Geohydrological Studies of the Primary Coastal Aquifer in Zululand

RICHARDS BAY REGION

Prepared for the Water Research Commission by

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EXECUTIVE SUMMARY

1 Preface

The competition for water in southern Africa together with changing demographics and social patterns are placing a huge burden on the water resources of most regions. The conservation and protection of these resources is a national responsibility that is being implemented through legislation covering the general environment and more specifically wetlands. These concerns also extend to the international community through Agenda 21 and ISO 14000 that regulate the exploitation of the environment. The protection of the environment, in particular the water resources, requires effective monitoring methods and programmes in order to implement the legal protection and conservation requirements.

The complexity of the environmental system, the limitations in knowledge about the system and the manner of its protection all require methods to assist in the management and planning of the utilization of these system. This report covers numerical methods used in systems analysis for effective management of groundwater resources.

2 Objectives

This report covers a three year project which aimed to establish **numerical methods** for determining the functioning of primary aquifers and to investigate some of the important processes governing these functions for specific water resources associated with groundwater systems. The largest primary aquifer in Southern Africa, along the Zululand Coast Plain (Figure A), was chosen as the principle location for the study but the results are applicable to many other regions of SA. The specific objectives were:

1. To develop suitable **numerical models of groundwater flow** for primary aquifers with emphasis on the Richards Bay area,
2. To develop a **conceptual model** of the geohydrology of the Richards Bay area for adaptation to numerical modelling of the groundwater.

3 To establish a Geohydrological **data base** for the Zululand Coastal Belt and in particular the Richards Bay area.

4 Combine the numerical models and database to form a decision support system (DSS) for the sustainable management of the regional groundwater resources which are affected by surface recharge through urban development that may have a major impact on the resources.

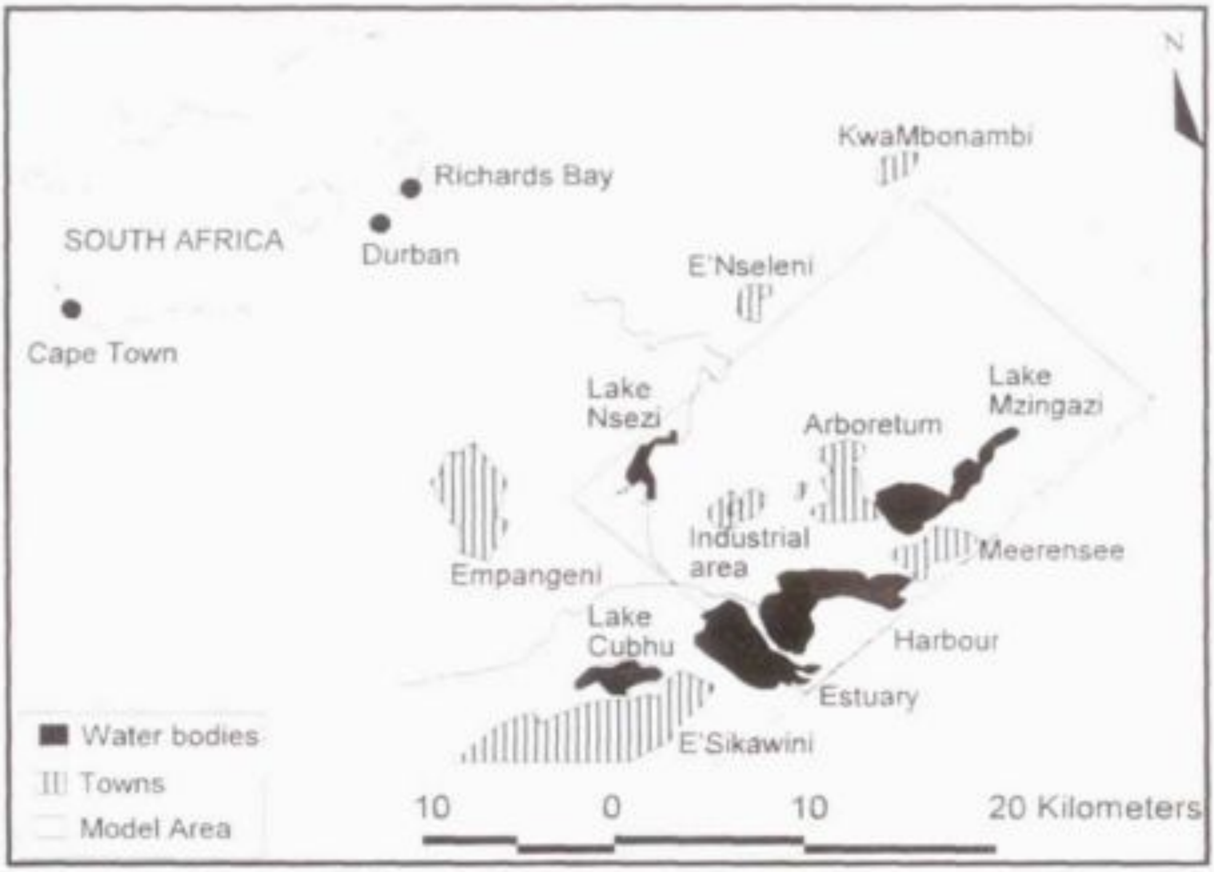

Figure A Location of the study sites.

The emphasis of the research is on the development of tools and methods for implementing numerical simulation solutions in primary aquifers in Southern Africa. The identification of relevant applications to solve particular problems is also considered. The basic approach has been to :

1 examine the regulations governing the utilization of groundwater resources,

2 describe the present knowledge of the water resources under investigation,

3 describe the investigative methods examined in the project and,

4 examine the information requirements for implementing the methods.

A summary of the level of protection offered by national and international legislation is presented as the introduction to the management tools for groundwater monitoring and utilization on a local scale. This includes the basics of the International regulations contained in ISO 14000 that cover the Environmental Management System as well as guidelines for environmental auditing.

Excerpts from the national legislation covering aspects of importance to groundwater exploitations and management are presented in the introductory sections. Sections of Environmental Conservation Act of 1989 and examples from Environmental Impact Assessments (EIA) involving groundwater analysis and management relate to detailed sections of this report. Numerical methods are discussed in detail in this report and several application offered as examples of their use in management and planning that are related to these EIA studies of water resources.

The methods described in the project are a gross simplification of complex environmental systems and consequently, their application and implementation involves considerable simplifications and the implementation of many assumptions about the environment. The application of these methods and the implications of some basic assumptions are examined in several case studies in the Richards Bay region. The basic resources which are examined in the region are described in a specific section that covers the principle resources and the main controlling factors (climate and geology).

2 Principle Environmental Resources

The successful application of numerical methods requires a considerable amount of information to configure the models to represent the environmental system adequately. Consequently, all the available knowledge of a system is required to establish the domain and constraints of the model before it can be used for analytical purposes. The source of this information and some of the methods of transforming it for use in the numerical models is described in the sections which cover the main components of the resources. The primary aquifer is controlled by geological features which are recharged from atmospheric processes and discharged through boundaries associated with many of the water resources of the regions (lakes, rivers and oceans). Consequently, these resources are described for the Richards Bay region as a background to the application of the numerical model which are presented as various case studies in latter sections of the report.

3 Atmospheric controls

The atmospheric conditions control the amount of water available for recharging the primary aquifer through precipitation processes and the evaporative losses from the system. The recharge is driven by rainfall which is affected by interception and runoff. The evaporation is controlled by available energy, atmospheric moisture content (relative humidity) and advection processes. These are all described by the local climate of the region in this section.

4 Water Resources

The main water bodies of the region are perceived to be intrinsically linked to the primary aquifer and respond directly to changes in the greater system. Consequently, knowledge of the main water resources of the region is required for configuring the conceptual and numerical models. Some of the descriptions are based on the results of the numerical methods described in later sections of the report which emanate from specific case studies. The principle water resources described are the coastal lakes which act as sources and sinks for the primary aquifer and are extremely important for regional water supply.

5 Geology

Primary aquifers are located within the unconsolidated geological formations in a region. The knowledge of these formations is based on few geological surveys that were not always designed for hydrogeological investigations. Consequently, there is a need to develop conceptual models of the region for the implementation of the numerical methods. The spatial extent and properties of the geological features are not well known and many assumptions are presented in the descriptions of the various features. The geological features, their inferred development and their spatial extent are described in this section of the report. The estimation of the stratigraphic sequence and the spatial mapping of the important surfaces are presented.

6 Groundwater Flow modelling concepts and modules

There are numerous methods and models which have been developed to investigate geohydrological systems. These are generally described in standard texts and are not described here. However, a description of the different modelling approaches and more specific details of the finite difference approach to groundwater flow modelling is introduced and a summary of the common models is listed for reference. The Modflow model was selected for detailed examination and a brief summary of the theory and parameterization process is presented. Considerable detail is offered for the conceptual modelling of specific processes not incorporated in the finite difference scheme of the numerical model. These include parameterization of the vertical processes involving recharge, evaporation, runoff, stream flow and abstraction. Details are presented of packages developed for use with the main Modflow programmes such as those developed to simulate the fluctuations of lake levels in response to the regional flow dynamics (Table a).

7 Parameterization and Sensitivity Analysis

The Modflow model and the associated packages require the specification of many sets of parameters (Table a). The initial estimation of these parameter values is based on available information of the system. Unfortunately this information is generally limited and in many cases

Table a Parameter set for model application.

Packages	Parameter set	Parameters
Modflow	Hydraulic Parameters	Permeability
		Storativity
	Vertical Fluxes	Evaporation rate
		Extinction depth
		Recharge
Stream Package	Streambed conductance	Permeability
		Thickness
Lake Package	Lakebed conductance	Permeability
		Thickness
	Inflow	Runoff and Abstraction
	Outflow	

nonexistent. Consequently, the estimation procedure must be supplemented by interpolation or extrapolation from other sources. These estimation procedures are mainly literature studies of other investigations in other regions which are often done under different circumstances and through calibrations. A range of values has been derived for most parameters in order to constrain the model parameters within acceptable limits in calibration routines. Consequently, a section on parameter estimation and calibration techniques has been described in this report.

An investigation of the application of **numerical** calibration techniques was conducted using CALIF (Häfner *et al*, 1996) for a study site in the coastal dunes to the north of Richards Bay. This was done because there was suitable information available for the calibration of the model. Since the numerical calibrations require large resources in time and computer hardware, only three objective criteria namely recharge, evapotranspiration and permeability, were used in the calibration procedure. These three criteria were based on the assumption that:

1. all the model layers were homogeneous and the numerical calibration was used to identify the optimum parameter value for each layer within specified limits.
2. heterogeneity existed which was derived by subdividing the layers into several homogeneous zones.
3. all layers are heterogeneous by subdividing each layer into four zones in successive calibration runs.

In all cases the model parameters were constrained within specified limits and were not permitted to reach their numerical limit of optimization. This study indicated that there were limitations to the use of numerical methods of model parameter calibrations. In nearly all cases the subjective calibration techniques usually produced parameter estimates that simulated the observations better than the numerical methods.

8 Case Studies

Numerical models play a large role in many water resources investigations that cover many different situations. This section of the report presents the application of the groundwater model in studies of regional systems and specific local resources. These applications are presented as a series of case studies which cover the role of modelling in groundwater monitoring, water budget estimation and the use of models as research tools for monitoring aquatic systems. The case studies have been conducted in the Richards Bay Area (Figure A) and cover many areas of concern involving the primary aquifer. The investigations chosen as case studies involve regional flow nets, conceptualisation of vertical discretization, coastal lake interactions with the primary aquifer, land use impact on aquifer dynamics, recharge parameterization and what-if scenarios.

Capacity development formed a very large component of this project. Students participated at MSc, BSc, Honours and undergraduate level. Foreign students also participated in collaborative work with local students from the University of Zululand, most of whom came from previously disadvantaged backgrounds. One MSc thesis resulted directly from this project. Postgraduate students participated in a national conference and Mrs Germishuyse delivered a paper at an international conference in Greece as well as two papers at national conferences. She also completed two internet courses in hydrological modelling and a three month scholarship at the Technical University of Freiberg in Germany.

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LIST OF ABBREVIATIONS

AMSL:	Above Mean Sea Level
CCWR:	Computing Centre for Water Research
CMA:	Catchment Management Agency
DSS:	Decision Support System
DWAF:	Department of Water Affairs and Forestry
EIA:	Environmental Impact Assessment
EPE:	Environmental Performance Evaluation
EWR:	Estuary Water Requirements
GIS:	Geographical information System
HRU:	Hydrological Research Unit, University of Zululand
IFR:	Instream Flow Requirements
IOF:	Indian Ocean Fertilizers
ISO:	International Organization for Standardization
ITCZ:	Inter-Tropical Convergence Zone
LWR:	Lake Waterlevel Requirements
MAP:	Mean Annual Precipition
MAR:	Mean Annual Runoff
MW:	Mhlathuze Water
RBCAA:	Richards Bay Clean Air Association
RBM:	Richards Bay Minerals
RDMS:	Relational Database Management System
RDP:	Reconstruction and Development Program
SAWB:	South African Weather Bureau
SDI:	Spatial Development Initiative
SEA:	Strategic Environmental Assessment
TLC:	Transitional Local Council
UZ:	University of Zululand
VTI:	Variable Time Interval

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PART 1

PREFACE
AND
INTRODUCTION

PREFACE

SECTION 1 INTRODUCTION

SECTION 2 SCOPE

PREFACE

Southern Africa lies at the same latitudes as all the major deserts of the world and shares many of the problems of arid countries with limited water supplies. It is a developing region with a rapidly increasing demand for water from all sectors of society. Huge international efforts, like the Lesotho Highlands Project, are well advanced to provide water for the industrial needs of South Africa. National programmes have been established to provide the basic needs of society. Many large dams have been developed for agricultural irrigation schemes. There is an afforestation permit system to conserve water. There are frequent water supply restrictions in all the major cities. These and other demands on a limited resource requires careful management and planning for long-term sustainability and development of the resource.

International requirements and national legislation of environmental resources generally address the control and regulation of limited environmental resources such as water. However, the implementation of these controls on the utilization of environmental resources involves suitable methods of monitoring and assessment. Consequently, the effective management and planning of environmental resources requires an understanding of the regulations and controls together with the implementation of adequate methods of monitoring to evaluate and assess the sustainable utilization and development of the resource. A brief summary of recent legislation and regulations are presented as a prelude to the description of methods for assisting in the monitoring and assessment of the water resources of a primary aquifer.

Management and planning of the utilization of environmental resources involves financial resources which are often lacking for effective monitoring and assessment. Consequently, the development and implementation of affordable methods are required to assist in the management of the resources. While it should be realized that the measurements and observations of a system are fundamental to assessment, the use of alternative methods to supplement them can reduce cost and enhance the knowledge of the resource. Numerical methods for interpolating and extrapolating observational measurements play an important role in enhancing the monitoring and assessment of limited water resources. These numerical methods have a large role to play in understanding the processes and interactions of the system and in assisting in the development of an effective observation monitoring programme.

The Zululand region of South Africa has the largest primary aquifer in the country and it supports a large population density. It has one of the fastest growing industrial centres in the country and has a thriving agricultural sector. All these sectors have a demand on the limited water resources and they all impact on the water quality. Consequently, there is a need to understand the hydrological system of the region and to develop methods to assist in the management of this resource.

Numerical groundwater models have played a major role in understanding the functioning of large primary aquifers in many countries (Townley *et al*, 1993). They were also used in studies of regional and local features within the Zululand primary aquifer. This project was initiated to investigate the use of the most reputable and appropriate numerical groundwater models for application in geohydrological studies of primary aquifers in southern Africa. The specific aim was to improve our knowledge of the system and develop methods for assessing the impact of developments on the aquifers in the region. The region chosen was considered to be representative of primary aquifers that are found in most of the coastal regions of southern Africa in order to facilitate technology transfer to the mutual benefit of all.

Section 1 INTRODUCTION

Water is essential for life on earth and is so important that it has been the cause of conflict in many arid regions of the world. South Africa is an arid country where the present water resources are expected to be depleted within the next few decades. These resources have been exploited over the past decades for select sectors of our society. However, there is now a strong emphasis on the equitable distribution of water for the entire population of South Africa without impinging on the environmental reserve which is required to sustain the resource for future generations. These developments are all embodied in the National Water Act promulgated in 1998.

The bulk of water exploitation in South Africa has concentrated on the surface water resources. The Lesotho Highlands Scheme to provide water to Gauteng from other regions of Southern Africa, is one of the largest water supply schemes in the world. The Tugela Transfer Scheme that takes precious water from KwaZulu-Natal to supplement the Gauteng region places a severe strain on the water resources of KwaZulu-Natal. The groundwater resources of KwaZulu-Natal are not utilized to the same extent as the surface water resources. However, groundwater provides the bulk of the water used by rural communities. During droughts groundwater is often the sole exploitable and reliable resource available for the survival of man and the environment (Bredenkamp *et al* 1995).

All water is contained within the Hydrological Cycle and is resident in the different storage compartments for varying lengths of time. The terrestrial branch of the cycle involves water which arrives through precipitation and returns to the oceans along various pathways that always involve BOTH the surface water and groundwater components except in extreme circumstances when it runs off in vast quantities through abnormal flood events. Consequently, it is difficult to distinguish exactly the interface between surface water and ground water. The National Water Act of 1998 recognizes that the water resources are intrinsically linked between the surface and subsurface components. Unfortunately, the water resources of the country have been conceptualized and categorically divided into surface and ground water systems and treated as totally separate entities which are divorced from each other (Water Act of 1956). However, there are many instances where the water table is exposed at the topographical surface and the distinction between the two water categories becomes difficult to qualify. These exposed groundwater components called "wetlands" are of immense ecological and social importance and require careful examination for their potential for exploitation and sustainability as a water resource.

Recent and proposed legislation in South Africa requires a greater understanding of the water resources and the processes that sustain them hydrologically and ecologically. This report examines a primary water resource in the coastal region of South Africa and some of the numerical methods that have been developed to examine and manage the hydrological component of the system.

1.1 ENVIRONMENTAL LEGISLATION

South Africa is a developing country with huge social problems that are the result of gross inequalities in basic living conditions. The Reconstruction and Development Progam (RDP) has been established to correct these imbalances in our society. South Africa is also dependant on international trade to maintain and develop its economy and must therefore also conform to the recognized standards set by international agreement. Consequently, South African resources development and exploitation are regulated by both national and international legislation and regulations. For the management of the natural resources to conform to national and international requirements, there is an urgent need to develop tools and methods to qualify and quantify the impacts of development on the country's environmental resources. The principle legislation which has direct impact on the utilization of the resources is summarized in this section.

1.1.1 INTERNATIONAL REQUIREMENTS

In its development, South Africa needs to create an equitable distribution of scarce water resources while maintaining economic development. To sustain economic development, South Africa must promote international trade. This development must adhere to recognized international standards which promote fair trade practices amongst competing industries and countries. Since all developments impact on the environment to varying degrees, international organizations have been set up to manage and control these developments and their impacts.

The need to protect the environment is recognized in nearly all countries. The International Organization for Standardization (ISO) is a worldwide federation of over 110 countries conforming to nearly 10000 voluntary consensus-based International Standards covering nearly every field of industrial, economic, scientific and technological activity. It is becoming more and more important for companies who trade internationally and are signatories to ISO, to become certified to globally acceptable environmental standard which are being set in ISO 14000.

ISO 14000 Environmental Performance Evaluation (EPE) is a process to measure, analyse, assess and describe an organization's environmental performance against agreed criteria for appropriate management purposes. Conformity to ISO 14000 promotes consistent and satisfactory adherence by an organization of its environmental obligations. The object is to encourage such programs to use certain procedures and principles to ensure due process, fairness to all stakeholders, and avoidance of trade barriers. The various national laws that serve to protect the environment are not the same for every country. ISO 14001 requires that organizations have knowledge of these laws, commit to comply, and establish process that bring and maintain such compliance.

1.1.2 NATIONAL LEGISLATION

The political and social changes in South Africa have provided the opportunity to make substantial changes in the management of the country. There has been a proliferation of legislative initiatives during the past decade that have been discussed in Green Papers and have now been proposed for promulgation as legislation in various White Papers. Several new laws have been passed and some of the White Papers on Government Policy are in the process of being promulgated.

Four important regulations governing the sustainable use of the water resources of South Africa are the Constitution, the National Water Act (1998), the Water Act of 1956, the Water Services Act (1997) and the Environmental Conservation Act (1989).

South Africa, as a signatory to the ISO convention, recognizes the importance of a healthy environment for sustaining life. The Constitution provides for the right to have the environment protected for the benefit of present and future generations as well as the right to sufficient water for basic domestic needs. In particular, the Constitution guarantees everyone the right to -

- an environment not harmful to health or well-being
- have the environment protected for the benefit of present and future generations
- access to sufficient water.

1.1.3 WATER SERVICES ACT (1997)

The Water Services Act (1997) provides for the right of access to basic water supply and sanitation. The Minister may set national standards for the quality of water taken from or discharged into any system, the requirements for persons who install and operate waste water services works.

The Act establish Water Boards to provide water services to other service institutions within a defined area. Mhlathuze Water is the designated water board in the Zululand region covered by this study. The executive authority of Water Boards vests exclusively with the Minister of the Department of Water Affairs and Forestry (DWAF).

Access to water for industrial use is regulated through the water services authority having jurisdiction in the industrial area. Industrial effluent must be disposed of in a manner approved by the water services authority and water services authorities must monitor the performance of water services providers and water services intermediaries within their jurisdiction to ensure compliance with the Act.

1.1.4 NATIONAL WATER ACT (1998)

The National Water Act (Act no 36 of 1998) recognises the "Fundamental Principles and Objectives for a new Water Law in SA"

These fundamental principles cover constitutional rights, ownership, management, access and basic rights. The management of water resources is aimed at achieving long term environmentally sustainable social and economic benefits for society (principle 7). The quantity, quality and reliability of water needed to maintain the ecological functions on which humans depend shall be preserved in order to manage the human use of water so that it does not compromise the long term sustainability of aquatic and associated ecosystems (Principle 9). Principle 10 defines the "Water Reserve" which shall enjoy priority of use by right. The use of water for all other purposes shall be subject to authorisation. The water quality and quantity are interdependent and shall be managed in a integrated manner which is consistent with broader environmental management approaches (Principle 15) while development must broadly conform to environmental management. ***In order to plan and manage these resources it is necessary to develop an understanding of the resources and to develop tools for analysing their resilience to change resulting from anthropogenic impacts.*** Since many land uses have a significant impact upon the water cycle, the regulation of land use shall, where appropriate, be used as an instrument to manage water resources within the broader integrated framework of land use management (Principle 21).

1.1.5 ENVIRONMENTAL CONSERVATION LEGISLATION

The Environment Conservation Act (Act No 73 of 1989) makes provision for the Minster of Environmental Affairs and Tourism to identify activities which will probably have a detrimental effect on the environment (section 21 of the act). This act prohibits a person from undertaking an activity which has been identified as having an impact. This involves undertaking Environmental Impact Assessments (EIA) or Strategic Environmental Assessments (SEA) prior to any developments in South Africa. Both EIA and SEA procedures require a detailed understanding of environmental processes operating and the interactions between systems. Most of the major developments in the coastal region requiring an EIA recognize the need for a detailed hydrological assessment. Proposed developments in the St Lucia area raised international concern which had a significant bearing on the outcome of the Assessment process.

The use of numerical methods had played a big role in these EIA processes. The need for improved numerical methods was one of the prime motivations behind the proposal for this project.

1.2 ASSESSMENT MECHANISMS

The implementation and control of the water resources of South Africa demanded by the legislation (Act 36 of 1998) requires suitable methods for investigating and monitoring the resources. Monitoring the impact of development is generally expensive and reactive. If the development is found to be detrimental to the environment it is extremely difficult to implement corrective action because it is generally very expensive and disruptive of society and consequently it is usually not implemented. Appropriate methods, that are proactive and cheaper, are required for management of the resource. Modelling techniques, where appropriate and effective are generally much cheaper to apply and they provide greater scope for the assessment of proposed developments. This project examines the use of numerical methods for describing the water resources of a region and for assessment of impacts on the resources by various developments. The application of modelling methods for designing expensive monitoring programmes is also presented in the report.

1.3 DEFINITIONS

The definitions in geohydrology and groundwater varies between the authors of most classical text books. In most cases the authors of text books specify the scope of the subject rather than the definitions. The numerical models presented in this study require conceptualization of processes, such as the recharge and evaporative losses from an aquifer, therefore some of the definitions for this project may differ from the more common definitions. These are indicated as project definitions.

Aquifer

Project definition: underground formation into which water flows and from which it can be withdrawn.

Bowen (1986) A permeable deposit which can yield useful quantities of water when tapped by a well.

Parsons (1995) Strata or a group of interconnected strata comprising of saturated earth material capable of conducting groundwater and of yielding usable quantities of groundwater to boreholes and /or springs. A supply rate of 0.1 ℓ/s was considered to be a usable quantity. It is implied that the quality of the water should be fit-for-use by the end user.

Todd (1980) A formation that contains sufficient saturated permeable material to yield significant quantities of water to wells and springs.

Base flow

Hatton *et al* (1998) Base flow is a purely conceptual quantity resulting from statistical or graphical methods of breaking up a stream hydrograph into components of quick and slow responses to rainfall. These are not directly equivalent to the amount of surface and subsurface (groundwater discharge) flow. Base flow is made up of several components, such as groundwater discharge, bank storage and lateral unsaturated flow. However, base flow is generally considered to arise to some significant degree from groundwater discharge to streams.

Todd (1980) Streamflow originating from groundwater discharge is referred to as groundwater runoff or base flow. During periods of precipitation streamflow is derived primarily from surface runoff, whereas during extended dry periods all streamflow may be contributed by base flow. Typically, base flow is not subject to wide fluctuation and is indicative of aquifer characteristics within a basin.

Capillary Zone

Bowen (1986) The belt of ground immediately above the water table, i.e. at the bottom of the zone of aeration and containing capillary water.

Todd (1980) The capillary zone (or capillary fringe) extends from the water table up to the limit of capillary rise of water.

Catchment

Project definition: The entire land area from which water flows into a system. The catchment boundaries for surface water processes are the topographical divides, while the catchment boundaries for groundwater processes are water table ridges.

Evaporation

Project definition: Loss to vapour from several locations, namely:

1) surface storage - loss from surface process including interception, ponding and runoff

2) soil moisture - loss from unsaturated zone

3) groundwater - the evapotranspiration from the capillary (and saturated) zone in contact with the water table.

Carageeg et al (1987) Evaporation occurs when water is converted from the liquid to the vapour phase and returned to the atmosphere. It occurs from open water surfaces, such as water intercepted by vegetation, ponded in depressions, flowing as surface runoff, or stored in wetlands or lakes. It also removes water directly from the soil. Its rate depends on atmospheric conditions (solar radiation, wind speed, temperature and humidity) and on conditions within the body of water (temperature).

Evapotranspiration

Carageeg et al (1987) Evapotranspiration is a collective term used to describe the combination of evaporation and transpiration, both of which depend on atmospheric conditions and on the availability of water.

Extinction depth

Project definition: Maximum depth to water table where evaporation ceases and equivalent to maximum rooting depth of vegetation.

Groundwater

Bowen (1986) Water in the zone of saturation.

Parsons (1995) All subsurface water occupying voids within a geological stratum.

Driscoll (1986) Underground water that can be removed by wells. All other water in the ground is termed subsurface water and is not available for man's use directly.

Fetter (1994) Water stored in the zone of saturation.

Todd (1980) Water occupying all the voids within a geologic stratum. This saturated zone is to be distinguished from an unsaturated, or aeration, zone where voids are filled with water and air.

Interception

Carageeg et al (1987) Interception occurs when roads, roofs or vegetation canopies catch rainfall and prevent its passage to the earth's surface. Intercepted water is usually returned directly to the atmosphere by evaporation. The amount of interception depends on vegetation type, canopy cover and rainfall characteristics.

Leakage

Anderson & Woessner (1991) Leakage refers to the movement of water through a layer of material that has a vertical hydraulic conductivity lower than that of the aquifer.

Rushton and Tomlinson (1979) Total leakage = base flow

Carageeg et al (1987) Leakage is the vertical flow of water from one aquifer to another. Its rate depends on resistance ot flow in the aquitard separating the two aquifers and on the difference between piezometric heads in the two aquifers.

Leakance

Cherkauer & Nader (1989) Leakance = hydraulic conductivity / sediment thickness

Rushton and Tomlinson (1979) Leakance: The flow rate between the aquifer and river is a direct function of permeability and head difference (Walton, 1970). Total leakage = base flow

Recharge

Project definition: The actual amount of water entering the saturated zone. This includes all water that returns to the surface or is lost to advection.

Bowen (1986) The difference between precipitation and runoff plus other losses, i.e. that part of precipitation which resides as groundwater, surface storage and soil moisture.

Rushton and Ward (1979) Groundwater recharge is that amount of surface water which reaches the permanent water table either by direct contact in the riparian zone or by downward percolation through the overlying zone of aeration. It is this quantity which may in the long term be available for abstraction and which is therefore of prime importance in the assessment of any groundwater resource.

Besbes & De Marsily (1984) Recharge is defined as the flux arriving at the water table, i.e. after percolation through the whole unsaturated zone. In this definition we assume that the transfer of the "effective rainfall" through the unsaturated zone is conservative. Average infiltration and average recharge are thus identical over a long period ... Implicit in this definition is the assumption that there is no upward migration from the water table to the soil surface.... This assumption is probably valid in temperate or dry climates, where the water table is deep and the delay between infiltration and recharge therefore significant.

Anderson & Woessner (1991) The volume of infiltrated water that crosses the water table and becomes part of the groundwater flow system. (Discharge refers to groundwater that moves upwards across the water table and discharges directly to the surface or unsaturated zone)

Dinçer (1982) ... it is necessary to study processes other than infiltration of the precipitation. A recharge possibility through wadi beds which absorb large quantities of flood waters must also be considered (Dinçer, 1980)

Runoff

Bowen (1986) That part of precipitation flowing from a catchment area and finding its way into streams, lakes, etc. Includes direct runoff and groundwater runoff. Total runoff includes both surface runoff and shallow percolation.

Carageeg et al (1987) Surface runoff occurs when water is unable to infiltrate and when the ground surface is sloping. Its rate depends on surface slope and roughness, soil moisture content at the surface, as well as on the rates at which additional water is supplied by rainfall and extracted by infiltration or evaporation.

Seepage

Todd (1980) Seepage areas indicate a slower movement of groundwater to the ground surface. Seepage is a general term describing the movement of water through the ground or other porous media to the ground surface or surface water bodies.

Townley et al (1993) ...the distribution of lake sediments plays a dominant role in controlling seepage through the lakebed...

Transpiration

Bowen (1986) The emission of water vapour by living plants into the atmosphere, almost always in daylight.

Roberts (1983) The transpiration component of evaporation is influenced by many ... factors; climate, forest age, species, structure and soil moisture conditions may well, a priori, produce large variations in forest transpiration. There is now accumulating evidence that soil moisture levels rarely limit transpiration in field-grown trees.

Balek et al (1983) The availability of water in the saturated zone increased significantly the amount of water transpired during the dry periods and after, while the transpiration of the plant of the soil profile without a saturated zone was much lower.

Carageeg et al (1987) Transpiration is the process by which plants take up water from the soil and return it to the atmosphere. Its rate depends on vegetation characteristics (species, root depth and density etc), atmospheric conditions and conditions within the soil (especially the distribution of soil moisture near the roots). Some plants, which are known as phreatophytes, have deep roots which intersect the water table and are capable of withdrawing directly from the saturated zone; the transpiration rates of phreophytes still depend on atmospheric conditions and conditions within the soil profile.

Water resource

Project definition: The water in the natural environment from which we draw the water required to meet human needs.

Zone of Aeration

Bowen (1986) Subsurface between the surface and the water table divisible into a belt of soil water, and intermediate region and a lowermost capillary fringe.

Zone of Saturation

Bowen (1986) The mass of water-bearing ground below the main water table comprising solid rocks and incoherent materials.

1.4 REGIONAL APPROACH

The largest primary aquifer in southern Africa is the extensive coastal plain stretching from Mtunzini on the Zululand coast up through Maputaland for the full length of the Mozambique coastal zone. This region is very flat with highly permeable soils that promotes a rapid recharge to the aquifer. The uppermost formation on this coastal plain is an unconfined aquifer which has as its upper boundary a "water table" that is the top of the saturated zone.

The region has many estuaries and coastal lakes which form part of tidal systems. Over the years many of these estuaries have been blocked off from the sea to form inland fresh water lakes (Sibaya, Bangazi, Cubhu and others).

This coastal plain supports large urban and industrial developments, extensive farming enterprises, mining and forestry industries and is fast becoming one of the prime tourist destinations in the subcontinent. The Maputaland SDI is proposing many developments along the coast from Richards Bay to Maputo which will have a huge impact on the water resources of the region. While this region has considerable national importance, the investigations conducted in this project can also be transferred to the other primary aquifers in Southern Africa. However, this project will focus primarily on the Richards Bay Area (Figure 1) where there are large industrial developments in very close proximity to the local water resources. Several problem areas have been identified in the region which need to be investigated. The use of numerical simulation models have been used in other studies to investigate some similar problems in the Zululand region. The application of similar methods using suitable models (tools) could be used to investigate some of the problem areas which have been identified in the Richards Bay area. These include:-

1) Saltwater intrusion into Lake Mzingazi (Rawlins, Kelbe and Germishuyse, 1996).
2) Industrial waste disposal site in Alton.
3) Mine waste disposal sites (Germishuyse, 1997b, Germishuyse and Kelbe, 1997).
4) Groundwater contamination from Industrial developments in Richards Bay.

5) Pollution monitoring from informal settlements on the shores of Lake Mzingazi.

6) Urban pollution in shallow coastal aquifer.

7) Lake Water Level Requirements for Mhlathuze. (Kelbe and Germishuyse, 2000).

8) Streamflow prediction for stream segments in flat groundwater dominating systems. (Kelbe and Germishuyse, 1999)

1.5 MODELLING APPROACH

To manage the resources of a region and determine the effects of development on these resources, the local and regional authorities, managers, planners, consultants and researchers all require suitable methods and tools. These tools must provide a synthesis of the system in an integrated manner and a means to check hypotheses on changes to the system. One of the most pragmatic and cost effective methods is the use of models. However, there are as many models of a system as there are people who are interested and involved in the system. These models, in a suitable form with relevant complexity, are the most appropriate methods of evaluating change and understanding the complexity of an interactive system without undue expense and time.

The numerical models investigated and chosen for application in this study are based on the finite difference approximation principle. They require an understanding of the structures and hydraulic properties of the aquifers, definition of boundary conditions and specification of the surface-groundwater interaction. Some of the boundary conditions, most notably lakes and rivers and the surface-groundwater interaction, require additional conceptual and numerical models for detailed applications.

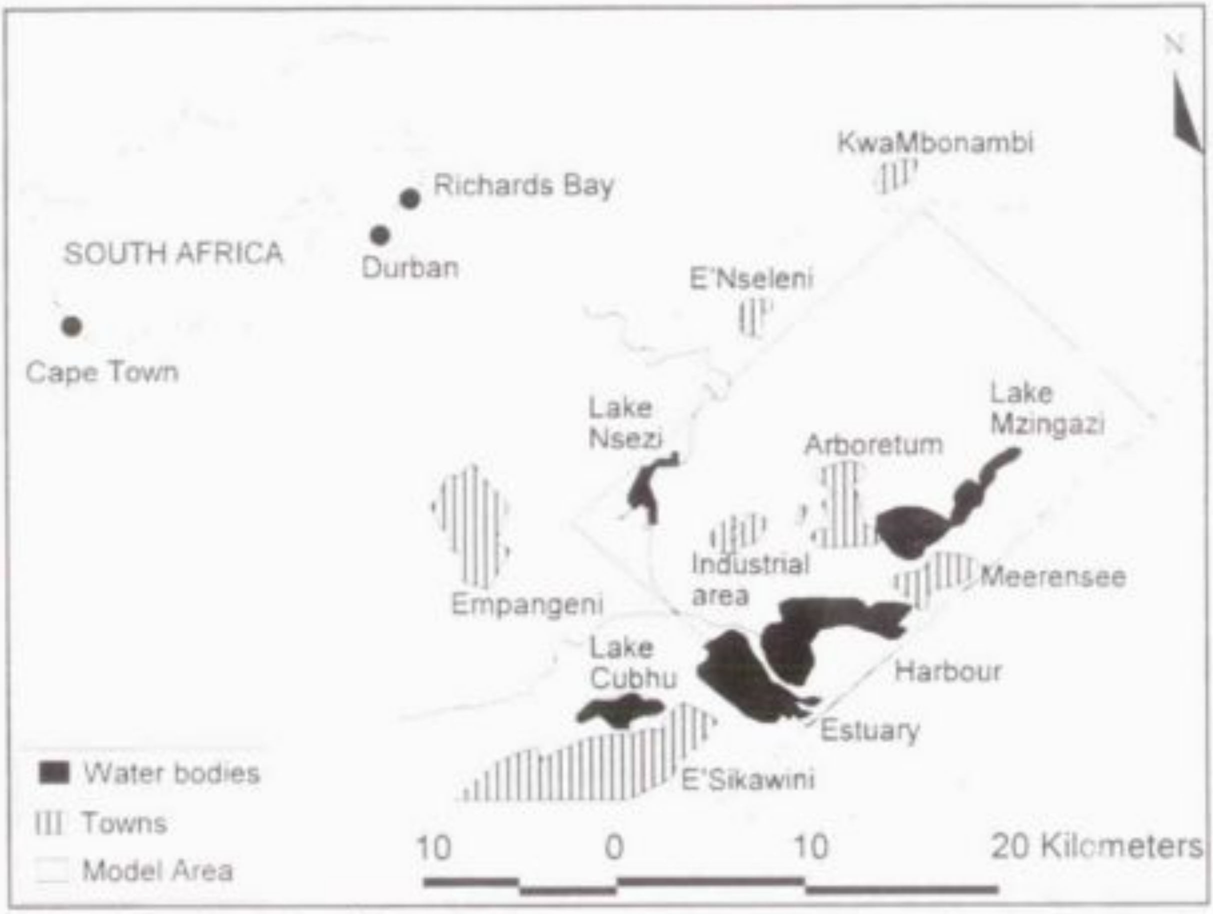

Figure 1 Location of the study area.

Section 2 SCOPE

The principal aim of the research project was to establish numerical methods for assessing the flow dynamics and solute transport processes of the geohydrological systems of the primary coastal aquifers along the Zululand Coast. The initial interest has focussed on the Richards Bay Area because of its national importance and rapid growth rate in a region with a high population density that is placing great demands on the environmental resources of the region.

2.1 OBJECTIVES

To investigate the application of suitable **numerical models of the groundwater flow** for the Richards Bay area to determine the hydraulics of the local aquifers

To investigate the use of a suitable **solute transport model** for the Richards Bay area to determine the dynamics of the primary aquifer for pollution monitoring and control.

To establish a Geohydrological **data base** for the Zululand Coastal Belt and in particular the Richards Bay area.

To develop a **conceptual model of the geology** of the Richards Bay area for adaptation to numerical modelling of the geohydrology.

Combine the numerical models and database to form a **Decision Support System (DSS)** for the sustainable management of the regional groundwater resources which are affected by surface recharge through urban development that may have a major impact on the resources.

2.2 METHODOLOGIES

The development of the hydrological data base and the Decision Support System (Kelbe, Snyman and Germishuyse, 2001) are also part of an ongoing project for the entire catchment area of the Mhlathuze River flowing into the Richards Bay Estuary. The data specific to this project and its structure for inclusion into a Decision Support System will be described as they play an important role in the application of numerical methods for water resources studies. However, this report mainly covers the numerical methods used and case studies of their application in the Richards Bay Area.

Numerical models for describing the flow dynamics of the groundwater are many and varied. Several models have been evaluated and these are described in the relevant section on modelling. Modflow and MT3D were chosen for applications in this study and their concepts are described in subsequent sections. The derivation and evaluation of methods for problem solving of specific conditions using numerical models is presented as a series of case studies. These case studies range in scale of application from regional flow dynamics to small detailed studies of waste sites. The Mhlathuze River is under investigation as part of an Instream Flow Requirement (IFR) study to determine the "Environmental Reserve" for the river. The lake and estuary water requirements (LWR and EWR) are also being examined for the same purpose. The numerical methods presented here have been used in the LWR and some of the results have been presented as case studies in this report and have been published by Kelbe and Germishuyse (2000).

The numerical methods have been used in this study to demarcate groundwater flow dynamics and the recharge and discharge zones for various types of investigations that are presented as case studies in this report.

2.3 DESCRIPTION OF THE STUDY AREA

KwaZulu-Natal, and particularly Zululand, is one of the fastest growing regions in South Africa. The harbour at Richards Bay was started in the early nineteen seventies and is now the largest bulk handling facility in Africa. The continued development at Richards Bay is crucial to the economic development of KwaZulu-Natal and South Africa. However, all developments have an impact on the environment and it is necessary to understand, monitor and manage the environment in order to minimize the negative impacts and enhance positive impacts of the existing and proposed developments. Several large industries have been developed or proposed for Richards Bay in the last 5-10 years. The aluminium processing capacity has expanded and the production of heavy minerals is expected to increase with the commissioning of new smelter facilities in the region. Changing legislation and the introduction of International Standards will require new standards and guidelines for acceptable limits of impact by industry on the environment. Consequently, there is a need for improved tools for evaluating and monitoring the impact on the environment of all present and proposed developments.

The high rate of development around the deep water harbour of Richards Bay is causing a serious threat to the environment. The major industries in the region have invested over R2 million to initiate the development of the Richards Bay Clean Air Association (RBCAA). This association has launched an atmospheric monitoring programme to determine the levels of pollution in the region and implement remedial actions when necessary. While the atmospheric pollution is causing serious concern, the impact of all developments in the Richards Bay area on the water environment is also becoming increasingly evident. The Department of Water Affairs and Forestry (DWAF) have found it necessary to close certain facilities because of pollution to the surface and groundwater. Mining concessions are required by law to implement an Environmental Audit and monitoring programme during operations and after closure. However, no other industry is required to undertake an environmental audit and provided they do not contravene effluent discharge regulation/legislation there is little control of their impact on the regional water resources.

2.4 DATA SOURCING AND CAPTURE

An understanding and management of the environment is critically dependent on information of the system which is derived and synthesised from field data and related studies. Consequently, considerable effort has been made to source, capture and assimilate all relevant geohydrological data in the region. Much of this data has been captured and configured in digital format for presentation in a Spatial Information system that is being developed along the lines of a Decision Support System (DSS). This DSS is being developed around an extensive Relational Database Management System (RDBMS) where possible which is accessible through spatial analysts programmes generally referred to as Geographic Information System (GIS).

Several database engines are commonly available and it has been extremely difficult to standardize the DSS on any one structure. ASCII, spreadsheet and RDBMS (.dbf) structured systems have been retained and others are being evaluated for use in a related project.

The data that has been identified, is derived from a very diverse source that is maintained on different platforms. The data are often confidential and derived at great cost. Consequently it is not always easily acquired. However, nearly all the large organizations in the region have released their geological data and some of their water quality data for inclusion in the database.

PART 2

GENERAL DESCRIPTION of the CLIMATE, WATER RESOURCES and GEOLOGY

SECTION 3	REGIONAL CLIMATE
SECTION 4	WATER RESOURCES AND WATER USE
SECTION 5	COASTAL GEOLOGY

Section 3 REGIONAL CLIMATE

The KwaZulu-Natal region covered in this project is located in one of the highest rainfall regions of South Africa (Schulze *et al*, 1996). This makes it a region with important water resources and a large diversity of ecosystems which are required to sustain a large proportion of the South African population. This summary of the climatic conditions for the region is presented as a background to quantifying the concepts and parameters of the modelling studies presented in subsequent parts of the report. Consequently it only covers these features of importance in hydrological studies.

3.1 GENERAL DESCRIPTION OF THE CLIMATE

The surface and groundwater regime in the Zululand coastal region is a direct response to local climatic conditions. Rainfall recharges the system while evaporation causes depletion of surface and subsurface moisture. The type of rainfall and its frequency of occurrence has a strong influence on the hydrological processes that determine the surface runoff rate and the groundwater recharge rate. Consequently it is important to understand the local weather conditions for hydrological studies.

3.1.1 WEATHER SYSTEMS AND CLIMATE

According to Money (1988), because of its location, Zululand has a unique "humid and wet" climate in comparison to other African regions (Figure 2). The rainfall over this region of South Africa is derived from both tropical and middle latitude weather systems. Tropical control is manifested in easterly waves which advect warm moist air from the Indian Ocean in association with equatorial troughs and the Inter-Tropical Convergence Zone (ITCZ). Low-level convergence in the presence of unstable atmosphere produces frequent cumulus convective rainfall during the summer months. However, extreme rainfall does occur when tropical cyclones occasionally move from the Indian Ocean over the area in their migrations toward the subtropics.

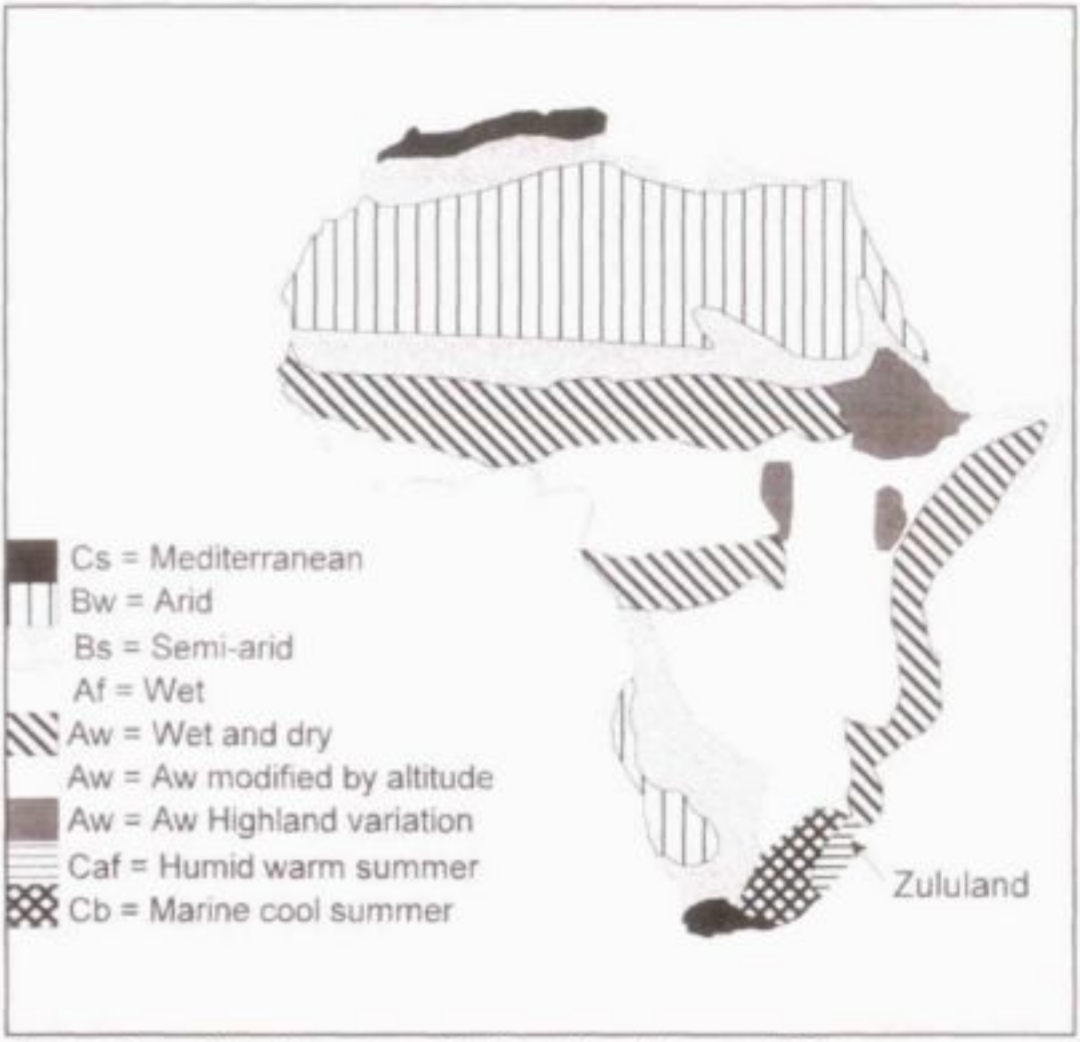

Figure 2 Climatic regions of Africa (from Money, 1988)

Westerly waves originating in the temperate middle latitudes, particularly if they are linked to tropical depressions over the subcontinent, produce widespread frontal precipitation along the entire east coast which is often preceded by thunderstorms that produce heavy localised rainfall. In conjunction with synoptic scale instability, these systems have produced extensive flooding in the region. All these extreme rainfall conditions have occurred along the east coast during the past two decades.

3.1.1.1 TROPICAL CYCLONES

Extreme rainfall has occurred on several occasions in the Zululand region from tropical cyclones which occasionally move close enough to the coast to produce extensive flooding with loss of life and property.

The occurrence, frequency and magnitude of these systems has been described in detail by Kovacs, du Plessis, Bracher, Dunn and Mallony (1985). The frequency of occurrence of tropical cyclones since 1927 is shown in Figure 3. Since 1950 there have been eight years when

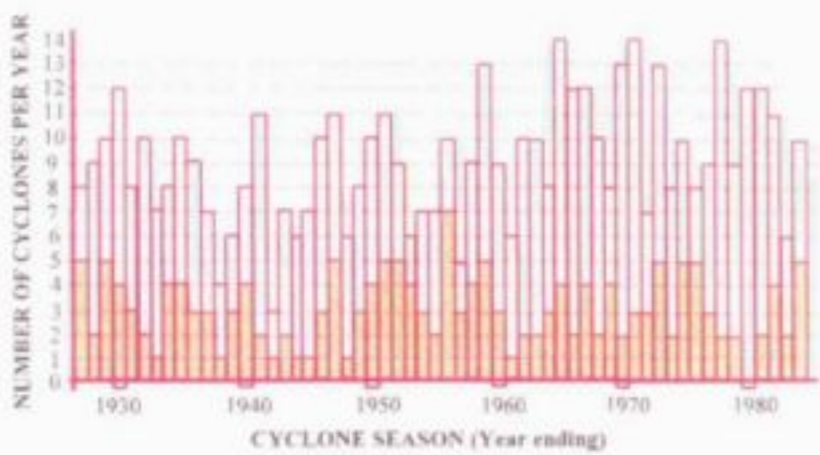

Figure 3 Annual frequency of tropical cyclones in the Indian Ocean (after Kovacs *et al* 1985). Shaded portion represents those cyclones moving West of Madagascar.

tropical cyclones have produced significant rainfall over the eastern seaboard but these constitute less than 5% of the number of tropical cyclones that have been recorded in the south-western Indian Ocean during this period. Two recent tropical cyclones (Domoina and Imboa) which struck the coast of KwaZulu-Natal within one month of each other in January and February, 1984, produced widespread rainfall. Extensive areas of Zululand (Figure 4) experienced >700mm of rainfall over a five day period (Jan 28 to Feb 2, 1984) which resulted in widespread destruction and loss of life.

3.1.1.2 MID-LATITUDE SYSTEMS

Extremely heavy rainfall can also be experienced as a consequence of temperate latitude systems advecting moist air from the Indian Ocean over the Zululand coast while under the influence of a cold upper air circulation (cut off low). Such a system, which produced

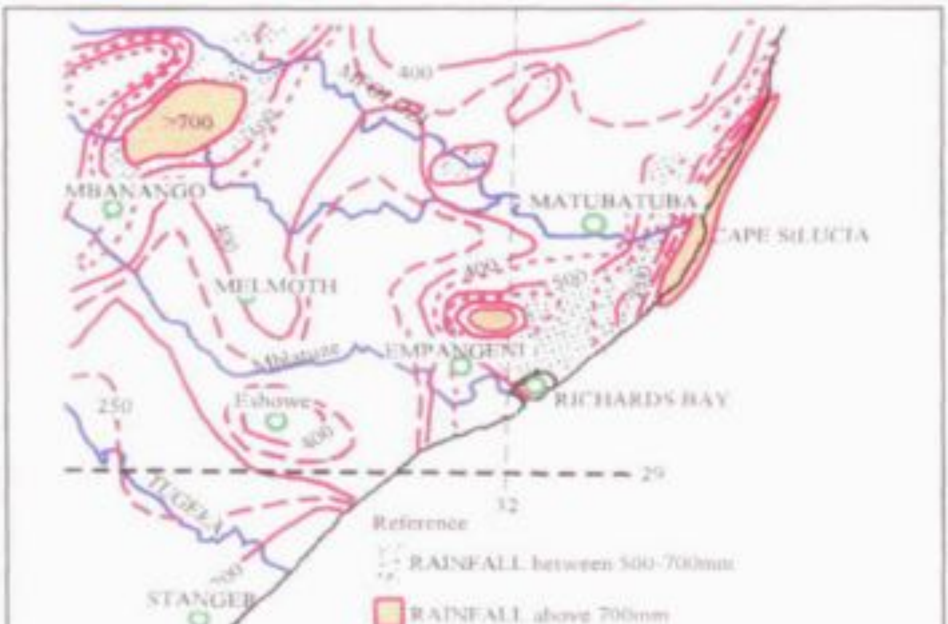

Figure 4 Spatial distribution of Rainfall for Domoina (after Kovacs *et al*, 1985).

substantial flooding along the KwaZulu-Natal coast during September 1987, has been described in detail by van Bladeren and Burger (1989). While the tropical cyclones originate to the north and therefore generally affect the more northern areas of KwaZulu-Natal, these temperate systems, propagating from the south, tend to affect the more southern areas of the region. However, both systems have produce extensive precipitation that is close to the maximum recorded pentad rainfall (world envelope in Figure 5).

The predominant mid-latitude synoptic system that produce significant rainfall in the Zululand region is associated with coastal Lows and frontal systems migrating round the southern coast of Africa ahead of an anticyclonic system. The dynamic mechanism associated with these systems and differences in the intensity of precipitation has been described by Kelbe (1987) and Garstang, Kelbe, Emmitt and London (1985) for the KwaZulu-Natal region.

