025	0	0.002	0
NgwodwanaDam	1	1	1	0	0.1	0.05	0	0	0.01	0.05	0	0.1	0	0	0	0	0
DDX21J-1	10	20	260	0	0.1	0.05	0	0	0.01	0.05	0.025	0	0	0.025	0	0.002	0
DDX21A-1	10	20	195	0	0.01	0	0	0	0.01	0.1	0	0	0	0.01	0	0	0
DDX21A-2	10	20	195	0	0.01	0	0	0	0.01	0.01	0	0	0	0.01	0	0.028	0
DDX21B-1	10	20	65	0	0.05	0	0	0	0.01	0.01	0	0	0	0.01	0	0.028	0
DDX21B-2	10	20	195	0	0.01	0	0	0	0.01	0.01	0	0	0	0.025	0	0	0

DDX21B-3	5	10	65	0	0.01	0	0	0	0.01	0.1	0	0	0	0.05	0.025	0	0
DDX21C-1	10	20	65	0	0.05	0	0	0	0.01	0.1	0.05	0	0	0.025	0	0	0
DDX21C-2	10	20	65	0	0.002	0	0	0	0.01	0.1	0	0	0	0.05	0.025	0	0
DDX21C-3	10	20	65	0	0.02	0	0	0	0.01	0.4	0.2	0	0	0.05	0.025	0	0
KwenaDam	5	10	65	200	0.05	0.025	0	0.8	0.08	0.4	0.2	0	10	0.005	0	0	0
DDX21D-1	10	20	225	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX21E-1	10	20	35	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX22A-1	5	10	35	0	0.005	0	0	0	0.01	0.1	0.05	0.002	0	0.001	0.001	0.012	0
DDX22B-1	0	0	0	0	0.2	0.1	0	0	0.01	0.8	0	0	0	0.2	0	0	0
DDX22B-2	0	0	0	0	0.2	0.1	0	0	0.01	0.8	0	0	0	0.025	0	0	0
DDX22C-1	15	10	55	0	0.15	0.075	0.05	0	0.01	2	0.001	0	0	0.04	0	0.002	0
DDX22C-2	15	10	55	0	0.15	0.075	0	0	0.01	0.8	0.2	0.002	0	0.04	0	0.002	0
DDX22C-3	200	400	250	0	0.2	0.1	0	0	0.01	0.8	5	0	0	0.01	0	0.012	0
DDX22D-1	10	20	32.5	0	0.05	0.025	0	0	0.01	0.025	0.015	0.1	0	0.005	0.003	0	0
DDX22D-2	10	20	32.5	0	0.3	0	0	0	0.01	0.5	0.2	0.1	0	0.2	0	0	0
DDX22E-1	10	20	35	0	0.005	0	0	0	0.01	0.3	0	0	0	0.05	0	0	0
WitklipDam	0	5	33	0	0.05	0	0	0	0.01	0.9	0	0	0	0.08	0	0	0
DDX22E-3	10	20	195	0	0.3	0	0	0	0.01	0.5	0.2	0.1	0	0.2	0	0	0
DDX22F-1	10	20	195	0	0.3	0	0	0	0.01	0.5	0.2	0.1	0	0.2	0	0	0
DDX22F-2	10	20	100	0	0.2	0.025	0	0	0.01	0.6	0.3	0	0	0.5	0.2	0.005	0
DDX22G-1	0	5	65	0	0	0	0	0	0.01	0.4	0	0	0	0.005	0	0	0
KlipkoppieDam	5	10	35	0	0.05	0	0	0	0.1	0.2	0.05	0	0	0.01	0	0	0
DDX22G-2	10	20	35	0	0.05	0.025	0	0	0.01	0.05	0	0	0	0.4	0.001	0	0
LongmereDam	5	10	35	0	0.2	0.025	0	0	0.1	0.05	0	0	0	0.005	0.001	0	0
DDX22H-1	5	10	195	200	0.01	0.005	0	0	0.01	0.002	0.001	0	0	0.01	0	0	0
DDX22H-2	10	20	195	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
PrimkopDam	10	20	35	0	0.05	0.025	0	0	0.01	0.6	0.025	0	0	0.01	0	0	0