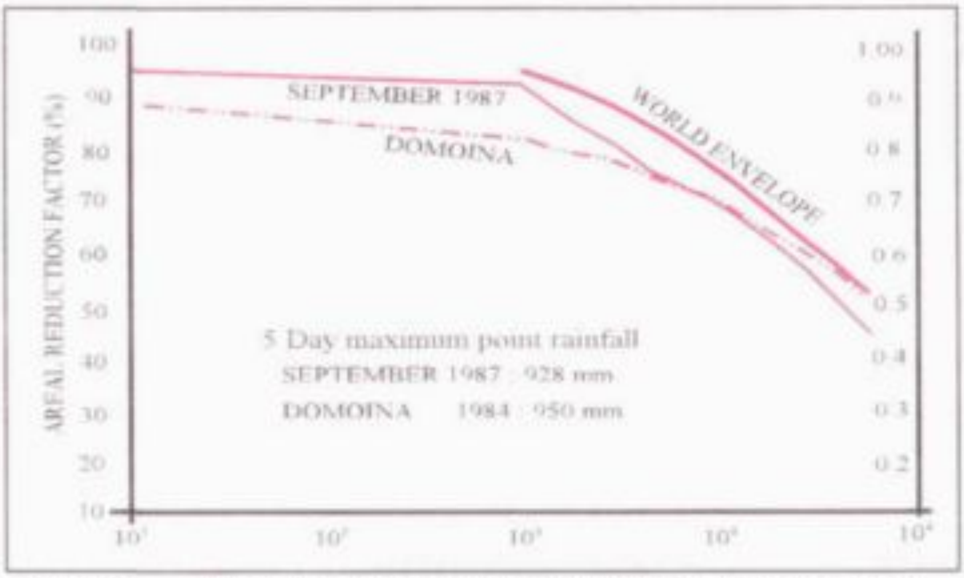

Figure 5 Extreme rainfall in KwaZulu-Natal relative to world maximum (after van Bladeren and Burger, 1989)

3.2 RICHARDS BAY CLIMATE

Climate has a strong influence on water resources of a region. Rainfall is the main form of recharge to the water resources and evaporation is a principle sink. Energy, usually in the form of radiation, affects the temperature of the land surface and the atmosphere that controls the rate of evaporation. The temperature and humidity of the air determine the moisture holding capacity of the atmosphere. Wind speed is an indicator of the advective properties of the atmosphere. Since rainfall and evaporation are very important components in the determination of the water resources of a region, the factors that have an influence on their variability and which play a role in estimating the appropriate parameters in the numerical modelling studies are examined in this section for the Richards Bay region.

There are several weather stations in the Richards Bay region which have records for various meteorological observations (Figure 6).

The Department of Hydrology at the University of Zululand had an automatic weather station which recorded all standard meteorological factors from 1988 to 1996 at hourly intervals. There were three automatic weather stations installed by RBM at Lake Nhlabane, RBM smelter and the Richards Bay Airport. The Lake Nhlabane station is still operational, the smelter and airport stations have been replaced by stations from the "Clean Air Association" monitoring network. There are rainfall stations at several sites which are monitored on a daily basis for the SA Weather Bureau (SAWB). The information from the "Clean Air Association" network is not available and has not been included in this project.

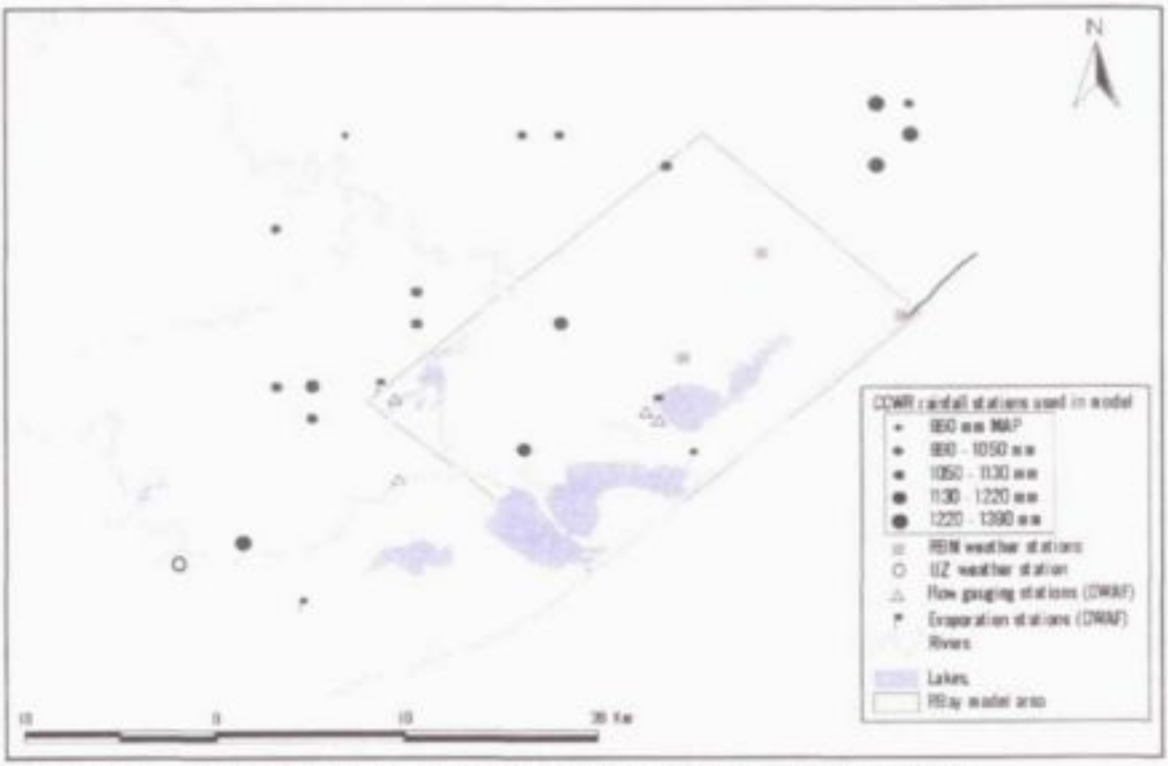

Figure 6 Hydrological monitoring stations around Richards Bay.

A summary of the weather information that is pertinent for hydrological studies is presented for the University of Zululand weather station, UZ304622 (Figure 7). This station is situated on the main campus just to the south of Empangeni near Felixton (Figure 6). Two years of the hourly observations have been published under HRU report # 2/88 and HRU report # 3/89.

3.3 RAINFALL

Rainfall is the principle recharge mechanism for the primary aquifers along the coastal region so considerably more emphasis has been placed on the analysis of its temporal and spatial variability in this section. The spatial distribution of rainfall on a monthly and annual basis for the whole of KwaZulu-Natal has been presented in Schultze (1982) and is available in a 1 minute x 1 minute grid from the CCWR.

Figure 7 Automatic weather Station UZ304622.

3.3.1 ANNUAL RAINFALL

Tyson (1986) identified isolated instances of secular trends in South African rainfall series but concluded that there was no evidence to suggest that South African rainfall was not stationary. No attempt has been made to verify this. There are several weather station in the Richards Bay region which are monitored by the South African Weather Bureau (SAWB), the Richards Bay TLC and private organizations (RBM, University of Zululand). The location of these is shown in Figure 7. The SAWB data is generally accessible from the Computing Centre for Water Research (CCWR) at Natal University, Pietermaritzburg (http://aqua.ccwr.ac.za).

3.3.1.1 SPATIAL DISTRIBUTION OF ANNUAL RAINFALL

All available daily rainfall stations with at least 30 years of data were used to estimate the spatial distribution of annual rainfall for the Richards Bay Region. All missing daily data were patched and then averaged over each hydrological year (1 October to 30 September). The data was interpolated using SURFER[1] and plotted in Figure 8.

There is a sharp gradient in the annual rainfall field from the coast to the hinterland. The mean annual rainfall is generally >1000 mm/year at the coast but decreases to less then 800 mm within 20 km of the coastline. While the 850 mm contour runs almost parallel to the coast there does appear to be a slightly lower rainfall aligned to the two principle valleys which may cause a reduced uplift for convective enhancement in these regions. This difference in rainfall is probably the reason for the major changes in land use patterns and crop water requirements of the region.

[1] Registered trademark for programme by Golden Software

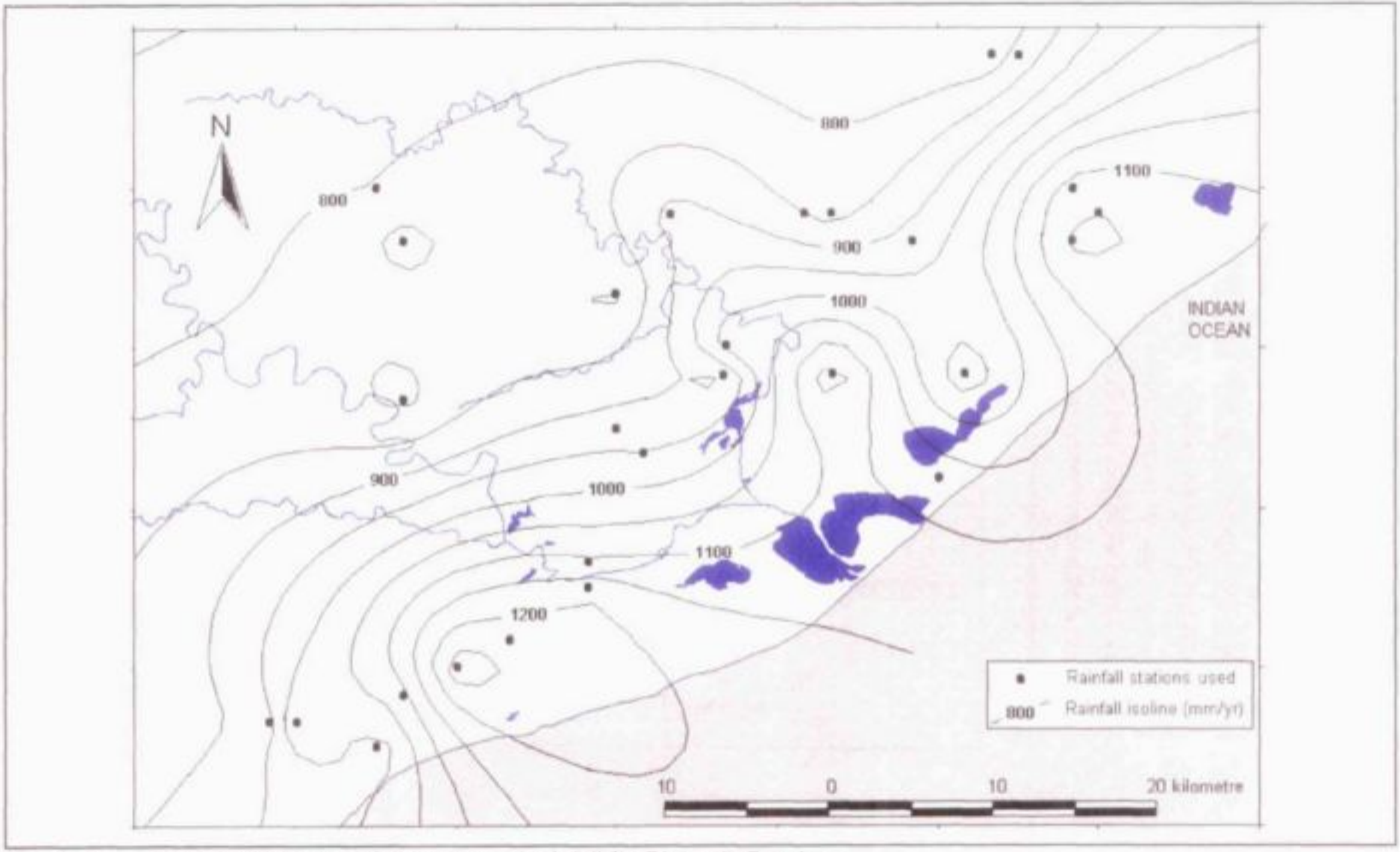

Figure 8 Spatial Distribution of mean annual rainfall for Richards Bay Area

3.3.1.2 TREND ANALYSIS

Spectral analysis of the annual series of rainfall for the whole of South Africa and for regions of the east coast have indicated significant periodicities in the rainfall patterns. Tyson (1986) detected a 18 year periodicity in South African rainfall series for the summer rainfall region of South Africa, while Dyer and Gosnell (1978) and Kelbe, Garstang and Brier (1983) found similar trends in the rainfall series along the eastern regions of Southern Africa. Spectral trends in the annual

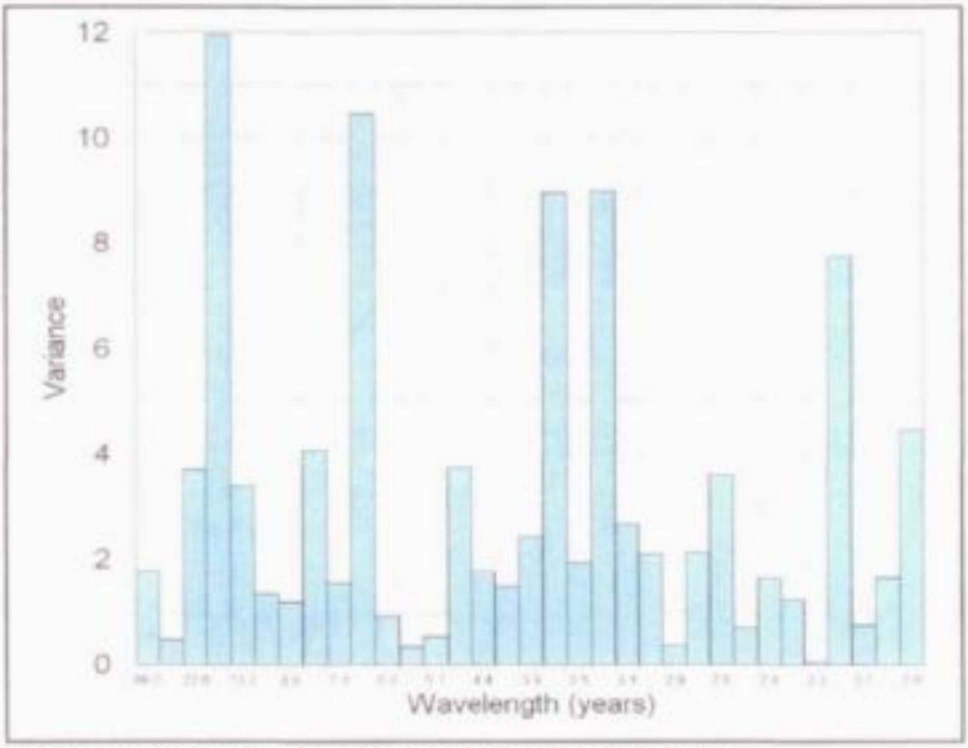

Figure 9 Spectral analysis of the annual rainfall series

rainfall for the long term series in Richards Bay are identifiable in the periodogram for Kwambonambi (Figure 9). The largest periodicity in the periodogram represents an 18 year cycle which has been observed and reported by many others. The quasi-biennial cycle (+2 years) is well documented in summer rainfall series but the other periodicities at 3.5 and 7 years are not well known.

3.3.1.3 FREQUENCY ANALYSIS of ANNUAL RAINFALL

The annual rainfall totals for the Kwambonambi Station with 66 years of data were used to represent regional rainfall frequencies. The depth duration curve for annual rainfall at this station is shown in Figure 10. Plotting position was derived using $\left\langle [\ln(^{x}/_{x-1})]^{-1} \right\rangle$ and plotted on a logarithmic scale.

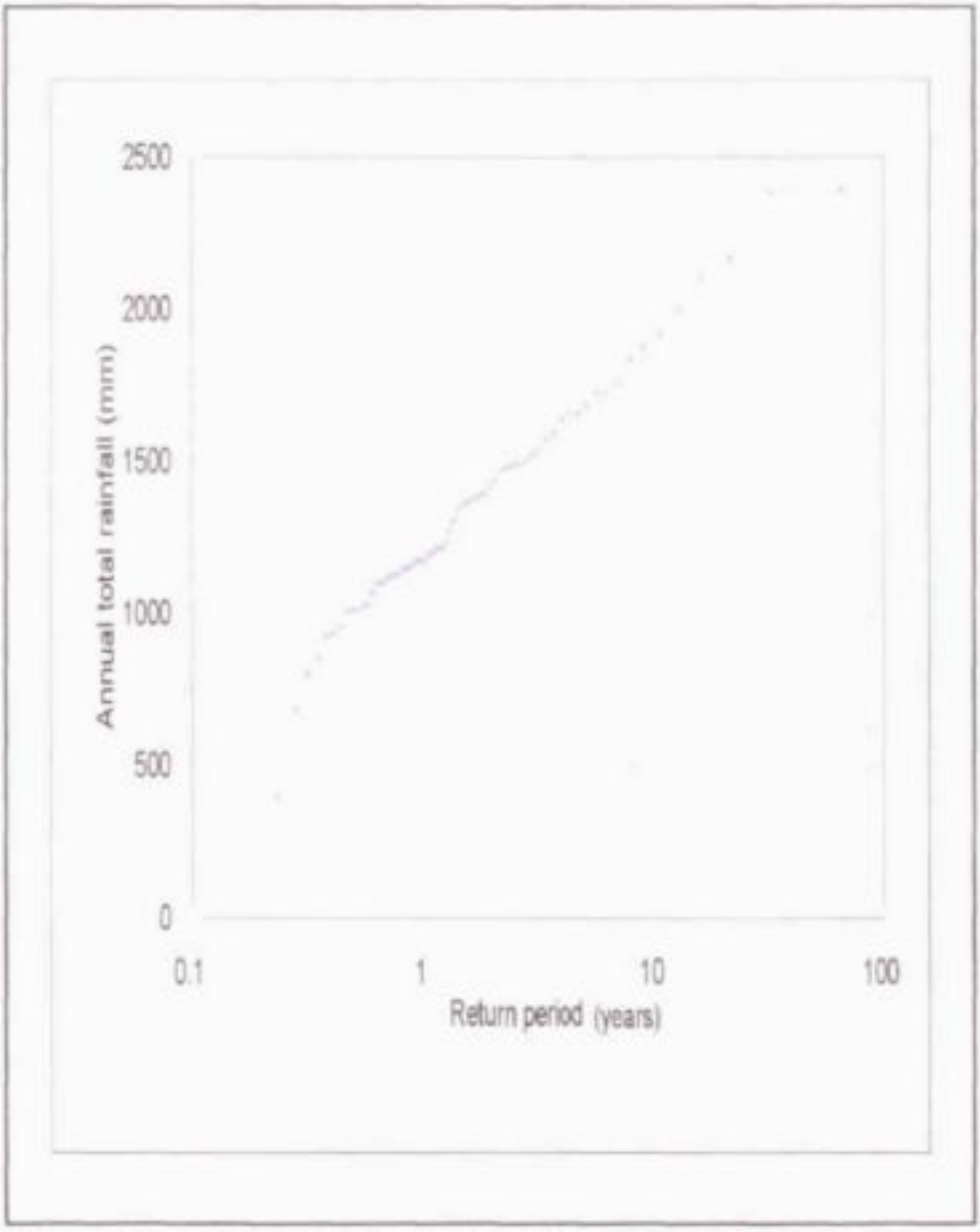

Figure 10 Frequency distribution of annual rainfall totals (in mm) for Kwambonambi.

3.3.2 MONTHLY RAINFALL

There is a definite annual cycle in the monthly rainfall series at the University of Zululand (Figure11). The wettest months are usually between January and March. Although there are extensive periods in winter when there is very little precipitation, the average rainfall in winter for this region is about 25 to 30% of the average summer rainfall.

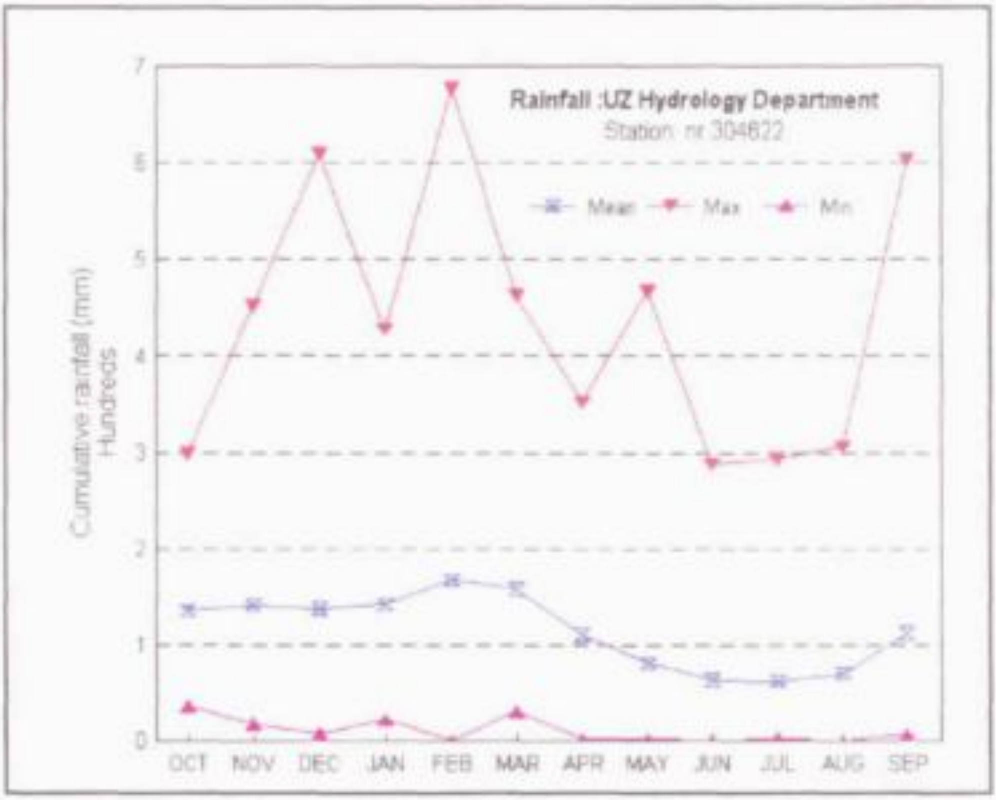

Figure 11 Maximum, Mean and Minimum monthly rainfall (mm) for University of Zululand station UZ 304622 from 1938 to 1997.

The frequency analysis for the annual series of <u>maximum</u> monthly rainfall for the Kwambonambi station is shown Figure 12. These frequency curves show the magnitude of the monthly rainfall that corresponds to a specified probability (return period).

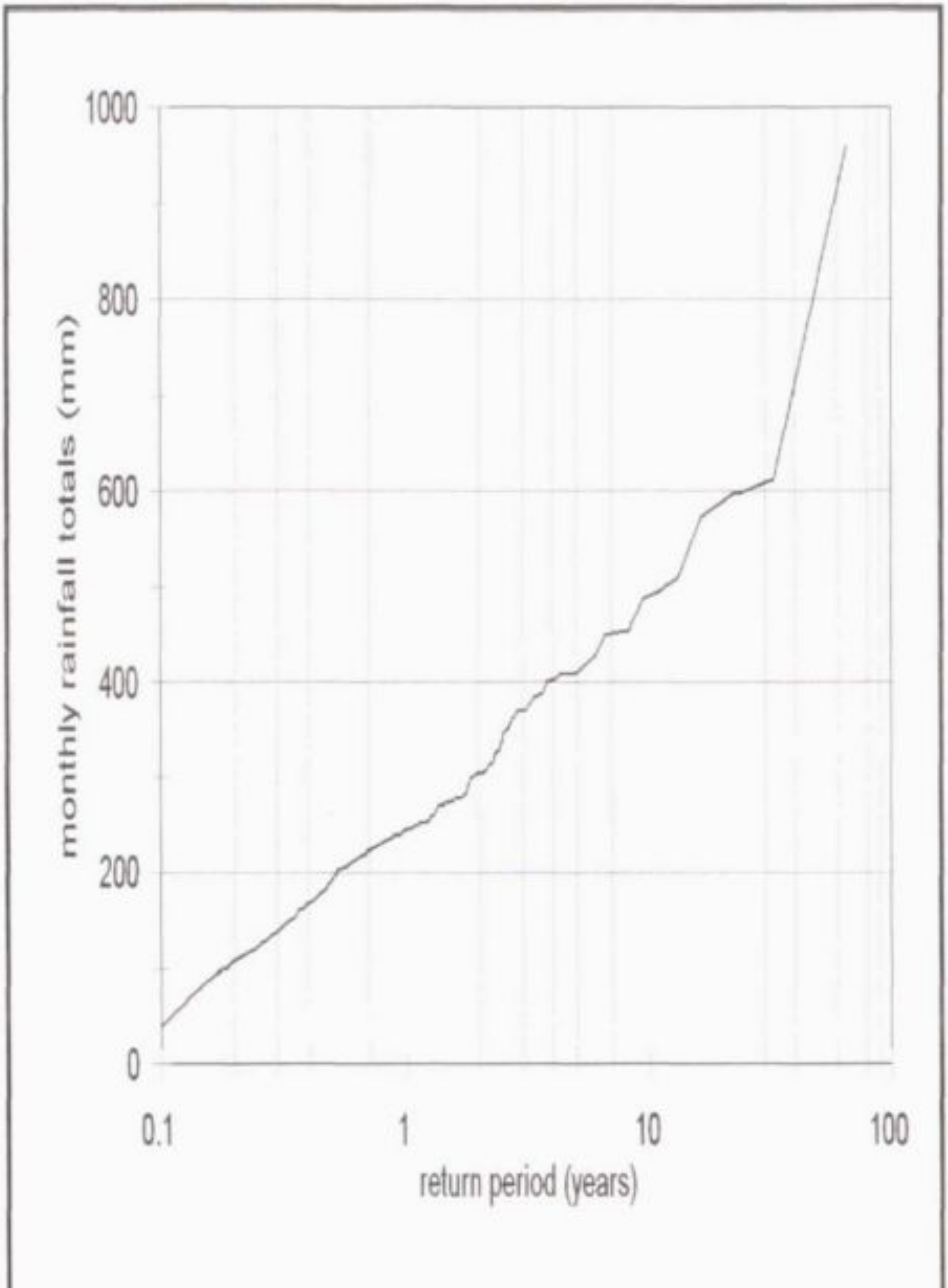

Figure 12 Depth duration curve for monthly rainfall at Kwambonambi Station.

3.3.3 DAILY RAINFALL

The mean annual rainfall at UZ304622 is approximately 1362 mm which occurs on an average of 99 days in each year. The 17 year mean monthly number of days with rainfall exceeding 5 and 10mm respectively for the University of Zululand weather station is shown in Figure 13. In summer there are generally about 4 days in each month with rainfall >10 mm. These storm events also occur in winter months with about half the frequency.

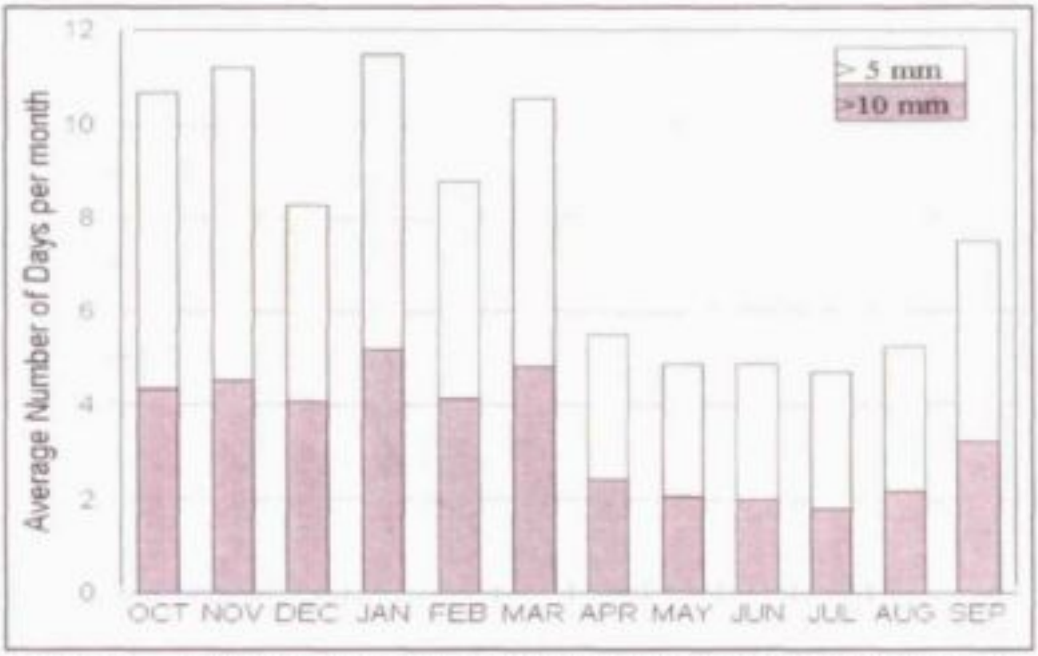

Figure 13 Number of days per month between 1975 and 1993 that there were more than 5 and 10 mm rainfall at UZ weather station (UZ304622).

While tropical and subtropical systems described above produce extremely high rainfalls, they occur infrequently. Approximately 1-2% of the precipitation events (rain-days) in this area have produced over 100 mm of rainfall in a 24 hour period. Most of the rainfall in this area is derived from localised convection or frontal systems that produce substantially less rainfall. Over 50% of events (days) produce daily rainfall rates of less than 10 mm per day. However, they only make up

24% of the total annual rainfall. These small amounts are shown later to have a minimal effect on groundwater recharge.

3.3.3.1 FREQUENCY ANALYSIS

The 1-, 3- and 5-day annual maximum rainfall for the Kwambonambi Rainfall station (WB305308) is presented in Figure 14. The largest extreme 3- and 5-day event is plotted at a return period of ~70 years which is the length of the record. It should be considered as a much less frequent event with a return period in excess of 100 years.

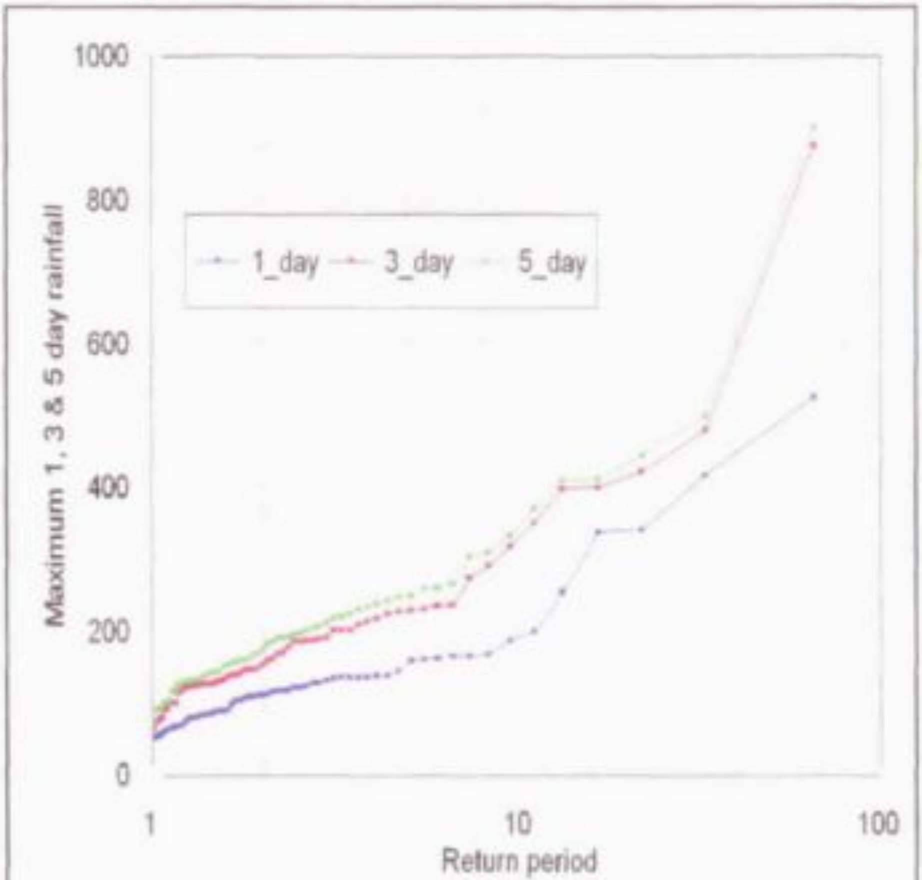

Figure 14 Annual Max 1, 3 and 5 day rainfall for Kwambonambi station.

In the assessment of runoff processes presented in latter sections, the recharge to groundwater is assumed to be derived from rainfall that does not exceed "infiltration rate" which is assumed to be approximately 50 mm/day. These events that are 50 mm/day or more are presented in Figure 15. They are assumed to represent those situations where surface runoff occurs in the numerical model simulation presented in subsequent sections. In the numerical simulations of groundwater, all the rainfall in excess of 50 mm is routed immediately to the boundaries and only 50 mm/day is assumed to recharge the aquifer.

3.3.3.2 RAINFALL INTENSITY

The regional rainfall is derived from several meteorological systems. The extreme cyclonic systems produce very high rates of rainfall which have been discussed in section 3.1.1.1.

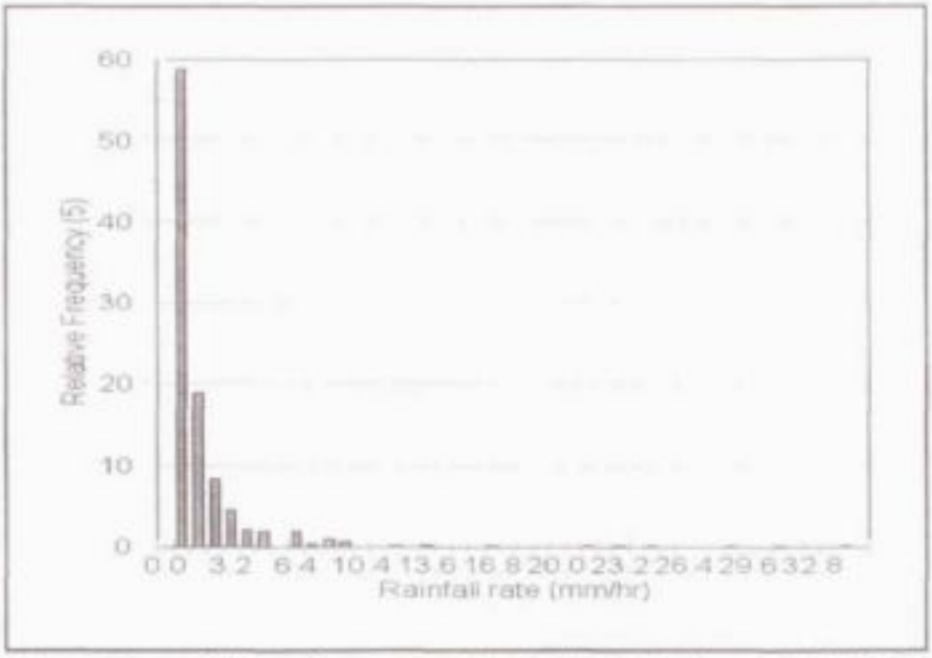

Figure 15 Relative frequency of rainfall rate for 4 month in 1995 at UZ304622.

Generally, however, the rainfall is derived from systems at a much lower intensity. Base on 5 minute rainfall observations the daily rainfall rate is generally less than 2 mm/hr (Figure 15). The rainfall rate exceeded 10 mm/hr on less than 2% of events during a 4 month observation period at the University of Zululand.

3.3.4 EVAPORATION

Evaporation and transpiration are primary mechanisms for the loss of water from the system. Estimates of the potential evapotranspiration (E_p) for the study area have been derived from measurements at the automatic weather station on the University of Zululand Campus and from measured pan evaporation at W1E009 at Lake Mzingazi. These observations are used in deriving estimates of other water balance components for specific resources and also for deriving model parameter values.

3.3.4.1 UNIVERSITY OF ZULULAND WEATHER RECORDS

Total monthly A pan measurements at the University of Zululand for 12 years from 1975 to 1988 are shown in Figure 16. Mid-summer monthly evaporation can range from less than 150 to more than 250 mm. Winter evaporation is generally <100 mm per month.

Evaporation at any given moment is a function of atmospheric water demand and soil water supply. The potential evaporation rate assumes adequate soil water supply and is only a function of the atmospheric demand. Atmospheric demand is driven by available energy (radiation), atmospheric temperatures and humidity and advection (wind speed). These can be integrated in the Penman model (Campbell 1977) to give an estimate of the atmospheric demand. Potential evaporation includes the biological characteristics of the vegetation (Leaf Area Index and Resistance Factor) which can be derived by the Penman-Moneteith model (Campbell 1977).

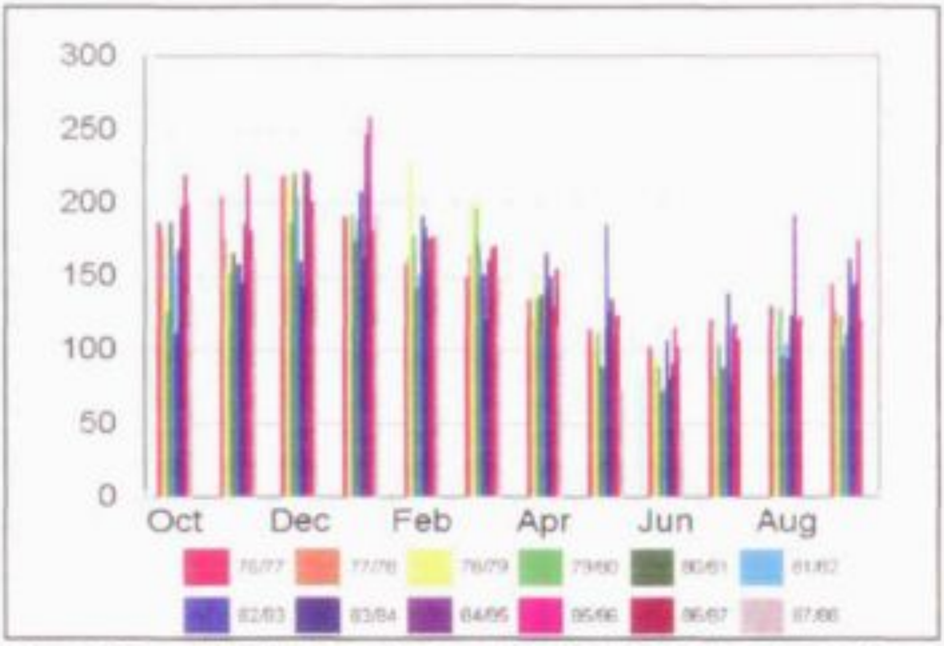

Figure 16 Monthly A-pan Evaporation for UZ weather station for 12 years from 1976 to 1988.

The meteorological weather station on the University of Zululand campus was operating from 1987 to 1991. This automatic weather stations provided hourly mean values of solar radiation, temperature, vapour pressure, and wind speed. The station also provided daily means, maxima and minima for these variables. From these measurement, hourly and daily estimates of the potential evaporation from grasslands were obtained using the modified Penman approach (Kelbe 1989, 1990). The estimated potential evapotranspiration is shown in Figure 17 for 1989 and indicate the same seasonality as the rainfall. The mean daily potential evapotranspiration rate for 1989 was 4.8mm/day.

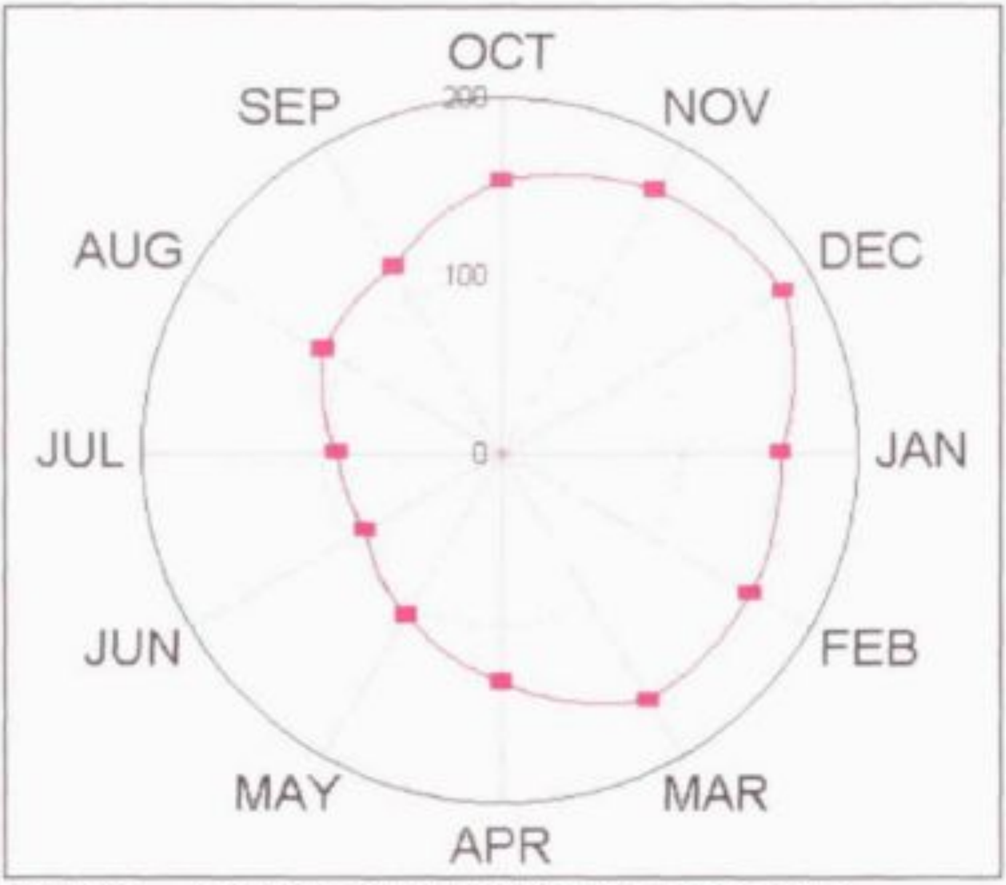

Figure 17 Variation in potential evaporation (in mm/month) at UZ304622.

Section 4 WATER RESOURCES AND WATER USE

The main water resources of the Richards Bay Area are associated with the coastal freshwater lakes of Mzingazi, Nhlabane, Nsezi, Cubhu and Mangeza, the Mhlatuze River and the extensive coastal primary aquifers. Abstraction occurs from all these resources (Figure 18) to sustain the local people, agriculture and industry through various local authorities. Water supply also involves inter-basin transfer to meet local needs during periods of high demand. There is a temporary transfer scheme at Middlesdrift on the Tugela river to augment the Mhlathuze River, regular transfer from the Mhlathuze River to Lake Nsezi, and there is abstraction from the Umfolozi to holding dams at Sokhulu to supplement the mining industry at Richards Bay.

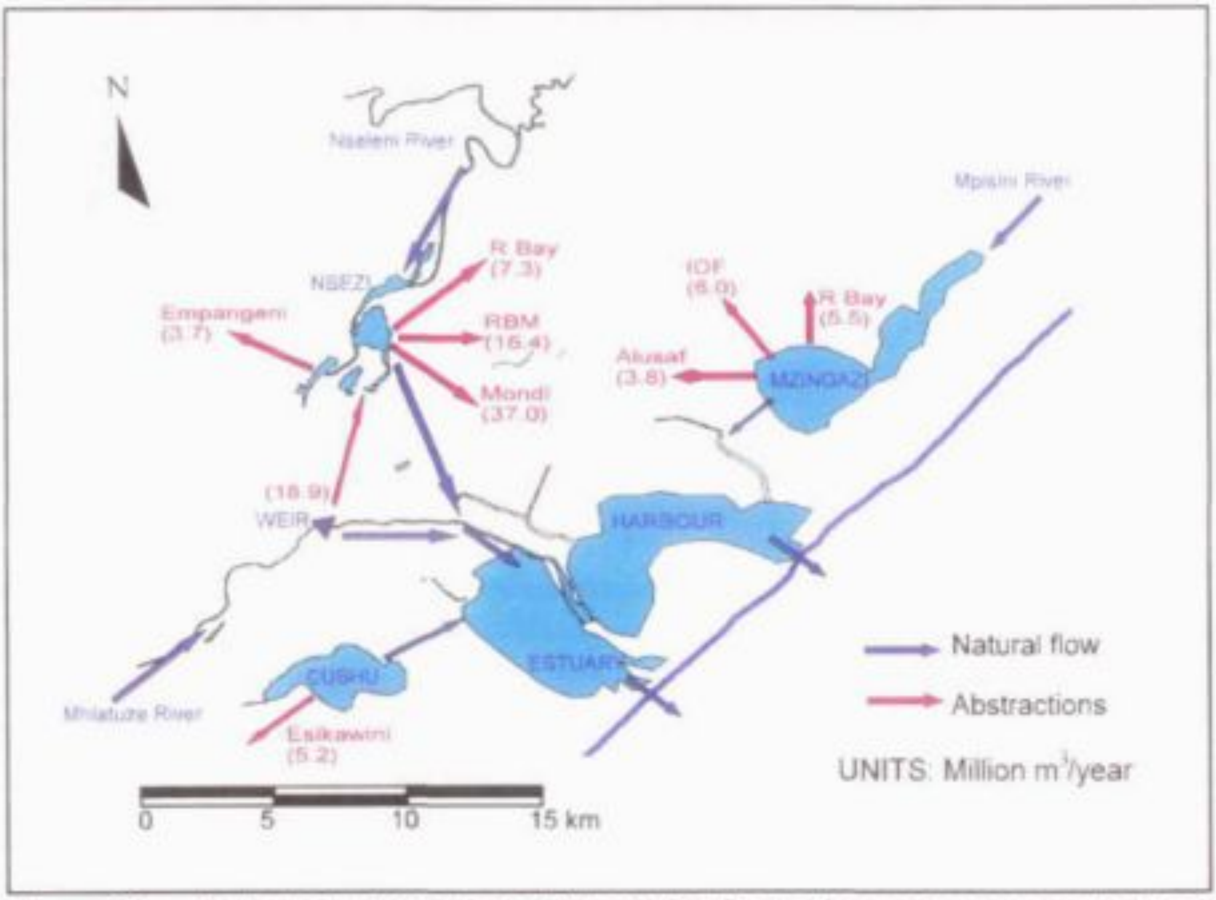

Figure 18 Estimated water use in the Richards Bay Region from various sources (adapted from the Iscor EIA by Kelbe, 1992).

These resources (Figure 18) are presently under the jurisdiction of several independent authorities who obtain abstraction rights (permits) from the Department of Water Affairs and Forestry, Regional Office, in Durban. The National Water Act (Act 36 of 1998) will delegate many of the management and administrative functions of the water resources to Catchment Management Authorities (CMA) in the near future.

At present the bulk water supply is controlled by the Mhlathuze Water whose jurisdiction covers most of the study area. Water rights are also vested in several local authorities and industries. Richards Bay TLC has abstraction rights from Lake Mzingazi; Empangeni TLC has transferred its rights to Mhlathuze Water; eSikhaweni Municipality has abstraction rights from Lake Cubhu which have also been transferred to Mhlathuze Water. Water is imported from the Umfolozi River by Richards Bay Minerals who also have abstraction rights from Lake Mzingazi and Lake Nsezi. There are also several irrigation control Boards operating along the Mhlathuze River with abstraction rights to "surplus" water from the Goedertrouw Dam.

MBB Consultants (1998) determined the storage capacity of dams in the Mhlathuze Catchment and the abstraction rates in the catchment area. They identified a catchment area of 404600 ha in size of which approximately 136000 ha consist of existing water control areas. The total abstraction rate utilised for agricultural purposes is 501811 m^3/day (5808 ℓ/s) which is made up of the contribution from each control area shown in Table 1 (MBB Consultants, 1998).

Table 1 Abstraction rates for the Mhlathuze Catchment (after MBB Consultants, 1998)

Control Area	Abstraction
	m^3/day
KwaZulu	37930
Lower Mhlathuze	10346
Richards Bay	21341
Nkwalini	156470
Mfule	67651
Heatonville	79142
Remainder	126230

The Mhlathuze catchment has a storage capacity of 5.2×10^6 m^3 (0.9% MAR) in small dams and an additional 304×10^6 m^3 (52.7% MAR) in the Goedertrouw Dam (Mhlathuze Water, 1998).

Details of the principle water resources are described in the following sections with particular emphasis on the coastal lake systems that form part of the primary aquifer. Several case studies of the flow dynamics and water balance for these lakes are presented in Part 3 of this report. The main lakes are all situated in the coastal plain where they form an extension of the local ground water aquifer. The shallow unconfined aquifer along the coastal plain has been used to supply water to local mining industries but these well fields have been closed in preference to surface water supplies.

4.1 WATER RESOURCES

The water resource features in this study are grouped into four distinct systems that need to be examined in different ways according to their interaction with the underlying aquifers. The systems that have minimal groundwater interactions and are dominated by river systems, are distinct from those resources that are often an extension of the groundwater. The four separate features are identified in the next sections.

4.1.1 MHLATHUZE RIVER

The Mhlathuze River flows into the Richards Bay Estuary which has been divided into two compartments by a berm wall. The northern part of the estuary has been developed as a deep water harbour while the southern section is retained as a natural estuary with the dredging of a new mouth directly opposite the river inlet. The Mhlathuze River is fed by three main tributaries, the Mhlatazana, the Mfule and the Nseleni Rivers, and regulated by the Goedertrouw Dam (Figure 19). This river is the focus of attention in a similar study still in progress.

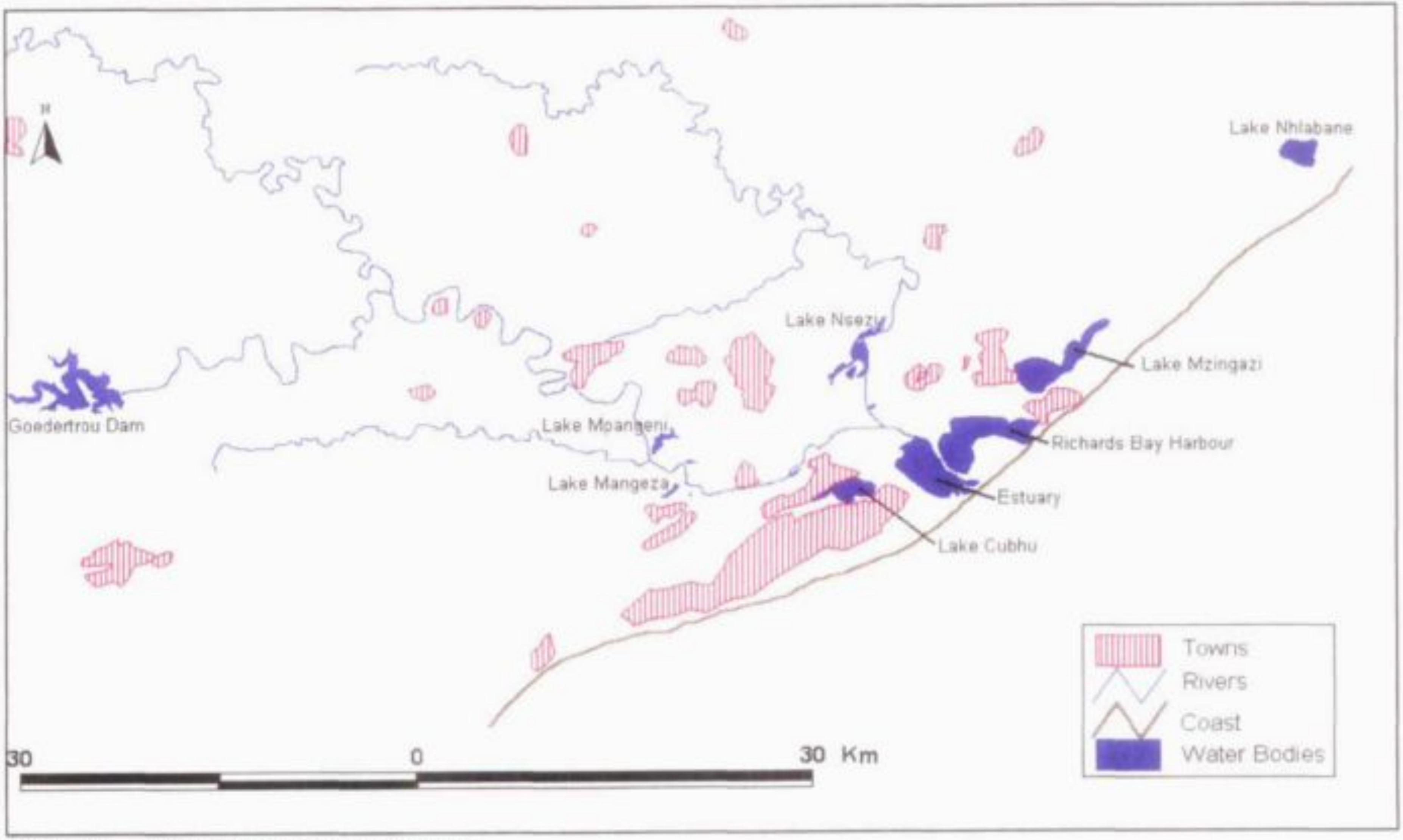

Figure 19 Map of regional water resources

4.1.2 COASTAL LAKES

Studies of coastal lakes on the Swan Coastal plain in Western Australia by Townley *et al* (1993) suggest that these coastal lakes have significant flow-through characteristics where there is generally continuous and simultaneous recharge and discharge through various parts of the lake bed to the aquifer. Generally, this seepage rate is greatest at the surface shoreline and decreases exponentially with distance underneath the lake. It has been assumed that the Zululand coastal lakes also have direct interaction with the aquifer and that they have similar seepage characteristics. Consequently, these lakes are assumed to be supplied through direct rainfall interception, surface runoff from riparian zones, streamflow and groundwater recharge. The Lakes in the Richards Bay area which are controlled by subsurface conditions, are shown in Figure 19 and include Lake Nhlabane, Lake Mzingazi and Lake Cubhu.

4.1.3 OFF-CHANNEL LAKES

Several small catchment rivers flowing into the Mhlathuze River just upstream of the old N2 road bridge, do not have sufficient flow to maintain an open channel connection. The lower reaches of these rivers in the Mhlathuze flood plain have been blocked by sand bars and have formed small lakes (Figure 20). These lakes have formed in the incised valleys with shallow soils overlying granitic formations. Consequently, these off channel lakes function in a different manner to the coastal lakes situated in a highly permeably sedimentary aquifer.

These off-channel lakes (Figure 20) along the Mhlathuze River are considered to be dominated by both surface runoff characteristics and groundwater seepage through the lake. The discharge is generally through groundwater into the Mhlathuze River.

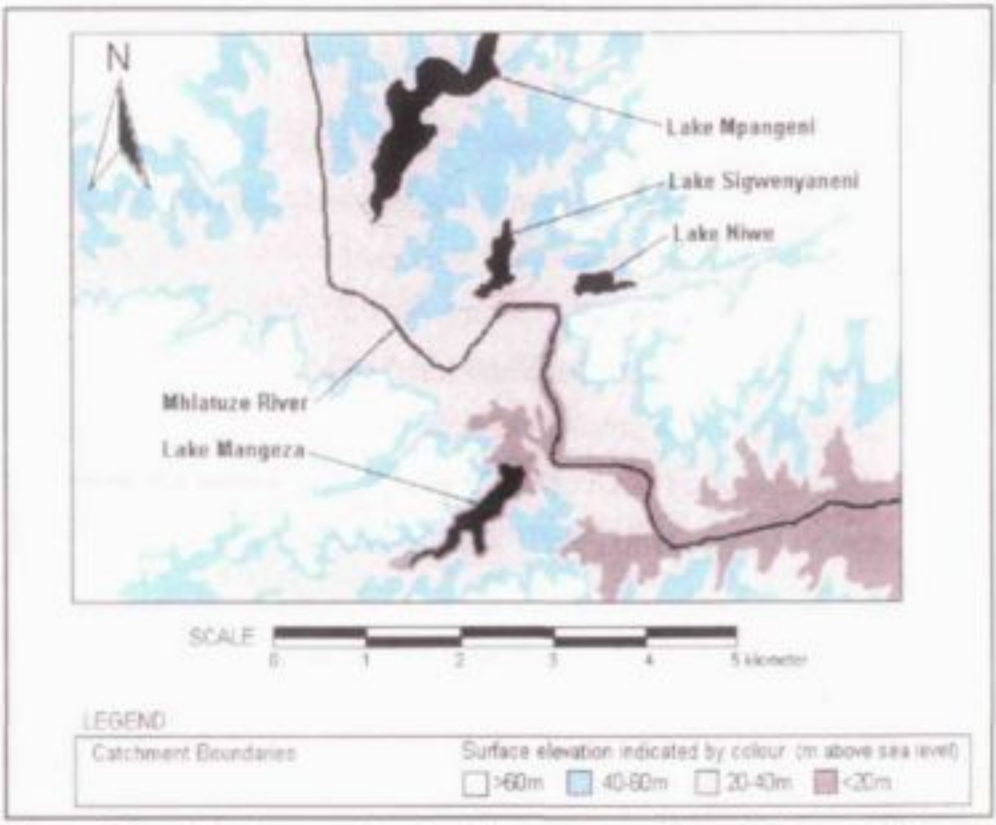

Figure 20 Study area showing the position of the off-channel lakes in relation to the Mhlathuze river and the main topographical features. Surface elevation indicated at 20 m intervals.

4.1.4 COMBINATION LAKES

Lake Nsezi, situated on the western edge of the coastal plain, is considered to have a significant groundwater component but is controlled to a large extent by the Nseleni river that has its origin in a very different geological region. Consequently, it is considered to be more appropriate to model this Lake system using both surface hydrological models (such as the Pitman or VTI models) and groundwater models. The groundwater component will be determined for the immediate vicinity of Lake Nsezi for comparative studies with the surface runoff component in the lake budget determinations.

4.2 LAKE MZINGAZI

Lake Mzingazi can be broken into two main compartments (Figure 21). The southern part of the lake is separated from the northern part by a very shallow and narrow section which is exposed during extremely dry conditions. The southern compartment is approximately 14 m below mean sea level at its deepest point and therefore susceptible to saline intrusion under adverse conditions. The problem of potential saline intrusion for Lake Mzingazi have been studied by Simmonds (1990), van Tonder, Botha and Muller (1986), Cyrus, Martin and Reavell (1997) and Rawlins, Kelbe and Germishuyse (1997).

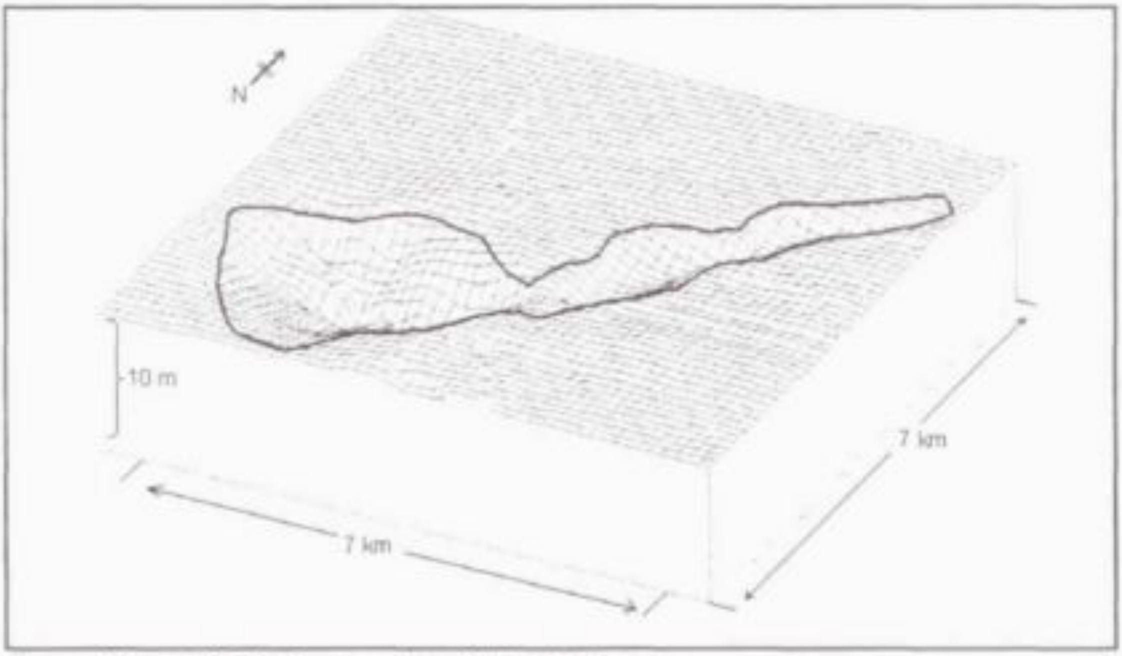

Figure 21 3D Surface profile of Lake Mzingazi

4.2.1 LAKE MZINGAZI WATER LEVEL AND DISCHARGE

The water level and discharge from Lake Mzingazi have been monitored since August 1978 at a small weir on the southern edge of the berm wall (Figure 22). The rating curve for this weir (W1H011) is shown in Figure 23. From the start of the monitoring program until 1992 the lake level remained fairly static between 3 - 4 m *AMSL* (Figure 24) with the exception of two short periods in 1981 and 1983 when the lake levels dropped below the present spillway elevation of 3.03 m *AMSL*.

Figure 22 Mzingazi weir W1H011

The major flood event in January 1984 following cyclones Domoina and Imboa showed as a significant increase in Lake level which reached a stage of more than 1.5m above the present spillway. This was followed three years later in September 1987 with even greater flooding when the Lake level reached an elevation of 2.85 m above the spillway.

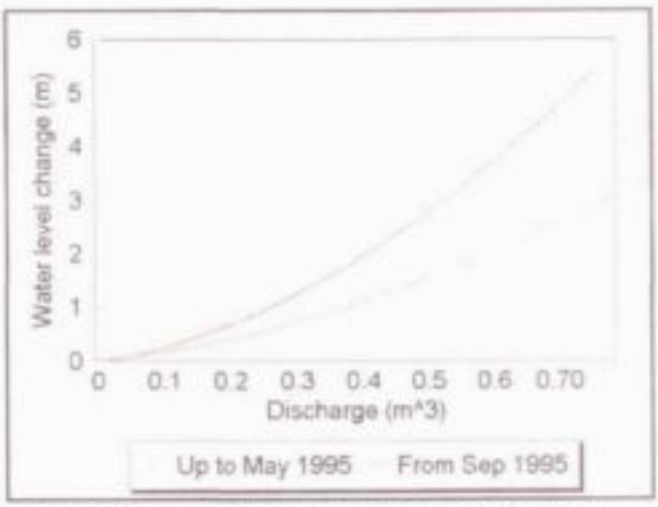

Figure 23 Rating curve for weir W1H011

Figure 24 Lake Mzingazi water levels since 1978

During the severe drought period from 1992 to the 1995, the lake level dropped continuously to a low level of 1.08 m *AMSL* at the end of the winter of 1993. There was a very slight recovery during the summer rainfall of 1994 but the lake level then fell even further to a low of 1.06 m *AMSL* in July 1994 and finally to 0.85 m in February 1995. Water restrictions were imposed in 1994 and only relaxed after heavy rains in 1996 when the lake started to overflow once more (Figure 24). The discharge from Lake Mzingazi during this period has been monitored intermittently by the Richards Bay TLC (Figure 25).

4.2.2 STORAGE CAPACITY

The capacity of Lake Mzingazi was derived from the bathymetric survey of the lake by Walmsey and Grobler (1986). Based on this bathymetric surface (Figure 21), the capacity of the lake, when full to the level of the spillway (3.03 m *AMSL*) is estimated to be approximately 43 $\times 10^6$ m^3 by Hattingh (1998) who has provided the rating table given in Table 2. The lake volume is estimated to reduced to 16 $\times 10^6$ m^3 when the lake level drops to mean sea level (0 m *AMSL*). The lake was reduced to an estimated available storage capacity of 22 x 10^6 m^3 when the lake level dropped to its minimum level of 0.85 m *AMSL*. However, the lake splits into two separate reservoirs below this level and the volume that is directly available is approximately halved.

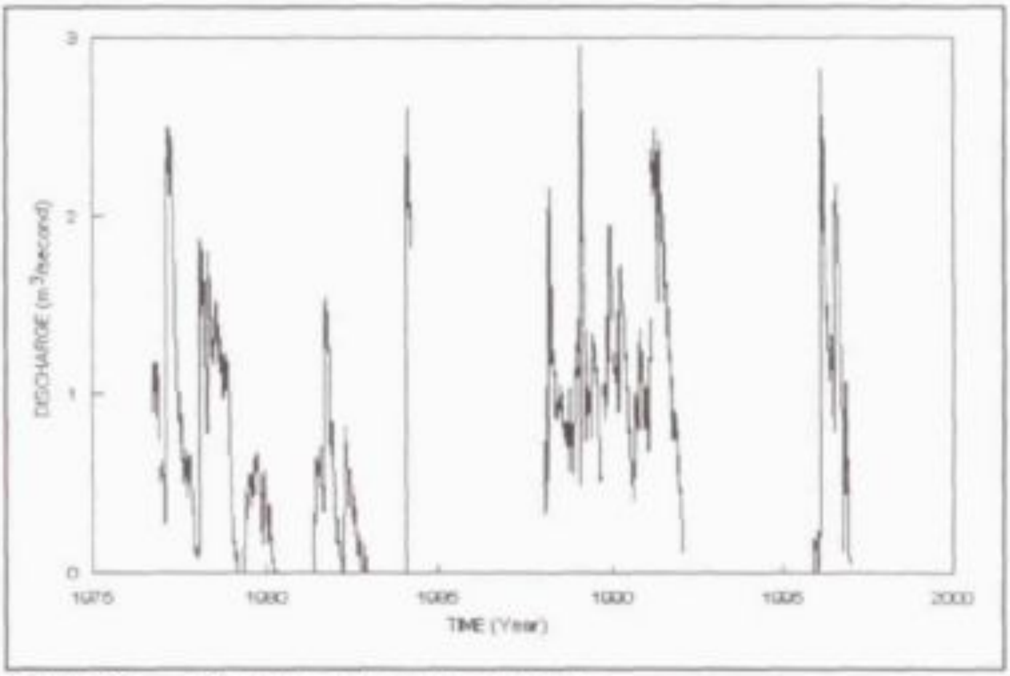

Figure 25 Discharge from Lake Mzingazi

4.2.3 ABSTRACTION

Richards Bay TLC abstract water from Lake Mzingazi (Figure 26) to supply water to the municipality of Richards Bay and Alusaf. RBM also has abstraction rights to withdraw water from Lake Mzingazi. Water is also used by the Richards Bay Country Club for the golf course and possibly by other small users situated directly next to the lake. Officially, water is only abstracted when the lake level is above a specified minimum stage (storage level) that is set to reduce the impact of saline intrusion (van Tonder et al, 1986).

Table 2 Lake Mzingazi perimeter, area and volume (Hattingh, 1998).

Water elevation	**Perimeter**	**Surface Area**	**Volume**
m - amsl	km	$10^{6*}m^2$	$10^{6*}m^3$
-1	8.30	4.03	10.11
-0.75	17.55	5.62	11.42
-0.5	18.03	6.09	12.89
-0.25	18.51	6.58	14.47
0	**18.99**	**7.08**	**16.17**
0.25	19.17	7.40	17.99
0.5	19.25	7.69	19.88
0.75	19.34	7.97	21.83
1	19.42	8.26	23.86
1.25	19.51	8.55	25.96
1.5	19.57	8.83	28.14
1.75	19.69	9.12	30.38
2	19.77	9.41	32.70
2.25	19.85	9.70	35.08
2.5	19.94	9.99	37.55
2.75	20.03	10.28	40.08
3 (weir @ 3.03)	20.11	10.57	42.69

The abstraction rates, as supplied by the Richards Bay TLC are shown in Figure 26. There are many impoverished rural people living in the immediate catchment area and consequently, the official abstractions are assumed to be a minimum rate for the purpose of calibrating the numerical models presented in subsequent sections.

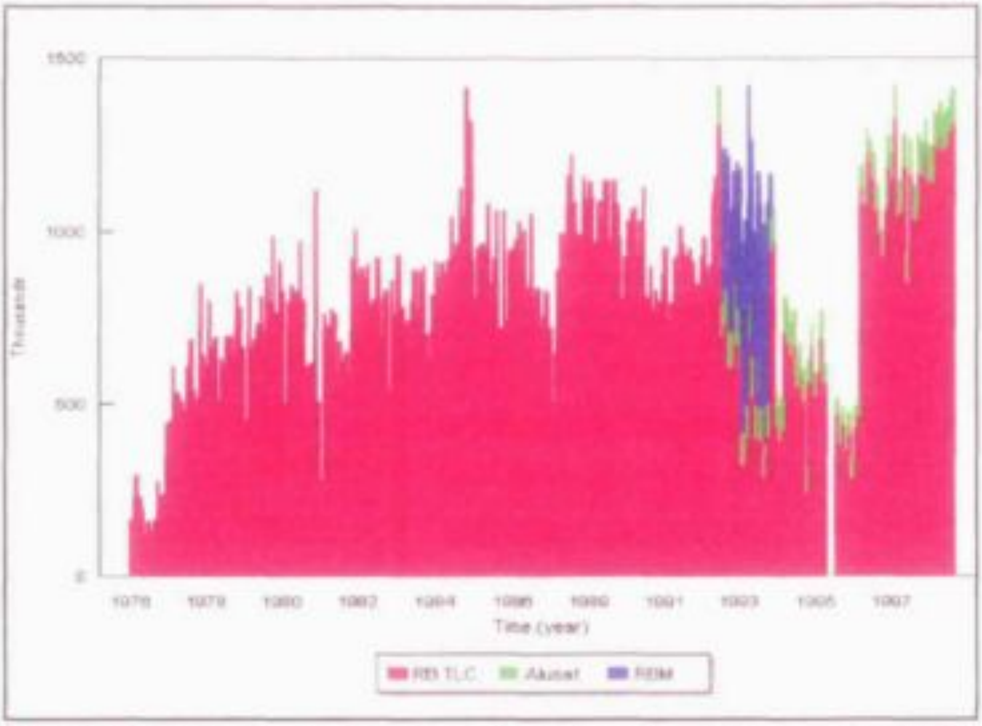

Figure 26 Abstraction rates from Lake Mzingazi (from Richards Bay TLC)

4.2.4 SALINE INTRUSION

Investigations of possible saline intrusion into Lake Mzingazi by Simmonds (1990) made recommendations on borehole monitoring between the lake and the Mzingazi Canal and also suggested the construction of a salt water barrier on the Mzingazi canal. A temporary barrier was constructed in 1992 and recently upgraded to a more permanent structure (Figure 27). Borehole monitoring in the area between the lake and the saltwater canal (Figure 28) started in 1983. The barrier has had a large effect on reducing the declining local water table elevation between the lake and the saltwater canal which has also reduced the threat of saline intrusion into the lake (Rawlins, Kelbe and Germishuyse, 1996).

The artificial barrier is located at the point on the Mzingazi Estuary where the greatest potential for saline intrusion is likely to occur. The barrier acts to retain fresh water at or above the saline water level (sea level) in the channel between the lake and the canal (Figure 28).

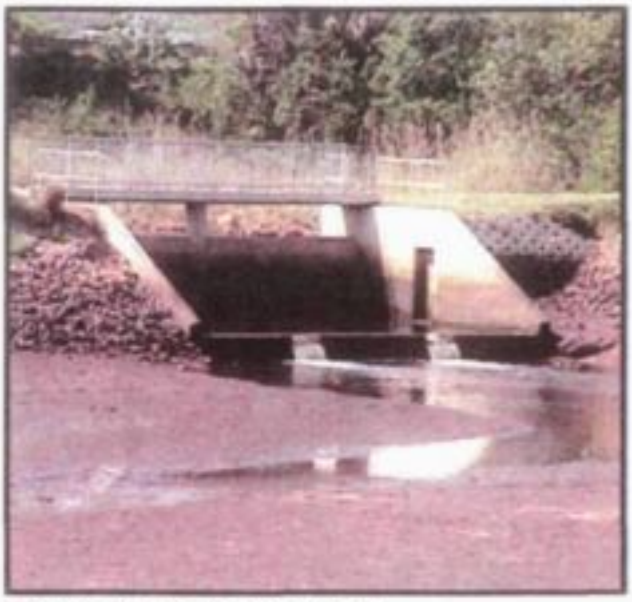

Figure 27 Saltwater barrier

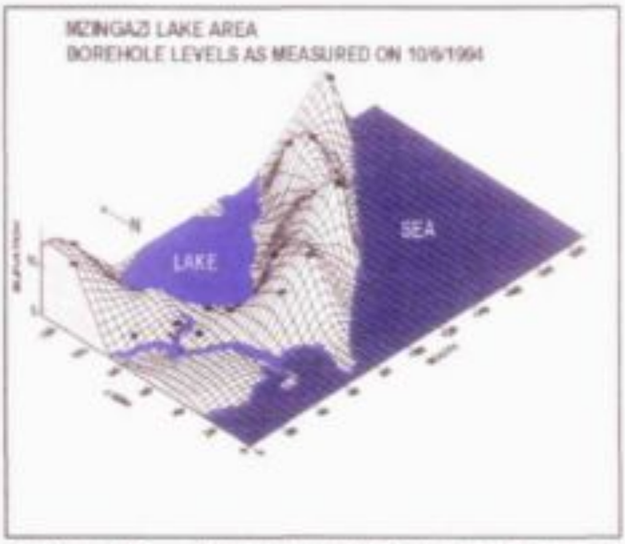

Figure 28 Borehole locations for Mzingazi and interpolated water table surface elevation

The effectiveness of the artificial barrier in restricting the water table decline between the lake and canal during severe drought periods can be assessed from Figure 29. The Lake level dropped to 0.85m at the height of the drought (Figure 24) but the water table between the lake and the salt water canal (0 m *AMSL*) was maintained at approximately the same elevation as the lake during the drought period (Figure 29) with the construction of the barrier.

Conductivity has been measured since 1990, at 5 m intervals down to varying depths, for most of the boreholes in the study area around the Mzingazi Canal. The conductivities at 5 m below the topographical surface for most of the boreholes around the perimeter of the lake are close to the measured conductivity value that was observed by van Tonder *et al* (1986) for Lake Mzingazi (45 mS/m).

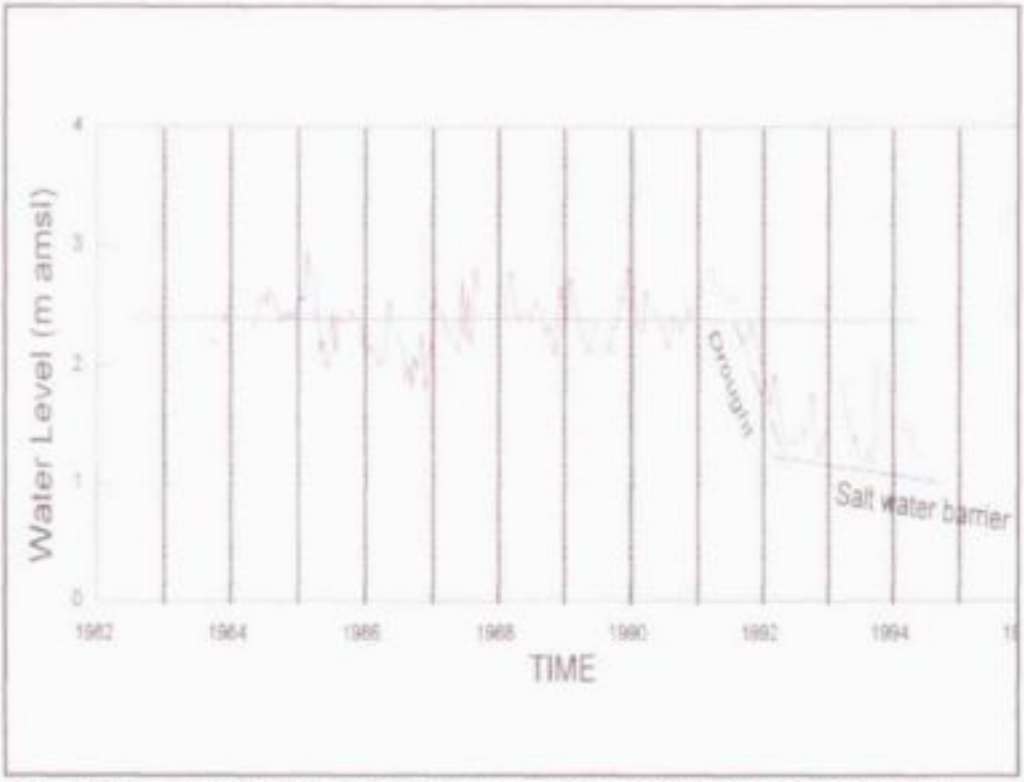

Figure 29 Water level elevation for Borehole "Q" from 1982 to 1994

The temporal variation in the conductivity at borehole "W2503", near the lake, shows that there have been no significant changes in concentration of dissolved solids (conductivity) at a 5 m depth since measurements commenced in 1990. However, the temporal variation in conductivity for boreholes "Q", which is midway between the lake and saltwater canal, shows an increasing trend from 1992 when the severe drought commenced and the water table elevation in the vicinity of this borehole dropped.

The spatial distribution of dissolved salts concentration at 5m depth before the saltwater barrier was installed is compared to the spatial pattern after the saltwater barrier was installed is shown in Figure 30. The difference in concentration is greatest in the section between the barrier and the lake.

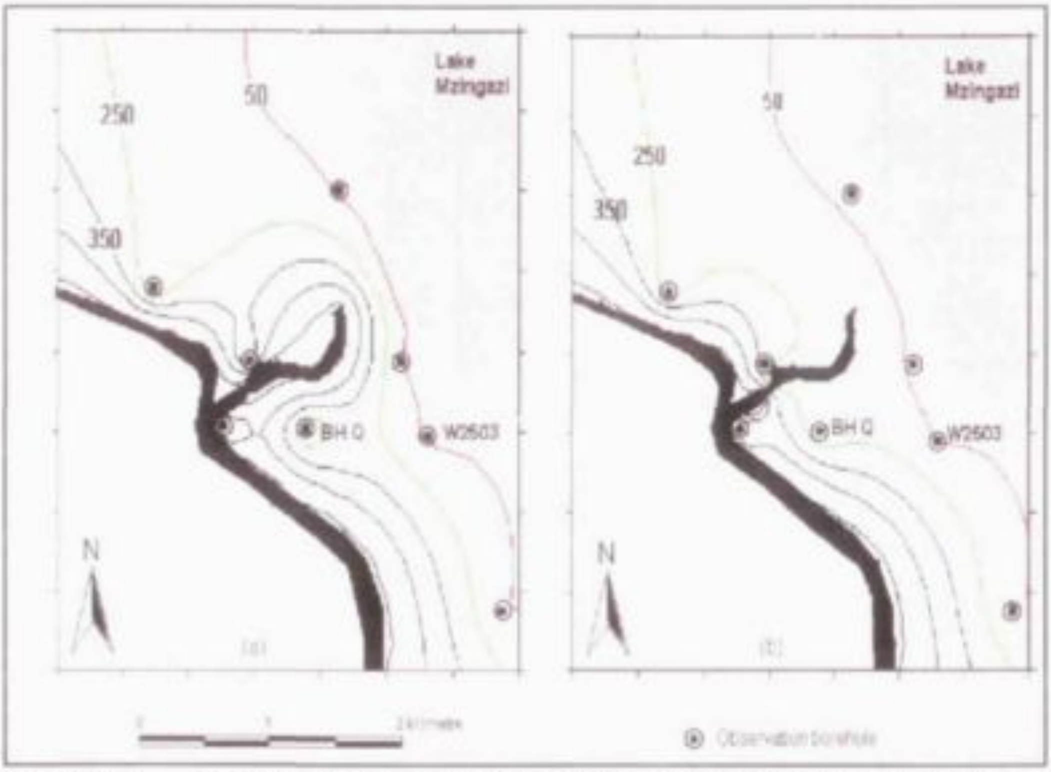

Figure 30 Contour values of conductivity (mS/m) between the lake and saltwater canal in (a) 1991 and (b) 1994

4.3 LAKE NHLABANE

Lake Nhlabane was an estuary draining directly into the Indian Ocean, but the construction of a weir has restricted the marine connection. The lake flows over the weir (Figure 31) and into the Indian Ocean through a tidal estuary. The lake has two main compartments separated by a narrow river section. A bathymetric survey of the lake was provided by Hattingh (1998) and is portrayed in Figure 32. The thick blue line represents the 5m contour (Hattingh, 1998) which is just 25 cm higher than the weir elevation. The weir has recently (Oct 1998) been raised by 1 meter and consequently the blue line in Figure 32 is now just below the spill way level.

Figure 31 Lake Nhlabane and estuary during high flow conditions. (Hattingh, 1998).

4.3.1 STORAGE CAPACITY

The bathymetric survey by Hattingh (1998) was used to estimate the rating table for Lake Nhlabane. The perimeter, surface area and volume of the lake are presented in Table 3. The volume of the lake has risen from 28 x 10^6 m^3 to nearly 40 x 10^6 m^3 with the raising of the new weir spillway. The lake has no storage below mean sea level and only 1.7 x 10^6 m^3 below the 1 m *AMSL* level.

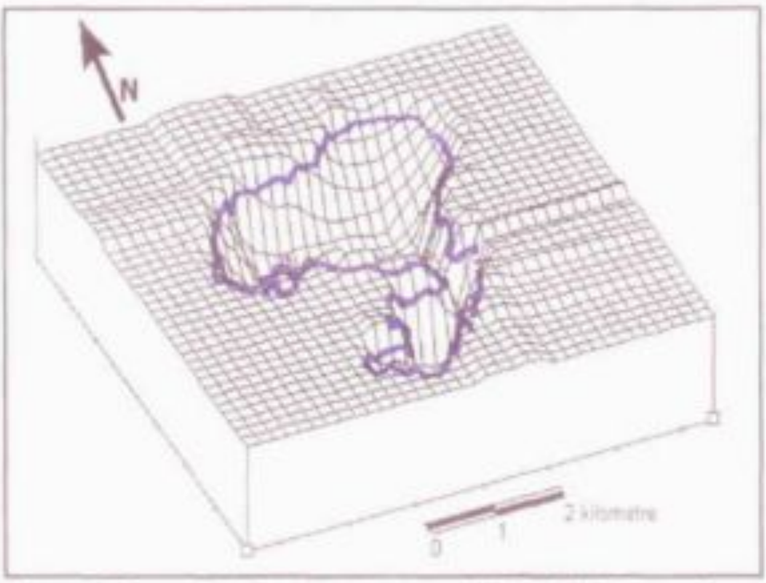

Figure 32 Surface contours of Lake Nhlabane (from Hattingh, 1998)

Table 3 Lake Nhlabane perimeter, surface area and volume (Hattingh, 1998)

Elevation	Perimeter	Area	Volume
m amsl	10^3 m	10^6 m^2	10^6 m^3
0.00	1.943	0.101	0.011
0.25	5.407	0.440	0.070
0.50	9.000	1.006	0.070
0.75	12.238	3.116	0.757
1.00	13.442	3.952	1.664
0.25	14.333	4.450	2.714
0.50	17.132	5.204	2.714
0.75	18.295	5.528	5.193
2.00	18.310	5.903	6.616
2.25	18.463	6.238	8.134
2.50	18.609	6.575	9.735
2.75	18.753	6.919	11.422
3.00	18.898	7.270	13.196
3.25	19.085	7.629	15.058
3.50	19.273	7.998	17.011
3.75	19.461	8.376	19.057
4.00	19.648	8.763	21.200
4.25	19.836	9.159	23.440
4.50	20.023	9.565	25.780
4.75 (weir)	20.211	9.980	28.223
5.00	20.399	10.405	30.771
5.25	29.481	11.625	33.627
5.50	30.513	12.048	36.585
5.75 (weir,1998)	31.546	12.491	39.652

4.3.2 WATER LEVEL

The lake water levels have been monitored by RBM for several years but the only information currently available is from November 1997 to April 1998 (Figure 33). Information on the lake level fluctuation is crucial for model calibrations over periods with extreme meteorological conditions. Unfortunately the lake levels during the extreme floods and droughts of the past two decades are not available and estimates from other sources have been sought. Because of their close proximity to Lake Nhlabane, the other lakes are likely to have experienced similar drought conditions and therefore the information derived for this period have been drawn from these other lakes. The best estimate presently available indicates that Lake Nhlabane water level dropped to almost 2 m *AMSL* during the drought period of 1994/95, but this could not be confirmed.

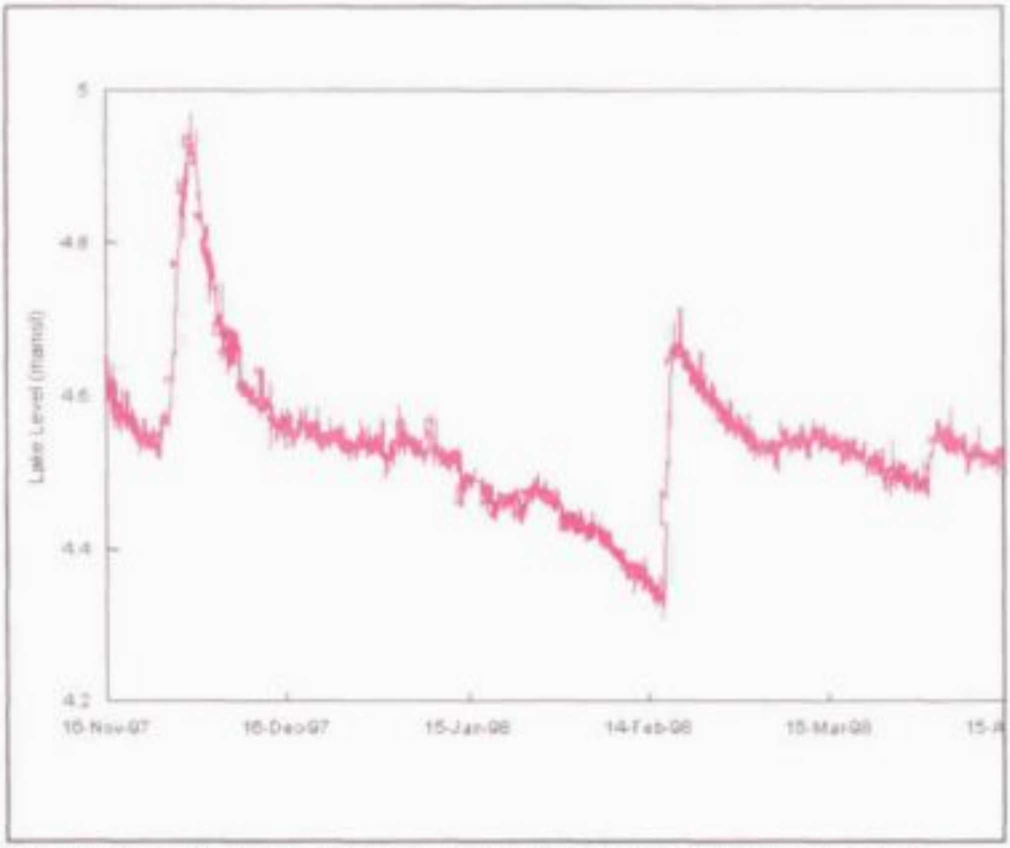

Figure 33 Water level observation for Lake Nhlabane (from RBM).

4.3.3 ABSTRACTION

The abstraction rate from Lake Nhlabane was provided by RBM and is shown in Figure 34. Withdrawal stopped in May 1994 and only resumed in January 1995 at a very reduced rate until June 1995. Normal abstraction only resumed in April 1996. This pattern is similar to abstraction rates from Lake Mzingazi (Figure 26).

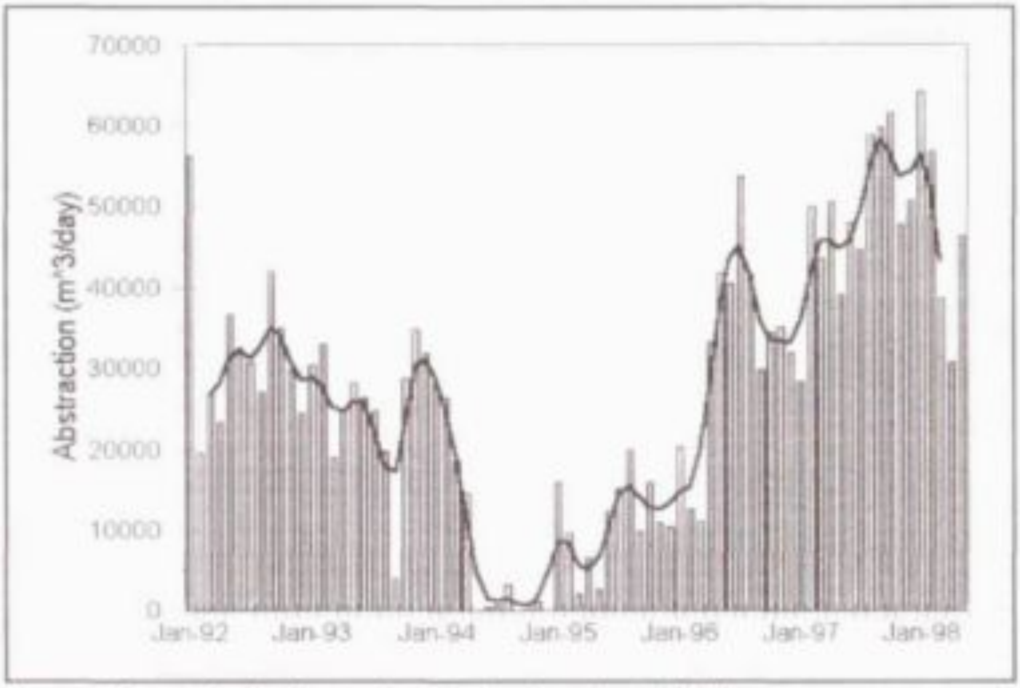

Figure 34 Abstraction rate of water from Lake Nhlabane.

4.3.4 SALINE INTRUSION

There are no known studies of saline intrusion potential for Lake Nhlabane. The lake volume is less 11×10^3 m^3 below mean sea level (Table 5) and consequently it is unlikely that there could be any significant problems.

4.4 LAKE CUBHU

Lake Cubhu is situated to the south of the Richards Bay Harbour and is assumed to have originally been part of the Mhlathuze Estuary but has become isolated by deposition processes on the northern sections of the lake (Figure 35). During flood events, the overflow from the lake is believed to flow through this section directly into the Mhlathuze estuary via a small channel linked to a series of canals on the Mhlathuze floodplain.

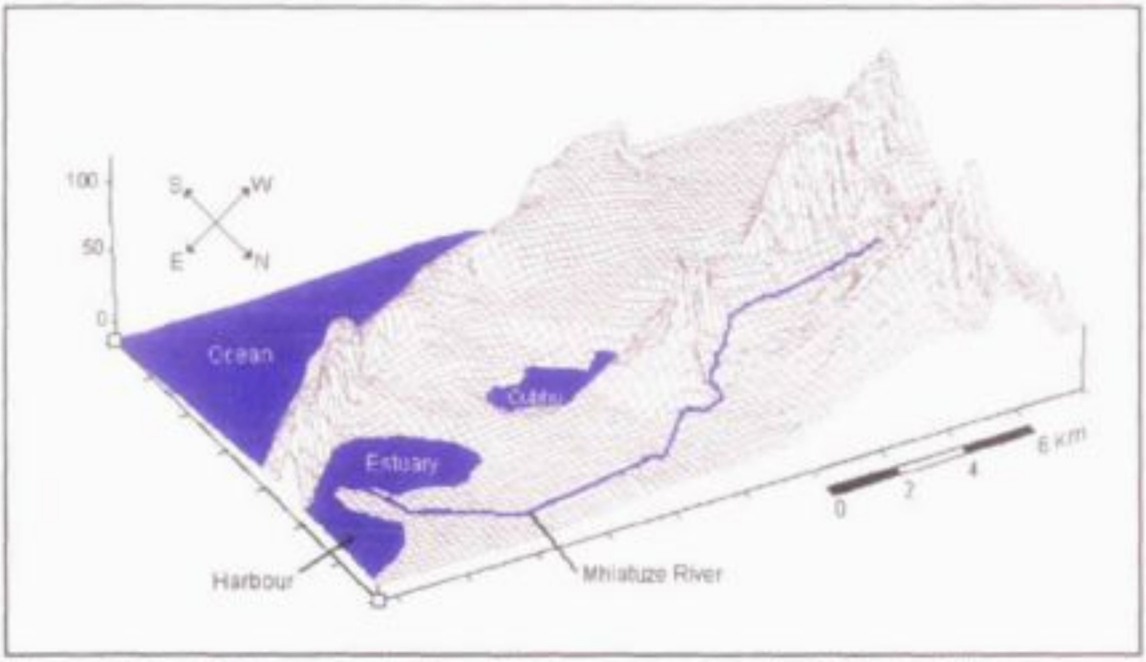

Figure 35 3 Dimensional view of the area surrounding Lake Cubhu

4.4.1 STORAGE CAPACITY

The bathymetric survey by Hattingh (1998) is portrayed by the 3D view in Figure 36. The storage capacity has been determined by Hattingh (1998) and is given in Table 4. The estimated level of the present outlet is assumed to be approximately 3 m *AMSL* which gives the lake a full capacity of roughly

$10.5 \times 10^6\ m^3$ (not indicated on Table 4) and a storage capacity of $0.7 \times 10^6\ m^3$ at mean sea level.

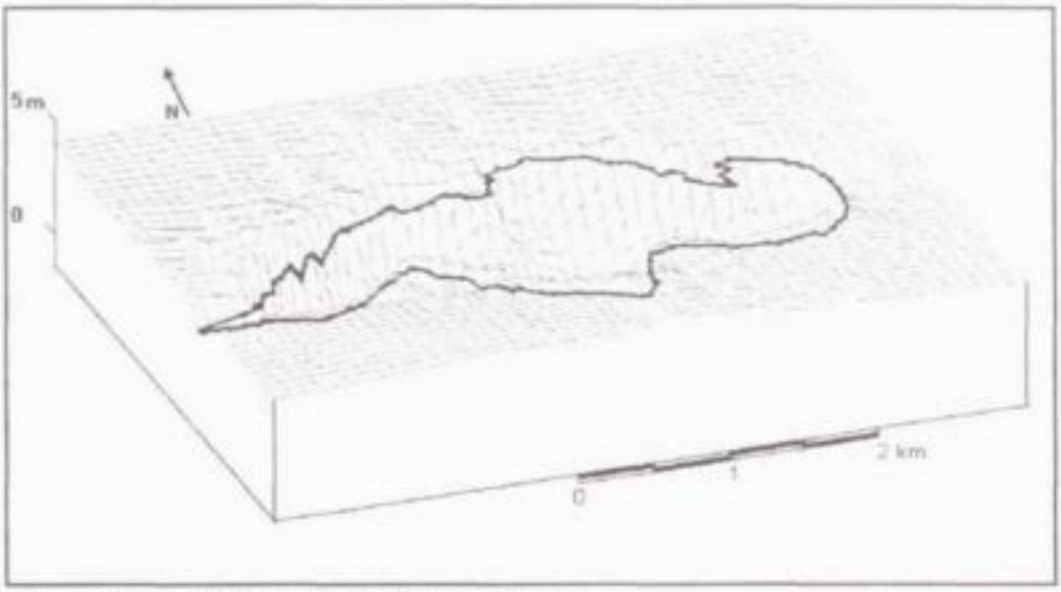

Figure 36 Bathymetry of Lake Cubhu.

4.4.2 ABSTRACTION

The rate of water abstraction at the Esikhaweni Water Treatment Works, provided by Otto Langenegger and Partners (1998), is given in Table 5. The peak rate of abstraction during the period of record was 17160 m^3/day in October 1997. However, it remains fairly regular at about 12500 m^3/day for most of the observation period.

Table 4 Lake Cubhu perimeter, area and volume (Hattingh, 1998)

Water elevation	**Perimeter**	**Surface Area**	**Volume**
m *AMSL*	km	$10^{6*}m^2$	$10^{6*}m^3$
-1	2.045	184310	0.032
-0.75	2.468	295559	0.091
-0.5	4.083	462655	0.184
-0.25	8.914	820273	0.335
0	**11.594**	**1821399**	**0.676**
0.25	12.261	2383110	1.207
0.5	12.004	2860863	1.866
0.75	12.478	3126396	2.614
1	13.605	3438812	3.435
1.25	13.709	3690215	4.327
1.5	13.061	3892080	5.277
1.75	12.804	4072550	6.272
2	12.458	4234005	7.311
2.25	12.231	4390209	8.389
2.5	12.005	4542136	9.506

4.4.3 WATER LEVEL

Lake levels have been recorded since October 1995 and are presented in Table 5. The lake has remained fairly static for the period of observation at about 3 m *AMSL*. Unfortunately the records do not cover the extreme floods of 1987 or the devastating drought of 1994/95. However, the abstraction during the drought remained consistently above 12 000 m^3/day which suggests that the lake had sufficient storage to sustain these levels of abstraction during dry periods.

Table 5 Lake surface elevation (m *AMSL*) and abstraction (10^3 m^3/day) from Lake Cubhu (from Otto Langenegger and Partners, 1998).

	1994		1995		1996		1997		1998	
Mon	Abstr	Lake Level	Abstr	Lake Level	Abstr	Lake Level	Abstr	Lake Level	Abstr	Lake Level
Jan			13.11		12.3	2.95	14.28	2.9	14.1	2.9
Feb			13.77		12.91	3	14.28	2.9	13.61	2.9
Mar	11.1		13.89		12.9	2.9	12.93	2.9		
Apr			13.41		12.45	2.9	12.61	2.9		
May			13.99		12.53	2.9				
Jun	13.11				11.75	2.9	12.49	2.9		
Jul	13.57				13.22	2.9	12.44	2.9		
Aug	12.77		12.47		13.83	2.9	12.44	2.9		
Sep	13.33		12.61		11.93	2.9	15.42	3		
Oct	13.05		12.38	2.85	12.03	2.9	17.16	3		
Nov					12.29	2.9	12.8	3		
Dec	12.88		12.96		12.86	2.9	12	3		

4.5 LAKE NSEZI

Lake Nsezi is the principle reservoir for water extraction by Mhlathuze Water (MW). The Empangeni TLC and many large industries are supplied with water by MW from this lake. The lake is fed by the Nseleni River (Figure 37) which passes just to the north of Empangeni and Nseleni. There is a permanent augmentation scheme which pumps water from the Mhlathuze River to the Lake. The lake is also maintained by some groundwater seepage from the local primary aquifer and direct recharge from rainfall.

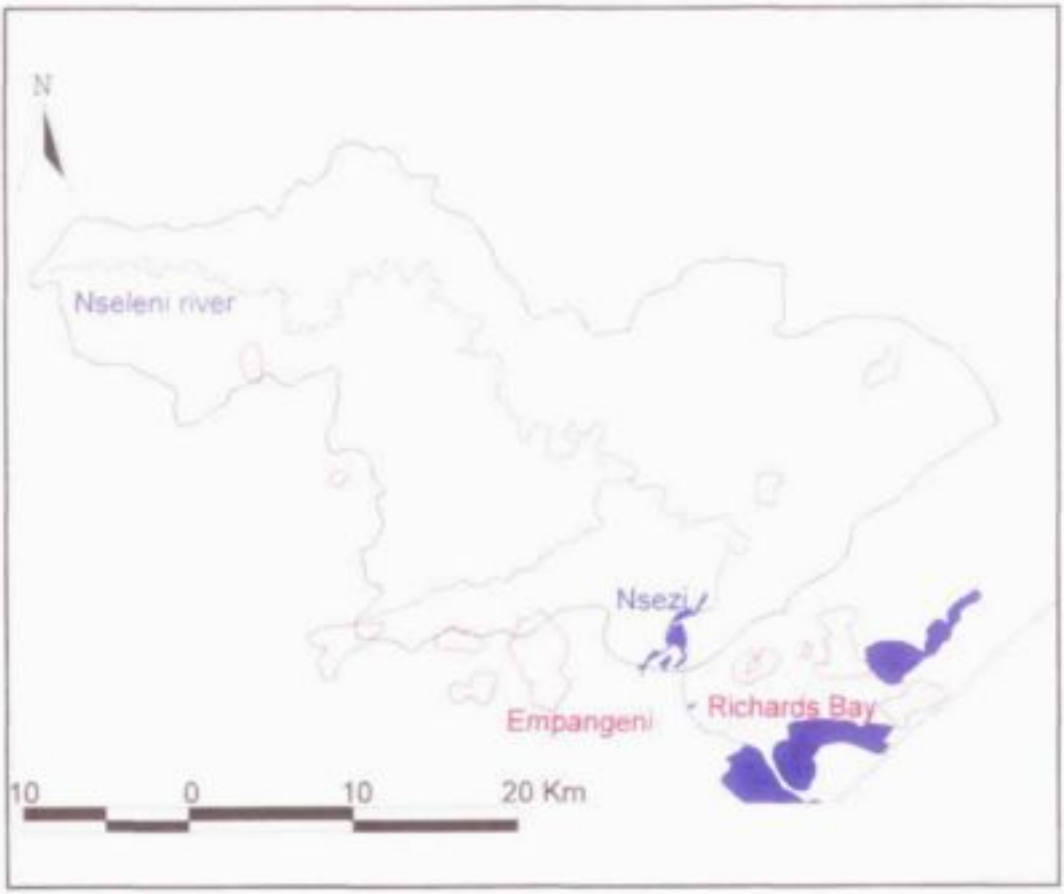

Figure 37 Nseleni catchment and lake Nsezi.

4.5.1 NSELENI RIVER.

The discharge from the Nseleni River has been estimated using [1] the Variable Time Interval Model in HYMAS that was developed by Hughes *et al* (1994) and [2] the WR90 data (Midgley *et al*, 1994). Since there are no observations of runoff from the river, the simulated discharge using both these models cannot be calibrated. However, they do differ and there is no basis for accepting one or the other. Both the WR90 and the VTI values are shown in Figure 38.

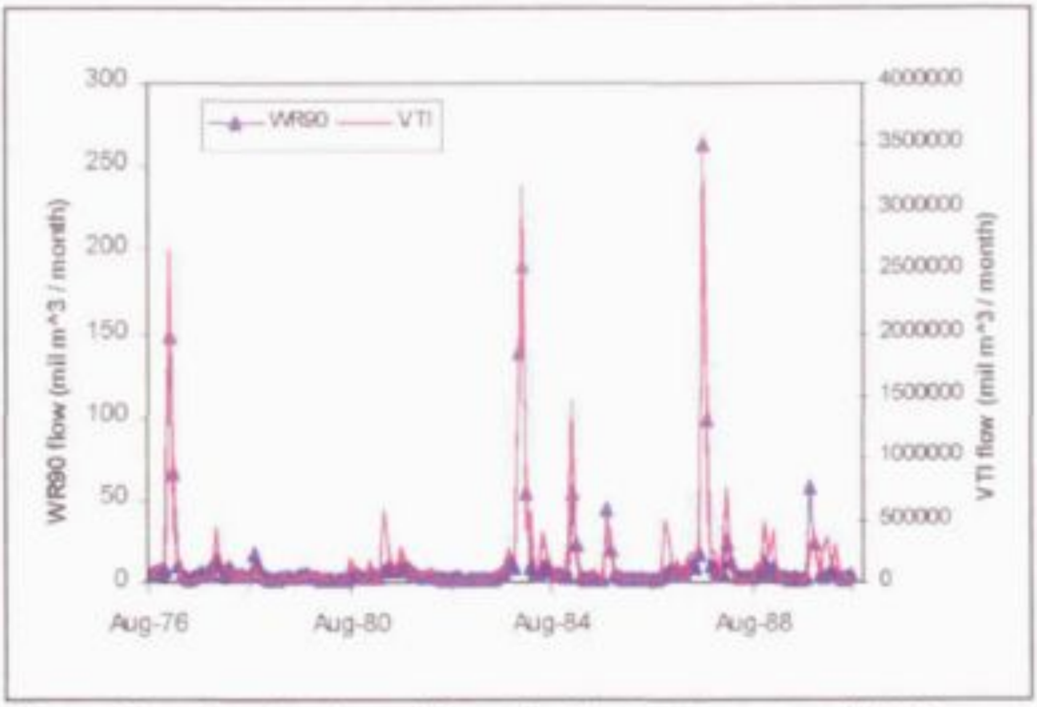

Figure 38 Simulated runoff from the Nseleni river using WR90 (Midgley *et al*, 1994).

4.5.2 LAKE LEVEL, AUGMENTATION AND DISCHARGE RATES

The level of Lake Nsezi is generally maintained at 6 m *AMSL* by the transfer of water from the Mhlathuze weir (W1H032). There are no regular recorded observations of lake level or the outflow from the lake. However, the transfer from the Mhlathuze river often continues even when the lake is overflowing in order to dilute the very high dissolved solids concentration in the lake (Botes, pers comm). Records of the water transfer from the river to the lake only commenced in October 1992 and are presented in Figure 39.

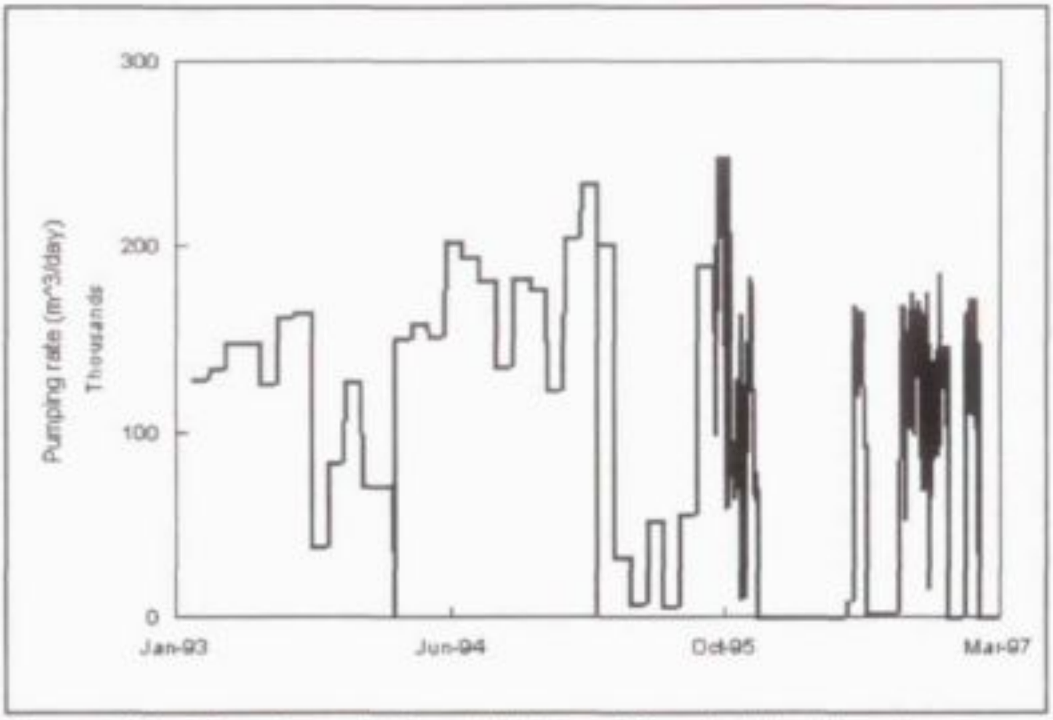

Figure 39 Transfer rate from Mhlathuze River to Lake Nsezi

4.5.3 STORAGE CAPACITY

The topographical 3D profile of the lake and surrounding areas is shown in Figure 40. The lake is maintained at a level of 6 m above mean sea level (*AMSL*) to sustain a reliable yield at all times for Mhlathuze Water (V Botes, pers com). However, DWAF indicate a sustained level of 6.2 m. The lake is generally about 1m deep and is covered in large sections by reed beds that make it difficult to identify the water surface from aerial or satellite photographs. However, it appears that the main channel of the Nseleni River enters the lake on the western sector and flows into the large reed mass. The inflow may act as a sediment source which is deposited against the vegetation in the main body of the lake. From aerial photographs, the flow then appears to travel along the south eastern shore. The upper reaches of the lake appear to be remnants of previous river channels. The storage capacity of Lake Nsezi was estimated to be 834000 m^3 for a lake level maintained at 6.2m amsl from the bathymetric survey data provided by Department of Water Affairs and Forestry (DWAF). This data has been updated by Hattingh (1998) for a Lake Water Requirement (LWR) study commissioned by DWAF. The Lake perimeter, area and volume for different water level elevations are given in Table 6.