DDX22H-3	10	20	295	0	0	0	0	0	0.01	0.8	0.6	0.4	0	0.005	0	0	0
DDX22J-1	10	200	175	0	0.8	0.6	0.4	0	0.01	1.8	5	0.2	0	0.01	0	0	0
DDX22J-2	5	10	175.5	0	0	0	0	0	0.01	3	1.5	0.2	0	0.002	0	0	0
DDX22K-1	75	100	300	0	0	0	0	0	0.01	0.05	0	0	0	2.75	0	0	0
DDX22K-2	100	100	300	0	0	0	0	0	0.01	0.05	0	0	0	2.7	0	0	0
DDX22K-3	10	20	450	0	0.075	0.005	0.005	0	0.01	0	0	0	0	0	0	0	0
DDX23A-1	10	20	85	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX23A-2	10	20	85	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX23B-1	50	25	500	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX23B-2	100	50	110	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX23B-3	50	25	430	0	0	0	0	0	0.01	0	0	0	0	0.005	0	0	0
DDX23C-1	10	20	35	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX23D-1	15	5	150	0	0.15	0.075	0	0	0.01	0.5	2	0	0	0	0	0	0
DDX23D-2	15	5	150	0	0.15	0.075	0	0	0.01	0.5	2	0	0	0	0	0	0
DDX23E-1	100	50	120	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX23F-1	100	50	350	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX23F-2	10	20	350	0	0	0	0	0	0.01	0	0	0	0	0.025	0	0.005	0
DDX23G-1	100	50	326	0	0	0	0	0	0.01	0	0	0	0	0.025	0	0.005	0
DDX23G-2	25	50	300	0	0	0	0	0	0.01	0.4	0.2	0	0	0	0	0	0
DDX23H-1	100	50	250	0	0	0	0	0	0.01	0	0	0	0	0.025	0	0	0
DDX23H-2	50	75	130	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX23H-4	50	75	250	0	0.075	0.05	0	0	0.01	0.18	0.02	0.04	0	0.005	0.005	0	0
DDX23H-5	100	50	250	0	0	0	0	0	0.01	0.4	0	0	0	0	0	0	0
DDX24A-1	100	50	135	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX24A-2	100	50	520	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX24B-1	100	50	1000	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX24B-2	100	50	1000	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0

DDX24B-3	100	50	1300	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX24C-1	100	50	530	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX24C-2	500	300	3000	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX24D-2	100	200	1400	0	0.075	0.05	0.005	0	0.01	0	0	0	0	0	0	0	0
DDX24E-1	2000	2000	850	0	0	0	0	0	0.01	0	0	0	0	0.005	0	0.027	0
DDX24E-2	100	50	740	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX24F	200	20	650	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0
DDX24H-1	10	20	650	0	0	0	0	0	0.01	10	0	0	0	0	0	0	0

Table E2. Reservoir water quality parameter values

Dam	Dam Starting algal concentration (mg/L)	Dam Starting DOM concentration (mg/L)	Dam starting POM concentration (mg/L)	Dam starting organic sediment load (kg)	Dam starting NO3 concentration (mg/L)	Dam starting ammonia concentration (mg/L)	Dam starting PO4 concentration (mg/L)	Dam starting inorganic sediment load (kg)	Dam starting TDS concentration (mg/L)	Dam starting hyacinth concentration (mg/m <sup>2</sup> )	Hyacinth mortality rate (day <sup>-1</sup> )	Hyacinth growth rate at Topt (day <sup>-1</sup> )	Hyacinth respiration rate at Topt (day <sup>-1</sup> )	Tmin for hyacinth growth and respiration (°C)	Top for hyacinth growth and respiration (°C)	Tmax for hyacinth growth and respiration (°C)	Partitioning coefficient for hyacinth mortality
NgwodwanaDam	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
KwenaDam	10	2	2	100	0.1	0.03	0.02	100	50	0	0	0	0	0	0	0	0
WitklipDam	1	2	2	4000	0.3	0.15	0.05	50	35	0	0	0	0	0	0	0	0
KlipkoppieDam	10	0	0	100	0.2	0.2	0.025	1	40	0	0	0	0	0	0	0	0
LongmereDam	1	2	2	4000	0.3	0.15	0.05	50	35	0	0	0	0	0	0	0	0
PrimkopDam	100	10	20	1	0.05	0.05	0.025	1	35	0	0	0	0	0	0	0	0