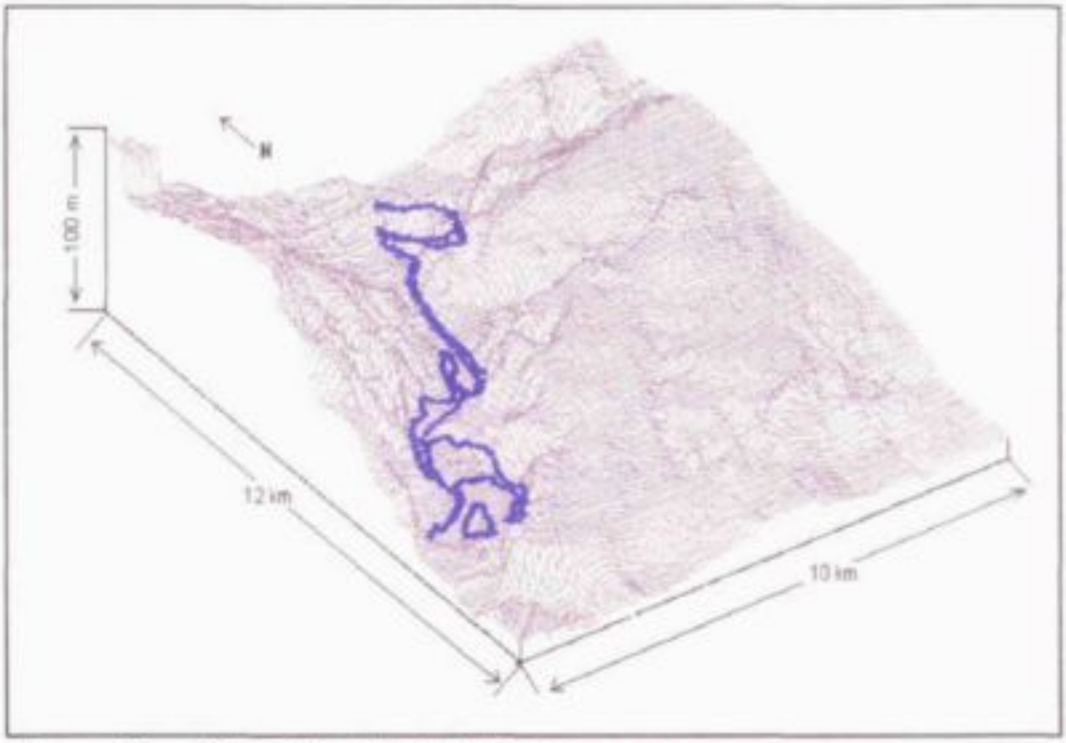

Figure 40 3D profile of Lake Nsezi.

4.5.4 WATER ABSTRACTION RATES

The abstraction rates for Lake Nsezi since 1994 are shown in Figure 41. These data have been supplied by Mhlathuze Water . There has been a large reduction in abstraction from 1996 which occurred when the Richards Bay TLC, RBM and Mposa river (upstream) abstractions all reverted to their previous water resources.

4.5.5 GROUNDWATER SEEPAGE

Groundwater seepage into the lake has been estimated from simulation studies using the Modflow groundwater model. The level of groundwater interaction for this lake is unknown, however, it has been treated in the same way as the other coastal lakes. The model simulations have been derived through the extrapolation of parameter values from the detailed calibration studies conducted on Lake Mzingazi. Because there are no discharge and lake level measurements for model parameter estimation, the values have been adjusted to achieve a water balance for the lake. It is assumed that Lake Nsezi groundwater interaction functions in a very similar fashion to Lake Mzingazi for the purposes of this study.

Table 6 Lake Nsezi perimeter, area and volume (Hattingh, 1998)

Water level	Perimeter	Area	Volume
m amsl	m	m^2	m^3
3	1385	21525	0
3.25	1585	35566	7106
3.5	1691	51042	17902
3.75	1844	67953	32747
4	7159	218779	32747
4.25	7505	279888	1144270
4.5	7851	343955	192189
4.75	8198	410978	286494
5	9363	517567	398751
5.25	20166	2276175	941195
5.5	20423	2493981	1537333
5.75	20680	2717805	2188664
6	20937	2981987	2896687

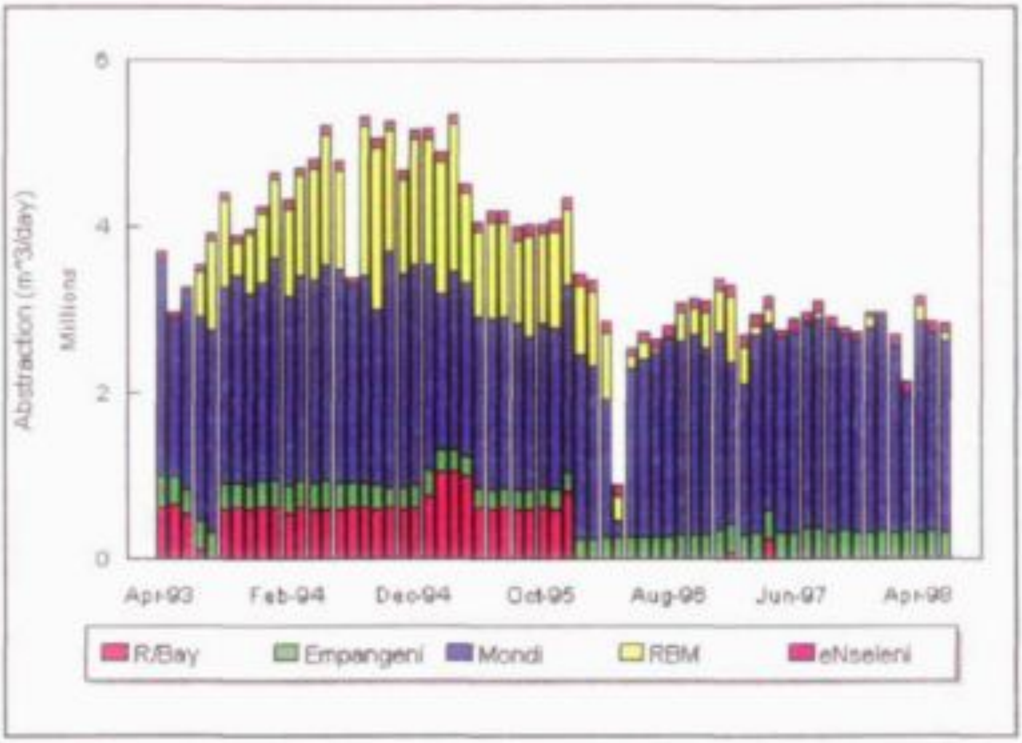

Figure 41 Abstraction rates for Lake Nsezi.

Section 5 COASTAL GEOLOGY

Richards Bay lies on the Zululand coastal plain which stretches from Umlalazi River, on the southern end of the plain, up the coast of Zululand and northward through Mozambique. This entire coastal plain was formed in recent Cenozoic time (post Cretaceous) through sedimentary erosion and deposition (Table 7). Consequently, all the information from various studies along the whole of the east coast of Southern Africa have been used to form a geological model of the Zululand and Richards Bay coastal plain area. From the classified geological formations that have been indicated in the various geological surveys of the region, those formations that have been recorded in Richards Bay are indicated in Table 7. The following sections of this report give a brief description of the different strata but concentrates on those strata that are important for the numerical studies presented later in the report.

Table 7 Summary of geological formations in the Richards Bay area (From Whitfield and Johnstone, 1993).

	Period	Epoch	Years	Lithology	Formation	Present at Richards Bay
CENOZOIC	Quaternary	Holocene		Sand, Silt Clay (alluvium)		yes
		Upper Pleistocene		Dune and beach sand		yes
				Sand and aeolianite	Kwambonambi	yes
		Middle - Upper Pleistocene		mudstone, shale, sandstone, lignite sand	Port Durnford	yes
				Berea red clayey sand, sand	Bluff	Only South of Richards Bay
	Tertiary	Miocene		calcareous sandstone	Uloa	yes
				Siltstone, sandstone	Richards Bay	??
	Cretaceous	Senonian		Siltstone, sandstone	St Lucia	yes
	Jurassic			Dolerite intrusions	KAROO	??
				Basalt		

5.1 EARLY GEOLOGY (PRE-CRETACEOUS)

Over a 100 million years ago, Natal was a smoothly undulating landscape of mainly volcanic rocks which was inherited from Gondwanaland (King, 1972). In Zululand, near Empangeni, the granite-gneiss basement was elevated between east-west crustal fractures to form the elongated fault block of the Ngoye Range. The basement rocks are overlain by the Natal Group. Upon this basement there is sandstones which in turn is overlain by sedimentary strata of the Karoo Supergroup and topped off with volcanic lava flows known as the Lebombo Group with attendant faulting. Both the sediments and the lava may be several thousands of metres thick (King, 1972). According to McCarthy (1961), jointing is poorly developed in the sequences of massive basaltic groundmass and there are no indications of intervening weathering and erosion between eastward-tilted amygdaloidal flows. These basaltic rocks are sub-horizontal throughout the Natal Midlands but they tilt between 5° and 15° in various directions in the coastal belt forming the Natal Monocline with some attendant faulting (King, 1972). These faults will have a profound impact on groundwater modelling and need to be identified before the conceptual models are used in the numerical simulations. The exposure of pre-Cretaceous granite-gneisss and Basalts to the west of the Zululand Coastal Plain is indicated by Worthington (1978) in Figure 42. This coastal plain stretches from Mtunzini through northern Kwazulu-Natal and Mozambique and is composed of post-Cretaceous sediments.

5.2 CRETACEOUS PERIOD

The Cretaceous sediments underlie the entire Zululand coastal plain. The lower layers of the Cretaceous consist of river and beach deposits where the main rocks are chalky sandstone, shale and limestone. However, the upper Cretaceous consists of deep water marine sediments that have been deposited on a seaward sloping continent. According to King (1972), during the

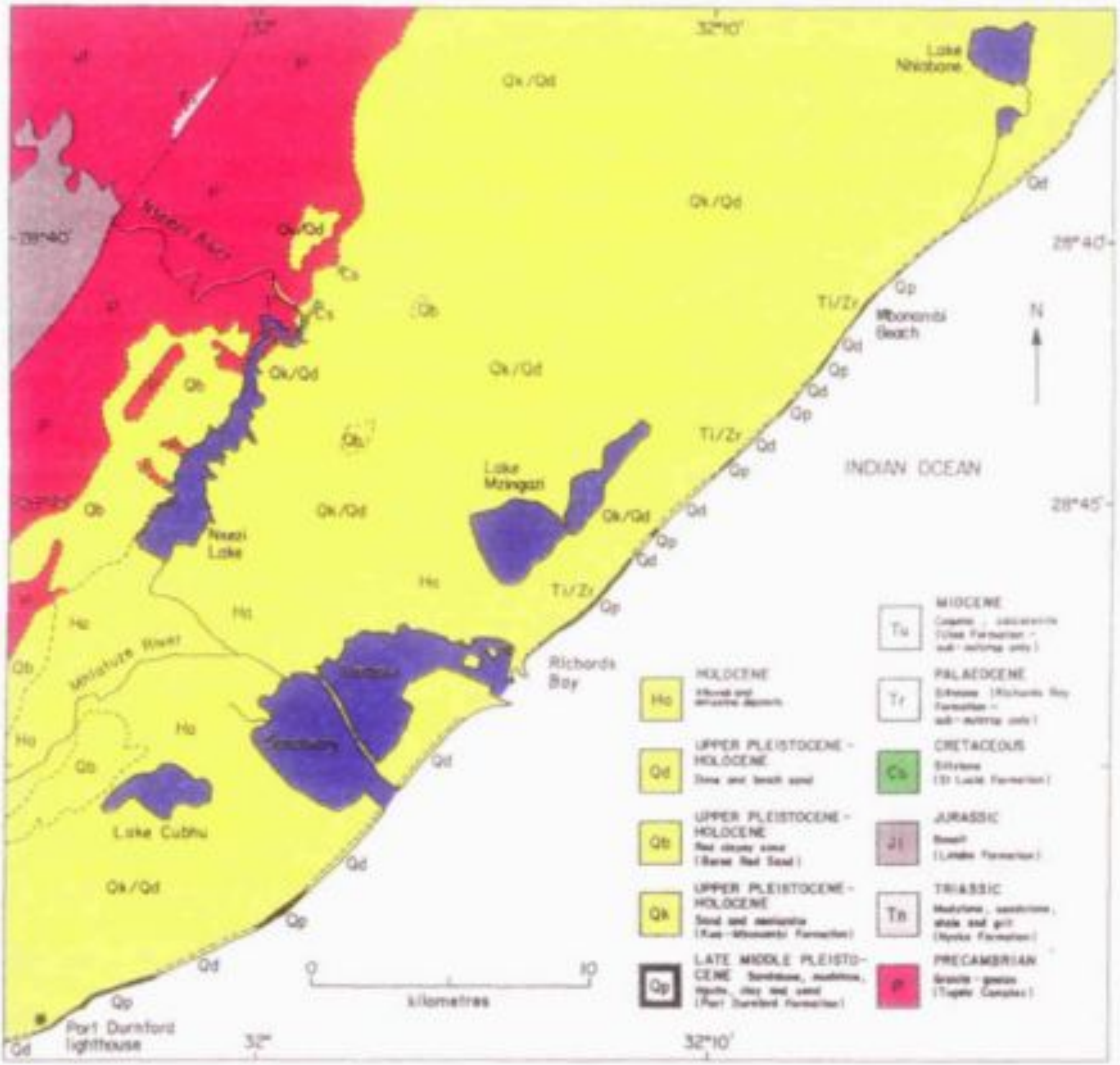

Figure 42 Simplified Geological map of Richards Bay region (after Worthington, 1978)

Cretaceous period, when the coastal areas of Natal were below sea level, sediments where deposited along the continental shelf to form siltstone and mudstone marine strata. Following coastal upliftment and declining sea level, these marine strata were elevated and eroded so that they are now exposed along the banks of the principal rivers in Zululand (Umfolozi, Hluhluwe, Umzinene and Mkuze) and around sections of the coastal lakes in the north. Several hundreds of metres of strata are represented (up to 2500 m in Mozambique) all dipping seaward at 1 to 3 degrees (Worthington, 1978).

This layer was exposed with a rich collection of marine fossils during the construction of the new harbour facilities. Examples of large ammonites and other fossils were observed in the spoils of the dredging at the new harbour docks.

5.3 TERTIARY PERIOD

After the deposition of the Cretaceous formations, which took place about 100 to 50 million years ago, the sea-bed was uplifted to form coastal lowlands for a further 30 million years before the coastal plain was again submerged during the Miocene period when further deposition occurred. The marine deposits during this period (Miocene), which are the richest fossil bearing deposits of South Africa (King, 1972), extend from Richards Bay through Uloa, on the Umfolozi River, to Hells Gate at False Bay on Lake St Lucia and as far as Kosi Bay (Meyer *pers comm*). However, since they are not specifically mentioned in the detailed geological survey of many areas, it is assumed that they are neither continuous nor are they well defined in this region.

These sediments comprise a hard coarse coquina of shell fragments (Uloa formation) and an aeolian cross-bedded calcarinite (termed Umkwelane formation by Botha (1997) in his stratigraphy of Figure 43). The Umkwelane has been interpreted as being of both Miocene and Pliocene age by Frankel (1968)

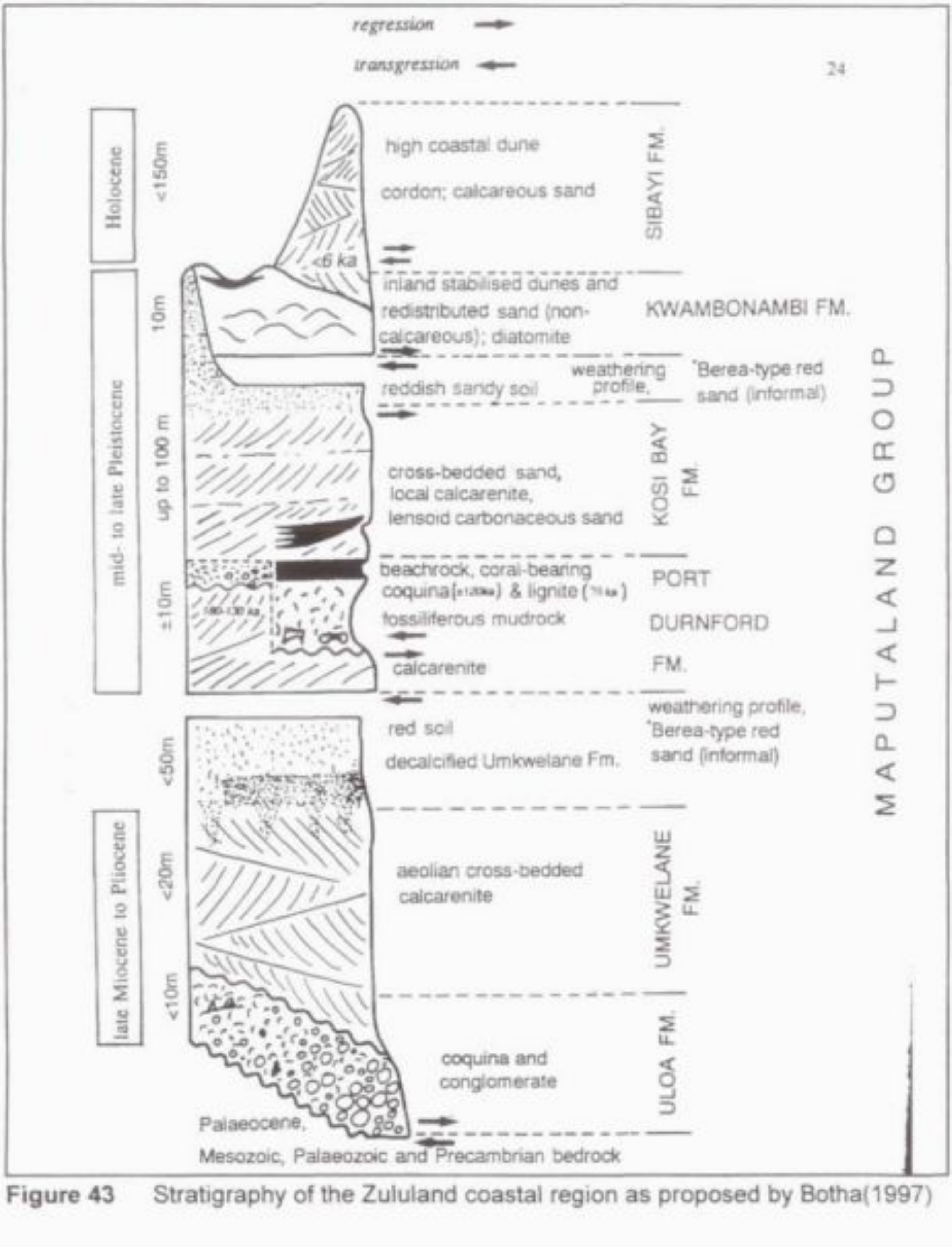

Figure 43 Stratigraphy of the Zululand coastal region as proposed by Botha(1997)

and King (1982).

Simmonds (1990) mentions the conspicuous absence of this layer in many places and Maud and Orr (1975) describe its erratic distribution. Worthington (1989) attributes the absence of this layer to drainage erosion while Hattingh (1997) proposes that the Miocene layer lies in confining beds which run parallel to the coast. Hattingh (1997) further suggests that these marine deposits are either reef relics or step faulting which caused preferential surface erosion due to accentuating drainage lines.

5.4 PLEISTOCENE PERIOD

The Miocene submergence was short and the coastal plains were again exposed for millions of year. According to King (1972), the sea returned about 5 million years ago, during the early Pleistocene Period, to transgress strongly over the land. It covered the surface of the present Zululand Coastal Plain across the soft Cretaceous and Miocene strata until the sea reached the Pre-Cretaceous bed rocks near Empangeni. As the water slowly deepened, the sea laid its own deposits of lime rich Pleistocene sandstone everywhere across the plain (King, 1972).

These Pleistocene strata were much more widespread than the Miocene but they were softer. When the sea receded in stages, towards the end of the Pleistocene, these deposits broke down into the loose sand which everywhere covers the coastal plain today. During phases of standstill in the regression of the sea, notches were cut by the wave action into the coastal plain surface and these temporary shore lines of reworked Pleistocene sands piled up into lines of coastal dunes that still trend for long distances north-northeast along the coastal plain (King, 1972). By the end of the Pleistocene retreat, the sea had continued well beyond the present shore line and the last of the Pleistocene coastal dune forms are still to be found as offshore shoals at Glenton reef

(Mtunzini) and Leven shoal (St Lucia).

These deposits, collectively known as the Port Durnford Formation, are preserved beneath the interlayered calcareous sandstone and uncemented sands. The upper surface of the Port Durnford varies considerably in elevation owing to post-depositional erosion, deposition and reworking (Davies Lynn and Partners, 1992).The Port Durnford is thought, by Maud (1968) to have been deposited at sea-levels of about 33-45 m above the present level while Hobday & Orme (1974) suggest levels of 8 m. However, Oschadeleus & Vogel (1996) suggest that this formation was deposited in a freshwater lake environment.

The Port Durnford Formation has been comprehensively studied by Hobday and Orme (1974) who found that this sequence consists of a lower argillaceous member overlain by an upper arenaceous member (Figure 44). Maud (1968) describes the stratigraphic succession of this Formation (from bottom to top) according to Table 8.

Table 8 Stratigraphic Succession of the Port Durnford by Maud (1968)

*	Red and yellow mottled consolidated sand
*	Yellow mottled consolidated sand passing downwards into strongly cross-bedded white consolidated sand (aeolian deposition)
*	Lignite or peat with admixed sand
*	Yellow brown ferruginised sandstone
*	Blue grey sandy mudstone with fossil remains

According to Maud (1968) and Hobday and Orme (1974) the lower more argillaceous member was deposited under transgressive conditions. This is evidenced by the presence of a truly blue-grey sandy mudstone with fossil remains. This lower layer of the Port Durnford Formation is overlain by a marine regressive member which was deposited under littoral and subaerial conditions as evidenced by the lignite bed and the cross-bedded aeolian consolidated sand. Maud (1968) reports that the thickness of these old red sand beds is 20 to 25 m. The lithology of these sediments is suggestive of a marine shallow-water, terrestrial and fresh-water lacustrine deposition (Maud, 1980 and Hobday, 1976). Good outcrops of this Formation are found along sea-cliffs (Maud and Orr, 1974) and isolated exposures also occur along the margins of Lake St Lucia.

These Pleistocene deposits are much more widespread than the Miocene and Pliocene deposits. It is present beneath most of the coastal barrier complex. The formation is exposed in some of the cliffs on the beaches north of Richards Bay. Hobday and Orme (1974) suggest that gaps in this formation were formed by the late Pleistocene streams breaching the coastal barrier.

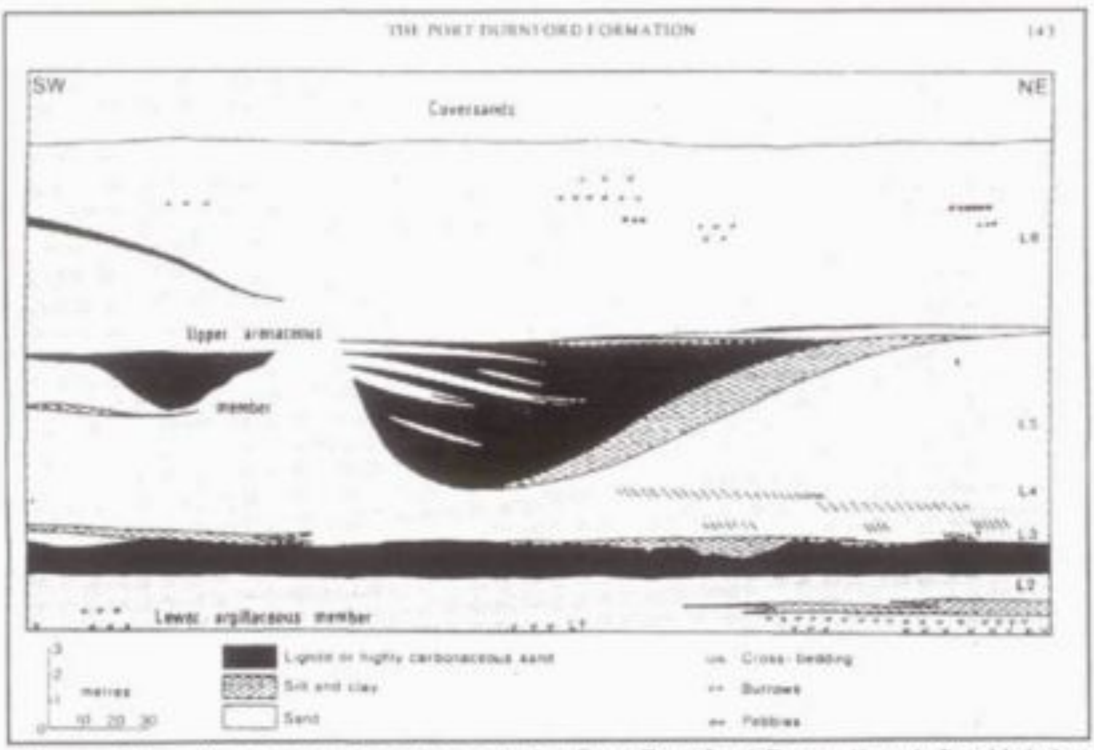

Figure 44 A cross-section through the Port Durnford Formation (after Hobday and Orme, 1974)

5.5 HOLOCENE EPOCH (RECENT)

The low level of the sea at the end of the Pleistocene Period caused lower courses of the Natal Rivers to become incised into the underlying strata giving rise to coastal lagoons when the sea returned to the present level (King 1972). The incisions cut deeply into all the strata including the Cretaceous in many areas. Figure 45 shows the deep incision into the Cretaceous for a transect from east to west just south of Lake Nhlabane (adopted from Whitfield and Johnstone, 1993). Another incision is apparent in the cross sectional transect through the Umfolozi valley (shown in Figure 46) and also the Mhlathuze Valley inland of Richards Bay. Similar paleo channels are found on the eastern shores of Lake St Lucia (Davies Lynn and Partners, 1992) and other KwaZulu-Natal estuaries.

These more recent sands that were deposited during the Holocene Epoch are comprised of successive units of boulder beds, old red sands, younger coversands, coastal dunes and calcarenites of aeolian, estuarine and alluvial origin (Hobday, 1979; Tinley, 1985). This lithology, according to Hobday (1979), reflects a complex history of erosion and sedimentation during the Quaternary Period. This view is supported by Frankel (1968) who observes that Tertiary and Quaternary shallow-water as well as dune sediments along the KwaZulu/Natal coastal region must have originated as a result of minor eustatic or epeirogenic movements which caused transgressions and regressions over large areas of the coastal region.

The Zululand coastal plain is characterized by the north-south trending coastal dune ridges. These dunes attain elevations of approximately 190 metres to the south of St Lucia Estuary and flatten out northwards into the very low hummocky structures of Maputaland (Hobday, 1976). The dune ridges consist of homogeneous sand which overlies boulder and pebble bearing deposits. Hobday (1976) attributes these sands to aeolian processes which accompanied marine regressions. He also ascribes the basal coarser (estuarine or beach) deposits to a transgressive-regressive couplet.

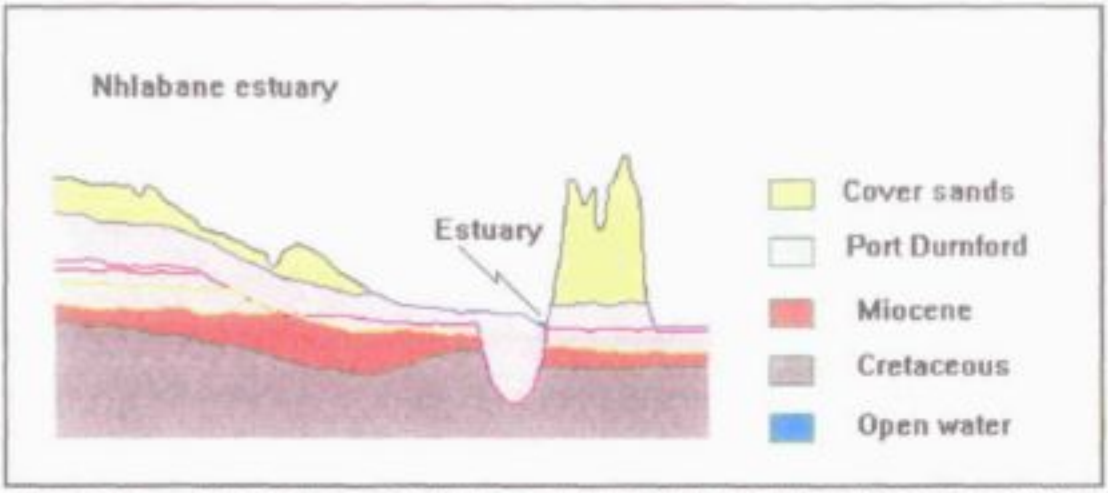

Figure 45 Transect across Nhlabane Estuary (adapted from Johnstone, 1992).

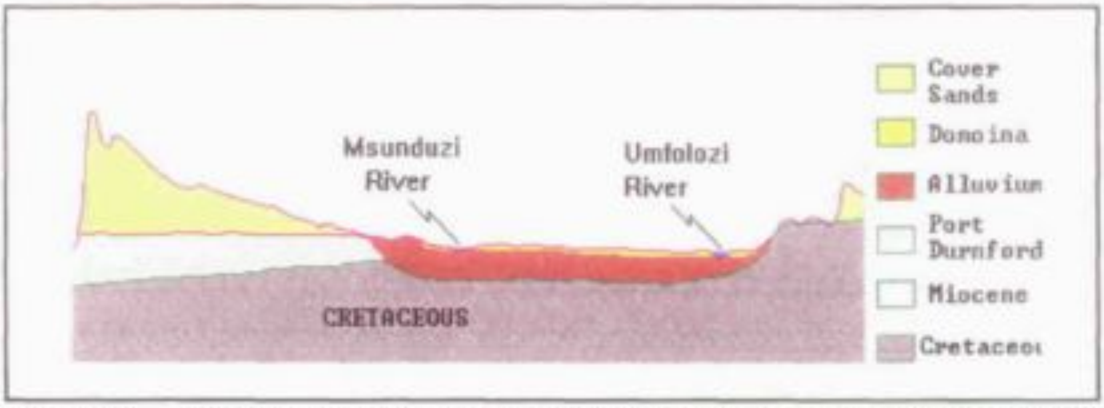

Figure 46 N-S transect through the Umfolozi valley in the southern section of the model domain (adopted from Maud and Orr, 1975)

5.6 CONCEPTUAL GEOLOGICAL MODEL OF RICHARDS BAY

The geohydrological investigation of these coastal sedimentary deposits require an accurate determination of the various aquifers and their physical dimensions together with the hydraulic characteristics of the layers and the variability within the layer. This involves the derivation of a detailed conceptual model of the geological structure which becomes increasing important for the solute transport studies discussed in section 9. The regional assessment of the geological formation described above has been used together with all available information to construct a hydro-geological model of the Richards Bay Area for numerical studies.

5.6.1 GEOLOGICAL INFORMATION

All available borehole information has been sourced, and analysed through the use of Hydrocom (HydroSolutions Inc., 1993) and Groundwater for Windows (Braticevic and Karanjac, 1995). Borehole logs have been provided by most of the major industries in the region who have done geological surveys for various purposes. Worthington (1978) did a detailed survey around Lake Mzingazi and the harbour during the feasibility phase of development. RBM have an ongoing geological explorations along the entire coastal section which has been made available for this study. Alusaf, Mondi, and IOF conducted detailed soil and geological studies for construction purposes which they have made available. Portnet and Uthungulu Regional Council have also released some of their borehole information for these studies.

The location of all identified boreholes in the region are shown in Figure 46. Additional information is available from Portnet, but the number of their boreholes for the harbour in the database are considered adequate for the purposes of this study. However, there are still areas with very few boreholes which makes it difficult to determine the existence of certain geological features in these localities. There were also problems with a number of the borehole logs. More recent information has become available but was too late to include in this study.

The borehole information was checked for consistency in relation to the general geological description above. Several boreholes were identified with incorrect locations and these were corrected where possible or discarded from the data set.

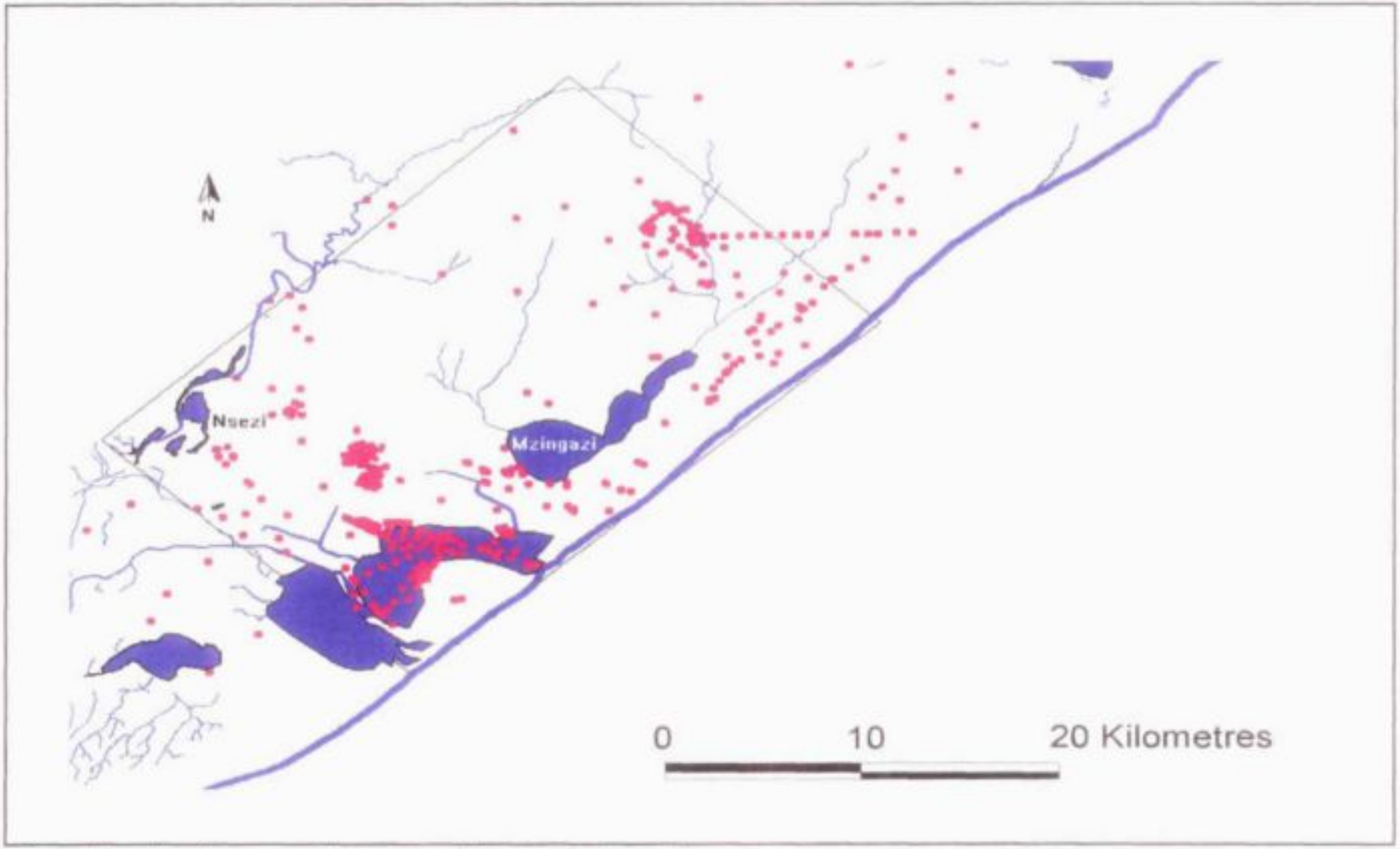

Figure 47 Location map of known borehole observation points.

The Interpretation of borehole logs and soundings provided a big challenge to this project. All borehole data were stored in the Hydrocom database. Several problems were encountered while trying to computerize the geological logs, namely:

- Hydrocom has a limited amount of geological descriptions.
- Locations of some boreholes were too vague to include.
- Some boreholes did not go deep enough to give the required information.
- Borehole log value of surface elevation did not always correspond with ortho photo contours.

5.6.2 STRATIGRAPHIC SURFACE LAYERS

Numerical modelling methods require the specification of the physical dimensions of the different aquiverous units. The upper and lower boundaries together with the hydraulic characteristics determine the transmissivity and yield of these units. Consequently, considerable effort has been made to estimate the surface profiles of all the important hydrogeological layers in the region.

5.6.2.1 CRETACEOUS LAYER

The Cretaceous is assumed to be the base of the primary aquifer in the region and its upper surface forms the lower boundary of the system under investigation.

All available borehole logs were used in conjunction with the previous studies of Worthington (1978) and Maud and Orr (1975) to derive an estimate of the surface contours. Several assumptions about the Mhlathuze River migration and erosion have been made to create cross-sectional profiles in regions where there is limited information. The following assumptions and procedures were applied in the construction of the Cretaceous surface profile:

- Boreholes that did not reach this layer were used to calibrate the contours (i.e. make sure that the contour value is at least lower than the deepest point of the borehole). Where this was not the case, a log was added to the model with a value that was 1m below the deepest point of the borehole to force the contours to fit this information.

- The Cretaceous contours from Webb (1972) and Worthington (1978) were digitized and added to the data together with the geophysical soundings from Worthington (1978). Sounding #20 was ignored, because 6 boreholes and 2 soundings around it had values at least 20m lower.

- The inland boundary of the coastal plain was assumed to have a Cretaceous layer at or near the topographical surface from geological maps.

- For the Nyokaneni river, located in the middle of the area, the Cretaceous layer was forced to the topographical surface.

- The geological data of borehole CA93 was unacceptable (granites and shale), but the deepest point of the borehole was used as the upper elevation of the Cretaceous.

- Boreholes in the area of the Nundwane river, indicated that the Cretaceous level is rather deep, but SURFER created separate holes instead of a more acceptable channel. Seven data points (three of which are along the river) were added to form a channel.

- The inferred paleo channels presented by Worthington (1978) were not used because there were more borehole logs in many of these regions.

In total 562 points were used to create this surface. The derived surface elevation of the Cretaceous and Paleocene siltstones were discussed with local geologists (Maud, Hattingh, Meyer, Rheeder & Barnes) before being accepted in this project.

The final estimated surface contour of the upper surface of the Cretaceous siltstone/mudstone deposits in the Richards Bay Study area is shown in Figure 47.

5.6.2.2 MIOCENE SURFACE

The late Miocene to Pliocene layer is composed of three units comprising the coquina & congromerates of the Uloa formation, the aeolian calcerenite of the Umkwelane Formation and the Berea-type red sands (Figure 43). The borehole logs are not always sufficiently detailed to identify these layers. There is also a considerable amount of subjectivity in the logging and consequently, the identification of this layer in the available data set is also subjective. These deposits are not continuous (Maud and Orr, 1975; Worthington, 1989; and Simmonds, 1990) but their suggested uniform orientation (Hattingh, 1998) has been used to estimate their spatial extent.

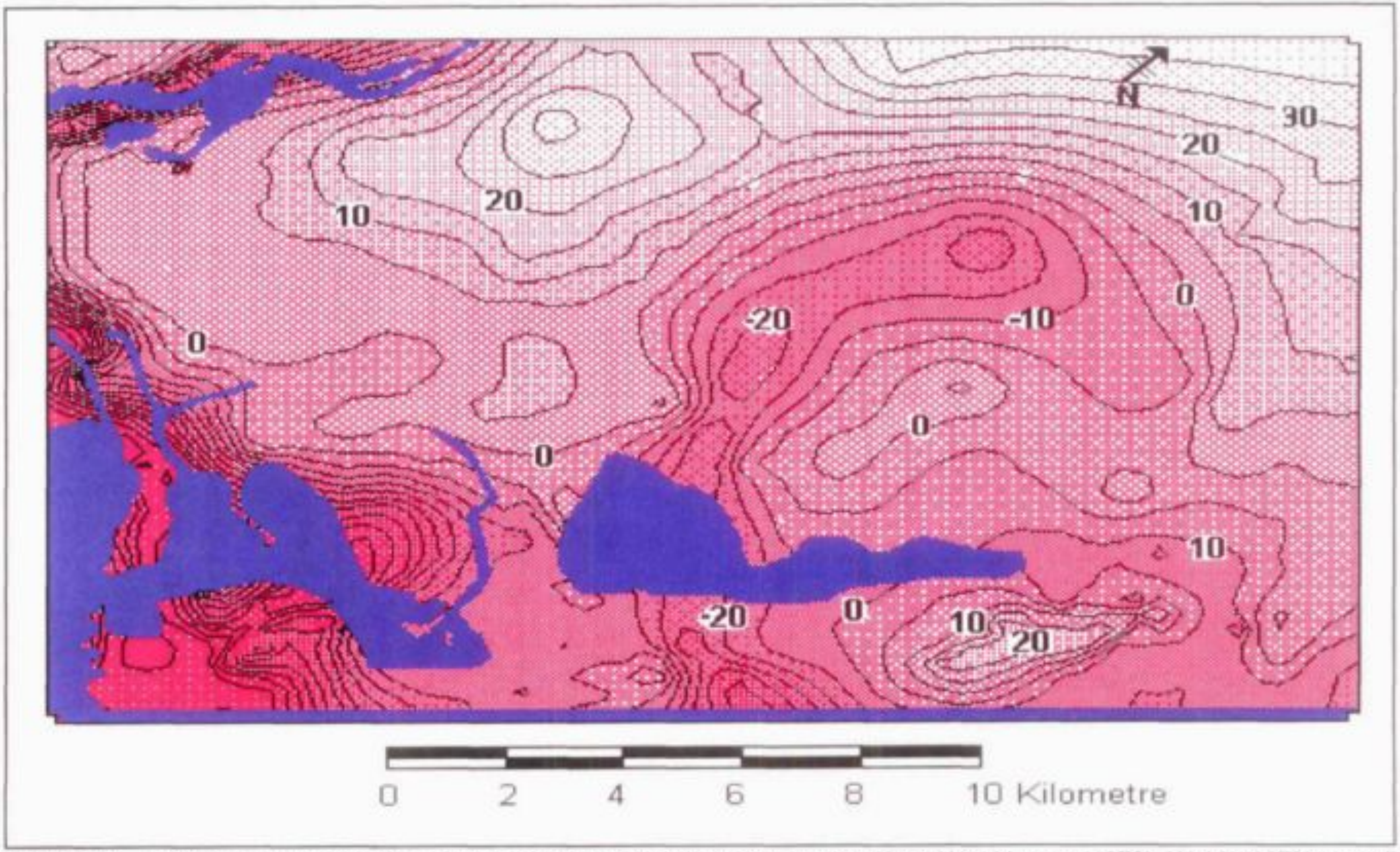

Figure 48 Upper surface of the Cretaceous siltstone formation reconstructed from Worthington (1978), Webb (1972) as well as all recent borehole logs.

The thickness of the Miocene deposits were determined by grouping the study area into regions where there was some mention of the Miocene stratum in the borehole logs. It was assumed that some areas in between were devoid of Miocene deposits. Subjective estimates were applied to the exact orientation and to the horizontal extent of the beds, particularly in those regions where there were few boreholes (marked with "?" in Figure 49). The location of all those borehole logs with Miocene sediments (□) and those without Miocene sediments (x) layers is shown in Figure 49. The more recent information is identified as a separate colour with the same symbols .

The surface contour elevation of the Miocene layer was estimated by superimposing the observed thickness of this layer on top of the Cretaceous layer upper surface. The resulting contour map is shown in Figure 50. In general, the Miocene deposits do not correspond with the incisions (paleo channels) in the Cretaceous layer but occur mainly on the higher elevations.

5.6.2.3 PORT DURNFORD

The Port Durnford formation is comprised of the lower argillaceous member which is overlain by the upper arenaceous member. However, most borehole logs do not differentiate adequately between these layers or the more recent cover sands. Consequently it has been extremely difficult to derive reasonable estimates of the upper surface of these units. Because it is difficult to distinguish these layers or their hydraulic properties, they have been considered to be a single unit for the purpose of numerical studies.

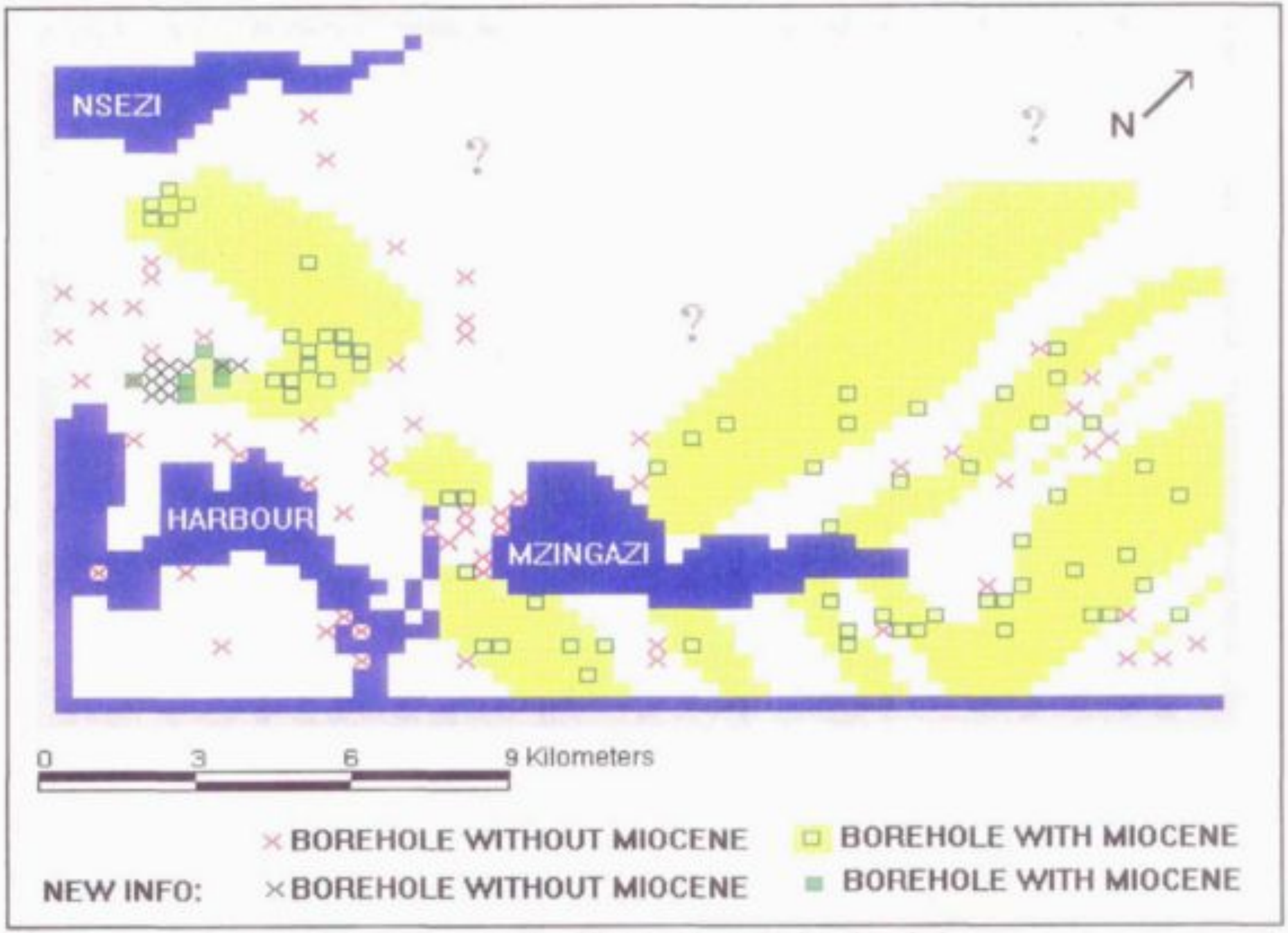

Figure 49 Estimation of the thickness of the Miocene deposits from boreholes

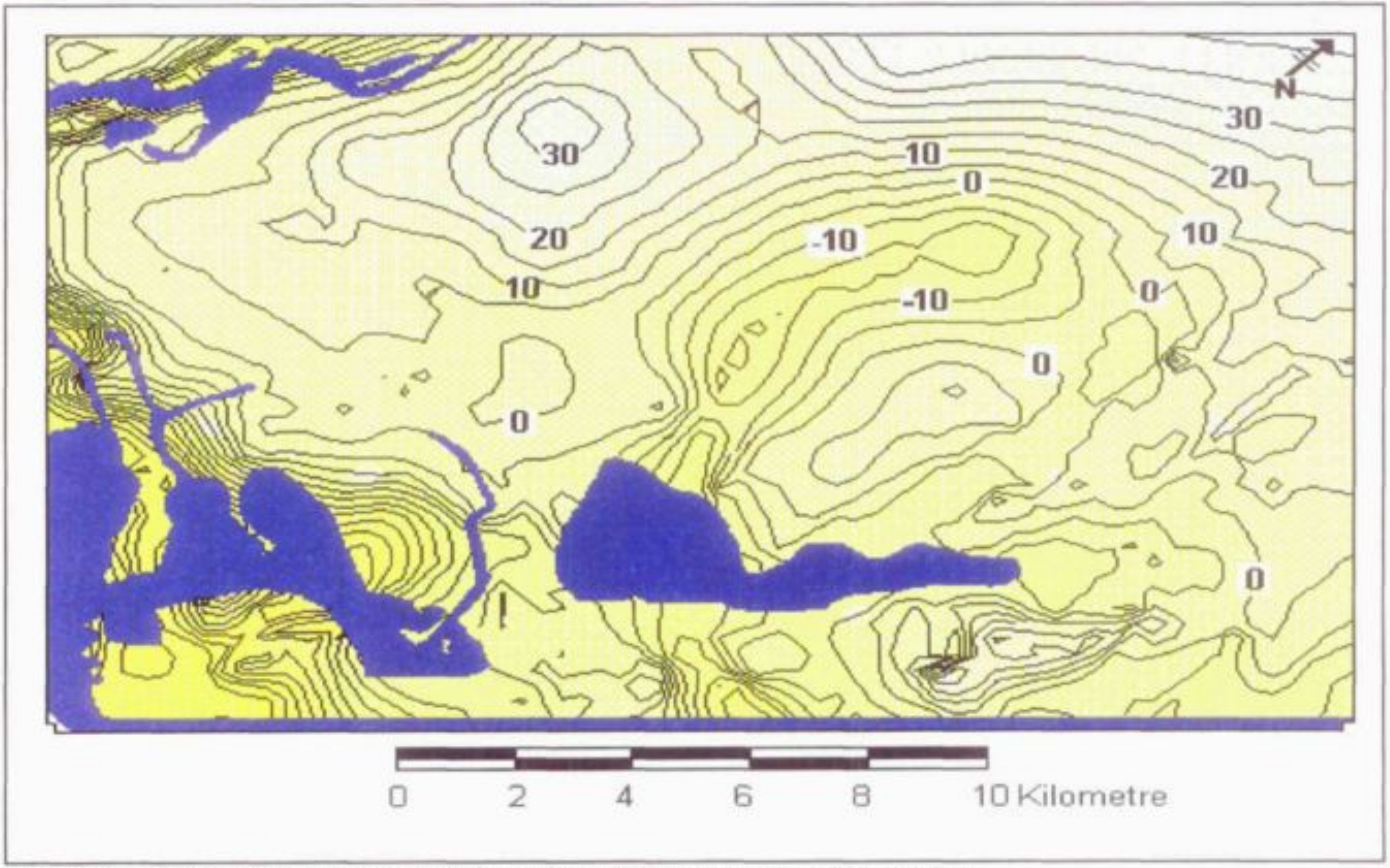

Figure 50 Estimated upper surface contours of the Miocene deposits in Richards Bay

5.6.2.4 TOPOGRAPHICAL SURFACE

The topographical surface of the region was derived from digitized contours of 1:50 000 maps. In the flatter regions, additional contours were digitized from ortho photos. A digital elevation model of the region is shown in Figure 51.

Three transects across the region indicating the borehole logs and inferred surfaces are shown in Figures 52, 53 and 54.

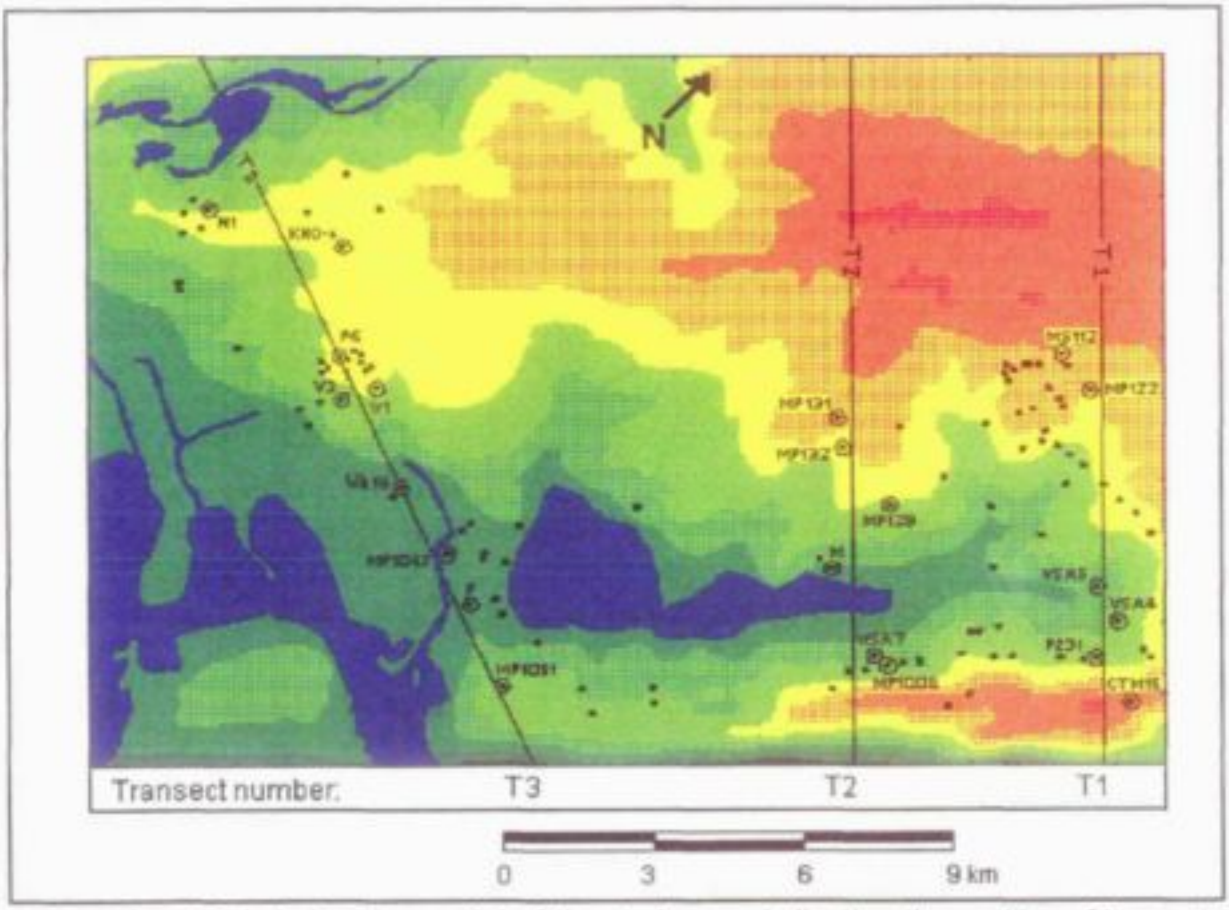

Figure 51 Digital elevation model of the study area indicating the position of transects shown in Figures 52 - 54.

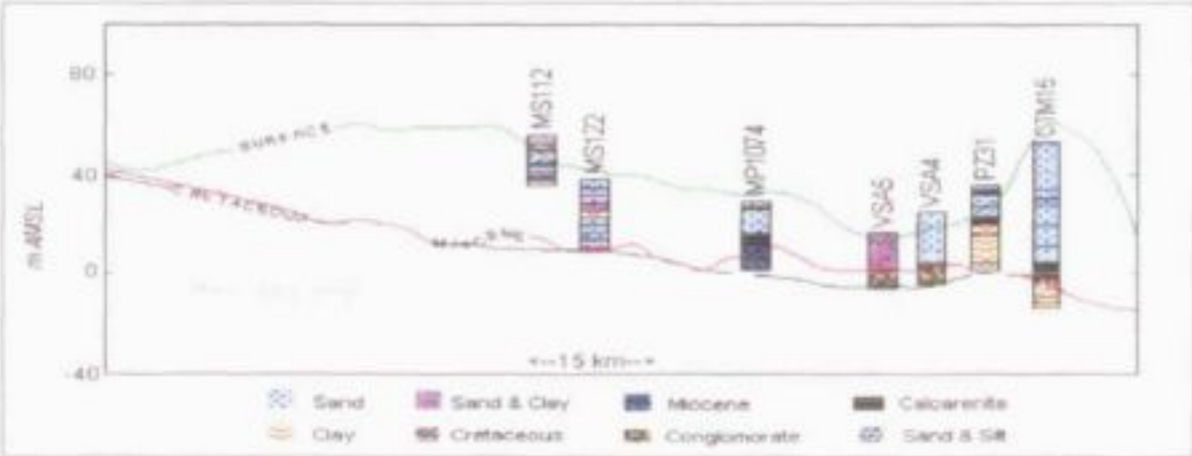

Figure 52 Cross section T1 (Figure 51) showing borehole logs and inferred surfaces.

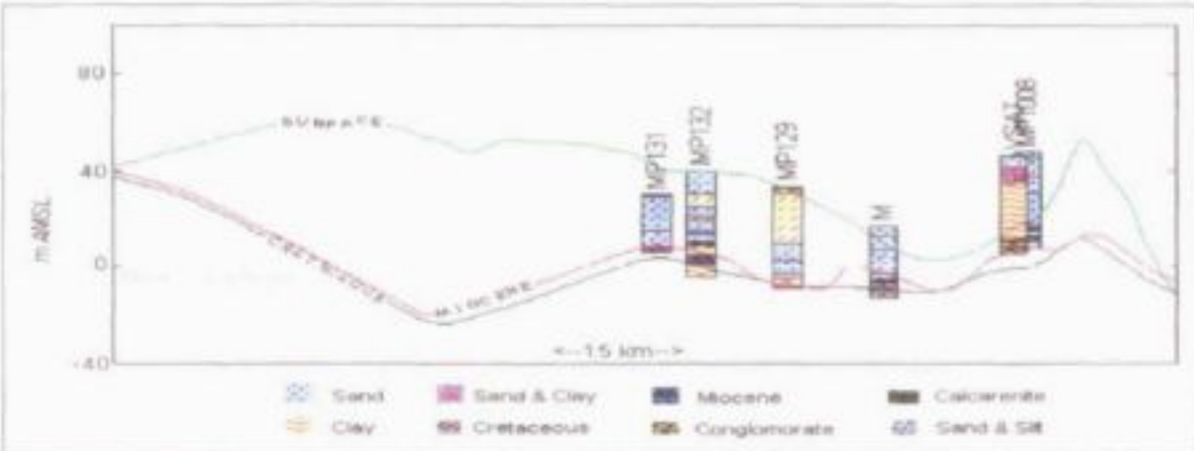

Figure 53 Cross section T2 (Figure 51) showing borehole logs and inferred surfaces.

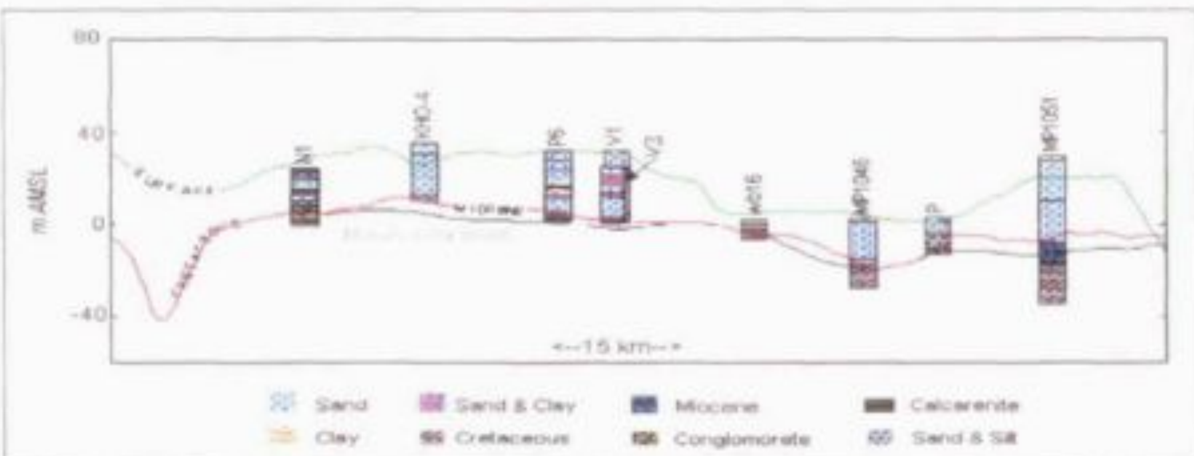

Figure 54 Cross section T3 (Figure 51) showing borehole logs and inferred surfaces.

PART 3

METHODS AND THEORIES FOR GROUNDWATER STUDIES

SECTION 6 GROUNDWATER FLOW MODELS
SECTION 7 PARAMETERIZATION, CALIBRATION AND SENSITIVITY ANALYSIS
SECTION 8 CASE STUDIES

Section 6 GROUNDWATER FLOW MODELS

Water resources are frequently analysed using numerical simulation models because of the extreme complexity of the non-linear processes and interactions involved in the flow dynamics which make it difficult to adopt physical or empirical models for all but the simplest situations. There is a huge range of numerical models available and they can be grouped into two fundamental classes that include multi-dimensional deterministic models and a group of stochastic of models. The multi-dimensional models can be subdivided into steady state and dynamic systems in 1- 2- or 3-dimensional space.

Surface water resources are generally simulated using lumped (1-dimensional) dynamic models that are often networked to form semi-distributed systems. This is a pragmatic approach because of the extreme variability of hydrological characteristics which influence the non-linear interactions. In groundwater systems where the flow is not constrained to defined channels, it is often necessary to use 3-dimensional models to determine flow paths. The MIKE-SHE model (Abbot et al, 1986) was an attempt to incorporate both the surface and subsurface hydrology into a fully 3-dimensional model. Unfortunately this model is expensive and requires considerable computer facilities and data for applications so it is considered to be unavailable for most studies of this nature.

The separation of the surface and subsurface hydrological processes requires very careful consideration in the estimation of model parameters which link the two systems. This chapter presents a description of the models and the concepts necessary for the application of groundwater flow simulations and the interactions with the topographical surface. The conceptual models required for solute transport simulations will be covered in a subsequent chapter. Unfortunately, there is no natural separation of the ground water and surface water conditions and consequently there is considerable discussion in the subsequent sections about the conceptual modelling of the interaction between the two components.

6.1 GROUNDWATER FLOW MODEL REVIEW

There are two basic types of groundwater flow models that are classified according to the numerical methods used. The finite element models use irregular arrays of elemental units to describe the dynamics of the system using triangulation techniques while the finite difference methods use regular rectangular elemental units. Finite elements define the variation of head within an element using interpolation functions while the finite difference method retains a step function between the average heads in the individual cells. It has been demonstrated that the finite difference method is a special case of the finite element grid (Anderson and Woessner, 1991 quoted Pinder and Gray, 1976 and Wang and Anderson , 1977).

These methods have been described in detail by Anderson and Woessner (1991). This project has concentrated entirely on the use of finite difference models and their application is described in detail in the following sections.

6.2 MODEL REVIEW AND SELECTION

There are numerous 3-dimensional finite difference models which have been developed that are similar to those which have been investigated in this study. Kelbe and Rawlins (1992) have used the INTERSAT model (Voorhees and Kirkner, 1986) to investigate the influence of proposed developments on groundwater systems as part of Environmental Impact Assessments in Zululand. Rawlins and Kelbe (1991) have used the same model to investigate the hydrological impact of land use on the shallow groundwater system near St Lucia. Germishuyse (1997) and Kelbe and Germishuyse (1997) used the CALIF model, developed by Häfner *et al* (1996), to investigate the dynamics of a waste site in a coastal aquifer. Numerous other models have been developed for various applications and some of these are listed in Table 9. Some of these models and their applications have been described by Anderson and Woessner

(1991).

Modflow is becoming established as a recognized standard in groundwater flow modelling. This model, developed by the USGS (McDonald and Harbaugh, 1983), has been adopted for this project and is discussed in this section. However, there are similar systems which are available together with several suites of models based on the Modflow computer code. The more common models are summarized below.

Table 9 Some groundwater models (1998)

FULL NAME	Type	Engine	2D / 3D
ASM	FD	ASM	2D
PLASM	FD	PLASM	2D
INTERSAT	FD	INTERSAT	Quasi 3D
Visual MODFLOW	FD	MODFLOW	Quasi 3D
Processing Modflow for Windows	FD	MODFLOW	Quasi 3D
Groundwater Vistas	FD	MODFLOW	Quasi 3D
ModIME	FD	MODFLOW	Quasi 3D
MS-VMS	FD	MODFLOW	Quasi 3D
Modflow Integrated Modeling	FD	MODFLOW	Quasi 3D
ModelGIS	FD	MODFLOW	Quasi 3D
Groundwater Modelling System	FE/FD	More than	3D / Q3D
Argus Open Numerical Environment	FE/FD	More than	3D / Q3D
FEMWATER	FE	own	3D
AUIFEM	FE	own	3D
AQUA3D	FE	own	3D
MICRO-FEM	FE	own	3D
Aquamod for Windows	FE	own	2D
SUTRA	FE	own	2D

6.2.1 FINITE DIFFERENCE MODELS

Some of the numerous finite difference models that are available for public use in either the commercial or public domain are summarized in Table 9. The models which have been examined are all based on conservation principles and Darcy's Law of flow in a porous media. The biggest difference is usually in the pre- and post-processors of the different models. Many have developed linkages to other programmes and some of them also have very elaborate graphical user interfaces for entering and displaying the data.

6.2.2 MODFLOW DERIVATIVES

Modflow is a 3-dimensional model written in Fortran 77 which requires a thorough understanding of the file structures and their role in the model for general applications. Because of the complexity in constructing the files for Modflow, several attempts have been made to improve the pre- and post- processing capabilities of Modflow in commercial programmes. Some of these programmes are reviewed in this section and compared for use in this project application of Modflow.

6.2.2.1 VISUAL MODFLOW

Visual Modflow was designed to facilitate a much easier method of pre-processing the data for application of Modflow. The programme has facilities to import data files in several formats (*.dxf) which can be created or processed by other programmes such as CAD and GIS. This greatly expands the pre-processing capabilities of the system and make it an ideal introductory programme for groundwater modelling. Version 2.70 (1998) combines recent versions of Modflow, Modpath and MT3D. It has intuitive graphical interface which provides a means for graphically assigning the necessary flow and transport parameters for large arrays of finite difference nodes. It has facilities for importing *.bmp and *.dxf graphical files for direct use in the model.

VisualModflow also provides adequate post-processor functionalities that allow graphical display of model results in three dimensions. It includes full support for MT3D96, automatic grid smoothing to optimize grid spacing, cell-by-cell anisotropy for hydraulic conductivity properties, WHS Solver, colour shaded contouring, and customizable display of contoured results. It also includes some calibration statistics and imports standard 3-D Modflow files.

The file structures of VisualModflow is different from Modflow file structures and the program translates its own files into the Modflow format before the model is run. Reverting back to Modflow is often necessary when additional modules or options are used.

6.2.2.2 OTHERS

The other programmes using Modflow as the principle hydrological engine are given in Table 10. Those that include MT3D are indicated. Further details of these models are available at http://www.scisoftware.com

Table 10 Programmes using Modflow

Model	Details and special features	Auto Calibration	MT3D
VisualModflow	Pre- and post processor. Very easy data input and output.	No	Yes
Groundwater Vistas	Pre- and post processor. Includes telescopic mesh refinements.	Yes	Yes
Modime	Pre- and post processor. Zoom capabilities using regional model as boundary conditions.	?	Yes
PM Win	Pre- and post processor. Includes all Modflow options.	Yes	Yes

6.3 MODFLOW

This section presents the theoretical **summary** of the MODFLOW programme because an understanding of the concepts is imperative for the correct estimation of boundary conditions and particularly for the use of these concepts to simulate the surface-groundwater interactions. Several conceptual models of the surface-groundwater processes and interactions are described, particularly the vertical fluxes. These include groundwater recharge, groundwater evaporation, stream flow and runoff into and out of wetlands as well as lakes and large water bodies. A full description of the Modflow theory is presented in the working manuals which are available from the US Geological Survey (MacDonald and Harbaugh, 1983).

Modflow is designed to simulate saturated geohydrological conditions and to determine the water balance of aquifer systems, including the effects of groundwater extraction. The model is capable of solving multi-layer *quasi*-three-dimensional problems using a variable grid network which allows for increased spatial resolutions of specific points of interest. The model includes very little support for preprocessing the data or for suitable display of the results. The use of other programmes is necessary to accomplish these tasks.

6.3.1 MODFLOW DESIGN STRUCTURE

Modflow is a computer simulation programme based on a main program linked to a number of highly independent primary and secondary subroutines called modules. The total simulation period is divided into a series of stress periods[1] within which specific parameters are kept constant. Within each stress period, the model simulates the flow

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1 In transient simulations the modeller specifies blocks of time (stress periods) of variable length during which all parameters will remain constant.

dynamics for each specified time step[2]. Within each time step a number of iterations are required to solve the set of finite-difference equations. The choice of the initial time step (Δt) often determines the stability of the iterative convergence.

The Modflow program calls several subroutines which are grouped into "packages" that represent certain hydrological processes or solutions to numerical methods. A list of the packages is given in Table 11.

6.3.2 INITIAL CONDITIONS

The initial conditions reflect the extend of knowledge about the system at a specific time that represents the start of the simulation. It is not necessary to know the conditions at the start of a simulation period but it is essential to know the conditions at some subsequent time in order to calibrate the model results. Initial conditions can be assumed for a model with known driving functions (recharge and discharge) so that an equilibrium (steady) state can be simulated for comparison with the known conditions. Generally the initial piezometric heads are unknown but assumed to be either a constant elevation or some function of the topography. Under steady state conditions the model simulates an average piezometric surface which is a reaction to the hydraulic gradients that create a balanced flow. These steady state conditions can be compared to known average geohydrological records.

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2 Subdivision of a stress period used in calculations (= Δt). Smaller time steps results in a better approximation of the partial differential equation.

Table 11 List of packages available with Modflow 96 (McDonald and Harbough, 1983)

Package Name	Package Description
Basic	Defines and sets key model parameters such as the grid and boundaries
Block-centred Flow	Sets grid parameters & calculates the conductance between cells (i,j,k)
Numerical Iteration Solvers	
SIP	Strongly Implicit Procedure Iterative solution
SOR	Slice successive Over-Relaxation Iterative
PCG2	
Stress Packages in Modflow	
Recharge (RCH)	Determines the rate of recharge to groundwater
Evapotranspiration	Determines vertical evaporation fluxes
River (RIV)	Determines flow into river nodes within cells.
Drain (DRN)	Determines flow out of drains into cells.
Well (WEL)	Specifies flow to wells
General-head boundaries	Specifies conductance between external sources and the cell
Separate packages from other developers	
Reservoir (RES1)	Simulates large water bodies
Lake (LAK1, LAK2)	Provides simulation of lake levels (Upgrade of RES1)
River Interactions	Made redundant by STR
Stream Routing (STR1, STR2)	Upgrade of RIV which routes water from cell to cell

6.3.3 NUMERICAL SOLUTIONS PACKAGES

Several iterative solution methods are presently available in Modflow. These include the Strongly Implicit Procedures (SIP) developed , the Slice-successive Over-Relaxation (SOR) Procedures and the PCG2. All three methods are described in detail by McDonald & Harbauch (1983).

6.3.4 PHYSICAL BOUNDARY CONDITIONS

Mathematical models require the specification of (1) the initial boundary conditions and (2) the physical boundary conditions. The physical boundaries may represent the full extremities of the model domain or internal features which inhibit or promote flow within the model domain. The application of the Modflow model is crucially dependant on the utilization of the transport mechanisms to represent the various internal and external boundary conditions. Therefore, considerable effort is made to describe the application of the different concepts in this report.

Kinzelbach (1986) and Anderson and Woessner (1991) have defined three boundary conditions which are distinguished by the flux across the boundary.

1 Dirichlet type boundary conditions of the first kind have a known fixed (constant) head

2 Neumann type boundaries of the second kind have constant fluxes across the boundaries (eg impervious boundaries have zero fluxes).

3 Mixed type boundaries of the third kind are a combination of the

first two kinds. These generally represent leakage boundaries such as rivers and drains.

The vertical fluxes have been identified for specific processes relating to the different recharge and discharge mechanisms and these are described in the next sections in great detail.

6.3.5 CONCEPTUAL BOUNDARY CONDITIONS

Modflow defines the flow dynamic equation for every cell but it is pragmatic to define the status of certain cells in advance in order to simulate boundary conditions. The two specific type of predefined cells used in Modflow are those with constant-head and those that are inactive (no-flow) cells. The inactive cells are usually specified to remove a portion of the mathematical array which is beyond the aquifer boundary. All other cells are described by a variable head conditions driven by vertical and horizontal forces.

6.3.5.1 BLOCK-CENTRED FLOW CONCEPTS

Modflow uses the Block-centred grid which simulates the flux boundaries along the edges of the grids.

Modflow provides the means for visualizing the vertical discretization in several ways. The vertical extent of the model can be viewed as an extension of the areal discretization where the flow is divided into flow system governed by the vertical resolution or by specifying the vertical extent of the individual aquifers (McDonald and Harbaugh, 1983). The first concept leads to a rigid superposition of an orthogonal 3-D array with varying hydraulic characteristics. The other extreme concept conceives each geohydrologic unit as a variable thickness layer. Each of these concepts has advantages and disadvantages in their application (McDonald & Harbaugh, 1983). The second concept is generally used in this study because the geological information that is usually available, provides an indication of the aquifer thickness rather than its hydraulic properties. However, a case study is presented where an adaptation of the first concept is applied to a specific problem in the Richards Bay area (see section 8.2).

The vertical boundary parameterization in Modflow requires specification of two components. The vertical flow is separated into the vertical recharge component (generally perceived to be the percolation from the soil moisture and artificial recharge) and the vertical discharge component (evaporation and abstraction) through the upper boundary surface. These two components represent the interaction between the saturated groundwater compartment and the unsaturated and surface processes in the zones above the water table.

Once a cell falls dry, it becomes an inactive cell. To overcome this problem McDonald et al (1991) developed an extra feature which will convert no-flow cells to variable head cells. This feature has two options in the Visual MODFLOW shell, namely cells will be re-wetted from the sides only or cells can be re-wetted from the sides and below. This feature is very important in aquifers where the water table is below the top layer.

6.3.5.2 VERTICAL CONDUCTANCE

The vertical conductance terms $Q_{vertical}$ is used to calculate the vertical leakance between two nodes according to the following equation:

$$V_{i,j,k+\frac{1}{2}} = \frac{1}{\dfrac{\frac{\Delta v_k}{2}}{K_{z(i,j,k)}} + \dfrac{\frac{\Delta v_{k+1}}{2}}{K_{z(i,j,k+1)}}}$$

where:
$V_{i,j,k+1/2}$ is the vertical leakance in cell (*i, j, k*)
ΔV_k is the thickness of model layer *k*
ΔV_{k+1} is the thickness of model layer *k+1*
$K_{z(i,j,k)}$ is the vertical hydraulic conductivity of the upper layer in cell (*i,j,k*)
$K_{z(i,j,k+1)}$ is the vertical hydraulic conductivity of the lower layer in cell (*i,j,k+1*)

In the case of a semi-confining unit, an additional term is included in the denominator to represent the conductance across the unit. McDonald and Harbaugh (1983) state that *"the options for calculating horizontal conductance under water table conditions, limitations on vertical flow under de-watering conditions and storage term conversion were all developed on the assumption that each model layer corresponds to a distinct aquifer or permeable horizon, and that these horizons are all separated by distinct units of low permeability. Use of these options where conditions are not satisfied may lead to a variety of problems and inaccuracies in simulation"*

6.3.5.3 STORAGE

The conservation of mass principle requires a specification of the storage of water in each cell. Modflow simulates both the confined and water table storage conditions which are described by a storage coefficient. When the water table is within a cell it is conceived as an unconfined aquifer. When the water table is located above the top of the cell (*i.e.* it is in higher layers) then the cell becomes confined. However, when the water table rises above or drops below the top of a cell then the status of the aquifer changes and the system converts to the appropriate type of aquifer. The storage term conversion requires user specification.

6.3.6 NATURAL RECHARGE

Bredenkamp *et al* (1995) presented a detailed study of many groundwater recharge methods. However, these methods are not usually designed for application in conjunction with numerical models which include some direct hydraulic contact with the surface vegetation. In this study, the effect of land use on the groundwater is considered and consequently it is necessary to develop suitable conceptual models of the surface groundwater interactions for inclusion in the model simulations.

The vertical recharge rate in Modflow is used to describe the processes of percolation and transmission losses from the stream bed when the water table elevation is below the level of the stream bed. The rate of recharge is dependent on the different boundary (surface) conditions associated with standing water (lakes, ocean, etc) and soil moisture fluctuations linked to rainfall and evaporation.

6.3.6.1 PERCOLATION FROM SOIL MOISTURE EXCESS

The processes and interactions influencing the percolation rate are shown diagrammatically in the conceptual model of Figure 55. Rainfall is derived from field measurements; interception is estimated for the different land use types; runoff is a function of rainfall intensity, soil conditions and land use practice; infiltration is dependent on soil moisture characteristics; and percolation represents the resulting influence of all these processes. The incident rainfall, as measured by a rain gauge, will not all percolate down to the water table as there are losses due to (1) interception by the vegetation, (2) evaporation (both from free standing water and from the vadose layer), and (3) the replenishment of the soil zone moisture content. It is extremely difficult to separate the interception, evaporation, infiltration and percolation components. The literature gives a wide range of values for these losses from different vegetation covers and soil types and additionally the depth to the water table will have an influence.

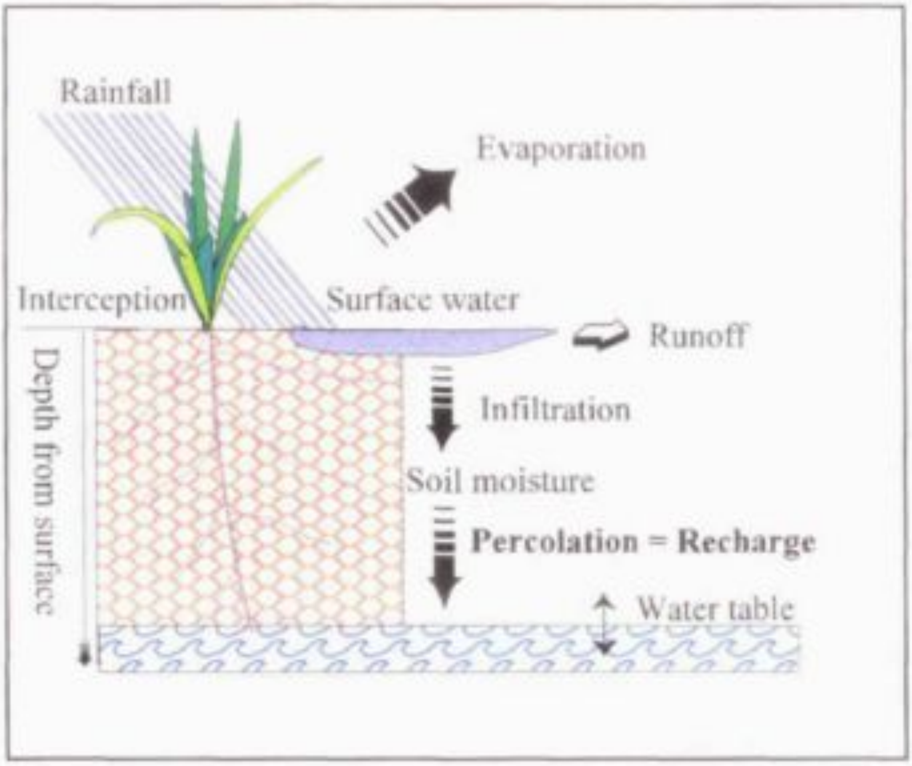


Figure 55 Diagrammatic representation of the mechanism considered in formulating recharge from rainfall.

Several methods have been used to estimate recharge in the Zululand Region. Bredenkamp *et al* (1995) have presented a detailed summary of these methods.

6.3.6.2 RAWLINS & KELBE MODEL

In an effort to obtain a relationship between the incident precipitation and the groundwater recharge in the St Lucia area, Rawlins and Kelbe (1992) made recourse to recorded measurements of rainfall and the corresponding water table response in an area with similar geological-soil conditions to the Richards Bay region. Measurements of the change in water table elevation following isolated rainfall events were examined and corrected for the expected lag between the rainfall and any subsequent response in the water table. This analysis indicated that the water table at a depth of 2-3 m below ground surface, will only respond to a rainfall event that exceeds approximately 10 mm (Figure 56) when the overlying vegetation is natural grassland. Rawlins and Kelbe (1992) incorporate the effects of antecedent

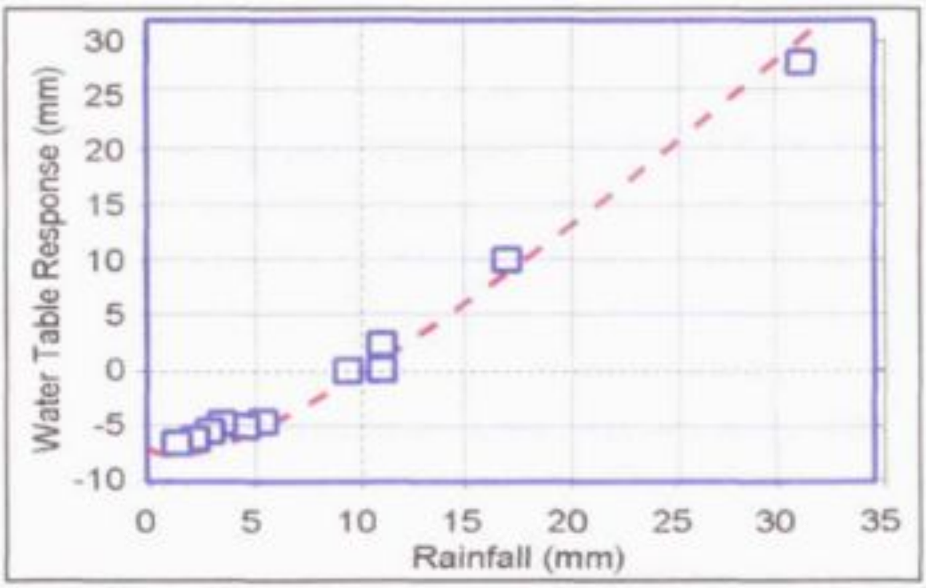


Figure 56 Volumetric response to incident rainfall on the eastern shores of Lake St Lucia.

depletion of soil moisture content by assuming that the soil moisture was depleted through evaporation at a rate of about 2 mm/day. This assumes that it would take five days to deplete the 10 mm of rainfall intercepted and stored in soil moisture before any groundwater extraction took place at the same rate of approximately 2 mm a day. Thus the 10 mm rainfall required before recharge includes proportional amounts from the previous four days.

In cases where there was no rainfall in the preceding four days, then the recharge amount equalled the rainfall event minus the initial 10 mm which was required to satisfy the interception, soil moisture replenishment and soil surface evaporation losses. In the case where the previous day had an excess of 10 mm (full profile), then the rainfall in subsequent days would be direct recharge to the groundwater. Proportional (w_i) amounts of the 10 mm used to replenish the soil (R_i) were integrated over the previous four day to determine the replenishment rate for the current event (R_0). That is, if the soil moisture was completely replenished yesterday, then it only required 2 mm to restore the evaporative loss of 20% per day. This model is shown diagrammatical in Figure 57.

This recharge model has been used successfully for groundwater simulation on the eastern shores of St Lucia by Kelbe and Rawlins (1992, 1993). However, this model may have limitations in coastal areas where there are well established streams which indicate substantial surface runoff for short duration, high intensity storms. This suggest that there may be more direct runoff than observed on the eastern shores region of St Lucia. Consequently, it was arbitrarily decided that all rainfall events of more than 50 mm/day for the Richards Bay region would lead to direct runoff and that only the initial 50 mm/day portion would infiltrate and contribute directly to percolation into the shallow groundwater system.

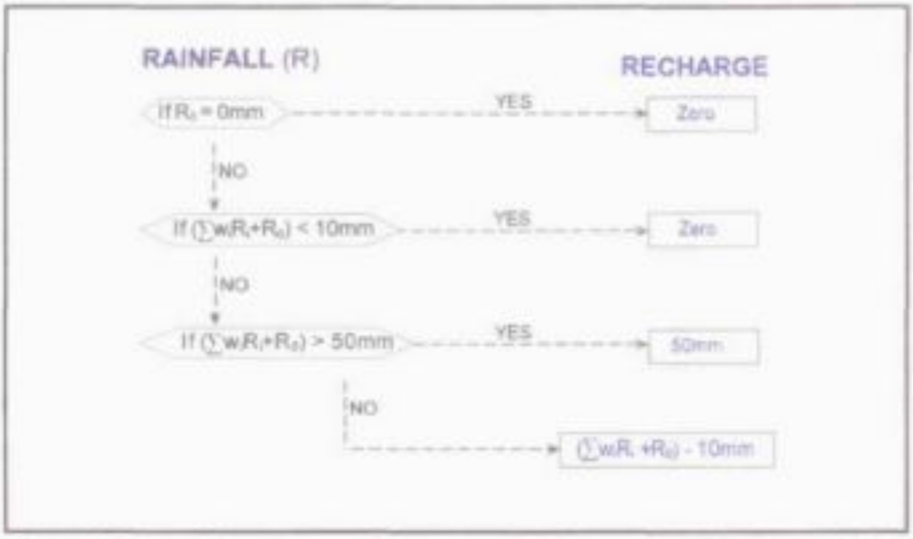


Figure 57 Diagrammatic representation of recharge model by Rawlins and Kelbe (1992).

6.3.7 EVAPORATION

It has been shown that it is necessary to make sure the processes which are responsible for the discharge (evaporation and transpiration) are considered when estimating the recharge. Many methods have been developed for estimating recharge which automatically account for all the discharge components (Bredenkamp *et al*, 1995). These methods cannot be used in this study where the evaporation component from the capillary fringe (groundwater) is modelled independently of the surface processes. Consequently, conceptual models of the vertical flow mechanisms have been included in this study.

Modflow assumes that a maximum evapotranspiration rate **from the groundwater** (E_{max}) is maintained when the water table elevation is at or above a lower limit (RD) relative to the earth surface. This maximum evaporation rate is **not** the same as the **potential evapotranspiration**

(E_p) which is defined by Campbell (1986) as "the rate of evaporation from a free transpiring short green grass with unlimited soil moisture". E_p has also been equated to the "atmospheric demand" - a measure of how much water can evaporate if there is no limitation from the soil and vegetation. All these definitions involve the soil moisture status. In Modflow, the maximum evaporation (E_{max}) is that evaporation component which is derived directly from contact with the groundwater or capillary fringe. This is a very difficult factor to define without a good estimate of the unsaturated zone processes. The conceptual model of the groundwater evaporation is a simple method for incorporating the surface interactions with the saturated zone through an assumed "capillary" zone which is within the rooting depth of the vegetation. It also assumes that the roots of plants can respond faster than the change in water level.

In Modflow, the "groundwater" evapotranspiration is perceived as a vertical flux of water from the topographical (upper model) surface when the water table is in direct hydraulic contact with the vegetation. The actual evapotranspiration rate (E_a) is reduced linearly from a user specified maximum rate (E_{max}) to a zero rate as the water table elevation declines in elevation to the point where there is no longer any hydraulic contact between the vegetation and the groundwater. At this point the "groundwater" evapotranspiration ceases. The upper elevation of the water table which sustains a maximum "groundwater" evapotranspiration is term $ET_{surface}$ and the depth below this where E_a becomes negligible is defined by the rooting depth of the vegetation (Extinction level). This conceptual model is shown diagrammatically in Figure 54.

It is therefore necessary to define values for maximum groundwater evaporation rate (E_{max}), the maximum rooting depth (Extinction depth) and the elevation of the water table ($ET_{surface}$) above which there will be sufficient water to maintain E_{max}.

The influence of different land use types on the groundwater system is effectively simulated using the evapotranpiration model described above in conjunction with conceptual models of recharge which account for interception of rainfall. The conceptual evaporation model is shown diagrammatically in Figure 58 for the four main land use types in the Richards Bay area. The urban environment is assumed to be a combination of these four types that is interspersed with areas of impermeable surfaces which have no evaporation. The proportion of each land use is used to estimate the representative parameter value under these circumstances.

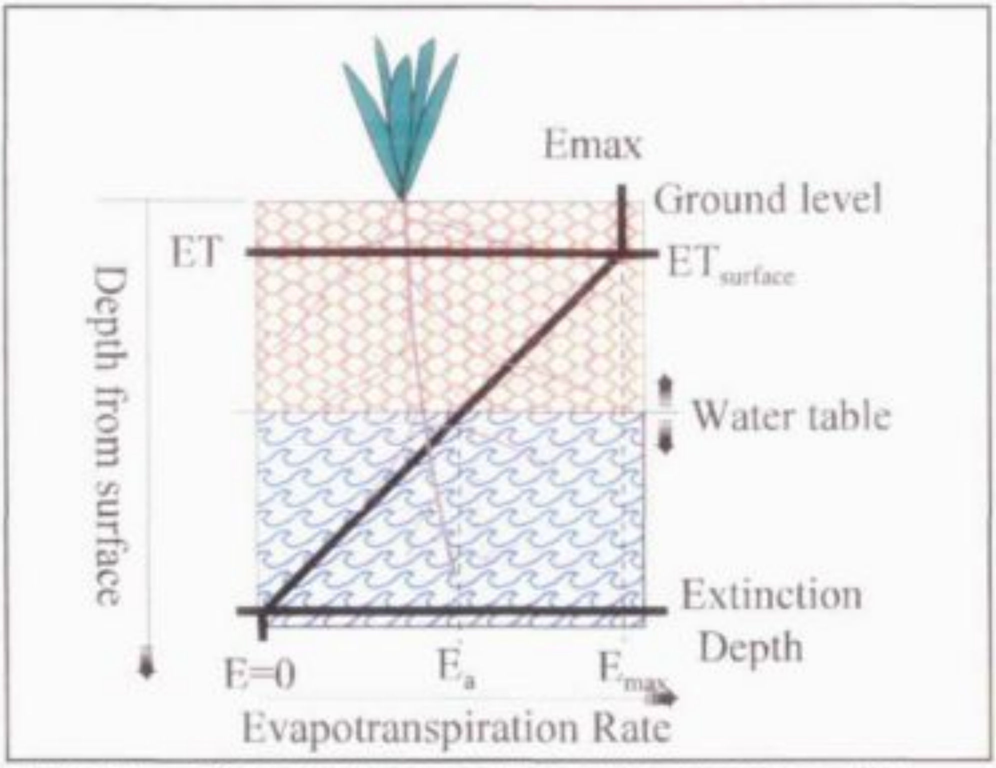


Figure 58 Diagrammatic representation of the evaporation model.

6.3.8 RIVERS AND DRAINS

Two packages which simulate the seepage of water to or from surface features are described in this section. These packages involve the transfer of water from surface water bodies such as rivers and drains when the surrounding water table is above or below the level of the surface water body (wetland). Modflow assumes that the vertical flow rate is represented by a conductance through a constraining layer. This layer can be visualized as a section with low vertical permeability which separates the surface water from the groundwater. Conductance of the section is dependent on the area, thickness and hydraulic conductivity of the low permeability layer as well as on the difference in head between the surface water body and the water table.

6.3.8.1 RIVER FUNCTION

Modflow assumes a reversible river function which allows vertical **discharge** from groundwater into the river (base flow) when the surrounding groundwater elevation is above the surface water body and a **recharge** (transmission loss from the river into the groundwater) when the water table is below the elevation of the river bed. This conceptual model is shown diagrammatically in Figure 59.

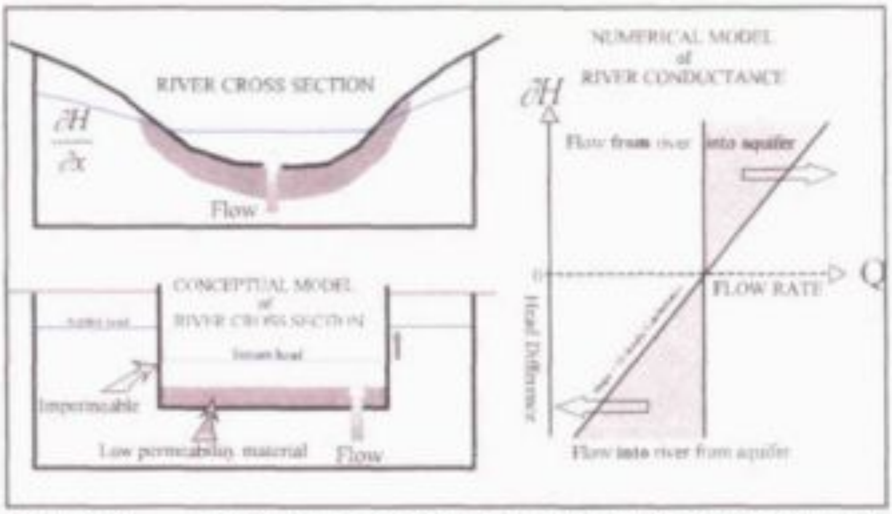


Figure 59 Conceptual model of vertical river transmission processes (adapted from McDonald and Harbaugh, 1983).

The river is assumed to be separated from the groundwater system by a layer of lower permeability material. The river is conceived as conductance block which occupies a proportional section of the cell it crosses. The length of the river covers a discrete number of cells forming river "reaches" which have a width (W) that is a proportion of the cell dimension. The flow in the rivers is assumed to be generated by the vertical discharge from the groundwater through the streambed with a known thickness (M) and hydraulic conductivity (K). The flow between the groundwater and river in each cell is described by

$$Q_{River} = \frac{KLW}{M}\left(h_{River} - h_{i,j,k}\right)$$

where Q_{river} is the hydraulic conductance. It is assumed that the cell remains fully saturated and the water level does not drop below the bottom of the cell. The package also assumes impermeable sides to the river channel so that there is only vertical flow.

6.3.8.2 STREAM ROUTING FUNCTION

The Stream Routing function (Prudic, 1989) is an upgraded version of the River function with the routing of water downstream added.

6.3.8.3 DRAIN FUNCTION

There are many instances when **drains** are installed to remove groundwater from local aquifers. The drain package removes water at a rate that is proportional to the difference between the head in the cell and some fixed head or elevation (representing the drain). The head in the aquifer (cell) must be above the level of the drain. However, the package assumes no interaction when the aquifer is below the level of the drain.

The drain does not characterize a cell as a whole, but assumes that the drain head prevails only locally (Figure 60). The packages assumes three local flow processes that involve head losses in the drainage process. These are convergent flow toward the drain, flow through varying conductivity material and flow through the pipe wall.

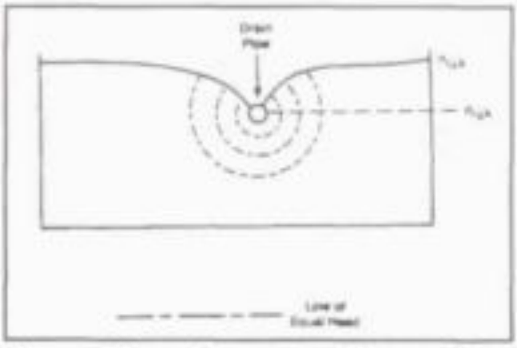


Figure 60 Conceptual model of drainage process.

6.3.9 CONSTANT HEAD

Kinzelbach (1986) implies that lakes be modelled as constant heads, in which case pathlines will progress towards the lake, but not further. All pathlines will stop at the edge of the lake. This is an adequate assumption under certain circumstances. It has been used to determine the water balance of specific water bodies such as the coastal lakes. However, it is not suitable for simulating the response of the lakes to changes in catchment conditions.

6.3.10 LAKE FUNCTIONS

Several efforts have been made to simulate the groundwater interactions with coastal lakes. Where the lakes are very large water bodies that control the interaction with the groundwater, they may be conceived as constant head system with unlimited storage capacity. However, for lake with significant response to changes in groundwater flow, the lake level respond may be simulated using a separate lake function.

The Lake Packages used in this project was developed by Council (1997) from earlier models which were developed by Cheng and Anderson (1993) and later by Fenske *et al* (1996). The Lake Package was acquired for the specific purpose of simulating the varying lake levels which these earlier models were not able to calculate.

The Lake Model utilises a specific **river package** which was also provided with the module. This river package was developed by Prudic (1989) to simulate the stream-aquifer interactions. This stream module functions in a similar manner to the concept described in the previous section. In this module the stream is assumed to be rectangular with greater width than depth. The stream-bed conductance is assumed to be constant for each stress period and the leakage from the stream to the aquifer is assumed to be instantaneous. The package also makes assumptions about the downhill flow of the stream bed elevation and cannot exchange water when cells become dry.

The Lake Package is shown diagrammatically in Figure 61. The hypsometric profile is required to determine the volumetric capacity of the lake to formulate a water budget driven by surface and subsurface flow components.

The Lake is conceived as a leakance boundary between the open water body and the aquifer. The leakance is described by the hydraulic conductance of the lakebed sediments which determine the groundwater flux into and out of the lake. The conductance is described by the following equation:

$$\text{Conductance} = K * \frac{A}{M}$$

Where K = hydraulic conductivity
A = area of cell occupying the lake regions
M = thickness of the lakebed sediments

The flow from the lake to the groundwater is controlled by the elevation of the head in the cell as described by:

$$\text{Velocity} = \frac{K_{ii}}{\phi} \frac{\partial h}{\partial x_i}$$

where ϕ = porosity
$\partial h/\partial x$ = head gradient

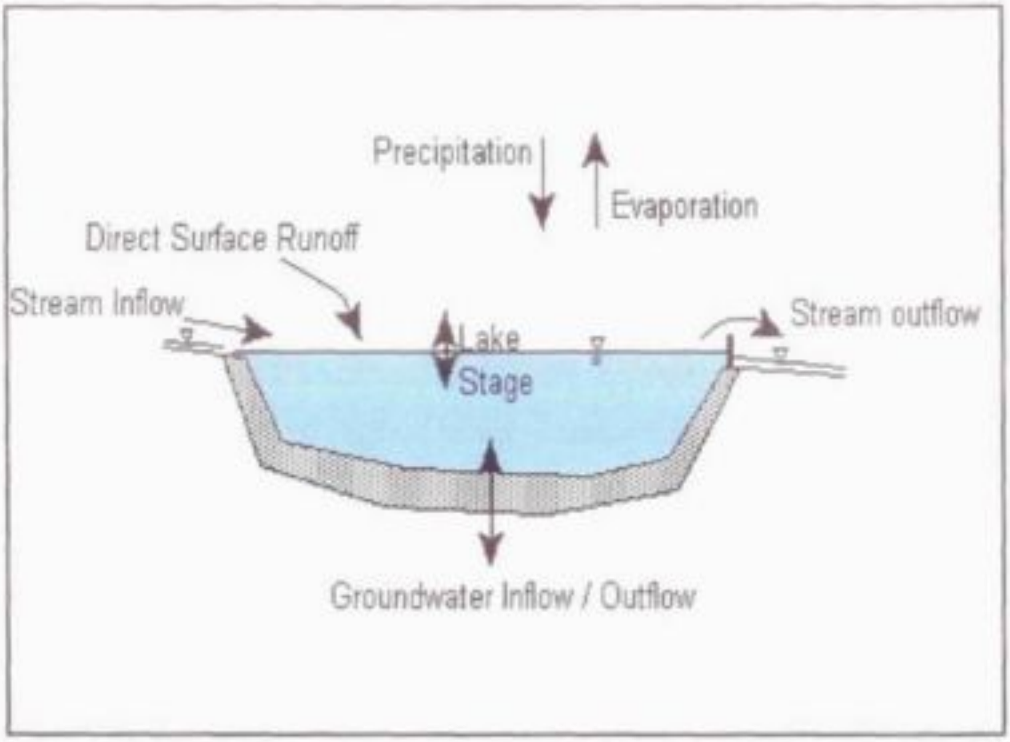


Figure 61 Diagrammatic representation of the Lake Package Model (after Council, 1997)

The relevant inflows and outflows to the lake are simulated by Modflow and integrated by the Lake Package. The outflows from the lake are incorporated as a variable function in the Streamflow Routing package (STR2). A steady state solution is balanced after each head solution approximation. This keeps the stage in balance with successive approximations of groundwater head until the head solution converges. The steady state stage is computed after each timestep, with increasing head when inflows exceed outflows and *vice versa*. For the first timestep, Modflow solves for the potentiometric head, using the initial lake stage as boundary condition. After the head solution is complete, lake inflows and outflows are integrated to determine the volume change for the lake (DV) during the timestep (Dt). This change in volume is added to the original volume to obtain the total volume for the next timestep. If the new volume is less than zero, the lake is dry and a warning is issued in the output file (the simulation continues and rewetting may occur in subsequent simulation periods). The stage is set by an iterative method to a value that gives the approximate volume in a similar way to that used in solving the steady state solution.

6.3.11 COMPARISON OF SEEPAGE

A purely hypothetical model of a pond in a surface depression was run in order to compare the seepage output from different simulations. The model dimensions were 1.4 km x 1.7 km divided into 28 x 34 cells of 50 m x 50 m each. The surface topography is indicated in Figure 62. No recharge was added to the aquifer, except to the pond cells in three scenarios. An extremely high recharge value was used in order to get an output that could be compared.

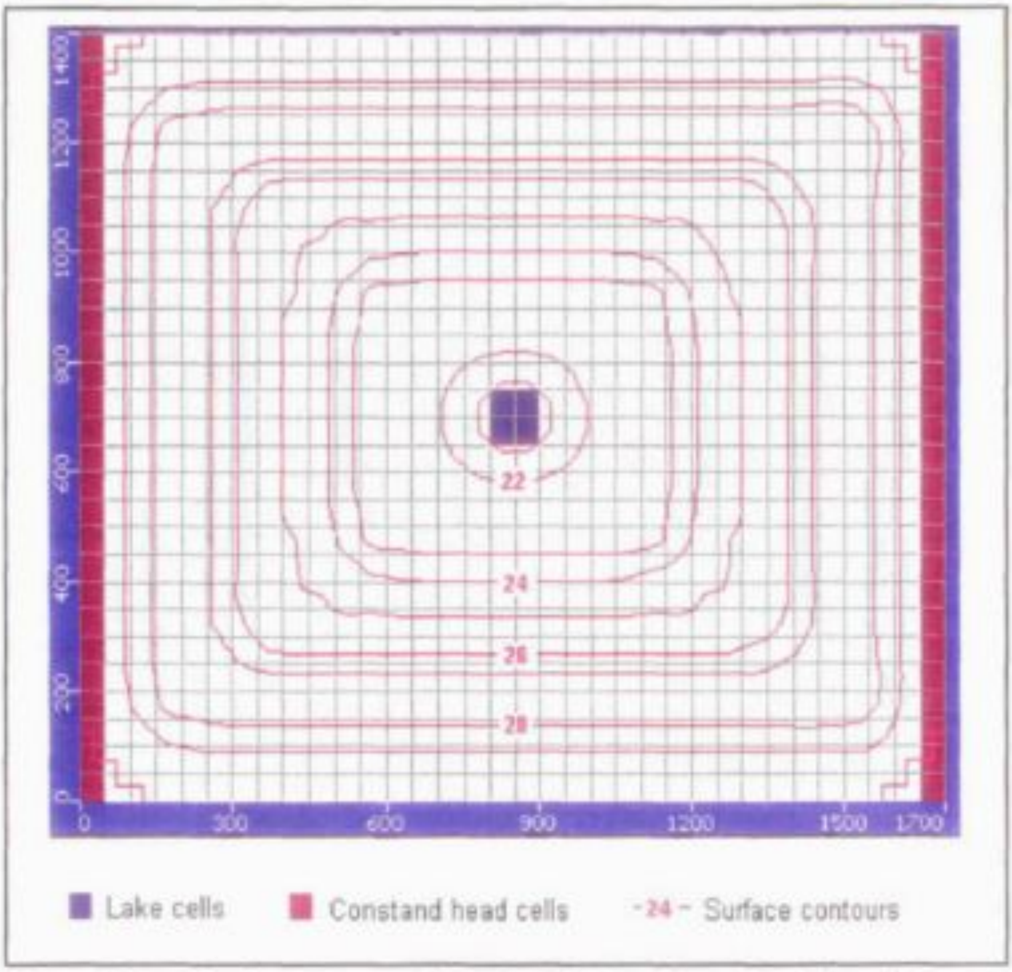


Figure 62 Surface topography and grid size of hypothetical model.

The different scenarios were: (A) A recharge of 150 000 mm/year to the 4 pond cells, (B) Pond cells were set as constant heads with NO recharge and (C) Lake package used with a recharge of 150 000 mm/year to the 4 pond cells.

The seepage and lake levels are listed in Table 12 and a cross section through the model area is shown in Figure 63. The results clearly indicate that the different models produce roughly the same seepage rate for these three different numerical conditions.

Table 12 Simulated seepage rate using different models

SCENARIO	RECHARGE (mm/year)	LAKE LEVEL (m *AMSL*)	SEEPAGE RATE (m/day)
A	150 000	20.56 (simulated)	4119.7
B	0	20.00 (given)	3937.3
C	150 000	20.00 (simulated)	3840.3

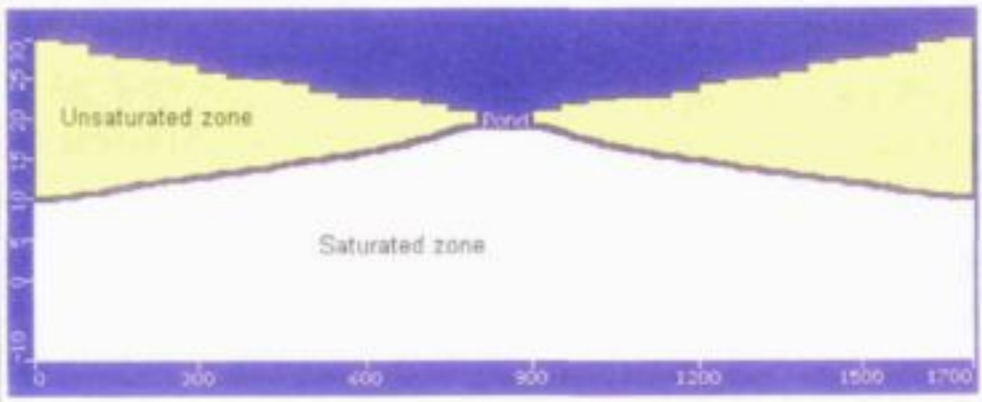


Figure 63 Simulated water table

Section 7 PARAMETERIZATION AND CALIBRATION

The numerical model is described by a set of finite difference equation together with several empirical equations based on conceptual models of various flow processes. These equations require specification of a set of parameter of both the spatial and temporal fields. These parameters have been defined in Section 6. However, it is necessary to determine estimates of these parameters for initial (starting) conditions, adjust them in some manner through calibration according to their sensitivity to the conditions under investigation. The parameters are calibrated against known conditions (field observations) by adjusting their values until the simulations agree with appropriate observations. The most common method of calibration is through subjective (trial and error) adjustment of single parameters within a range of values which are considered appropriate for the conceptual model. The other method of parameter calibration is using numerical techniques to achieve the convergence of prediction with observation. In both cases, the initial parameters must be estimated from observation or extrapolated from other measurements which are generally published from studies in other regions under. The initial part of this section present the known and estimated range of values for the parameters set used in the flow models. This is followed by a brief description of the numerical calibration methods examined in the case studies.