Table E3. Water quantity parameter values

Node	Antecedent Precip. Factor	Antecedent Precip. Threshold	Gauge1 Weight	Gauge2 Weight	Gauge3 Weight	Monthly to Daily FDC Conversion: A	Monthly to Daily FDC Conversion: B	Monthly to Daily FDC Conversion: C	BF Parameter (Interflow)	BF Parameter (GW)	hasStorage	isIncremental Node	isReturnFlow Node	Dam full supply cap (Mm <sup>3</sup> )	Dam full supply area (km <sup>2</sup> )	Power for calculating area	Reach Length (km)	Reach average biologically active width (m)
X21F-1	0.98	5	1	5	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	3.08	5
X21F-2	0.98	5	1	5	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	17.28	5
X21G-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	1	0	0	0	5.31	5
X21G-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	25.86	5
X21H-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	11.69	5
X21J-1	0.995	2	10	10	10	1	-0.1	0.3	0.95	0.92	0	1	1	0	0	0	26.66	5
X21J-2	0.995	2	10	10	10	1	-0.1	0.3	0.95	0.92	0	1	0	0	0	0	8.9	5
X21K-1	0.995	2	10	10	10	1	-0.1	0.3	0.95	0.92	0	1	0	0	0	0	19.92	5
X21K-2	0.995	2	10	10	10	1	-0.1	0.3	0.95	0.92	0	1	1	0	0	0	13.95	5
X21K-3	0.995	2	10	10	10	1	-0.1	0.33	0.95	0.92	0	1	0	0	0	0	15	5
EWR1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	1.41	3
X21A-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	1	0	0	0	40.8	3
X21A-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	1.41	3
X21B-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	10.99	3
X21B-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	10.72	3
EWR2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	10.7	3

																		2	
X21B-3	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	0	19.76	3
X21C-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	0	30.02	3
X21C-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	1	0	0	0	0	7.09	3
X21C-3	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	0	50.3	3
X21D-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	1	0	0	0	0	26.5	3
X21D-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	0	18.23	3
X21E-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	0	15.13	3
EWR3	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	0	23.58	3
X21E-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	0	16.44	3
MontroseFalls	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	1	0	0	0	0	0.61	3
X22A-1	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	0	10.38	5
X22A-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	0	9.65	5
X22BTributary	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	0	9.65	3
X22B-2	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	1	0	0	0	0	14.33	5
X22CTributary	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	1	0	0	0	0	36.62	3
X22C-3	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	1	0	0	0	0	25.11	5
X22D-1	0.985	3	10	10	10	1	-0.3	0.62	0.95	0.92	0	1	0	0	0	0	0	11.25	3
X22D-2	0.985	3	10	10	10	1	-0.3	0.62	0.95	0.92	0	1	0	0	0	0	0	11	3
X22D-3	0.985	3	10	10	10	1	-0.3	0.62	0.95	0.92	0	1	0	0	0	0	0	22.64	3
X22E-1	0.985	3	10	10	10	1	-0.3	0.62	0.95	0.92	0	1	0	0	0	0	0	3.19	3
X22E-3	0.985	3	10	10	10	1	-0.3	0.62	0.29	0.95	0	1	0	0	0	0	0	5	5.515
Spare	0.985	3	10	10	10	1	-0.3	0.62	0.95	0.92	0	0	0	0	0	0	0	5.515	3

X22F-1	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	17.0 4	5
X22F-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	31.2 3	5
X22H-3	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	1	0	0	0	12.4	5
X22J-1	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	1	0	0	0	8.25	5
X22J-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	7.9	5
X22K-1	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	1	0	0	0	3.8	5
EWR4	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	3.8	10
X22K-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	8.01	5
X22K-3	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	9.4	5
X23A-1	0.985	3	1	5	10	1	-0.3	0.62	0.95	0.92	0	1	0	0	0	0	9	3
X23A-2	0.985	3	1	5	10	1	-0.3	0.62	0.95	0.92	0	1	0	0	0	0	18.5 4	3
X23B-1	0.985	3	10	10	10	1	-0.3	0.62	0.95	0.92	0	1	0	0	0	0	6	3
X23B-2	0.98	5	1	5	10	1	-0.2	0.38	0.95	0.92	0	1	1	0	0	0	23.3 3	5
X23B-3	0.98	5	1	5	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	13.2 7	5
X23C-1	0.98	1	1	10	10	1	-0.1	0.26	0.95	0.92	0	1	0	0	0	0	10.7 45	3
X23C-2	0.98	1	1	10	10	1	-0.1	0.26	0.95	0.92	0	1	0	0	0	0	10.7 45	3
X23D-1	0.98	5	1	5	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	12.1 6	5
X23D-2	0.98	5	1	5	10	1	-0.2	0.38	0.95	0.92	0	1	0	0	0	0	7.68	5
X23E-1	0.99	3	10	1	10	1	-0.35	0.55	0.95	0.92	0	1	0	0	0	0	19.7 4	3
X23E-2	0.99	3	10	1	10	1	-0.35	0.55	0.95	0.92	0	1	0	0.02	0.08	0.65	10.0 4	3
Barbeton	0.99	3	10	1	10	1	-0.35	0.55	0.61	0.95	0	1	0	0	0	0	5	13.57
X23F-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	0	1	1	0	0	0	17.0 9	3
X23G-1	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	8	3
EWR7	0.995	5	10	10	10	1	-0.1	0.29	0.55	0.95	0	1	1	0	0	0	8	24.24

X23Hkaap	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	1	0	0	0	7.65	3
X23H-2	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	3	3
X23H-3	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	3	3
X23H-4	0.995	5	10	10	10	1	-0.1	0.29	0.92	0	0	1	0	0	0	0	3	3
X23HGuage	0.995	5	10	10	10	1	-0.1	0.29	0.92	0	0	1	1	0	0	0	3	3
X24A-1	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	20.2 2	3
Phola	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	0	0	0	0	0	13.2 2	3
X24A-2	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	12.4 2	3
X24B-1	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	9.99	3
X24B-2	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	8.76	3
Lundi	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	0	0	0	0	0	3.87	3
X24B-3	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	12.4 7	3
X24C-1	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	25.4 8	3
X24C-2	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	1	0	0	0	7.84	10
X24D-1	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	0	0	0	0	12	3
EWRS	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	0	1	1	0	0	0	15.4 9	10
X24D-2_ [Extra]	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	0	1	1	0	0	0	10	5
X24E-1	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	0	1	0	0	0	0	6.73	10
X24E-2	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	0	1	0	0	0	0	8.28	10
X24F	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	0	1	1	0	0	0	16.5 6	10
X24G	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	0	1	0	0	0	0	61.8 7	3
X24H-1	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	0	1	1	0	0	0	7.73	10
EWRS6	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	0	1	1	0	0	0	36.5 1	10
Mozambique2	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	0	1	0	0	0	0	12.9 2	10

End	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	0	0	0	0	0	0	1	1
DDX21F-1	0.98	10	1	5	10	1	-0.2	0.38	0.95	0.92	1	1	0	2.93	1.48	0.67	0	0
DDX21F-2	0.98	5	1	5	10	1	-0.2	0.38	0.95	0.92	1	1	0	1.3	0.41	0.67	0	0
DDX21G-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.39	0.12	0.67	0	0
DDX21G-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.58	0.19	0.67	0	0
DDX21H-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.1	0.02	0.67	0	0
Ngwodwan aDam	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	10.4	0.87	0.67	11.0 4	3
DDX21J-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.37	0.09	0.67	0	0
DDX21A-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	3.44	1.27	0.67	0	0
DDX21A-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.88	0.34	0.67	0	0
DDX21B-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	1.28	0.46	0.67	0	0
DDX21B-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.84	0.27	0.67	0	0
DDX21B-3	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.28	0.11	0.67	0	0
DDX21C-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.41	0.17	0.67	0	0
DDX21C-2	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.44	0.18	0.67	0	0
DDX21C-3	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	0	0	0.03	0.01	0.67	0	0
KwenaDam	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	0	1	158.9 3	12.5	0.67	0	0
DDX21D-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.3	0.07	0.67	0	0
DDX21E-1	0.98	5	10	10	10	1	-0.2	0.38	0.95	0.92	1	1	0	0.1	0.03	0.67	0	0
DDX22A-1	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.13	0.03	0.67	0	0
DDX22B-1	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.1	0.03	0.55	0	0
DDX22B-2	0.995	5	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.01	0.01	0.55	0	0
DDX22C-1	0.995	2	10	10	10	1	-0.2	0.29	0.95	0.92	1	1	0	0.62	0.22	0.55	0	0
DDX22C-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.81	0.27	0.55	0	0
DDX22C-3	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	1.57	0.53	0.55	8.25	5
DDX22D-1	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.3	0.07	0.67	0	0
DDX22D-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.57	0.12	0.55	0	0