7.1 PARAMETER ESTIMATION

There are two basic sets of parameters described for the Modflow model, those hydraulic parameters associated with the flow dynamics described by the finite difference equation, and those parameters associated with the boundary conditions.

7.1.1 HYDRAULIC PARAMETERS

In Modflow, the flow dynamics are described by the finite difference equation that requires the specification of parameters associated with the aquifer thickness, the storage coefficient in the aquifer for both confined and unconfined conditions, the permeability (transmissivity) and parameters describing the vertical flow rates for different processes. These parameters are estimated from the available information which is extremely limited. Consequently it is necessary to calibrate the model under known conditions where possible for sections of the model's spatial and temporal domain. This calibration process requires an estimation of the range of values for presenting the parameter values. This generally involves a large degree of subjectivity.

7.1.1.1 PERMEABILITY

Probably the single most limiting feature of this modelling study has been the uncertainty involved in estimating the hydraulic properties of the different layers. Anderson and Woessner (1983) have published a range of permeability (hydraulic conductivity) values that have been observed for many of the common rocks and soils (Figure 64). The coastal primary aquifer is composed of unconsolidated (loose) sands with varying amounts of clay and silt. In Figure 64, the range of "expected" values for permeability covers more than three orders of magnitude for each of these soils. For most of the consolidated (hard) rock aquifers, this range increases by at least another order of magnitude. However, this range of values may be considerably reduced within a local area or aquifer.

Davies Lynn and Partners (1992) conducted permeability tests on two of the important geological formations in a geological surveys of the eastern shores of Lake St Lucia. They obtained permeability values which varied by more than one order of magnitude within each layer (Table 13). Some published values in the common hydrology text books for the rock and soil types of interest are shown in Table 14. These published values do not show quite the same range of values but there is still a large spread. This indicates the difficulty in estimating the initial values and more specifically the possible range of values. Even with field observations in the same aquifers, the range is still enormous (Table 13).

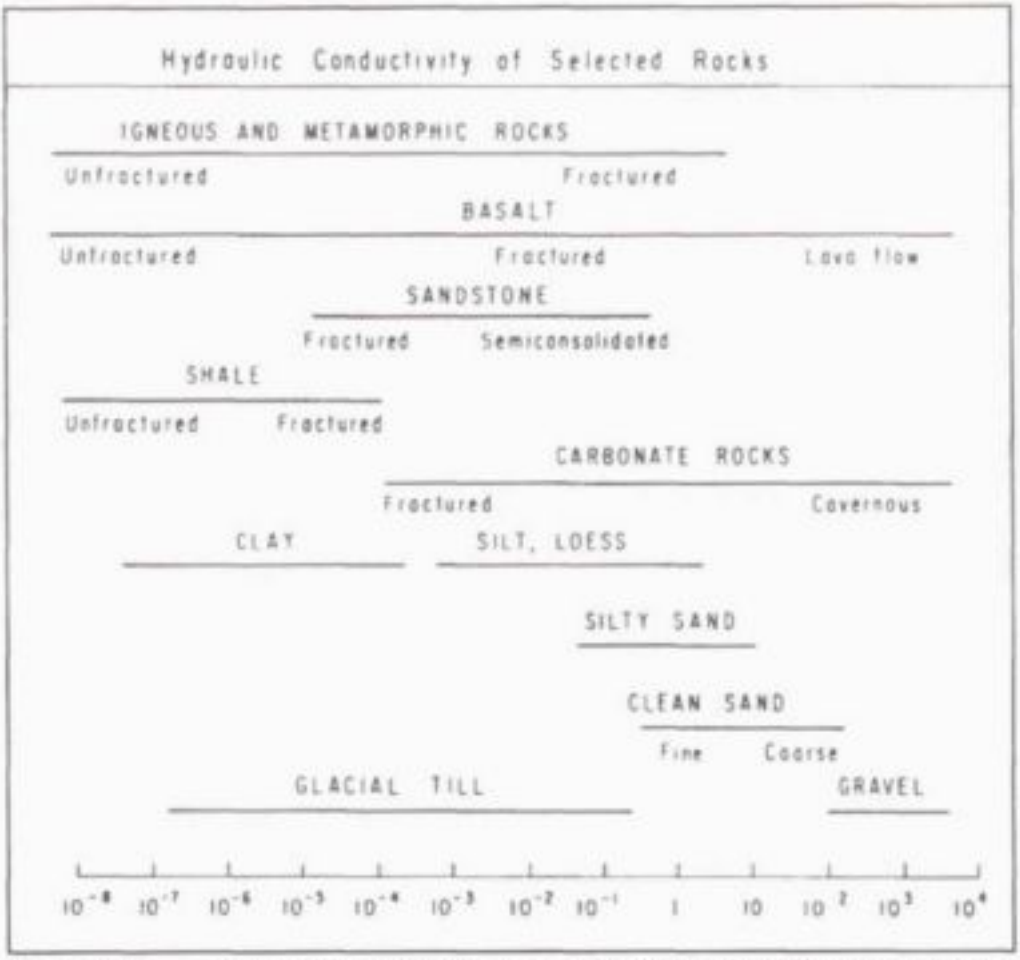


Figure 64 Range of Permeability values (in m/day) for different geological units (after Anderson and Woessner, 1991).

Table 13 Soil properties for eastern shores of St Lucia (Davies *et al*, 1992)

SOIL TYPE	PERMEABILITY		POROSITY (%)
	in cm/sec	in m/day	
Cover sands (site 1)	3×10^{2}	26	38.3
Cover sands (site 2)	1.81×10^{2}	15	37.9
Older cover sands	1.76×10^{2}	15	38.8
Older aeolian sands (site 1)	1.0×10^{3}	0.88	35.8
Older aeolian sands (site 2)	9.6×10^{4}	0.83	36.0
Port Durnford sands	8.64×10^{3}	7.5	42.3
Grey Port Durnford	6.8×10^{4}	0.59	42.3
Yellow Port Durnford	1.3×10^{4}	0.11	42.3

In order to derive representative values for permeability of this region, the published observations for the study area (Table 15) were used in conjunction with range indicated above have bee taken into account. The estimated values from Meyer and Godfrey (1995) were derived from laboratory samples for a wide range of soils throughout Zululand. Worthington (1978) estimates were derived from pumping tests at some boreholes around Lake Mzingazi. His estimates were based on transmissivities of 0.2 - 0.5 m^3/day/m for the Port Durnford (Worthington, 1978). Other studies indicated transmissivities of 10 m^3/day/m for the Nhlabane area (Martinelli, 1988) and 16.7 m^3/day/m for the Mzingazi area (Simmonds, 1990) .

Table 14 Permeability estimates from published geological surveys (m/day).

MATERIAL	Heath (1983)	Kruseman *et al* (1994)	Shaw (1983)
Fine Sand	0.5 to 200	1 to 5	12
Medium Sand		5 to 20	
Course sand		20 to 200	
Silt	0.001 to 5		0.08
Clay	10^{7} to 10^{3}	10^{4} to 10^{2}	10^{4}
Sandstone	10^{5} to 1	0.001 to 1	3.1
Limestone			0.94

Table 15 Permeability values in m/day as determined by different authors.

<table>
<tr><th></th><th>Davies et al 1992</th><th>Meyer et al 1995</th><th>Worthington 1978</th><th>Simmonds 1990</th></tr>
<tr><td>METHOD</td><td>LAB</td><td>LAB</td><td>PUMPING</td><td>LAB</td></tr>
<tr><td>Cover Sands</td><td>15.6 - 25.9</td><td rowspan="2">15.6</td><td rowspan="5">0.5 - 34.6</td><td rowspan="5">0.11 - 2^{*}</td></tr>
<tr><td>Older Cover Sands</td><td>15.2</td></tr>
<tr><td>Older Aeolian Sands</td><td>0.83 - 0.87</td><td>0.87</td></tr>
<tr><td>Port Durnford Sands</td><td>7.46</td><td rowspan="2">4.3</td></tr>
<tr><td>Port Durnford</td><td>0.11 - 0.59</td></tr>
</table>

7.1.1.2 POROSITY

The porosity values are much more uniform with far less variability (Table 13). Consequently, the estimates for the Richards Bay stratigraphic units have been selected with greater confidence from published values (Table 13). They have been adjusted over a fairly narrow range of values in the calibrations when other hydraulic parameter limits were reached.

7.1.2 BOUNDARY PARAMETERS

The Modflow model requires the specification of parameters for both the external and internal boundaries. These boundaries have been classified by Kinzelbach (1988) according to their characteristics as (1) no flow boundaries, (2) constant flux boundaries or (3) specified flux boundaries. The selection of these boundaries is done in the conceptual model of the study area. Large scale regional studies provide estimates of catchment divides which can be specified as no flow boundaries in smaller scale studies (see case studies in next section). Where the internal boundaries (such as rivers) isolated the external boundaries from an area of interest in the model domain, then the external boundaries have little influence and the choice is not important. The internal boundaries are presented in subsequent sections according to their conceptualization (rivers, lakes, drains etc).

7.1.3 LAYER THICKNESS

The three dimensional finite difference equations in Modflow involve the specification of both horizontal and vertical dimensions. The horizontal dimensions are set in the specification of the model domain (Δx and Δy). However, the vertical dimensions (Δz = m) are set by specifying layers with variable thickness. The vertical dimensions seldom exceed the horizontal dimensions, but are often an order of magnitude smaller.

The layer thickness is defined by the different aquifers identified in the conceptual geological model and generally conform to the local stratigraphy. The layer is usually identified as a stratigraphic unit which is assumed to be a homogeneous media with a single representative hydraulic characteristic. It is common, therefore, to create the numerical model with vertical layers which have homogeneous hydraulic properties. However, the use of heterogeneity in layer properties is considered in this report and a case study is presented in the next sections.

The assumption of uniform hydraulic characteristics in the model layers requires a considerable effort in the identification of the stratigraphy of the Richards Bay area. Two methods of specifying the stratigraphy in Modflow have been developed for this study.

7.1.3.1 HOMOGENEOUS LAYERS

The most common method of layer specification in numerical modelling is to assume a continuous stratigraphic unit with homogeneous hydraulic properties. The layer varies in thickness across the model domain in direct response to geological formations which have common hydraulic properties. In these conditions it is necessary to identify the upper and lower surfaces of the aquifer layer and then estimate a single representative hydraulic parameter for the whole layer or sections of the !ayer.

The conceptual geological model described in section 5 identified three main aquifers for the Richards Bay region. The Cretaceous mudstone-siltstone deposits were assumed to form the base of the primary aquifer. The discontinuous layer immediately above the Cretaceous deposits, the Miocene deposits are composed of calcareous conglomerate and has been described as the main aquifer in the region (Botha, 1997). Above this layer are the argillaceous deposits of the Port Durnford formation which has a much higher clay content, lower permeabilities and storage coefficients. Overlying these are the more recent arenaceous cover sands.

7.1.3.2 HETEROGENEOUS LAYERS

The second method assumes an identifiable layer thickness with specified upper and lower surface elevations and known hydraulic characteristics. In this case the layer thickness is specified at each node and the hydraulic properties vary throughout the model domain. The method developed for the application of this technique requires a considerable amount of effort in linking the stratigraphy with the varying hydraulic characteristics.

A spreadsheet model was constructed (Figure 65) to convert the stratigraphic sequence in a borehole log to the "arbitrarily" assigned layers in this conceptual model. The borehole information available in the regular data bases used for this region (Hydrocom) are shown in the example of Table 16. The information at each borehole location was used (in the spreadsheet model) to estimate the permeability of the "arbitrarily" assigned layer based on the proportion of each stratigraphic unit within the layer. The assumed values for the logged parameters as well as the calculated permeabilities for the three layers, are shown in Table 16.

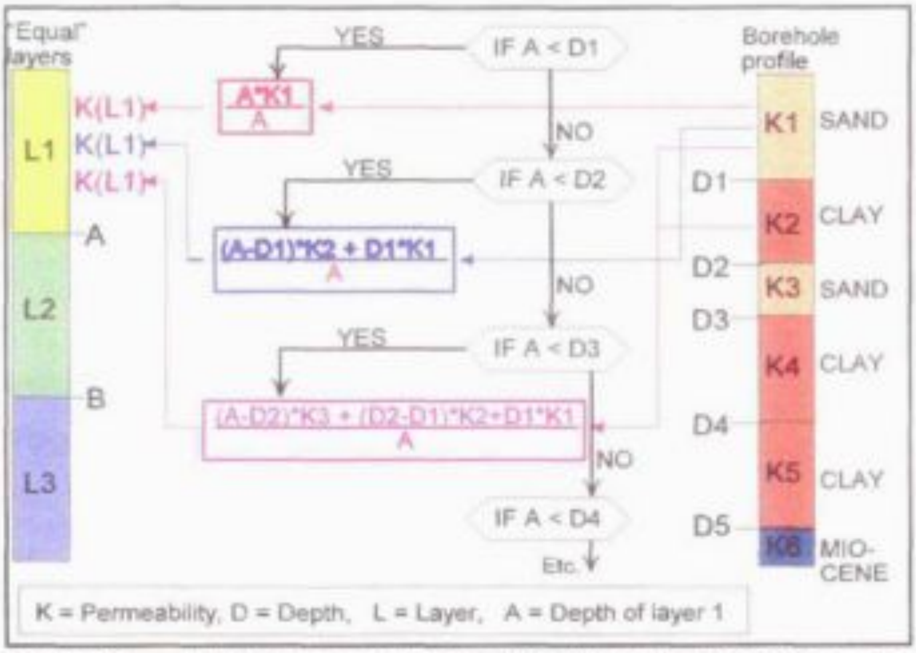


Figure 65 Model for estimating the hydraulic parameters in a heterogeneous layer from borehole logs. Example borehole used here.

The "arbitrarily" assigned layer of equal thickness at the location of each borehole were determined and then used to estimate the hydraulic properties of the layer from the proportion of the layer that is occupied by the stratigraphic units identified in the borehole log. The left hand column in Figure 65 represents the "arbitrarily" assigned layers with vertical dimensions which are indicated as A and B (10 m and 20 m respectively in the example in Table 16). The vertical extent of the layer in Figure 65 indicates its thickness in direct proportion to the borehole layers derived from the logs (portrayed in the column on the right hand side of Figure 65). The borehole logs have the stratigraphic units identified on the right hand side together with elevations of their horizons. The spreadsheet model provides the method for determining the proportion of the stratigraphic unit within the model layers. The method adopted here required the identification of stratigraphic units with assumed homogeneous qualities which where identifiable in the borehole logs. The individual logs were transposed to a spatial array in direct relation with the proportion of the different units located within the specified layer. A diagrammatic representation of the method is portrayed in Figure 65.

Table 16 Example of borehole information as used in a spreadsheet to calculate average permeabilities for arbitrarily assigned layers

Borehole:	MP1065		Depth of layer 1	Depth of layer 2	Depth of layer 3
X:	3174156		10	20.0	30.0
Y:	81297				
Elevation:	30.32				
Depth from top	Lithology: code	Permeability for soil type	Permeability for layer 1	Permeability for layer 2	Permeability for layer 3
0	SAND	25	20.1	25.0	14.9
3.2	CLAY	10			
6.5	SAND	25			
20.7	CLAY	10			
25.4	SAND	25			
28	CLAY	10			
31					

In the spreadsheet model, K_i represents the hydraulic property estimated (or assumed) for each stratigraphic unit (i) in the borehole log (*i.e.* the permeability in the example of Table 16). D_i indicates the depth of each stratigraphic unit (i) in the borehole log. For the first model layer (left hand column), the spreadsheet model determines which stratigraphic unit overlaps the lower boundary of the model layer. In the example in Figure 65, Layer L1 properties would be derived from the following equation because the depth of layer 1 (A) is between D2 and D3.

$$K_1 = \frac{\left(A - D_2\right)K_3 + \left(D_2 - D_1\right)K_2 + D_1 K_1}{A}$$

For the second layer the spreadsheet model would search for the stratigraphic unit in the borehole log which is shared with the third layer (K4) and estimate the hydraulic properties in the same manner. This procedure is then repeated for all the boreholes. This model was used to create heterogeneous layers which were compared to the homogeneous layer model in one of the case studies presented in the next section.

7.1.4 RECHARGE

The recharge mechanism and parameterization has been described in detail in section 6.3.6. The recharge parameter chosen for any model simulations will depend on the extent that the other hydrological processes are incorporated in the simulations. If evapotranspiration is included then the recharge that would have led to the evaporation must be retained in the model input. Consequently, the recharge model for each case is presented where necessary.

7.1.5 EVAPOTRANSPIRATION

Evaporation in the Zululand region has been described in Section 3. Models for estimating potential evaporation from vegetated surfaces has also been described in that section. The conceptual evaporation model has been described in section 6.3.7. Initial estimates of the parameters that need to be specified (E_p and Extinction Depth) are given in Table 17. The concept of a groundwater maximum rate of Evapotranspiration was discussed in section 6.3.7. The values chosen for any model application will depend on whether the evaporation from the groundwater is included in the recharge.

There is no information on the extent of partitioning of evaporation between the various hydrological pathways. Consequently, these parameters require calibration. Unfortunately there is no information available for comparison with prediction that will afford the calibration of the evaporation components. Table 17 indicates the values that were used by Kelbe and Rawlins (1992) for the eastern shores of Lake St Lucia. Kelbe and Rawlins (1992) assumed that the maximum groundwater evaporation (E_{max}) was one quarter of the regional estimate of Penman Potential Evapotranspiration (E_p).

Table 17 Evaporation parameter values from Kelbe and Rawlins (1992)

Vegetation Type	E_p (mm/day)	Extinction depth (m)
Grasslands	2	2
Scrub and indigenous forest	2	6
Plantation forest	2	12

Pine trees have been known to transpire at a rate in excess of 1100 mm/year (Lindley and Scott, 1987). Other species of fast growing trees, notably Eucalyptus, have had recorded transpiration rates as high as

2700 mm/year (Greenwood *et al*, 1985). Afforestation appears to have a significant influence on the water balance of a region by increasing evapotranspiration rates and thereby reducing runoff and groundwater storage (Bosch and Hewlett, 1982). Studies by Rawlins and Kelbe (1991, 1992) suggest that the pine forest situated in the Eastern Shores of St Lucia transpires water at a rate 150 mm/year higher than the surrounding natural vegetation. Consequently there is a major influence on the water table elevation of this region. Under the pine plantation, there is a recorded steady decline of the water table during the dry winter period of about 5 mm/day. Assuming a porosity of about 45%, this corresponds to a water loss of approximately 2 mm/day, which is due mainly to evapotranspiration but also to some lateral seepage flow to the lake and swamp. However, the hydraulic gradient in the vicinity of the weather station is very low and the seepage rate is considered minimal in comparison with the evaporation rate. Consequently, it is important to include the effects of evaporation and vegetation type in these numerical simulations. The estimated difference in evaporation parameters for the different vegetation types used in this study are given in Table 18.

Table 18 Evapotranspiration parameters for various landuses.

LANDUSE	E_v (mm/d)	Extinction depth (m)
Trees	3	12
Bush	2.5	10
Sugar	2	6
Subsistence	1.5	4
Grasslands	2	2
Wetlands	2	2

The extinction depth is assumed to be related entirely to the rooting depth of plant

Table 19 Correction factor in evapotranspiration parameters for three classes of soil depth (Kelbe, Rawlins and Nomquphu, 1997).

Layer thickness (m)	Factor
< 5	0.5
5 to 15	1.0
> 15	1.5

species. Since the rooting depth is affected by the soil thickness and composition, these parameters should also be adjusted for the soil types. Table 19 gives the correction factors used by Kelbe, Rawlins and Nomquphu (1997) for the Lake St Lucia region.

7.1.6 SURFACE ELEVATIONS

All the surfaces of the different hydrogeological layers (stratigraphic units) were created from available borehole information and published commercial maps as described in section 5.

7.1.7 WATER TABLE HEADS

Various methods were used to estimate the initial heads but the most pragmatic approach was generally to set the water table at the same elevation as the topographical surface.

7.1.8 RIVER CONDUCTANCE

None of the parameters used to simulate the river or lake bed conductance were known. The lake bed conductance is essential if the interaction between the aquifers and coastal lakes is to be determined. A case study based on the calibration of the lake package is presented in section 8.3.

7.2 CALIBRATION

Numerical models seldom have sufficient information to determine representative values of model parameters. Consequently, it is usually necessary to "improve" the parameter estimates through calibrations. However, Kelbe and Rawlins (1992a) used a detailed geological survey which provided adequate information to determine the hydraulic features for a hydrological study in the eastern shores of Lake St Lucia that did not require further calibrations. Nevertheless, wherever there is any uncertainty in parameter values, it is necessary to calibrate the model against observed conditions. When there is uncertainty and there is no information on the system then the model application becomes extremely tenuous.

The easiest and most common observation of the groundwater system is water table or piezometric surface elevation. Consequently, the initial calibration is usually based on a comparison of simulated and observed heads. While single observations do provide some measure of convergence, the transient changes in head are usually needed for reasonable calibrations.

The comparison between measured and predicted heads is used as the principle means for calibrating parameter values in this study. However, water balance of selective boundary conditions is also considered in several cases.

7.2.1 TRIAL AND ERROR CALIBRATION

The trial and error method of calibration is outlined by Anderson and Woesner (1991). In this method the numerical model parameters that have been estimated from some source are used to simulate the observations. The parameter values are adjusted individually in a trial and error approach to achieve an acceptable comparison between the prediction and observation. This method does not seek to achieve the "best estimate" but rather an acceptable (subjective) estimate. This is the most common methods employed in groundwater studies and it has been found to give the more reliable results in the case studies presented in this report. An example of a comparison of observed and simulated heads for a regional model is shown in Figure 66 for the Richards Bay area. There are several boreholes which exceed simulated levels and *vice versa*. To improve the prediction of these boreholes it would be necessary to adjust smaller scale features that affected only these boreholes.

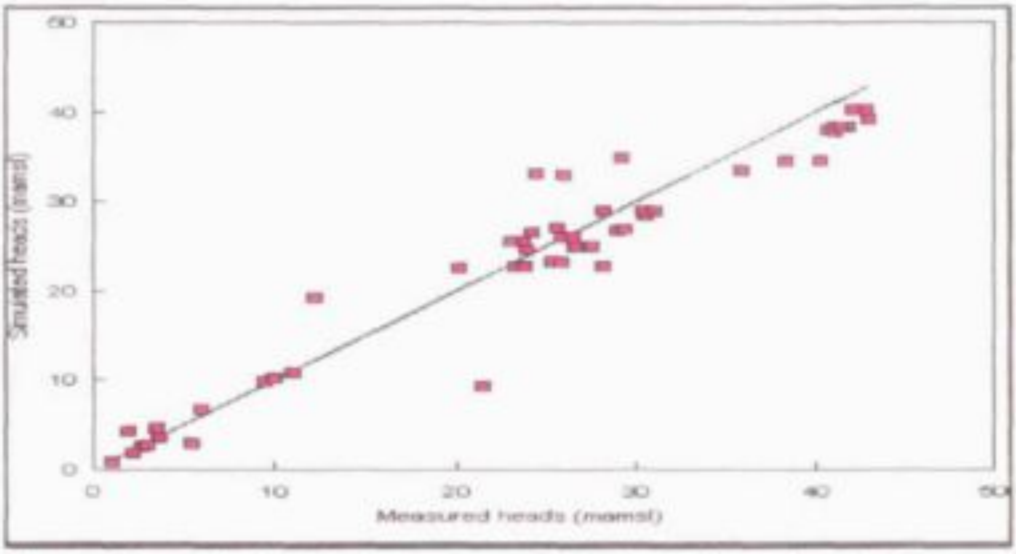


Figure 66 Simulated versus measured water levels after calibration. The grey lines indicate a 3m (level 1) difference.

7.2.2 AUTOMATIC CALIBRATION METHODS

The only numerical methods investigated in this project for calibration of parameters was CALIF (Häfner *et al*, 1996). This method uses a search pattern to find a set of parameters to minimize the sum of squares of the differences between simulated and observed values. In CALIF the sum of squares of the difference between simulated (C_i) and observed (C_i^{obs}) value is minimized in the calibration procedure using different iteration techniques. The three iteration methods used were (1) Gauss-Newton iteration technique, (2) the Powell's method and (3) the Levenberg-Marquardt method (Häfner *et al*, 1996).

CALIF partitions the model into "zones" for identifying appropriate parameter values in the calibration procedure. The programme is only capable of adjusting four zones in each iteration. Consequently the partitioning of the model domain into four zones requires careful consideration. In this study, it was realized that this technique of applying zones in the calibration model could have a definite influence on calibration results. Sonnenborg *et al* (1996) suggests that the identification of an optimal zonation structure of the permeability field seemed to be a critical factor in calibration method. They also suggest that in an attempt to improve the fit to observed data, a modeller may choose too many zones which may lead to poor parameter estimates. The calibration procedure requires:

- *the specification of specific zones where parameters are assumed to be homogeneous,*
- *the initial parameter values in each zone that are to be optimized in the calibration procedure,*
- *the range of values for each parameter which restricts the changes that the program can apply in the search for better values. This range is specified as a multiplication factor. For example a minimum of 0.1 and a maximum of 5 means the optimized value may be anything from 10 times smaller to 5 times bigger than the given starting value. This range should be small for the program to search effectively.*

Experience with the CALIF model shows that some of these calibration procedures require large resources in time and hardware. Therefore one needs to set objective criteria for the procedure. In this study the permeability parameters were optimized for flow simulations and the retardation factor was optimized for transport simulations. These two cases have been presented in separate case studies in sections 8.6 and 11.1 respectively.

7.2.3 SENSITIVITY

In the process of changing the parameters during a calibration study, the sensitivity of the predictions to parameters can also be determined for the case in particular. Consequently, the calibration and sensitivity processes generally are combined. During a sensitivity analysis the calibrated parameters are changed systematically (one at a time) and the magnitude of each change is observed. An example is shown in Table 20 for a three parameter assessment where the values of the recharge, hydraulic conductivity and evapotranspiration have been halved and increased by 1.5 times according to the sequence shown in Table 20.

The simulated change in head between the control and the "sensitivity" scenarios A - F (in Table 20) was quantified by averaging the water level in 49 observation points for each of the runs. The percentage change between the control run and each sensitivity run (shown in Figure 67) indicates that recharge is the most sensitive parameter and evapotranspiration the least.

Table 20 Parameters used for different sensitivity runs

	RECHARGE (mm/year)	EVAPOTRANSPIRATION (mm/year)	HYDRAULIC CONDUCTIVITY (m/day)
CONTROL	1000	1000	10
A (Recharge)	**500**	1000	10
B (Recharge)	**1500**	1000	10
C (Hydr.Cond)	1000	1000	**5**
D (Hydr.Cond)	1000	1000	**15**
E (Evap)	1000	**500**	10
F (Evap)	1000	**1500**	10

Another way of displaying sensitivity results is to choose some observation points which have a very good agreement between measured and simulated head values for the calibrated model and plot absolute changes for each sensitivity run for each of these points (see Figure 68). The distribution of the five boreholes chosen are indicated in Figure 69. In the case of these five boreholes, the C scenario produced the largest change.

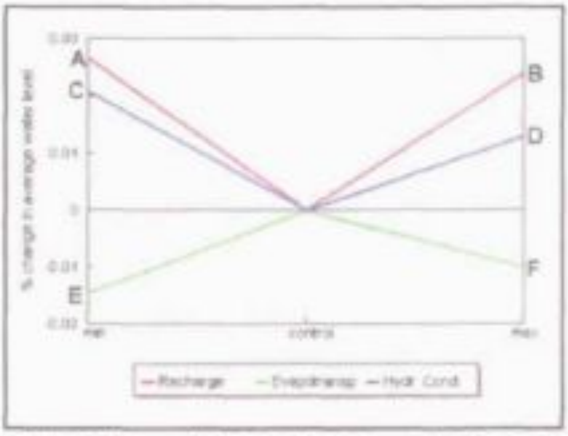


Figure 67 Percentage change in average head between the calibrated model and different "sensitivity" models

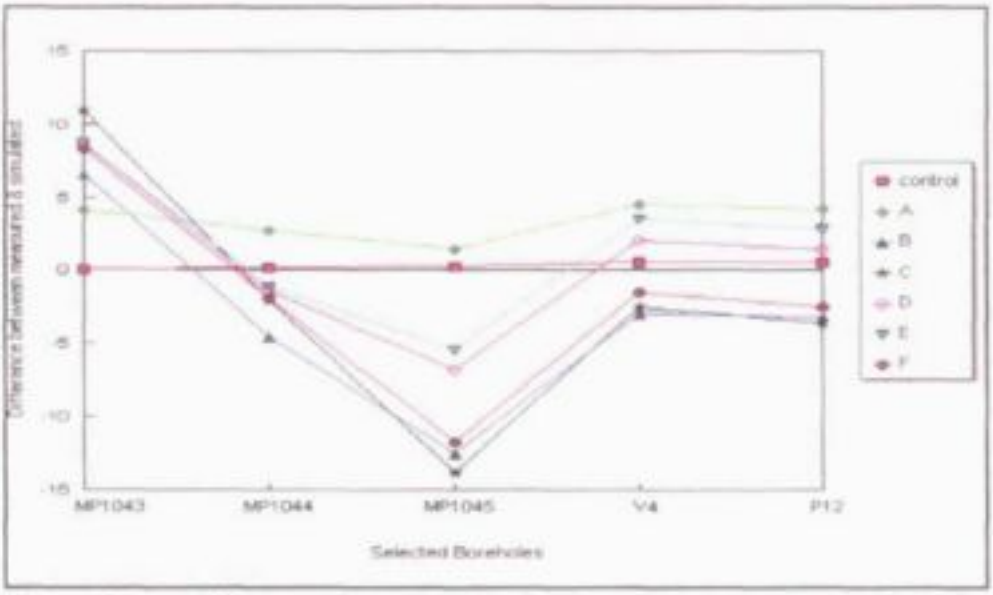


Figure 68 Difference between simulated and measured water levels for selected boreholes. A - F are the different "sensitivity" runs indicated in Table 20.

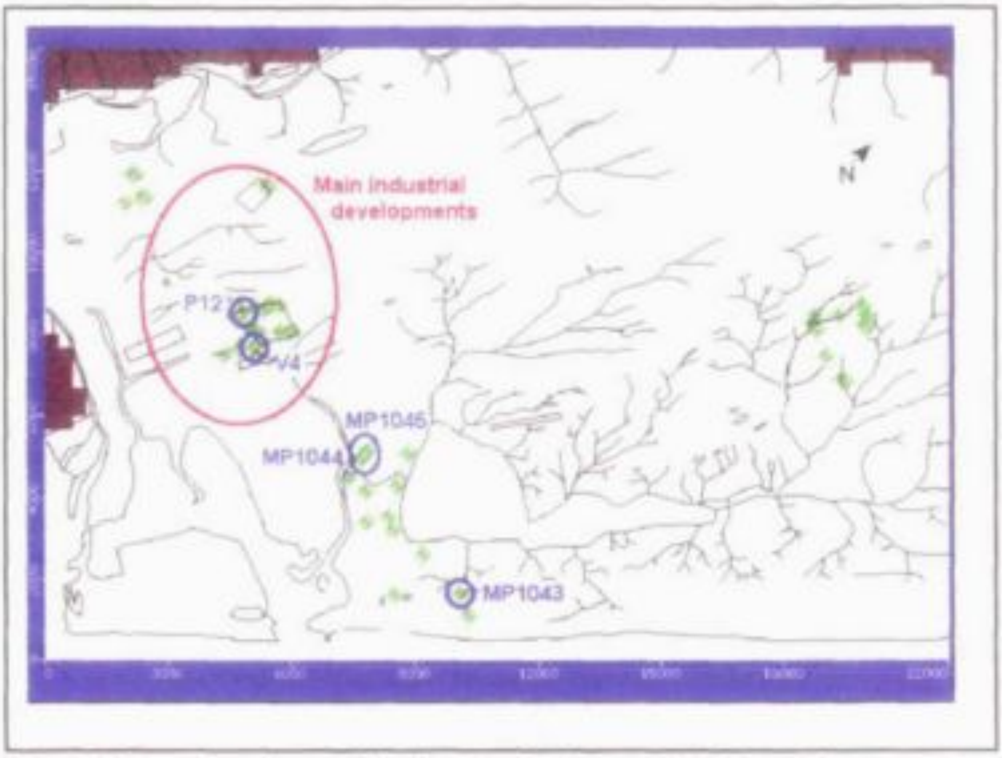


Figure 69 Locations of the five boreholes used in Figure 68.

Section 8 CASE STUDIES

The previous sections have outlined the numerical methods for groundwater simulation studies and some of the numerical models that are currently available for use in these studies. These models are all similar and have been tried and tested under different conditions in many parts of the world. This study was initiated to develop the means and experience in applying these models in the unconfined aquifers of the Zululand Coastal Region where there is rapid developments which are impacting on the primary aquifer. The numerical methods have been used by Kelbe, Rawlins and Nomquphu (1995) to determine the groundwater contribution to Lake St Lucia and by Kelbe and Rawlins (1992) in the assessment of the likely impact from dune mining on a sensitive region of the eastern shores section of Lake St Lucia. This section of the report presents several case studies of specific studies which have been conducted during the last three years of the study programme in the Richards Bay area using these numerical methods.

1 The first case study (REGIONAL GROUNDWATER DYNAMICS) involves a regional assessment of the groundwater dynamics that was undertaken to determine the areas contributing to the recharge of the important water resources of the region. The study has identified the regional flow pattern and the catchment divides for the main water bodies. In order to develop these simulations a considerable effort was made to construct the best geological model of the region which has been described in detail in Section 5 and used in all case studies.

2 The second case study (MULTI-LAYERED REGIONAL MODEL) describes the impact of multi-layered models in simulation studies of regional flow patterns. The difference in simulated results between a one, three and four layer model are examined in the region.

3 The third case study (WATER RESOURCES STUDY OF LAKE MZINGAZI) was undertaken to determine the water balance of the primary coastal lakes in the region. The study estimated the various flow contributions to all the lakes. However, this report has been restricted to a description of Lake Mzingazi. The study describes the simulated changes in Lake level as part of the Lake Water Requirements (LWR) study being conducted for Mhlatuze Water (1998). The results have been published by Kelbe and Germishuyse (2000).

4 The fourth case study (LAND USE ASSESSMENT) is an extension of the LWR study which evaluates the effects of land use on the water balance of the Lake systems. The extensive afforestation in the region is thought to have had a large impact on the water resources of the region. Rawlins (1992), Rawlins and Kelbe (1991) and Kelbe *et al* (1995) have examined the impact of extensive afforestation in the St Lucia region. This case study examines the effect of afforestation in the Richards Bay region.

5 The fifth case study (COMPARISON OF CALIBRATION TECHNIQUES) describes a test site that was used to test automatic calibration techniques. Both a two-layer and a five-layer model were used to test different scenarios in order to find the best calibration of the models. The complexity and uncertainty of automatic calibration is highlighted in this case study.

8.1 CASE 1 : REGIONAL GROUNDWATER DYNAMICS

A sequence of dry years in the early 1990's resulted in concern for the water resources of the Richards Bay area. The principle water resources in the region are the network of coastal lakes which are considered to be an extension of the unconfined aquifer. This study was initiated as a project to establish methods for determining the dynamics of the groundwater system to assist in the regional water resources management. This section of the report covers the initial assessment of the regional groundwater flow dynamics.

8.1.1 CONCEPTUAL GEOLOGICAL MODEL

The regional study area was confined by physical boundary considerations. The area chosen is shown in Figure 70. The Indian Ocean was assumed to form a constant head boundary along the south eastern section of the area. Lake Nsezi and the Nseleni river were chosen to form the north-western boundary while the Richards Bay Estuary and Harbour and the Mhlatuze River formed the south-western Boundary. The north-eastern boundary was created as a no flow section because it was assumed that the drainage in this region was topographically driven and would generally be parallel with the physical model boundary. It was also assumed to be a distant boundary (Anderson and Woessner, 1991) which was sufficiently removed from the main regions of interest.

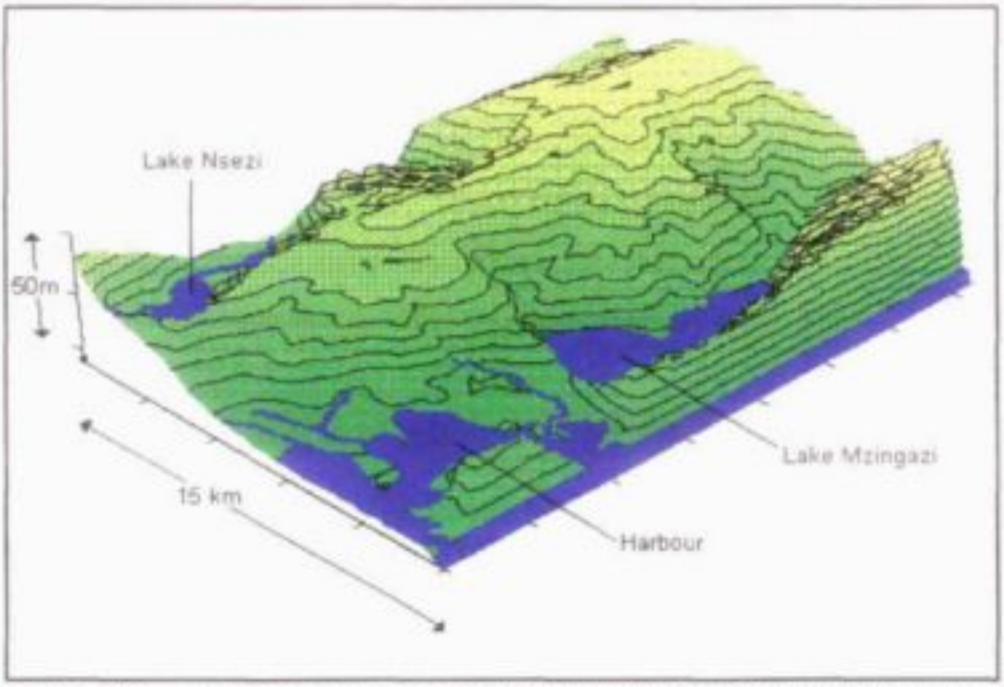


Figure 70 Model domain for regional groundwater studies (vertical scale exaggerated)

The geological transects through the study area (Figures 52 to 54) shows the main stratigraphic units described in section 5.6.2. The Cretaceous siltstone was taken as the impermeable lower boundary of the aquifer. The Miocene is confined by the overlying Port Durnford which is topped by the unconsolidated cover sands. As a final stage assessment, it was assumed that the regional groundwater flow dynamics could be simulated as a single unconfined aquifer controlled by the main surface water bodies shown in Figure 70, because all the layers were unconsolidated sand deposits with varying final content.

The derivation of the upper (topographical) surface and the lower (Cretaceous) surface boundaries are explained in Section 5.6.2. Homogeneous hydraulic properties were assumed for the model layer which were initially derived from reviews of previous studies (section 7.1) and adjusted in the calibrations described in the next sections.

8.1.2 CALIBRATION AND SENSITIVITY ANALYSIS

The simulated flow for the region was compared to all the available water level observation provided by the various organizations. The location of known water level information is shown in Figure 71.

8.1.2.1 STEADY STATE CONDITIONS

To calibrate the Modflow simulations using observed water level measurements it was necessary to evaluate the model results generated under similar meteorological conditions to the observation. The initial calibration was conducted using observations from an assumed "mean" meteorological conditions of rainfall and evaporation. The model simulations representing long term average meteorological conditions were assumed to represent the mean hydrological state. The long-term "mean" recharge and groundwater "potential" evaporation (see Section 6.3.6 for definitions of the meaning of these parameters) used in the simulation are given in Table 21.

Table 21 Calibrated parameters representing the "mean" meteorological state.

Parameter	Value (mm/year)
Recharge	~800
Potential Evaporation	1000

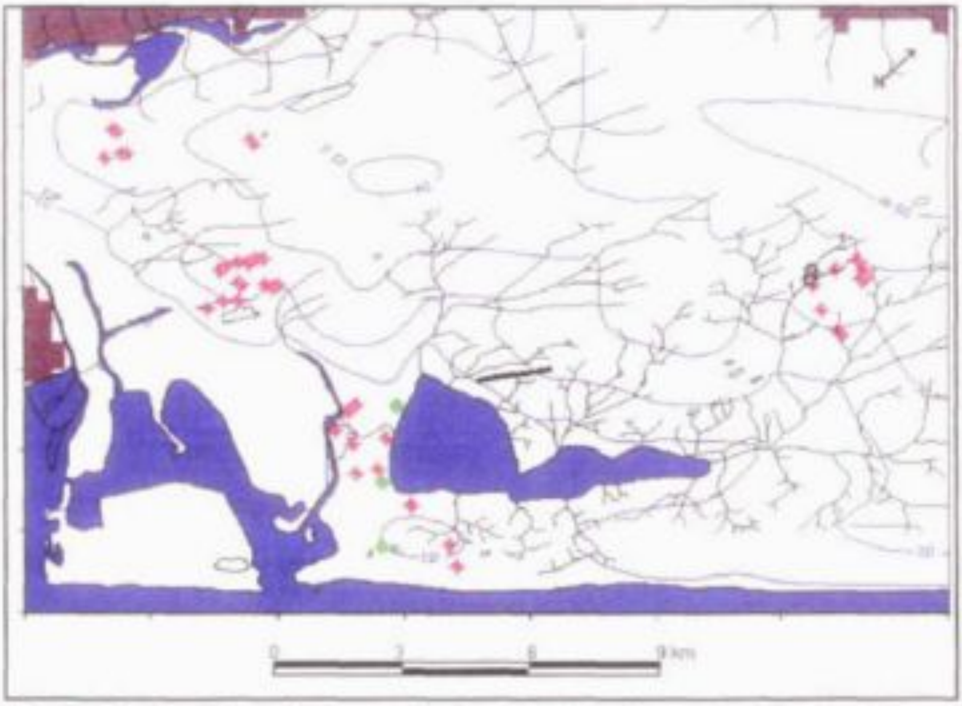


Figure 71 Location of observation boreholes referred to in the text.

The hydraulic parameters (permeability and storage coefficient) during the calibration of the model were adjusted subjectively to achieve the best fit between the simulated and observed water level observations. The comparison between the simulated and observed water levels for the assumed mean hydrological conditions derived from the steady state model are shown in Figure 68. The difference between the observed and simulated is generally less than 3 m. This is considered acceptable for this regional assessment of the flow dynamics.

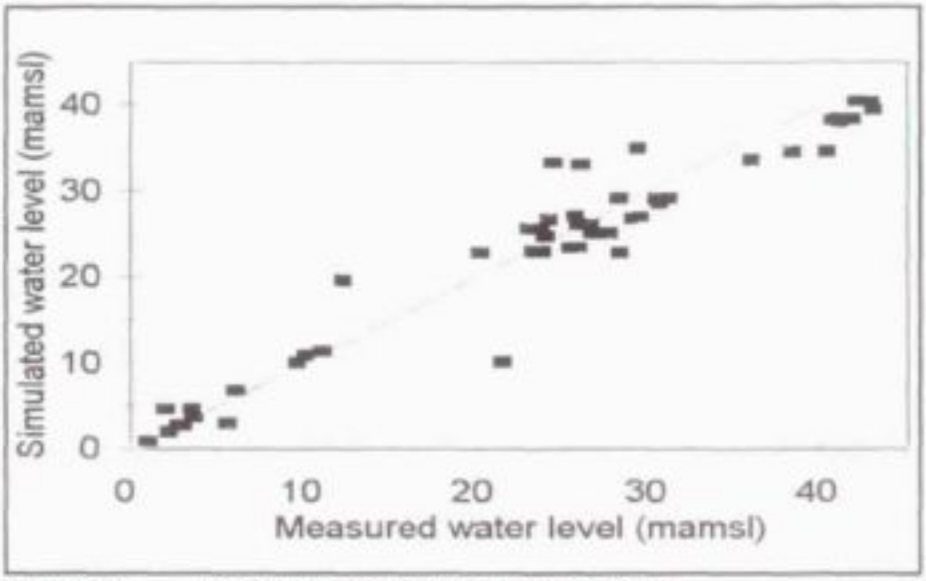


Figure 72 Observed -vs- simulated water levels

8.1.2.2 TRANSIENT CONDITIONS

The simulated conditions for the stress periods with known recharge (rainfall) and evaporation were compared to the available observations using the same hydraulic parameters calibrated in the steady state model simulations above. The parameters were again adjusted to suit BOTH the steady state and the transient flow calibrations to achieve the ultimate set of hydraulic parameters shown in Table 22.

The transient flow simulations for selected nodes corresponding to observation boreholes are compared in Figure 73. The initial straight line represents the steady state mean hydrological conditions followed by the period of observation. The borehole labelled MP1041 is situated in the dunes between the Indian Ocean and Lake Mzingazi where the greatest fluctuations in water are expected to occur. The other two series represent boreholes between Lake Mzingazi and the saltwater canal.

Table 22 Hydraulic parameters for the calibrated 1 layer model

Parameter	Layer 1
Permeability (m/day)	10
Storage Coefficient (m^{-1})	0.2

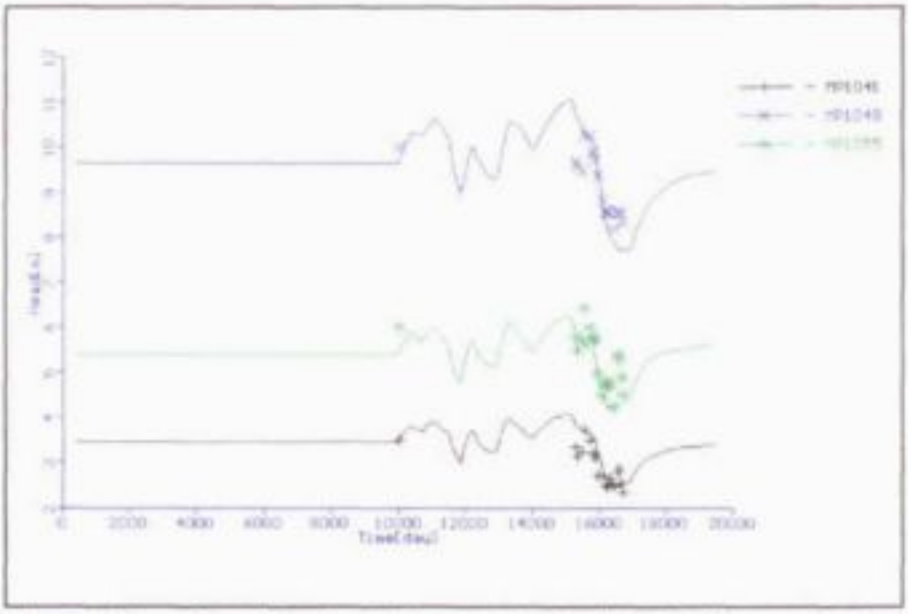


Figure 73 Simulated and observed water levels at three selected boreholes located at the sites shown as red circles in Figure 71.

The simulated results do not correspond as well for two boreholes in the northern section of the study area (Figure 74) which are located at the two black circles in Figure 71. These two boreholes are situated very close together but have very different water table elevations. A single layer model is unable to simulate this difference as the two boreholes may represent different aquifers. Since the numerical model is configured for one layer, it cannot simulate confined aquifers. Similarly, the simulated values are likely to be similar to each other because the internal boundaries formed by some of the local streams have not been included and they may have a much larger influence than the model predicts. However, the variations in water table elevations have been adequately simulated in both series (Figure 74) although the absolute elevation is in error by 6 - 8 m.

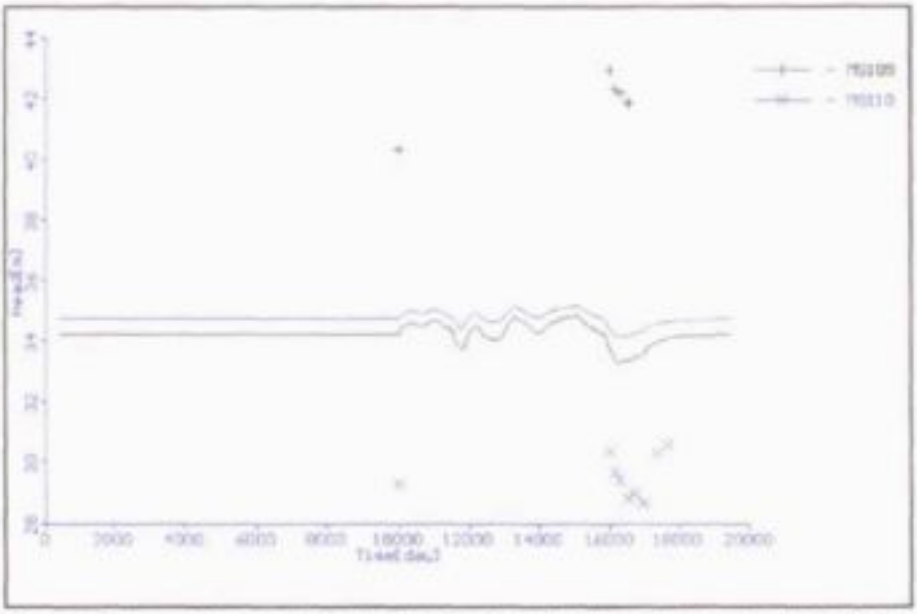


Figure 74 Comparison between simulated and observed heads for two sites with poor relationships that are located at the black circles in Figure 71.

The calibrated results are considered adequate for a regional scale assessment of the groundwater resources for Richards Bay.

8.1.3 REGIONAL STEADY STATE FLOW PATTERN

The calibrated flow pattern for the region is shown in Figure 75 and 76. The direction of flow at each node is indicated by the arrow in Figure 75. The flow velocity at each node is indicated in Figure 76 by the length of the arrow. Also shown in Figure 76 is the simulated water table elevation contours. The flow pattern in Figure 75 indicates the groundwater divides that separate flow into the main boundaries (lakes and rivers). These groundwater divides represent the recharge area for each of the main water resources.

8.1.4 SUMMARY AND CONCLUSION

This case study provided an indication of the regional groundwater flow pattern around Richards Bay. This flow pattern was used to evaluate those section of the topographical surface where groundwater recharge occurs in order to identify the land use type which could impact on the recharge, evaporation and contamination of the aquifers. Figure 77 provides an indication of the dominant land use types within the receiving catchment of the main water bodies in Richards Bay. This shows that large sections of the urban community and all the peri-urban (informal) settlements are located in the catchment area for Lake Mzingazi. On the other hand, nearly all the industrial complexes are located in the area discharging into the harbour.

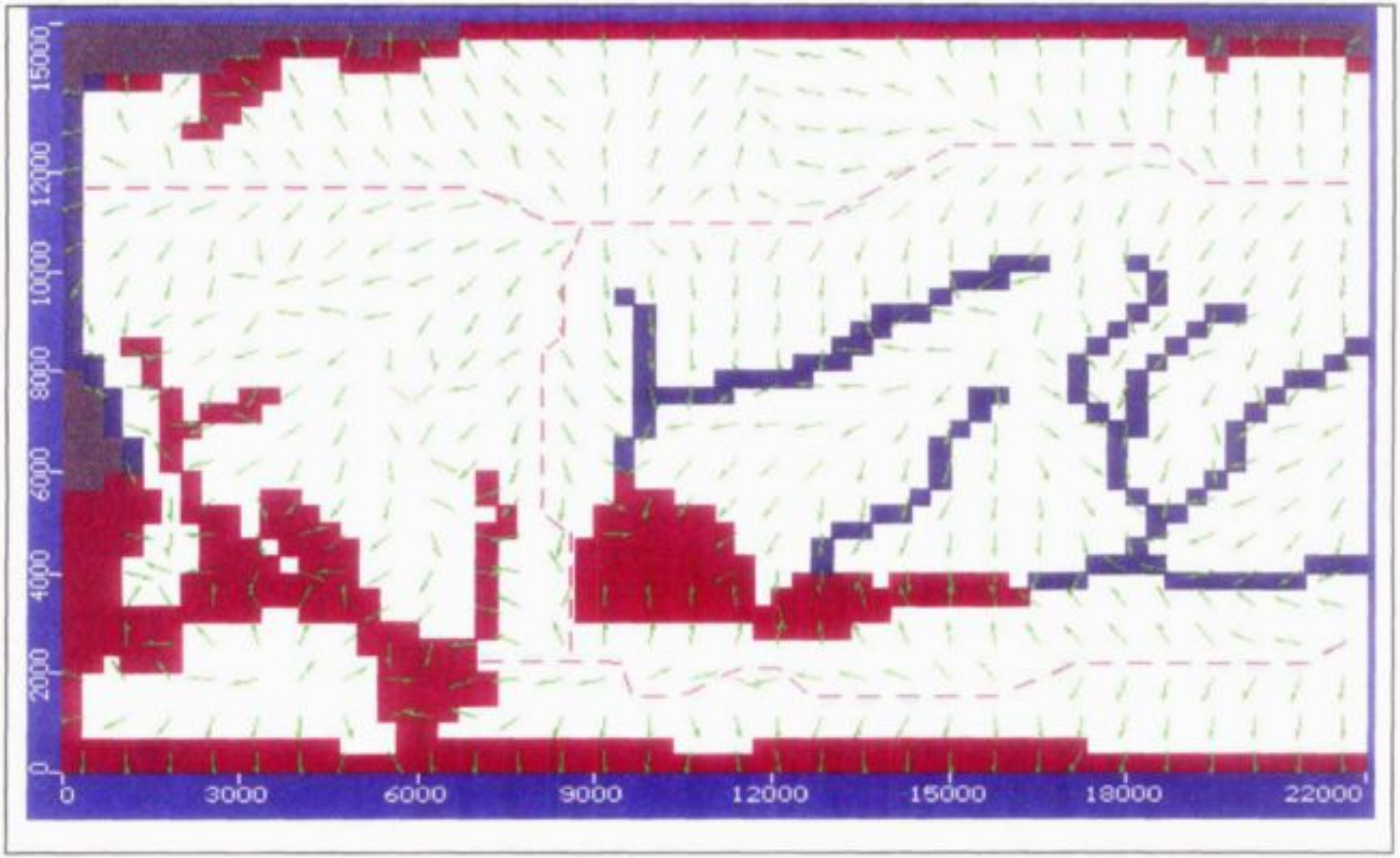


Figure 75 Simulated flow path for the regional groundwater model of Richards Bay. This flow pattern indicates the surface recharge area for all the major water bodies in the region.

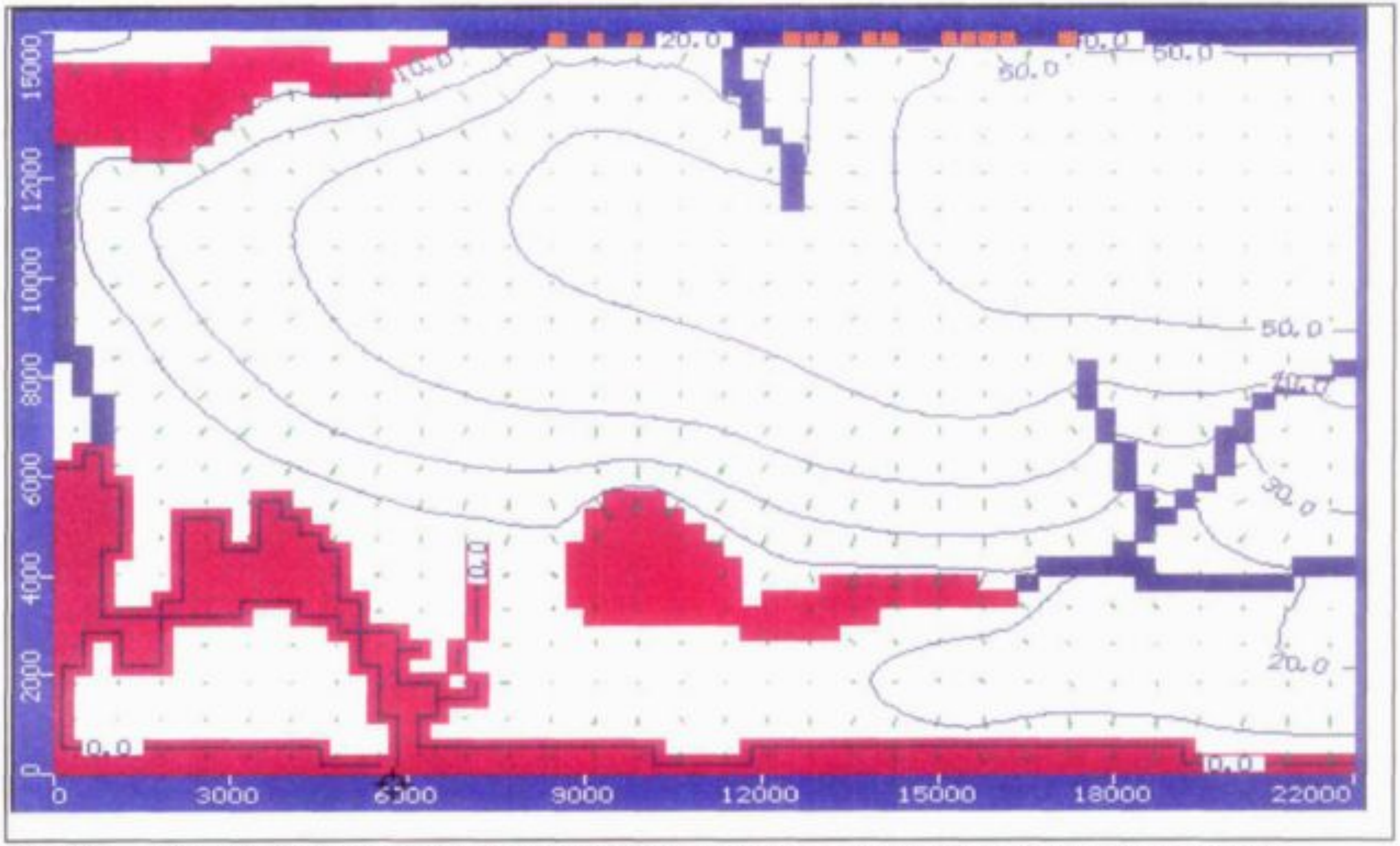


Figure 76 Simulated flow path and velocities for the regional groundwater model of Richards Bay. The water table elevations are shown as 10 m contours. Water bodies shown in red were simulated as constant heads and streams (in blue) simulated as head dependent boundaries.

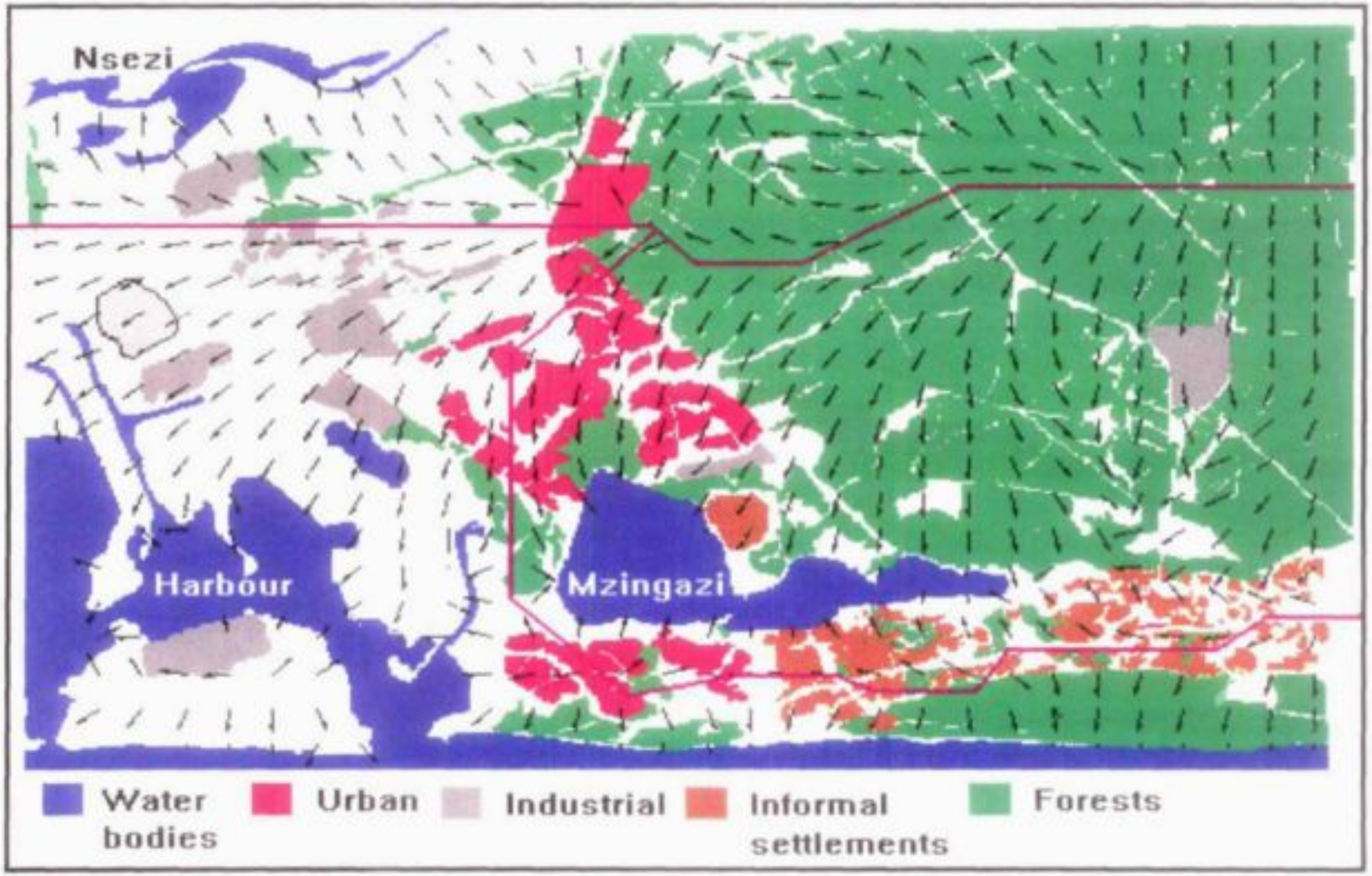


Figure 77 An example of the Identification of groundwater divides for the modelling of the major water bodies in Richards Bay for possible contaminant monitoring studies.

8.2 CASE 2 : MULTI LAYERED REGIONAL MODEL

In the development of the 3D Modflow groundwater model, McDonald and Harbaugh (1983) describe two extreme vertical discretization concepts for the model application. The application of these two extreme concepts is examined in this case study using the Richards Bay area described in the first case presented in section 8.1

8.2.1 HOMOGENEOUS PERMEABLE ZONES

This concept is based on the representation of separate aquifers or permeable zones defined by individual layers of the model with uniform or homogeneous properties. Since geological surveys of a region seldom have sufficient information to identify the variability of aquifer properties it is common to apply uniform characteristics over the full extent of these layers. Consequently, these permeable zones are assumed to be homogeneous layers with a single set of parameters.

8.2.2 ARBITRARY HETEROGENEOUS ZONES

The other extreme conceptual model suggested by McDonald and Harbaugh (1983) involves the more or less arbitrary process of dividing the vertical flow system into segments which are defined in part by the vertical resolution of the information (borehole logs). Most geological investigations (surveys) that determine the stratigraphy seldom have any information on the variability of aquifer properties. The borehole logs from these surveys differentiate the stratigraphy on the basis of soil texture and composition. The hydraulic properties of these layers are seldom determined. However, independent laboratory studies have derived a range of hydraulic properties of sedimentary layers for various compositions. Consequently the borehole log description of layer composition (sand, loam and clay content) and published hydraulic properties were used to describe the varying nature of the model layers.

The two extreme approaches to vertical discretization are shown in Figure 78. The first cross section shows the stratigraphy derived from the geological survey. The second cross-section shows four layers with assumed homogeneous properties that represent separate aquiferous units where the Cretaceous siltstones represent the basement material. The third cross-sectional model is based on arbitrary layers of relative uniform thickness with heterogeneous hydraulic properties. The derivation of the heterogeneous layers and a comparison between the simulations with this model and a model with homogeneous layers are presented in this case study for Richards Bay.

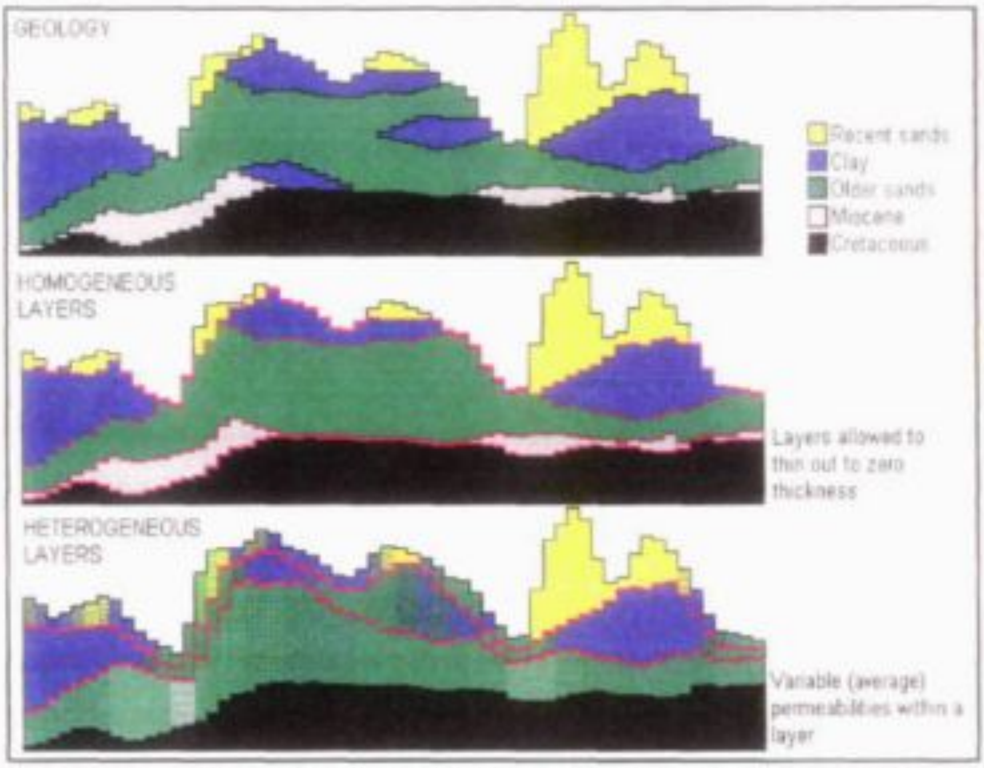


Figure 78 Example of contrasting numerical models of geological stratigraphy.

The conceptual geological model for this study was derived in a similar manner to that described in the first case study presented in section 8.1. The numerical model presented in section 8.1 was used as the initial starting condition in this study. However, these vertical discretization methods were adopted to compare the influence of vertical stratification and heterogeneous conditions in model predictions. The comparison involved a one layer model, a four layer model with homogeneous properties and a three layer model with heterogeneous layer properties. In all three simulations the lower and upper boundaries were the same and only the layer configurations in between were adjusted to conform to three different conceptual models of the region. The base of the system is formed by the very low permeable siltstone of Cretaceous Age described in section 5.6.2.1. The topographical surface forms the upper surface boundary as described in section 5.6.2.4.

8.2.3 ONE LAYER MODEL (METHOD 1)

The single layer model with uniform properties that was presented in Case Study 1 described in section 8.1 was used for comparison with the multi layer models presented here.

8.2.4 HOMOGENEOUS FOUR LAYER MODEL (METHOD 2)

The four principle aquifers which could be identified from the available information in the borehole logs were used as the model layers. These layers were not continuous and the surface fitting interpolation methods caused some vertical overlapping to occur in places. To prevent these situations in the model, the interpolated data (grid files) were imported into a spreadsheet and the different layer elevations were subtracted. Negative values were eliminated and the new grid files were restored in the model.

A serious problem in identifying the boundary between the layers from borehole information was the loosely defined terms "sand" which made no distinction between older and more recent sands. Consequently the sand layer was often divided into two units where the identification of the argillaceous and arenaceous units were determined.

8.2.4.1 MIOCENE UNIT

These were the highly permeable coquina and calcarenite deposits which were usually identified in the borehole logs. This layer was derived from borehole logs as described in section 5.6.2.2. Because the layer is not continuous the model layer was reduced to zero thickness in many areas.

8.2.4.2 ARGILLACEOUS UNIT

The argillaceous unit forms the lower member of the Port Durnford Formation. This unit consists of silty sands and a pronounced lignite band which overly the Miocene deposits. Where clay was present in the boreholelogs, it was assumed that this formed the boundary between the argillaceous member and the more recent sands of the arenaceous unit.

8.2.4.3 ARENACEOUS UNIT

The arenaceous unit forms the upper member of the Port Durnford Formation. This unit consists of medium to fine aeolian sands with good aquifer characteristics. These aeolian deposits were identified in the borehole logs as those layers of sand which were separated from the Miocene or Cretaceous by a layer (argillaceous) with some clay content.

8.2.4.4 HOLOCENE UNIT

The layer of recent cover sands over the entire region were assumed to form the fourth layer. These sandy deposits have been separated into two groups with different properties. The Holocene deposits underneath Lake Mzingazi and in the Mhlatuze Flood Plain generally have higher clay contents which may cause a semi-confining layer over the Port Durnford. For this study the Cover sands in the top layer were assumed to have uniform properties and the distinction between the two groups were ignored.

These aquifers were not continuous and the model layers were not always present in each cell. Consequently, this example was also used to examine the effect of zero thickness layers in the numerical model simulations.

8.2.5 THREE LAYER HETEROGENEOUS MODEL (METHOD 3)

For this model the aquifer was subdivided into three layers of approximately equal thickness within each vertical column. The minimum layer thickness was approximately one metre were the Cretaceous was close to the topographical surface.

In the homogeneous layer model (8.2.4) the layers were derived from the geological units in the borehole logs. In this heterogenous layer model the layers were constructed arbitrarily and the properties were derived from weighted proportions of the composition of the geological unit in the layer (Figure 65).

In the homogeneous model, each layer represented one geological unit and was therefore assigned the same hydraulic properties as the geological unit. In this heterogeneous model, the same properties were assigned to each geological unit, but the layer properties were derived from weighted contributions of each unit.

The model layers were constructed according to Section 7.1.3.2 to convert the stratigraphic sequence, from borehole logs, to the arbitrarily assigned layers in this conceptual model. The estimates of the hydraulic properties for each geological unit in the borehole log were derived from the stratigraphic sequence described in the four layer homogeneous model. In most cases no distinction could be made between older and more recent sands. However, where clay was present, it was assumed that the clay separated older and more recent sands. Where no clay was present, the thickness of sands were divided into two strata of equal thickness, the top part recent sands and the bottom part older sands. Layers were forced to a minimum thickness of at least 2 m where ever it was thinner than 2 m or absent. Where the layer protruded at the surface, the layer between the surface and bottom of the layer was divided into two parts of equal thickness. The derived profiles, using this model, for each borehole location were used in SURFER to create a spatial distribution of the properties of each layer for use in Modflow. The spatial distributions for the three derived layers are shown in Figure 79.

A transect through the heterogeneus model domain is shown in Figure 80.

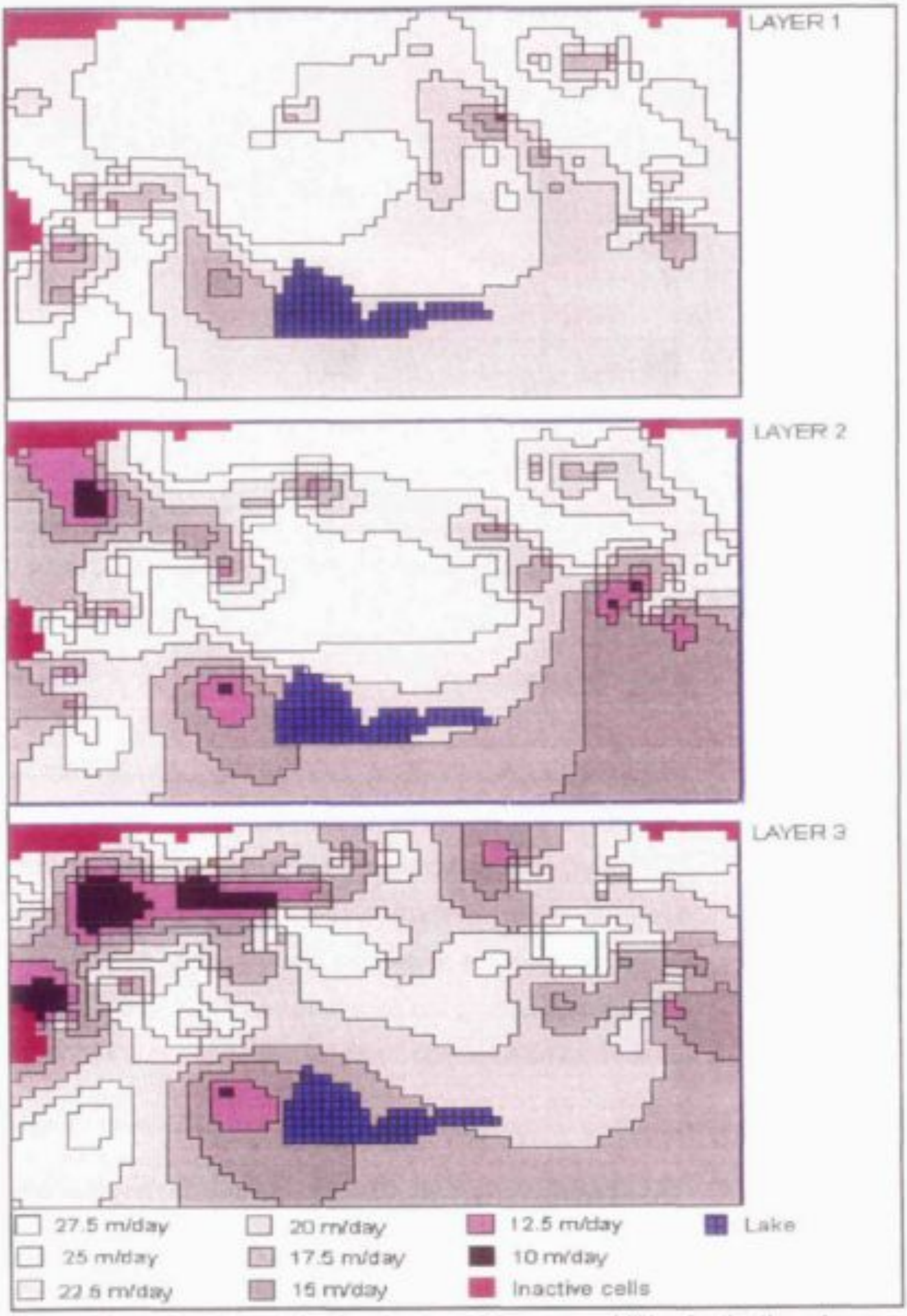


Figure 79 Spatially derived estimates of the permeabilities for the three layer heterogeneous model of the Richards Bay region described in the text.

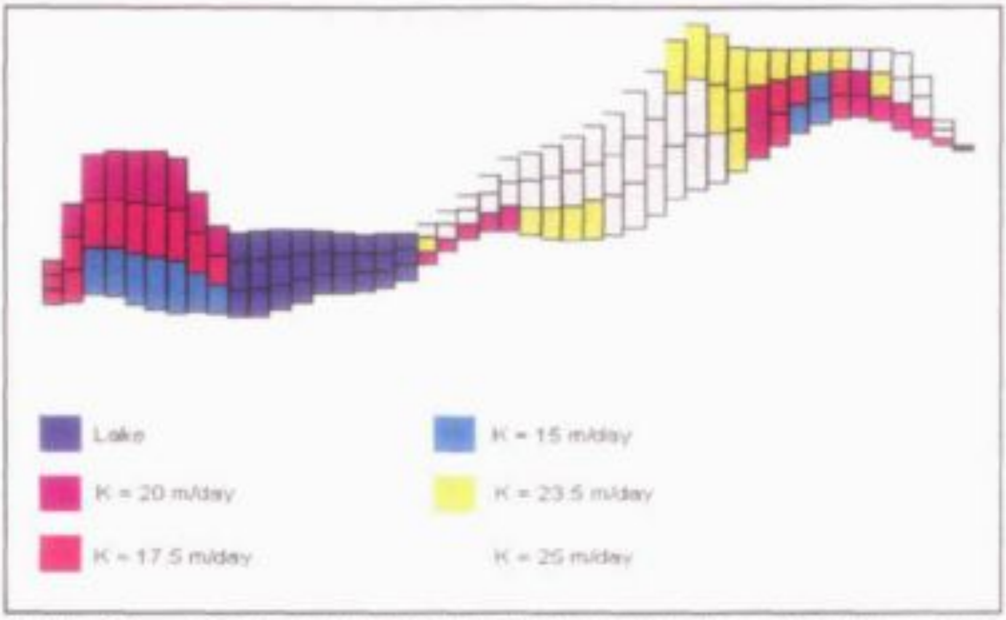


Figure 80 Cross-sectional profile of the assigned permeabilities for the three layer heterogenous model described in the text.

8.2.6 CALIBRATION

While it is relatively easy to change the parameter values using the spreadsheet model, the calibration of this model is problematic because there is a large range of values for the hydraulic parameters which need to be adjusted within each layer to achieve an acceptable temporal and spatial agreement between observations and simulations. The simulation run using the parameter set determined from the geological units in the borehole logs was compared to the few observation values available for the region as part of a subjective calibration procedure.

The comparison between the simulated water levels and the observed water levels for the available boreholes is shown in Figure 81. The simulations were done for assumed average hydrological (climatic) conditions and compared to the mean borehole observations. Because these observations are not evenly distributed spatially the comparison may not be representative of some areas where there is a paucity of information. However for a regional assessment of flow dynamics the model is considered acceptable for these comparative studies.

The regional one layer groundwater model produced a simulated water table between the other two cases. Generally, the simulated water table elevation of the homogeneous four layer model was slightly higher than that for the other conditions.

8.2.7 COMPARISON OF VERTICAL DISCRETIZATION METHODS

The simulated water table elevation contours for steady state conditions are presented in Figure 82 for all three models. The figure shows little difference between the three models at many nodes that are controlled by some boundary condition, usually a surface stream or water body. The largest difference is observed in the region furthest from these internal boundaries. However, these differences could be reduced through further calibrations. This would suggest that the specified boundaries have a much greater impact on model simulations than the vertical discretization method.

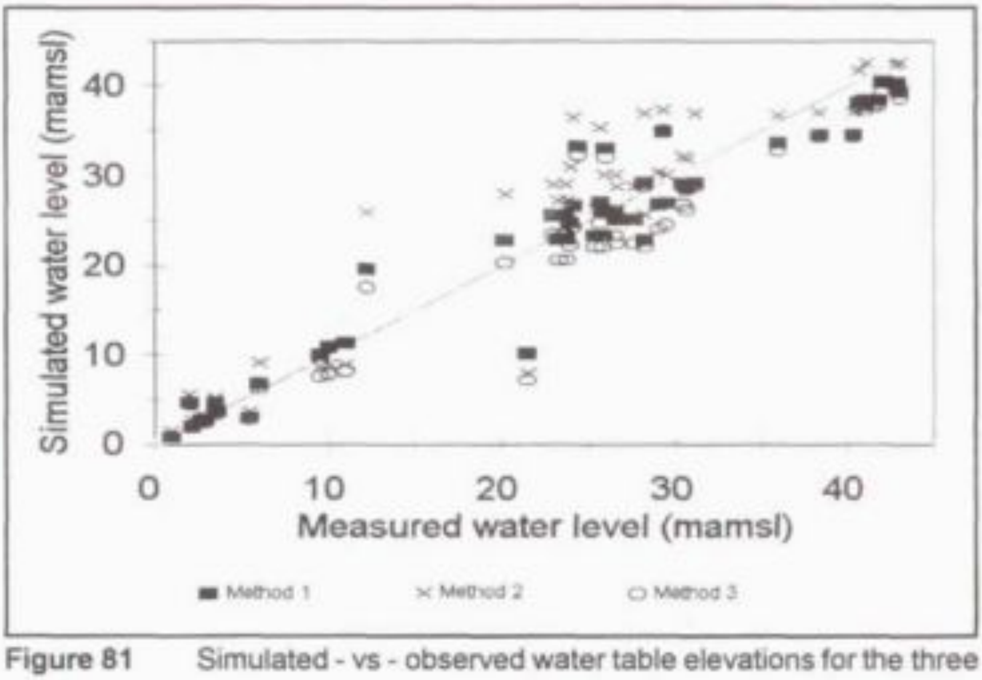


Figure 81 Simulated - vs - observed water table elevations for the three conceptual models of vertical discretization.

The similarity between the three cases suggest that a one layer model is adequate for regional studies of the flow dynamics. This is not surprising for this case where the horizontal dimension of the model nodes is more than an order of magnitude greater than the vertical dimension.

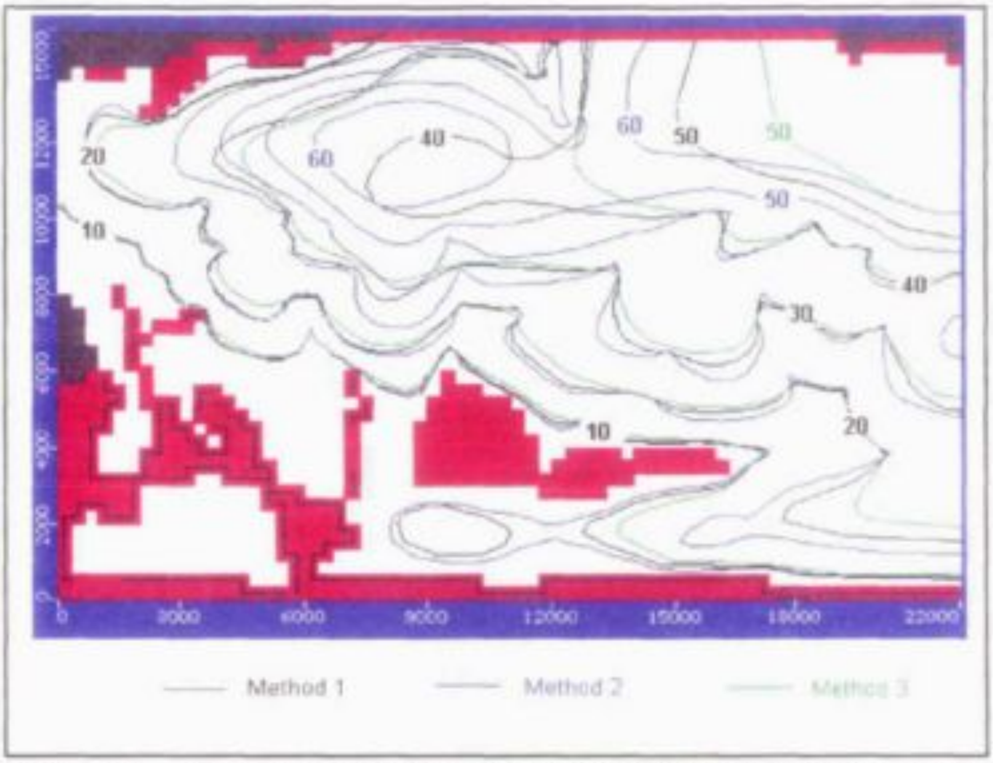


Figure 82 Simulated water table elevation for the 1, 4 and 3 layer model described in the text.

8.3 CASE 3 : WATER RESOURCES STUDY OF LAKE MZINGAZI

The lakes of the Zululand Coastal Plain are affected by and affect the behaviour of the regional unconfined aquifer. Kelbe, Rawlins and Nomquphu (1995) and Krikken and van Nieuwkerk (1997) examined the interaction between the local unconfined aquifer and Lake St Lucia and Lake Mzingazi respectively. In these studies, the lakes on the coastal plain of Zululand were assumed to be an extension of the unconfined groundwater system. In general those lakes that form part of the water table have been classified into three groups according to their level of interaction with the groundwater (Born *et al*, 1979 cited in Townley *et al*, 1993). The lakes either

(1) **receive** groundwater over their entire lake bottoms;
(2) **release** water to the aquifer over the whole bottom; or
(3) **receive and release** water over their bottoms.

These are classified by Townley *et al* (1993) as discharge, recharge and flow-through lakes respectively. The studies of the coastal lakes of the Swan Coastal Plain in Western Australia by Townley *et al* (1993) found that they were all flow-through lakes which received and discharged water through their bottoms. The simulation methods used in this study must be able to represent the assumed lake system. For recharge or discharge lakes it may be acceptable to adopt a constant head system where the lake acts as a infinite storage system. However, in this study it has been assumed that the coastal lake in the Richards Bay area are similar to the Swan Coastal Plain lakes in their interactions and have been modelled as flow-through lakes with head controlled functions.

Townley *et al* (1993) suggest there is little or no underflow for lakes embedded in regional flow systems. In these lake systems the flow is greatest along the shoreline and decreases approximately exponentially with distance from the shoreline (McBride and Pfannkuch, 1975 cited in Townley *et al*, 1993). Townley *et al* (1993) showed that these lakes can be modelled as no flow boundaries **beneath** the centre of the lakes. Lee *et al* (1980) observed an exponential decay in seepage from the lake shoreline using tracer studies. Consequently, it is assumed that the coastal lakes near Richards Bay can be simulated by a one layer model above the bedrock Cretaceous siltstone.

Rushton and Tomlinson (1979), Mishra and Seth (1988) and others have identified the important role that leakage factors make in controlling the rate of seepage of water through the sediment of rivers and lakes in the surface-groundwater interactions. The interaction of the aquifer and lakes in the Richards Bay area are examined in this case study with particular emphasis on the role of groundwater seepage in the water balance of coastal lakes.

8.3.1 LOCATION AND SETTING

As described in previous sections, the soils and geology of the coastal plain are predominantly composed of unconsolidated recent sands which are extremely permeable. Consequently, most of the rainfall infiltrates and the hydrology of the lakes is assumed to be controlled by the groundwater system. Modflow was chosen with stream and lake modules to simulate the flow dynamics of the main lake systems in the region. Lake Mzingazi is the only lake in the region with data that may be sufficient to calibrate the model. Consequently, this lake is presented in this case study. The main features of the lake have been described in Section 3.3. The main land use features surrounding the lake are described in section 8.4. The predominant land use is urban and industrial complexes, informal settlements, afforestation and areas of natural forest.

8.3.2 CONCEPTUAL MODELS OF THE SYSTEM

Lake Mzingazi formed part of the Richards Bay Harbour/Estuary system that was created in recent geological times from erosion during coastal upliftment and declining sea levels and deposition associated with marine submergence with the changing sea levels described in Section 5.2. The siltstone of the Cretaceous period is assumed to form the base of the unconfined aquifer. The unconsolidated sedimentary deposits of the Tertiary period form the composition of the one layer model in which is situated below Lake Mzingazi. Cross-sectional transects through the region are shown in Figures 52 to 54.

The Miocene deposits (Figures 49 and 50) were, in all likelihood, continuous throughout the lake region but it has been assumed that they were eroded during the formation of Lake Mzingazi (see section 5.3). The Miocene is likely to be exposed to the lake in sections so it has been assumed for this study that the surface-groundwater system remains a flow through lake. However, it is assumed that the sediments are the main controlling factor. Consequently, the system is simulated as a one layer model with several stream functions feeding into the lake module.

8.3.3 BOUNDARY CONDITIONS

A comparison between single and multi layer models has been described in the case study presented in section 8.2. This comparison suggested that the model was more sensitive to boundary conditions and that a one layer model was acceptable in the initial stadium. The one layer regional model described in section 8.1 was used as the basis for this case study.

The system was configured using VisualModflow and all files translated into Modflow in order to accommodate the inclusion of the lake package. The Lake package system described in Section 6.3.10 was used to simulate the lake reactions and interactions with the unconfined aquifer.

8.3.3.1 LAKE MODULE CONFIGURATION

The lake model configuration in relation to the lake shoreline and contributing streams is shown in Figure 83. The very small streams on the eastern shores and the many of the small ones on the western shores were not simulated as separate entities. The outlet to the lake is controlled by the weir on the southern extremity of the lake which is included as an outflow stream.

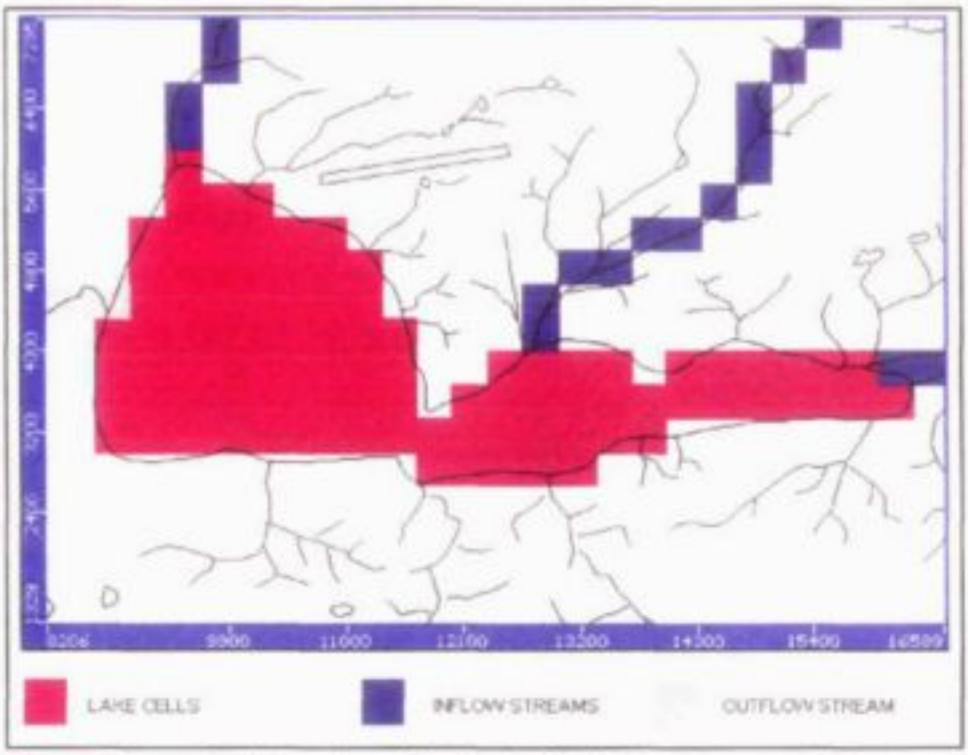


Figure 83 Configuration of the Lake Model boundary conditions.

The recharge in the lake cells was set to zero in the Recharge Package in Modflow and reassigned to the Lake Package cells. Similarly the evaporation was also reassigned to the Lake Package cells representing the lake.

Two surface elevations are required for the lake cells in the Lake Package. These indicate the top and bottom of the confining sediments forming the base of the lake. The upper surface of the lake sediments was derived directly from the bathymetric map shown in Figure 21 of section 4.2. No information is currently available on the thickness of the lake bed sediments and consequently, the confining layer in the lake model was arbitrarily set to 1m.

The Lake Package requires specification of the following parameters: lake bed conductance, recharge (rainfall) and discharge (evaporation and runoff). The recharge and evaporation parameters are area dependent and specify the vertical fluxes. They were specified individually. The runoff component is a specified volumetric rate which was also used to define the abstractions from the lake. The abstractions are derived from the information provided by the Richards Bay TLC and shown in Figure 26.

The lake bed conductance controls the flow of water between the lake and the groundwater. Consequently, this parameter determines the degree of interaction. By reducing the parameter to low values the lake will function independently of the aquifer. Conversely, a high conductance infers a strong interaction controlled by the aquifer. The degree of interaction between the lake and aquifer is NOT known and needs further investigation.

8.3.3.2 STREAM CONFIGURATION

The lake is fed by several small streams and discharges into the Mzingazi Canal through a small stream monitored by weir W1H011. Three of the larger streams contributing to Lake Mzingazi have been configured using the Stream Package in the Lake model (Figure 84). Unfortunately, none of the streams flowing into Lake Mzingazi are monitored and consequently there is no information available on the surface runoff into the lake. Because of this, it is difficult to determine the exact role of the stream network in the functioning of the system. Consequently, it was assumed that those streams shown in Figure 84 were sufficient to simulate the functioning of the system using the Lake Package.

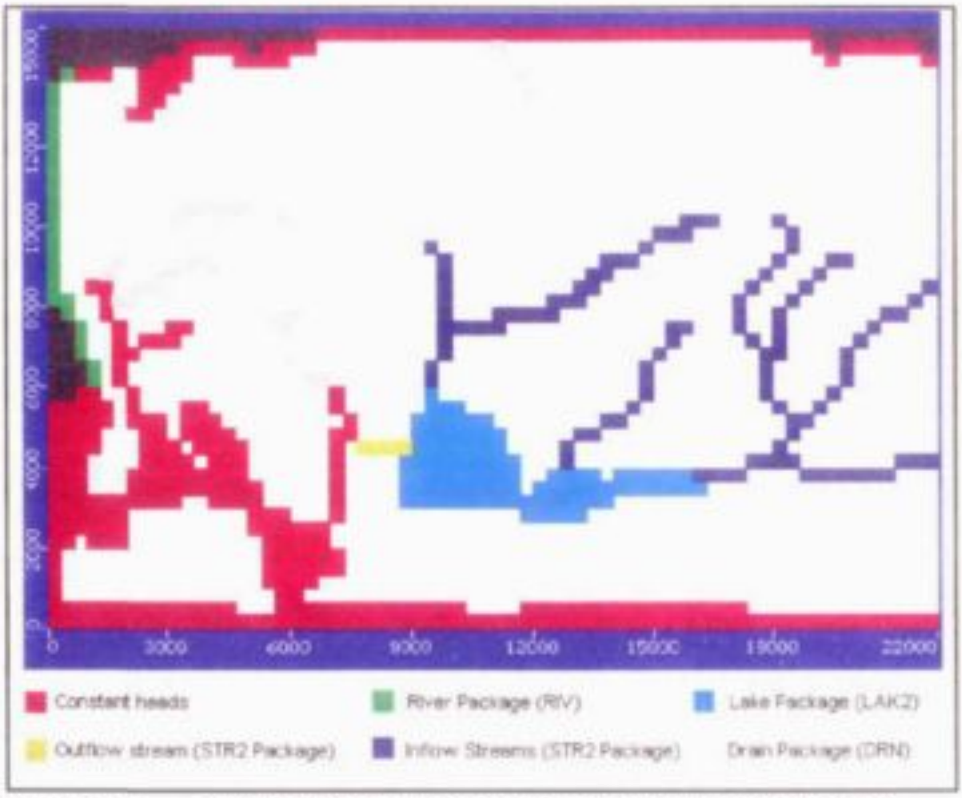


Figure 84 River segments used in the Lake simulation Package.

The Streamflow package described in Section 6.3.8.2 was used with the Lake Package. The rivers were included as internal systems which were assumed to be represented by head dependent boundaries with stream beds that had a vertical conductance of 1000 m^3/day. The Streamflow package was set up for 11 inflow segments with 108 reaches and 1 outflow segment with 4 reaches.

8.3.4 SIMULATION PERIOD

The simulation period was divided into 19 stress periods that represent variable length sections of the hydrological record that had relatively constant rainfall. The stress periods were subjectively chosen to coincide with relatively large changes in the rainfall conditions. Several extreme events, such as cyclones, were retained as separate stress periods in the record. The regional rainfall and evaporation records for this simulation period have been described in section 3. The stress periods chosen for these model simulations are given in Table 23 together with the available information on the rainfall, net lake evaporation (mm/year), official abstraction rates (m^3/day) as supplied by Richards Bay TLC (Figure 26 in section 4.2.3) and the surface discharge from the lake which was measured at weir W1H011 (Figure 25 in section 4.2.1).

8.3.4.1 MODFLOW PARAMETERIZATION

<u>**Recharge**</u> rate to the groundwater for the model domain was based on the model of Kelbe & Rawlins described in Section 6.3.6.2. This conceptual model assumes

(1) that 5 day accumulations of rainfall are lost to unsaturated surface

Table 23 Parameter values estimated for each stress period during the simulation series.

Stress Period	End Model Day	End Date	Net Evap (mm/yr)	Abstraction (m^3/day)	Surface Runoff (m^3/day)	Runoff Input (m^3/day)
1	1597	15-May-80	220	18594	169678	151084
2	1961	15-May-81	549	24253	5172	-19081
3	2511	15-Nov-82	367	25607	107579	81972
4	2648	01-Apr-83	739	24570	4593	-19977
5	2937	15-Jan-84	364	26671	78378	51707
6	3014	15-Apr-84	-1213	25159	901625	876466
7	3654	01-Jan-86	359	32101	69152	37051
8	4184	15-Jun-87	420	22186	83568	61382
9	4276	15-Sep-87	-118	22689	376729	354040
10	4292	01-Oct-87	-11411	29617	8127183	8097566
11	5737	15-Sep-91	245	32233	155139	122906
12	5966	01-May-92	777	36769	2931	-33838
13	6269	01-Mar-93	817	37755	8279	-29476
14	6361	01-Jun-93	953	35526	0	-35526
15	6544	01-Dec-93	692	29412	2292	-27120
16	7045	15-Apr-95	524	18063	13171	-4892
17	7122	01-Jul-95	353	10880	17432	6552
18	7320	15-Jan-96	697	18407	2980	-15427
19	10000	year 2002	220	40617	169678	129061

processes (interception and evaporation) at a rate of 2 mm/day so that all 5 day events exceeding 10 mm contribute to recharge

(2) all daily rainfall in excess of 50mm does not enter the groundwater system but is released through surface runoff processes.

All the remaining rainfall on a daily basis was assumed to recharge the groundwater where it was partitioned into lateral flow and vertical flow components (groundwater evaporation, lakes, rivers and drainage flow) by the model. The recharge record has been partitioned into the 19 stress periods listed in Table 24. The recharge for the Lake was assumed to be the total rainfall.

Table 24 Recharge averages for each stress period.

Stress period	Recharge (mm/yr)	Stress period	Recharge (mm/yr)
1	877	11	936
2	597	12	454
3	644	13	369
4	409	14	236
5	905	15	401
6	1779	16	458
7	89	17	1063
8	849	18	546
9	1082	19	877
10	4177		

Evaporation from the groundwater is defined by the vertical conductance through the maximum groundwater evaporation rate and rooting properties of the vegetation as described in section 6.3.7. These parameters are dependent on land use type and their estimated values for the Mzingazi area are given in Table 25. The estimated evaporation rate that comes directly from the lake surface is the total evaporation required in the Lake Package.

Permeability and **Storage Coefficients** for the model were derived from the calibrations in the case studies presented in sections 8.1 and 8.2. The permeability parameters from these applications were used without adjustment during the calibration of the Lake Model in this case study.

Runoff into the Lake from the surface and other sources. This function is not area dependant and consequently was used to model the excess rainfall contribution to the lake from the catchment area as well as abstraction rates. All rainfall event exceeding the recharge rate described above were routed directly into the lake (*Surface Runoff* in Table 23). However, antecedent moisture conditions were considered by reducing the total runoff during dry stress period. For all stress periods when the recharge rate was less than 4mm/day, the runoff was assumed to be 25% of the moist states. This was combined with the known abstraction rates (Table 23) to give the *Runoff Input* parameter (Table 23).

Discharge from the Lake was estimated from the observed overflow at weir W1H011. The discharge series is presented in Section 4.2.1 and shown in Figure 25. At very high level, the weir is overtopped and the spillway to the west of the weir also discharges water from the lake. Consequently, the high flows are likely to be underestimated. However, the discharge for low flows is considered to be reliable for the purposes of this study.

Table 25 Estimated evaporation model parameter values for various land use types.

Landuse type	Maximum Evaporation	Extinction depth
Grassland & Swamp	900	1.5
Urban areas	700	1.0
Informal settlements	800	5.0
Indigenous Forests	1000	10
Eucalyptus Plantations	1100	10

8.3.5 CALIBRATION OF THE MODEL

The groundwater model was configured the same as the one layer model presented in the first two case studies (sections 8.1 and 8.2). Consequently, the calibrated parameter values from these two studies were assumed to be adequate for this case study. Therefore the calibrations presented here refer specifically to the Lake Package parameters.

The Lake Package has been described in section 6.3.10. The flow between the lake and the groundwater is controlled by the conductance which is described by $\left\langle \text{Conductance} = K \bullet \frac{\text{Area}}{\text{thickness}} \right\rangle$ where K is the permeability of the confining layer. This parameter determines the level of interaction between the aquifer and the lake. For very large conductances the lake would act like a constant head boundary which is controlled by the aquifer properties. For very low conductances, the lake becomes an isolated system dependent only on the surface recharge and discharge conditions. Unfortunately there is no information to derive an estimate of this parameter. The area of each cell is known (333x333 m^2) but it is necessary to measure the thickness and determine the permeability of the sediments throughout the lake. In an effort to overcome this problem, the calibration studies have been used to derive an estimate of these parameter values.

8.3.5.1 INITIAL CALIBRATIONS

The estimation of the conductance parameters is critical in the determination of the level of interaction between the lake and the water table. Townley *et al* (1995) state that *"bottom sediments affect both the physical interaction between the lake and the underlying groundwater flow system and the chemistry of the lake water. The physical effect of bottom sediments is to add resistance along a flow path between the regional groundwater flow system and the body of the lake, thus tending to reduce the degree of inter-connection. The chemical effect is to provide surface area for sorption of phosphate and metal ions, thus acting to reduce their concentration in the water body, at least until sorption capacity of the sediments is exceeded"*. Unfortunately there is no information on the sediments of Lake Mzingazi and the estimation of these parameters for this study are based on a trial and error calibrations.

The initial parameter values for the lake bed conductance were estimated from the permeabilities in the literature (Figure 64) and an assumed sedimentary layer thickness of 1m. The estimated mean value and the upper and lower limits in the range of conductance values is presented in Table 26. Calibrations have been conducted across this range of values.

Table 26 Range of lake conductance estimates for Lake Mzingazi

Parameter	Permeability (m/day)	Thickness (m)	Conductance (m^2/day)
Lower limit	10^{-5}	1	1
Median	10^{-3}	1	100
Upper limit	10^{-1}	1	10000

The comparison between the simulated lake levels and observations was problematic. The simulated lake levels during the first twelve stress periods up to the start of the severe drought in 1992 were relatively close to the observed stage values (Figure 85). However, the comparison became progressively worse as the drought intensified after approximately 6000 days of the simulation period (Figure 85). The model was **unable** to simulate the draw-down in the lake with the initial mean parameter for the Lake bed conductance of 100 m^2/day. Consequently, the interaction with the groundwater was investigated through the range of conductances shown in Table 26. The simulated lake stage series for the upper and lower conductance series are also shown in Figure 80. There is little change for the upper range of seepage values (conductance of 10000 m^2/day) but a significant improvement in comparisons with the lower seepage rates (conductance of 1 m^2/day).

The series of water balance components for the simulations with a lake bed conductance of 1 m^2/day for the 19 stress periods is given in Table 27. Also shown in Table 27 is the seepage through the lake bed relative to the surface inflow components of rainfall and

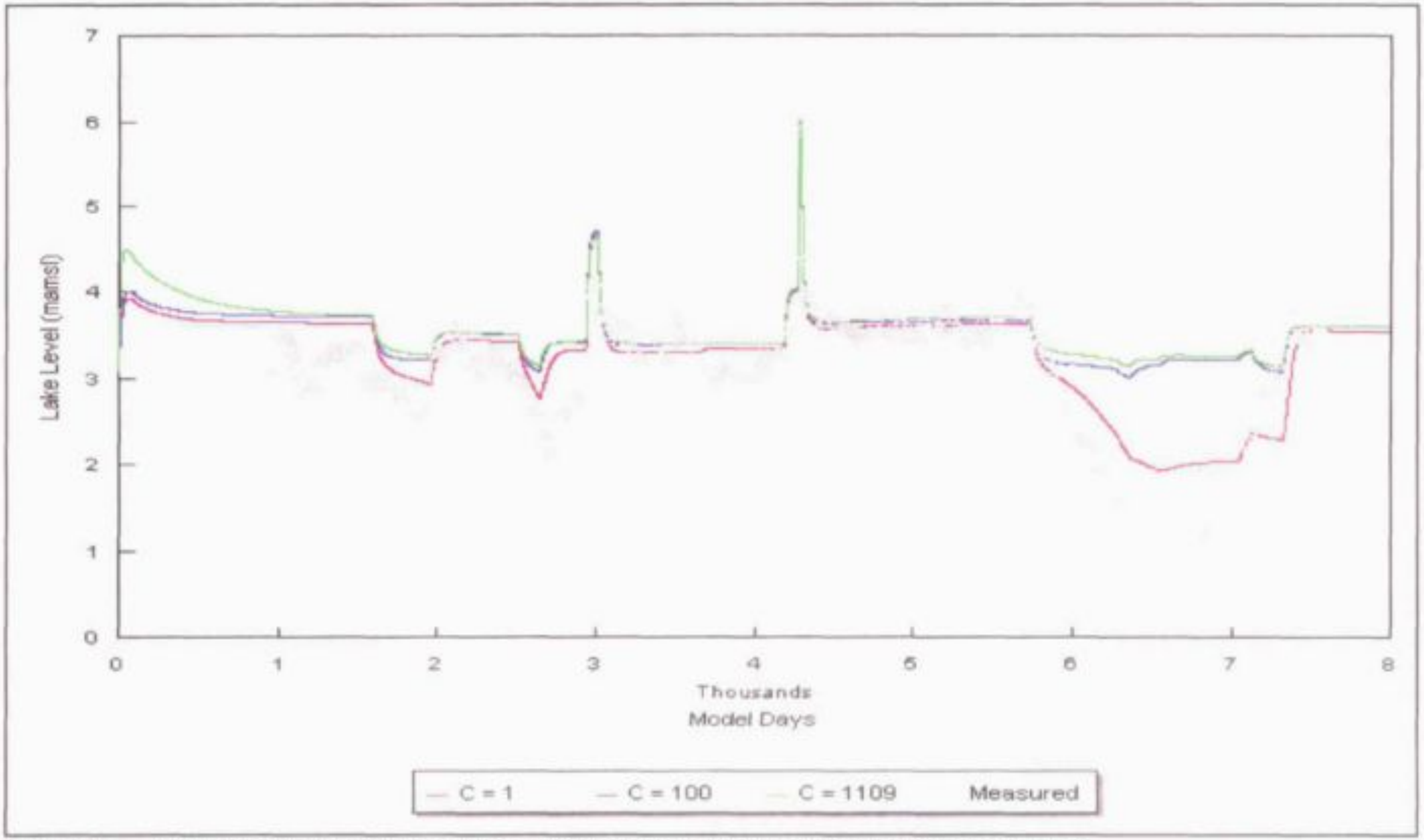


Figure 85 Observed and simulated lake levels for various paramterizations of the lake bed conducatnces.

streamflow.

It is unlikely that this lake is totally isolated from the primary aquifer and consequently the conductance value of 1 m^2/day is perceived to be the lowest limit of groundwater seepage. This lower limit effectively removes any significant contribution of the local aquifer to the lake recharge. If this assumption holds, then it is necessary to reduce the lake level through other sources of water losses. Because of the uncertainty in the total water abstraction and use by riparian users, an **unaccountable water loss** is introduced to achieve further improvements in the calibration.

8.3.5.2 UNACCOUNTED LOSSES

A preliminary water balance of the lake is based on the components shown diagrammatically in Figure 86. The individual components for each stress period are given in Table 27 for the simulations based on a very low lake leakance values in the model (conductance = 1 m^2/day).