DDX22E-1	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.02	0.01	0.55	0	0
WitklipDam	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	12.64	1.9	0.55	6.55	3
DDX22E-3	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	1.97	0.28	0.55	10	3
DDX22F-1	0.995	2	10	10	10	1	-0.2	0.29	0.95	0.92	1	1	0	0.59	0.2	0.62	0	0
DDX22F-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.48	0.15	0.62	17.04	5
DDX22G-1	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.39	0.12	0.67	0	0
KlipkoppieDam	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	12.26	2.35	0.62	5	3
DDX22G-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.13	0.12	0.62	0	0
LongmereDam	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	4.2	0.94	0.62	5	3
DDX22H-1	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	1	0.82	0.28	0.62	5	3
DDX22H-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	3.03	1.08	0.62	8.25	5
PrimkopDam	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	1.93	0.41	0.65	12	3
DDX22H-3	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	1	0.37	0.65	12.4	3
DDX22J-1	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	2.35	0.77	0.65	3	5
DDX22J-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.62	0.19	0.65	0	0
DDX22K-1	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.83	0.16	0.65	3.8	3
DDX22K-2	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	0.62	0.14	0.65	0	0
DDX22K-3	0.995	2	10	10	10	1	-0.1	0.29	0.95	0.92	1	1	0	1.39	0.37	0.65	9.4	10
DDX23A-1	0.985	3	1	5	10	1	-0.3	0.62	0.95	0.92	1	1	0	0.2	0.07	0.65	0	0
DDX23A-2	0.985	3	1	5	10	1	-0.3	0.62	0.95	0.92	1	1	0	0.33	0.12	0.65	0	0
DDX23B-1	0.985	3	10	10	10	1	-0.3	0.62	0.95	0.92	1	1	0	0.18	0.04	0.65	0	0
DDX23B-2	0.985	3	10	10	10	1	-0.3	0.62	0.95	0.92	1	1	0	0.6	0.25	0.65	0	0
DDX23B-3	0.985	3	10	10	10	1	-0.3	0.62	0.95	0.92	1	1	0	0.41	0.16	0.65	0	0
DDX23C-1	0.985	3	10	10	10	1	-0.3	0.62	0.95	0.92	1	1	0	1.83	0.19	0.65	0	0
DDX23D-1	0.985	5	10	10	10	1	-0.3	0.24	0.95	0.92	1	1	0	0.92	0.41	0.65	0	0
DDX23D-2	0.985	5	10	10	10	1	-0.3	0.24	0.95	0.92	1	1	0	0.74	0.34	0.65	0	0



DDX23E-1	0.99	3	10	1	10	1	-0.35	0.55	0.95	0.92	1	1	0	0.26	0.07	0.65	0	0
DDX23F-1	0.99	3	10	10	10	1	-0.35	0.55	0.95	0.92	1	1	0	0.64	0.28	0.65	0	0
DDX23F-2	0.99	3	10	10	10	1	-0.35	0.55	0.95	0.92	1	1	0	0.42	0.18	0.65	0	0
DDX23G-1	0.99	3	10	10	10	1	-0.35	0.55	0.95	0.92	1	1	0	0.39	0.08	0.65	0	0
DDX23G-2	0.99	3	10	10	10	1	-0.35	0.55	0.95	0.92	1	1	0	0.99	0.23	0.65	0	0
DDX23H-1	0.99	3	10	10	10	1	-0.35	0.55	0.95	0.92	1	1	0	0.17	0.04	0.65	0	0
DDX23H-2	0.99	3	10	10	10	1	-0.35	0.55	0.95	0.92	1	1	0	0.46	0.13	0.65	0	0
DDX23H-4	0.99	3	10	10	10	1	-0.35	0.55	0.95	0.92	0	1	0	0	0	0	3	3
DDX23H-5	0.99	3	10	10	10	1	-0.35	0.55	0.95	0.92	1	1	0	0.36	0.15	0.65	0	0
DDX24A-1	0.99	10	10	10	10	1	-0.39	0.61	0.95	0.92	1	1	0	0.12	0.03	0.65	0	0
DDX24A-2	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	0.12	0.06	0.65	0	0
DDX24B-1	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	0.26	0.1	0.75	0	0
DDX24B-2	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	0.06	0.02	0.75	0	0
DDX24B-3	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	0.05	0.02	0.75	0	0
DDX24C-1	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	0.42	0.18	0.75	0	0
DDX24C-2	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	0.03	0.01	0.75	0	0
DDX24D-2	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	1.98	0.71	0.75	0	0
DDX24E-1	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	1.01	0.31	0.75	0	0
DDX24E-2	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	2.18	0.87	0.75	0	0
DDX24F	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	2.75	1.08	0.75	0	0
DDX24H-1	0.99	10	10	10	10	1	-0.39	0.62	0.95	0.92	1	1	0	5.21	1.65	0.75	0	0