At the height of the drought indicated by the stress period 17, the lake received an average rainfall contribution to lake storage of 35712 m^3/day. The evaporation during this period reduced this contribution to 11799 m^3/day which was increased to 16351 m^3/day from runoff and 812 m^3/day due to groundwater seepage. Since there was NO discharge from the lake and the lake level was maintained at a relatively constant level, this inflow to storage had to be balanced by losses from the system. There is a deficit in outflow from the system of about 10000 m^3/day which is unaccounted for in the model

Table 27 Water Balance components for each stress period

Stress	Rainfall	Evaporation	StreamFlow	Discharge	Seepage	Volume	Abstraction	SfcRunoff	Unknown	Storage
Period	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day
1	40873.7	-43718	36374.1	-185287	541.319	6.322672E+07	-18594	169678	0	-132
2	28337.7	-46562.3	29572.9	0	614.442	5.577188E+07	-24253	5172	0	-7118
3	35185.1	-41295.1	21312.4	-98025.4	571.162	6.109062E+07	-25607	107579	0	-280
4	21174.3	-61626.6	21214.8	0	635.365	5.401452E+07	-24570	4593	0	-38579
5	35395.8	-39925.6	13525.6	-61419.8	580.795	5.996747E+07	-26671	78378	0	-136
6	95231.5	-46878.3	17953.6	-940725	450.82	7.433085E+07	-25159	901625	0	2499
7	34553	-45087.5	27685.4	-54676.9	585.095	5.973367E+07	-32101	69152	0	110
8	33288.9	-49828	19398	-65006.6	585.641	6.008766E+07	-22186	83568	0	-180
9	53620.4	-29601.8	17814.7	-394590	522.89	6.708744E+07	-22689	376729	0	1806
10	482583	-42875.2	20225.8	-	333.459	8.810137E+07	-29617	8127183	0	6115902
11	39820.2	-43612.6	66099.3	-185574	621.441	6.323293E+07	-32233	155139	0	260
12	19699.4	-48563.8	48836.8	0	699.833	5.602974E+07	-36769	2931	0	-13166
13	18119.3	-49828	35896.4	0	767.54	4.999047E+07	-37755	8279	0	-24521
14	12957.4	-46351.6	33672	0	798.344	4.692448E+07	-35526	0	0	-34450
15	22859.8	-37502.7	30364.8	0	818.561	4.526716E+07	-29412	2292	0	-10580
16	29285.8	-51724.2	26612.5	0	817.765	4.651538E+07	-18063	13171	0	100
17	35711.8	-23913.2	24191.7	0	788.736	4.986797E+07	-10880	17432	0	43331
18	23070.5	-42875.2	31486.2	0	798.976	4.908571E+07	-18407	2980	0	-2947
19	40873.7	-43718	19343.4	-146417	688.211	6.234043E+07	-40617	169678	0	-169

simulations.

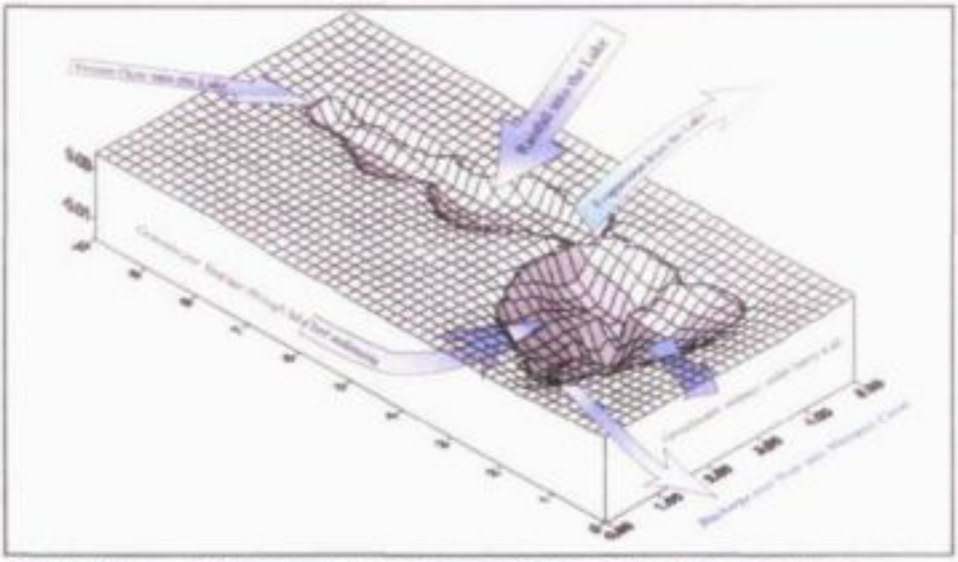


Figure 86 Diagrammatic representation of the water balance components used for calibrating the Lake Model of Mzingazi.

The RAINFALL RECHARGE rate was specified from observed rainfall records. The STREAM DISCHARGE was controlled by the rating equation for weir (W1H011). The EVAPORATION rate for an open water body was derived from WR90 and data measured at station W1E009 near Lake Mzingazi. The RUNOFF accounts for the surface contribution from the groundwater model and was derived from the measured rainfall events exceeding 50 mm while taking into account the antecedent moisture conditions in the catchment (see section 8.3.4.1) as described above. The groundwater seepage rate has been reduced to a minimum. All these parameters and data sets are derived from measurements and offer little scope for major changes during simulations studies. Consequently, the contribution from the other sources needs be examined further in this calibration of the Lake Model. There is also a need to identify the possibility of unaccounted losses such as additional abstraction for irrigation.

The initial effort to achieve a closer correspondence between the lake elevations and simulated heads tested the sensitivity of the recharge and evaporation values in determining the lake levels with little improvement in the stage comparisons. Similarly, changes in the Runoff function caused unacceptable simulations in the peak stages during very heavy rainfall events. The lake bed sedimentary conductance was reduction to a value of 1 m^2/day (*ie* a permeability of approximately 0.0002 m/day typical of a 2 m impervious layer). This very low permeability would effectively isolate the lake from the aquifer (see Table 27). This low lake bed conductance produced groundwater seepage in most stress periods that was less than 10% of the other water balance components.

In an attempt to determine the magnitude of possible LOSSES in the system, several constant rates of water loss from the lake system have been included in the model simulations to achieve a better comparison with the observed lake levels during the entire simulation period. Fixed daily water losses from the system covering a range from 1000 to 20000m^3/day have been included in the model simulations to determine the effect on the simulations with no interactions between the lake and groundwater. The range of scenarios is presented in Table 28.

Table 28 Water Loss scenarios for Lake Mzingazi water balance studies.

Scenario	Water Loss (m^3/day)
1	1 000
2	4 000
3	10 000
4	20 000

The comparison between the simulated lake elevations and the observed levels are shown in Figure 87 for the three scenarios with minimal seepage rates. The series of crosses indicate the observed lake elevations. The other three lines represent the simulated lake levels. The thickest (lower) line represents the best fit during the drought period and is derived from an additional unaccounted water loss of 10 000 m^3/day from the Lake system. The middle and upper series shown during the drought period indicate the 6000 and 1 000 m^3/day unaccounted loss simulations respectively.

The water balance components for the 10 000 m^3/day water loss scenario is presented in Table 29. The change in lake storage for each stress period was estimated from the components according to the following equation:

$$\Delta S = R_{ain} - E_{vap} + S_{tream\_IN} - D_{ischarge} - S_{eepage} + \left\{ R_{unoff} - A_{bstraction} \right\}$$

The MEAN change in volume of the lake is also presented in Table 29 for comparisons. Figure 88 shows the relative contributions of all the main water balance components during the simulation period. Those with negative contributions signify losses from the lake system.

The fit between simulated and observed lake levels during the drought period suggests that the unaccounted loss of 10 000 m^3/day is the best estimate for the Lake Mzingazi study with minimal groundwater interaction (conductance 1 m^2/day). To increase the groundwater interaction, the unaccountable water loss scenario was doubled (20 000 m^3/day) and the seepage rate increased to obtain a similar fit between the simulated and observed water levels during the

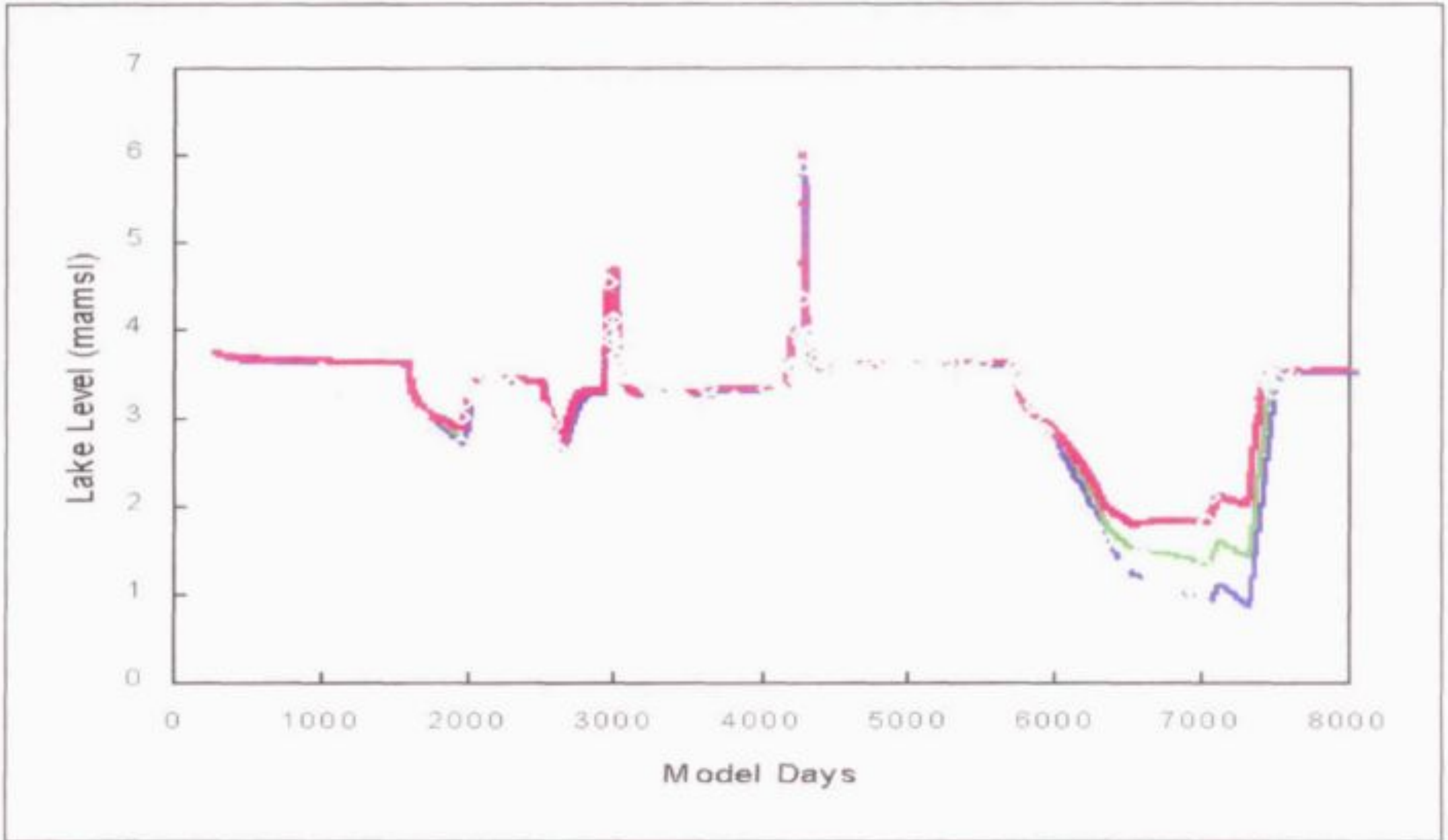


Figure 87 Observed and simulated lake levels for various additional losses and a lake bed conductance of 1 m^2/day.

Table 29 Water Balance components for minimal seepage (Conductance = 1m^2/day) and unaccountable losses of 10 000m^3/day

Stress	Rainfall	Evaporation	StreamFlow	Discharge	Seepage	Volume	Abstraction	SfcRunoff	Unknown	Storage
Period	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day
1	40873.7	-43718	36374	-175292	543.301	63006570	-18594	169678	-10000	-130
2	28337.7	-46562.3	29572.8	0	638.719	53079580	-24253	5172	-10000	-17030
3	35185.1	-41295.1	21312.2	-88039.7	573.724	60803960	-25607	107579	-10000	-270
4	21174.3	-61626.6	21214.6	0	646.68	52756730	-24570	4593	-10000	-48510
5	35395.8	-39925.6	13525.4	-51230.6	583.974	59609750	-26671	78378	-10000	10
6	95231.5	-46878.3	17953.3	-930609	451.81	74215480	-25159	901625	-10000	2750
7	34553	-45087.5	27685.2	-44668.8	588.372	59364140	-32101	69152	-10000	120
8	33288.9	-49828	19397.8	-55021.8	588.658	59745920	-22186	83568	-10000	-240
9	53620.4	-29601.8	17814.5	-384418	524.309	66922860	-22689	376729	-10000	2040
10	482583	-42875.2	20224.6	-2441931	333.393	88101370	-29617	8127183	-10000	0
11	39820.2	-43612.6	66099.1	-175570	623.355	63012700	-32233	155139	-10000	280
12	19699.4	-48563.8	48836.5	0	713.271	54531420	-36769	2931	-10000	-23160
13	18119.3	-49828	35895.9	0	808.205	45470300	-37755	8279	-10000	-34490
14	12957.4	-46351.6	33671.5	0	847.259	41488360	-35526	0	-10000	-44400
15	22859.8	-37502.7	30363.9	0	883.859	38011450	-29412	2292	-10000	-20450
16	29285.8	-51724.2	26611.3	0	927.74	34293100	-18063	13171	-10000	-9870
17	35711.8	-23913.2	24190.4	0	905.556	36884310	-10880	17432	-10000	33450
18	23070.5	-42875.2	31484.9	0	933.376	34146790	-18407	2980	-10000	-12820
19	40873.7	-43718	19341.6	-136422	690.073	62097750	-40617	169678	-10000	-230

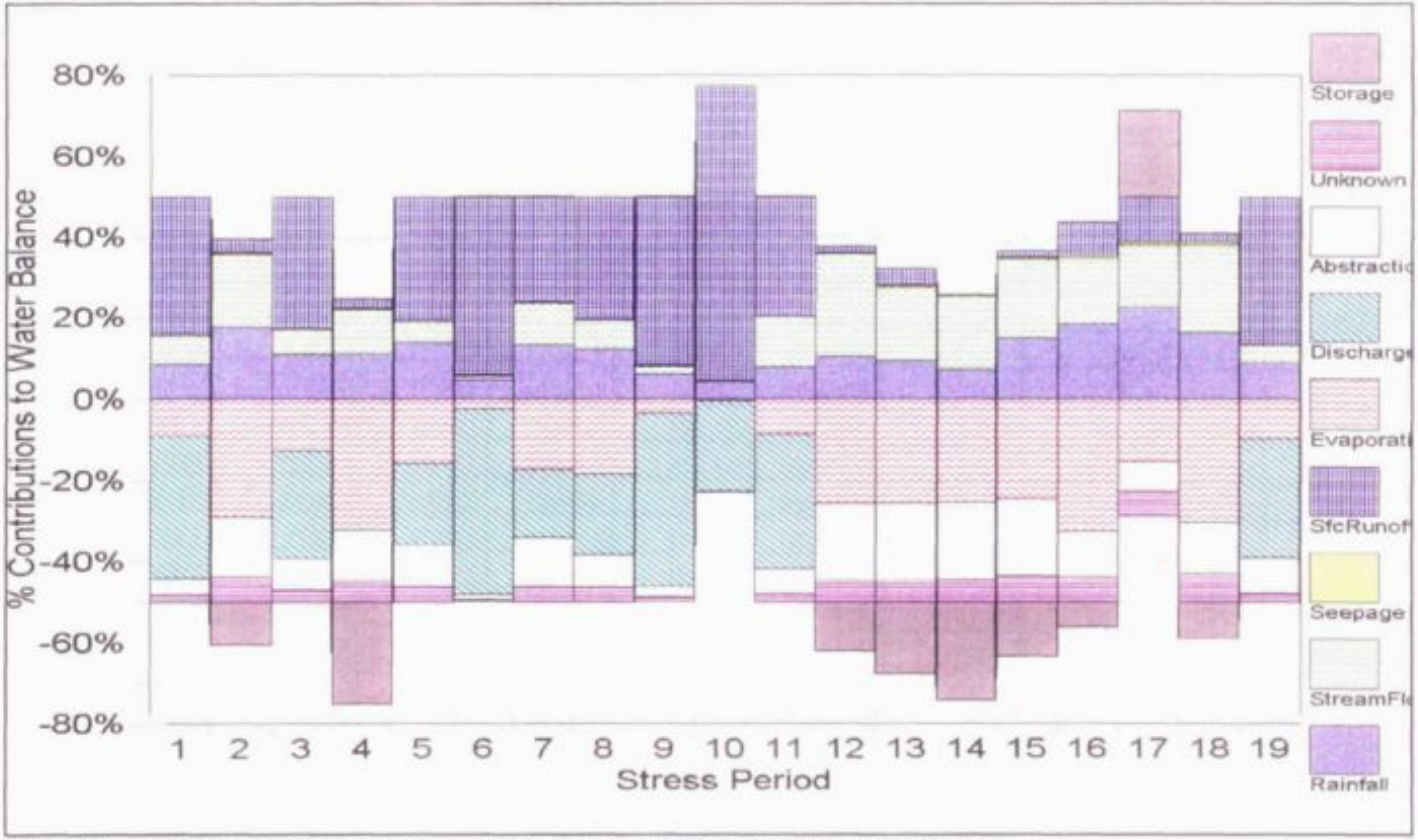


Figure 88 Water balance components for limited seepage and 1000 m^3/day unaccountable losses

drought period. A further set of simulation series were conducted using the 20 000 m^3/day water loss and the lake-bed conductance given in Table 30.

Table 30 Assumed Lake bed conductance range in calibrations

Scenario	Permeability (m/day)	Conductance (m^2/day)
1	1×10^{-6}	10
2	1×10^{-5}	100
3	1×10^{-4}	1000

The simulation series of lake elevations have been compared to the observed lake levels in Figure 89. Once again the observed series is shown by the crosses while the bottom line in the drought period indicates the best fit for a 20 000 m^3/day water loss with seepage rates derived from a lake bed conductance of 10 m^2/day.

The differences are marginal between the simulated series with minimal seepage (conductance = 1 m^2/day: losses of 10 000 m^3/day) and the simulations with slightly higher unaccountable losses with increased groundwater interaction (conductance = 10 m^2/day: losses of 20 000 m^3/day). Consequently, these two scenarios have been examined on the assumption that they represent the best estimates of the groundwater-lake interaction. Without additional information on the sedimentary layer or seepage rates, it is not possible to determine the system dynamics with any greater level of assurance. The complete water balance components for the second series with 20 000 m^3/day unaccountable losses and groundwater interaction simulated with a lake bed conductance of 10 m^2/day are given in Table 31 and Figure 90.

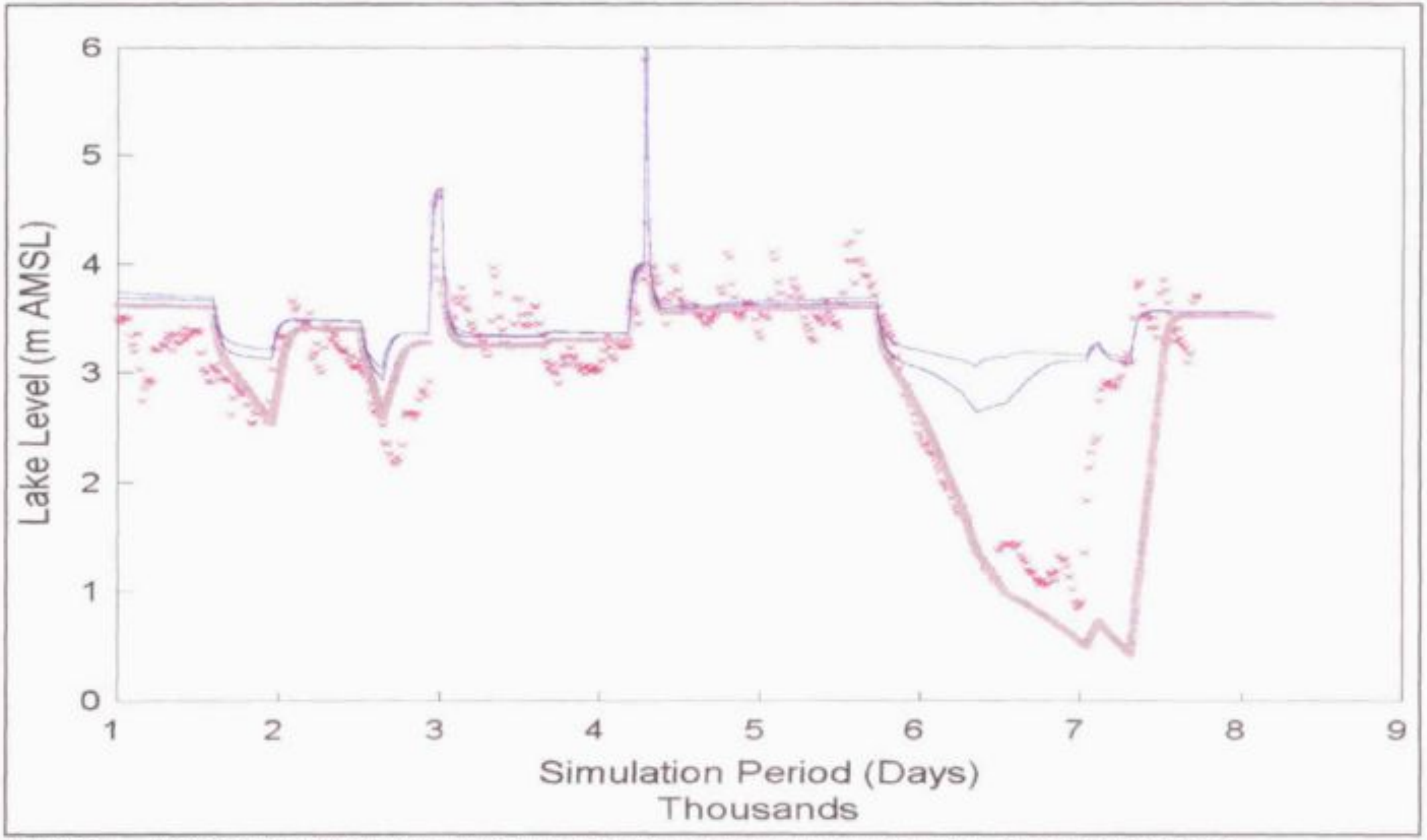


Figure 89 Comparative series of observed (X) and simulated lake water levels for three cases of varying seepage rates.

Table 31 Water balance components for limited seepage and 1000 m^3/day unaccountable losses

Stress Period	Rainfall	Evaporation	StreamFlow	Discharge	Seepage	Volume	Abstraction	SfcRunoff	Unknown	Storage
	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day	m^3/day
1	40874	-43718	36252	-169898	5270	62885720	-18594	169678	-20000	-50
2	28338	-46562	29418	0	6304	51637340	-24253	5172	-20000	-21580
3	35185	-41295	21107	-82756	5489	60647020	-25607	107579	-20000	-270
4	21174	-61627	21002	0	6249	52108140	-24570	4593	-20000	-53200
5	35396	-39926	13340	-45740	5556	59405180	-26671	78378	-20000	360
6	95232	-46878	17712	-924070	4220	74140760	-25159	901625	-20000	2850
7	34553	-45088	27421	-39357	5547	59154510	-32101	69152	-20000	120
8	33289	-49828	19088	-49628	5509	59550980	-22186	83568	-20000	-230
9	53620	-29602	17507	-378345	4852	66823720	-22689	376729	-20000	2180
10	482583	-42875	19929	-2441931	2934	88101370	-29617	8127183	-20000	0
11	39820	-43613	65774	-170365	5757	62896140	-32233	155139	-20000	260
12	19699	-48564	48497	0	6700	53745250	-36769	2931	-20000	-27460
13	18119	-49828	35506	0	7728	43487100	-37755	8279	-20000	-37980
14	12957	-46352	33264	0	8136	39201330	-35526	0	-20000	-47500
15	22860	-37503	29885	0	8530	35170030	-29412	2292	-20000	-23330
16	29286	-51724	26132	0	9025	30130280	-18063	13171	-20000	-12160
17	35712	-23913	23702	0	8811	32530520	-10880	17432	-20000	30870
18	23071	-42875	31016	0	9108	29319330	-18407	2980	-20000	-15120
19	40874	-43718	18718	-131302	6202	61970730	-40617	169678	-20000	-110

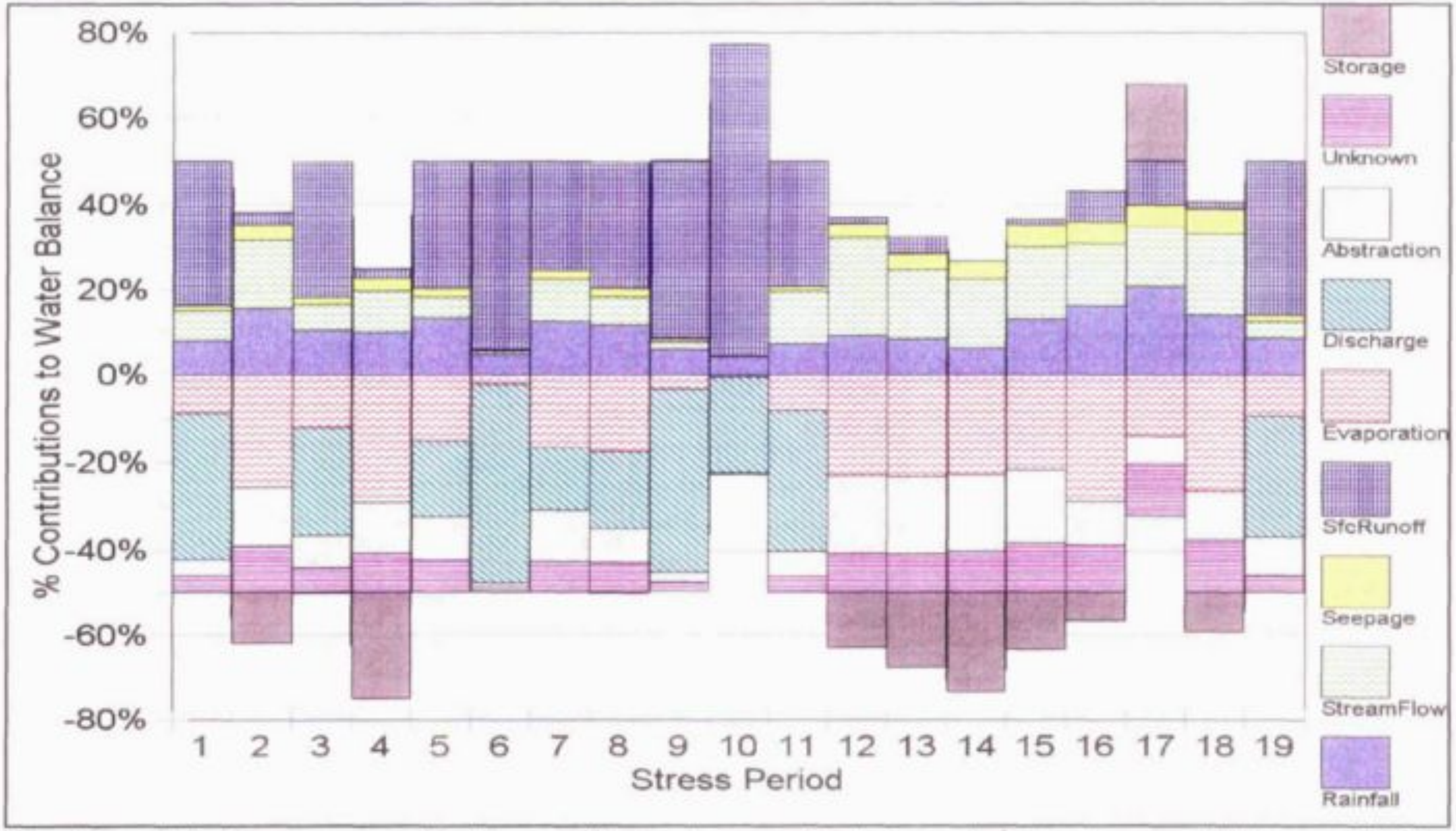


Figure 90 Water balance components for the case with minimal seepage (Conductance = 1m²day) and unaccountable losses of 10 000 m³day.

During the drought periods when there was no discharge from the lake system, the unaccountable losses reached approximately 10% of the total water budget for the case with increased seepage (Figure 90 and Table 31). The seepage rate was generally about half of this unknown loss. The largest proportion of the total water budget was the contribution from the evaporation and abstraction rates which made up nearly 40% of this budget and was responsible for the very large deficit in the lake storage volume.

There were larger deficits in the lake storage during the 4'th stress period (15 Nov 1982 to Apr 1983) but this was not sustained for very long and was followed by a period of good rainfall. The large storage deficit during the severe drought was sustained for a long period which led to the serious draw-down in the Lake elevation.

The change in lake level was compared to the changes in water table elevation at nearby boreholes. Figure 91 shows the change in elevation for common periods of observation (during the severe drought conditions) for the lake and a borehole in the high dune areas (between the lake and the ocean (B/H 2506)). Also shown is the difference between these water levels for this observation period. The groundwater system responded to the drought much slower than the lake which created a larger head gradient that would assist the seepage rate from groundwater into the lake during this period, as predicted by the model simulations (Figure 91).

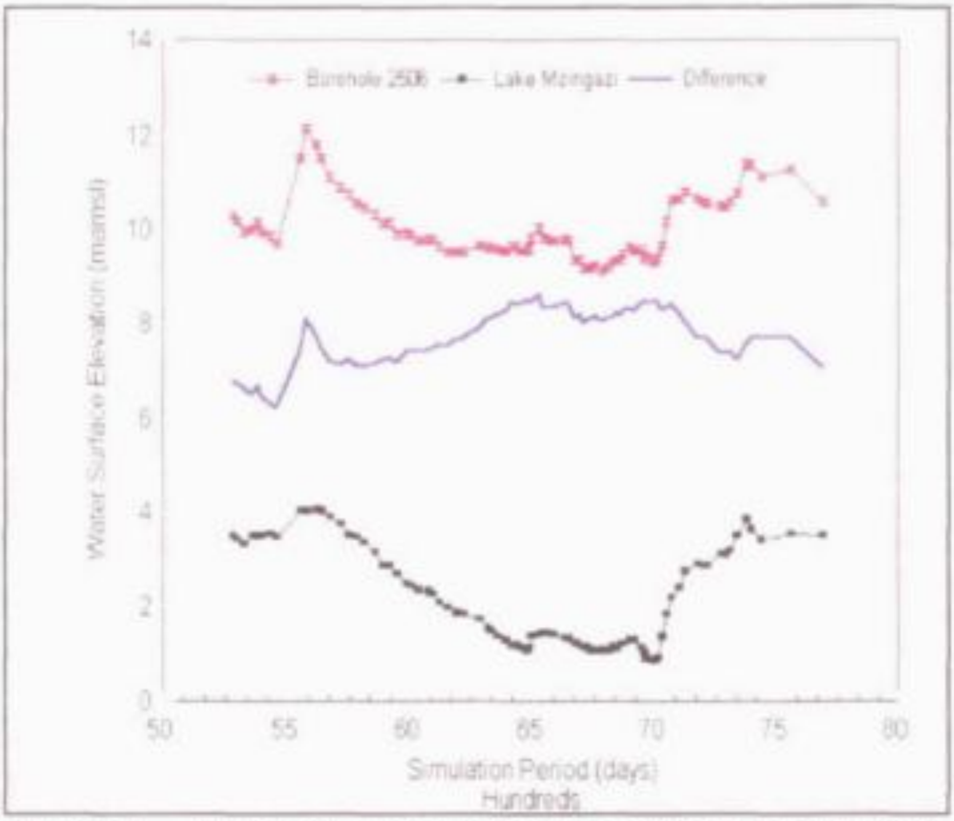


Figure 91 Water level comparison for Lake Mzingazi and B/H 2506

8.3.6 SIMULATED RESPONSE TO ANTHROPOGENIC EFFECTS

Two possible lake scenarios have been described in the previous calibration section. Both these cases are examined in this section for responses to proposed changes in the physical environment of Lake Mzingazi. Environmental concern for the sustainability of Lake Mzingazi require estimates of the lake system under natural conditions for direct comparison with the anthropogenic effects derived from changing the storage capacity of the lake and eliminating abstraction. The effects of changing land use are described in a separate case study described in section 8.4.

8.3.6.1 NATURAL ENVIRONMENT

The natural flow dynamics of Lake Mzingazi were simulated by assuming that there were no official abstraction and the unaccountable losses still occurred in the system. The comparison between the observed lake levels (with abstraction) and the two simulated series when there was no abstraction are shown in Figure 92. The difference is minimal between the two scenarios with assumed water losses of 10 000 and 20 000 m^3/day and different seepage rates. In both cases the lake is fairly static at about 3½ m for most of the simulation period. The lake is reduced to almost no outflow for most of the extreme drought. The difference between the simulated levels and the observed levels is an indication of the impact of abstraction.

The individual water balance compounds for each stress period are given in Table 31 for the case with no abstraction and an unaccounted loss of 20 000 m^3/day. The relative contributions of each water balance component are given in Figure 93. Without abstraction, the simulated change in storage is considerably reduced, particularly during times of severe drought.

8.3.6.2 HEIGHT ALTERATIONS OF OUTLET WEIR

The natural flow dynamics of Lake Mzingazi were altered by the construction and subsequent raising of the berm wall in the past. The possibility of additional increases in the height of the berm wall also require further investigation. Simulated increase and decrease of 1m in the height of the berm wall were conducted to evaluate the lake

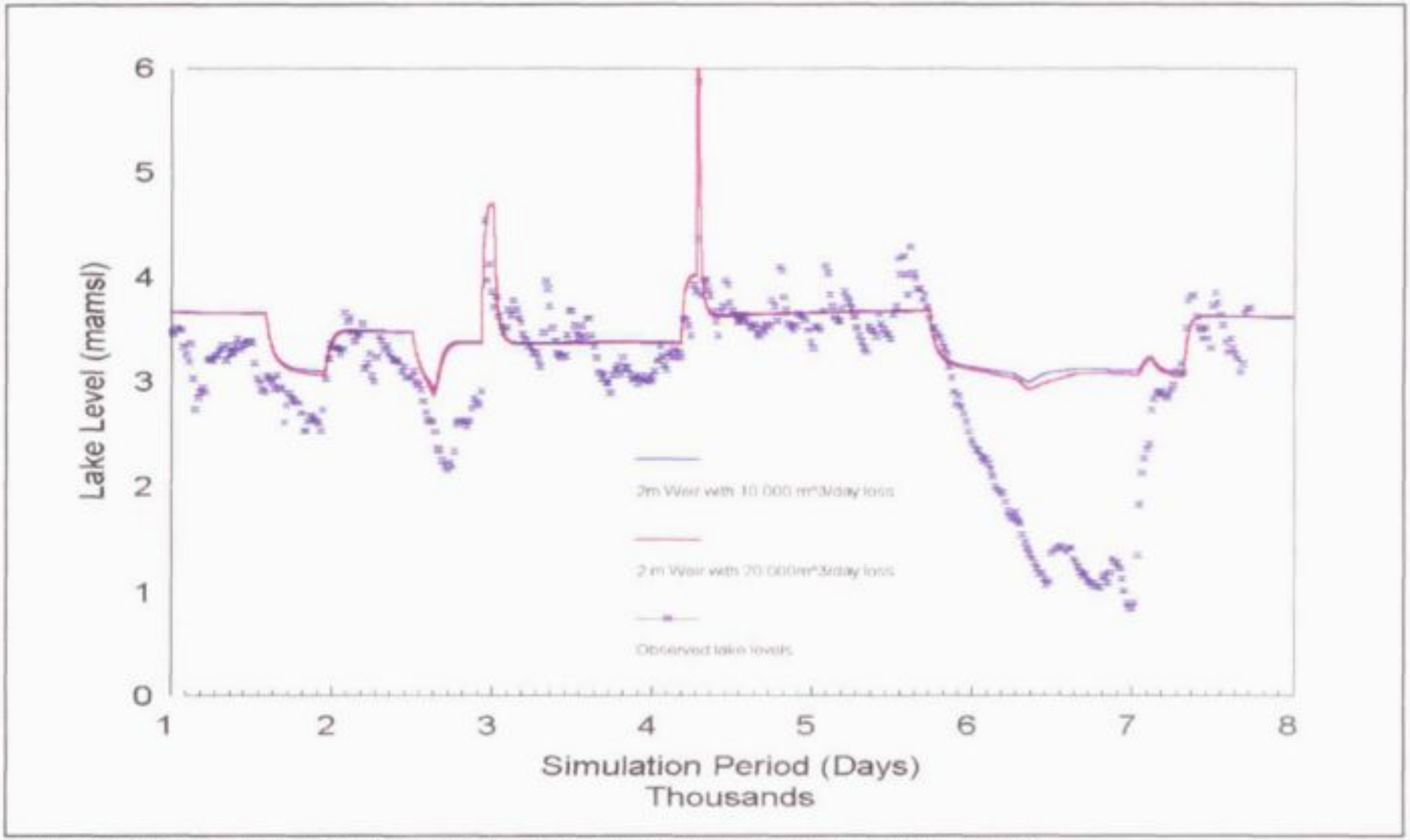


Figure 92 Simulated lake level fluctuations with no abstraction relative to observed levels (blue crosses).

Table 32 Simulated water balance components for the case with no abstraction, groundwater seepage and a system loss of 20000 m^3/day.

Time	Stress	Stage	Rainfall	Evaporation	StreamFlow	Discharge	Seepage	Volume	Runoff	Storage
Days	Period	*m*	*m^3/day*	*m^3/day*	*m^3/day*	*m^3/day*	*m^3/day*	*m^3/day*	*m^3/day*	*m^3/day*
1597	1	3.656	40874	-43718	36374	-193877	540	63412090	159678	-190
1961	2	3.098	28338	-46562	29573	-8107	599	57527610	-4828	-930
2510	3	3.476	35185	-41295	21313	-113613	567	61515700	97579	-260
2648	4	2.921	21174	-61627	21215	0	620	55693730	-5047	-23660
2937	5	3.380	35396	-39926	13526	-78133	576	60506320	68378	-230
3014	6	4.710	95232	-46878	17954	-956047	449	74504460	891625	2460
3654	7	3.377	34553	-45088	27686	-76787	578	60464790	59152	40
4184	8	3.378	33289	-49828	19398	-77177	582	60476910	73568	-140
4276	9	4.025	53620	-29602	17815	-407461	521	67293350	366729	1750
4292	10	6.000	482583	-42875	20226	-2441931	333	88101370	8117183	0
5737	11	3.684	39820	-43613	66100	-207814	617	63706150	145139	250
5966	12	3.150	19699	-48564	48837	-16539	681	58077210	-7069	-2930
6269	13	3.075	18119	-49828	35897	-5234	702	57289900	-1721	-2100
6361	14	2.991	12957	-46352	33672	0	713	56415510	-10000	-9050
6544	15	3.096	22860	-37503	30366	-7905	708	57512150	-7708	870
7045	16	3.101	29286	-51724	26614	-8636	718	57567400	3171	-610
7122	17	3.244	35712	-23913	24193	-36964	706	59056450	7432	7310
7320	18	3.085	23071	-42875	31487	-6374	724	57389390	-7020	-930
8191	19	3.621	40874	-43718	19345	-177018	682	63044950	159678	-130

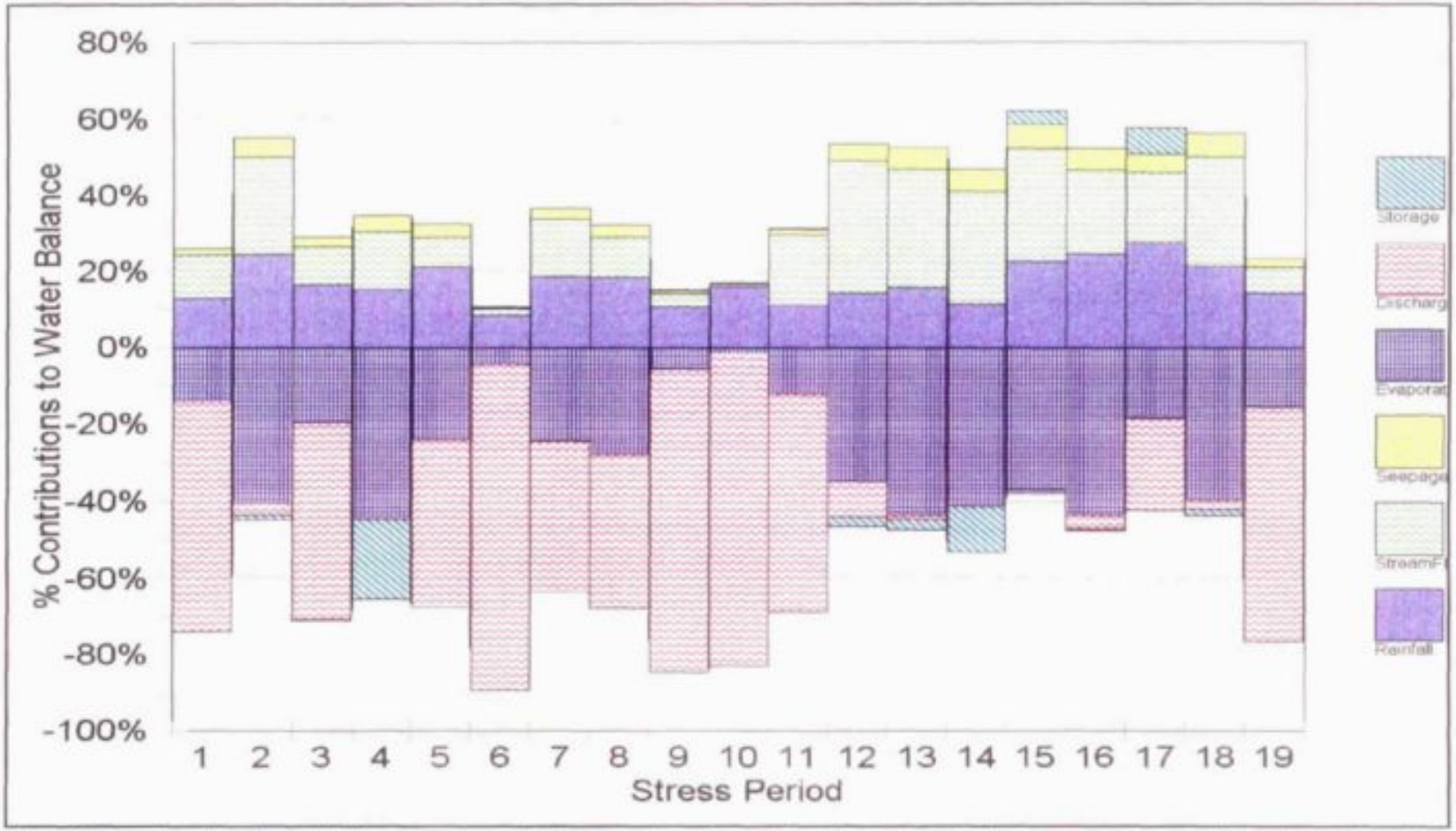


Figure 93 Simulated water Balance components for scenario with no abstraction, groundwater seepage and an unknown loss of 20 000 m^3/day.

response to these possible changes. The lower berm wall (2 m *AMSL*) would represent the possible natural system prior to the previous changes in the height of the weir.

Simulated series of lake levels were conducted to determine the response to changes in the height of the lake outlet. It was assumed that the discharge rating equation would remain the same and that the lake levels would be a response to changes in storage capacity of the Lake. The difference in Lake storage (Figure 94) is most noticeable during drought periods. The similarity in lake storage for stress period 10 is due to the model constraining the maximum lake elevation to 6 m and the limitations of the model.

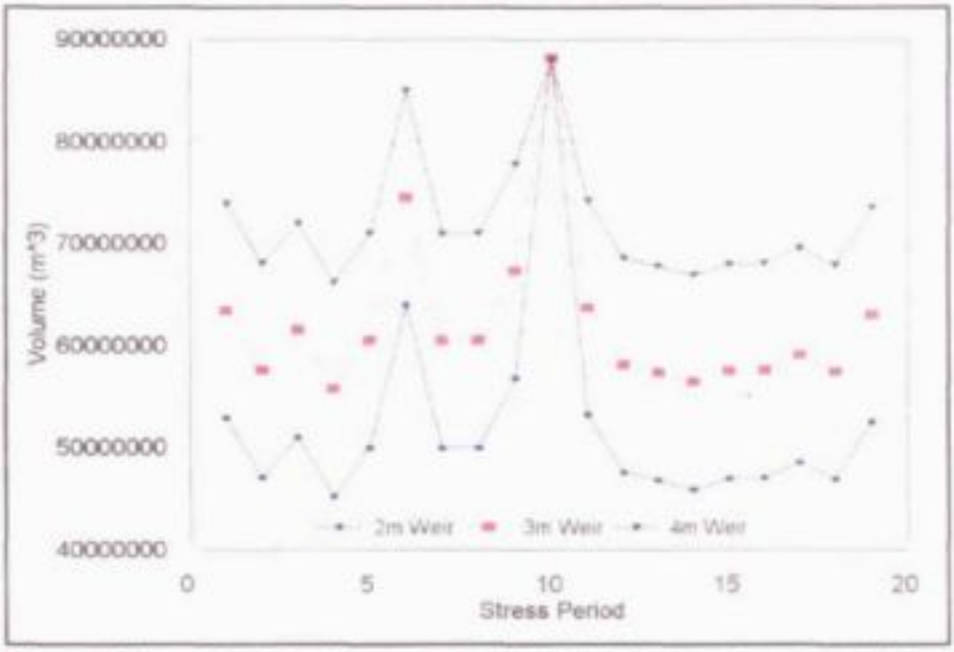


Figure 94 Simulated changes in the Lake Storage Capacity at the end of each stress period.

The simulated variation in the lake levels for the three weir heights during the series of stress periods is shown in Figure 95. There is very little variation between the series except in their overall magnitude.

8.3.7 SUMMARY AND CONCLUSIONS

This case study has simulated the flow dynamics of the groundwater in the vicinity of Lake Mzingazi. It has attempted to simulate the interaction between the lake and the aquifer but the calibration indicated that there was serious doubt about specific losses in the water balance of the lake information set. This uncertainty cause difficulties in determining the degree of interaction because the lake model could only be calibrated by introducing an unaccountable loss that could be part of the interaction.

The model calibrations could be improved with more information on the lake bed sediments and their conductive capacity as this would provide less reliance on the adjustment of the other factors in the calibrations. This would require field observations and increased monitoring around the lake perimeter. Tracer studies would also make a contribution to these studies. Groundwater flow rates are several orders of magnitude slower than the surface flow rates. Consequently, the parameterization of these processes needs careful consideration. The stress periods of recharge and evaporation are generally adequate for the groundwater slow simulations, but may be seriously in error for the lake level simulations.

ADDENDUM

Further studies of the lake have indicated that a two layer model could provide discharge conditions that are able to account for the unknown losses (Kelbe and Germishuyse, 2000b)

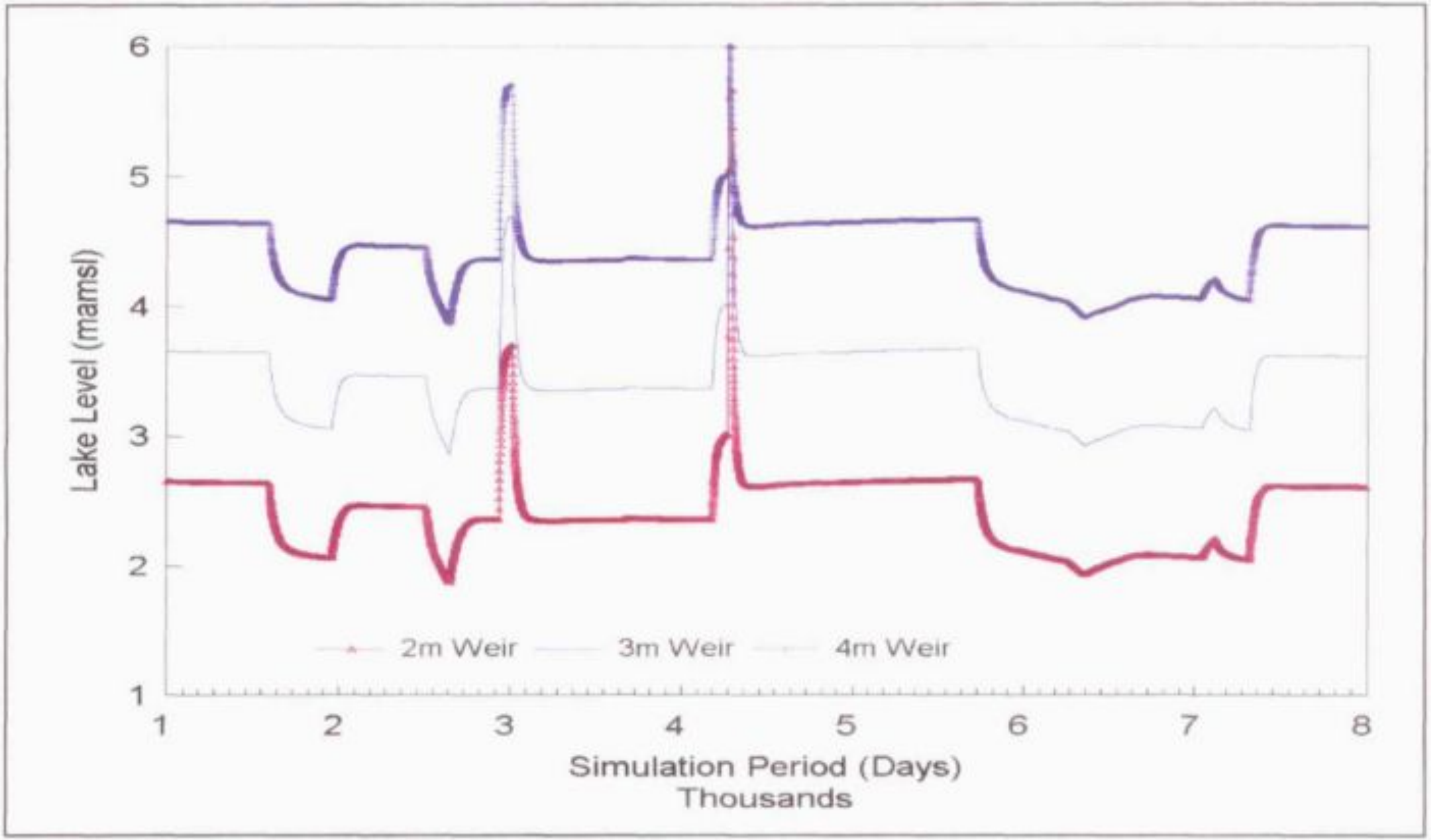


Figure 95 Simulated response to changes in the height of the Lake outlet

8.4 CASE 4: LAND USE ASSESSMENT

Rainfall is the principle recharge process for sustaining the watertable in phreatic systems. Evaporation is the other main surface process for controlling the discharge. Both of these processes are strongly affected by surface land use. Impervious road surface and deep rooting trees will greatly influence the water budget of an unconfined shallow aquifer. This study examines the influence of changes in land use on the water balance of Lake Mzingazi which has been described in the third case study in section 8.3.

The conceptual model and the calibration of the parameters have been described in detail in section 8.3. Because of the uncertainty in the abstraction rates and the level of groundwater leakance in the lake model, two different scenarios were presented in section 8.3 for the present conditions of land use in the region. However, the model with minimal groundwater interaction has **not** been used in this case study because it is unlikely that there will be any significant changes when the lake is effectively isolated from the aquifer. The model with a lake bed conductance of 10 m^2/day has been used to investigate changes in lake seepage for different land use scenarios. This level of interaction may be sufficient to mask the land use effect. However, the results are presented here as an initial estimate.

8.4.1 LAND USE

The impact of land use on groundwater system is modelled through changes in the recharge and discharge parameters. In natural grasslands, the rainfall-groundwater interaction has been described by Kelbe and Rawlins (1992) for the shallow aquifer on the eastern shores of lake St Lucia. This model is supported by rainfall-vs-water table response for other regions on the coastal plain shown in Figure 96. Under mature forests, it is assumed that a significant proportion of the rainfall would be intercepted (and then evaporated) so the recharge would be reduced in comparison with grasslands. However, this may be compensated by a reduced runoff rate in heavily vegetated surface in comparison to the grasslands. Consequently, it was assumed that the recharge was not altered for all the different land uses. For urban, industrial and commercial sectors it was assumed that the impervious surfaces (roads and rooftops) reduce recharge.

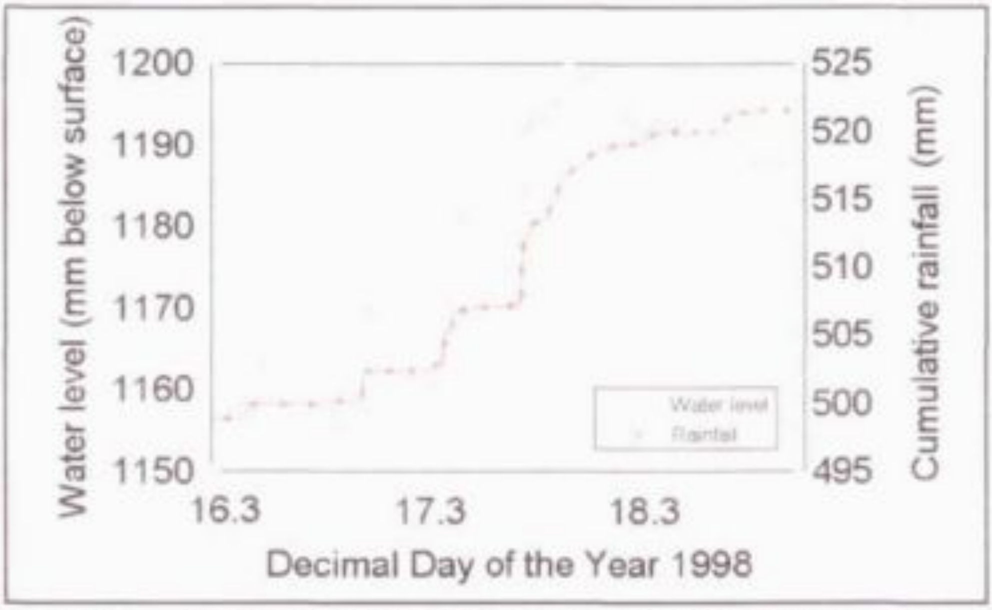


Figure 96 Cumulative rainfall and water table elevation during four rainfall events.

The largest impact on groundwater from vegetation is considered to be through evapotranspiration. This is modelled using two parameters that specify the maximum groundwater evaporation rate and the maximum (extinction) depth from which this occurs. This is assumed to vary considerably between the various land use types in this case study.

8.4.1.1 PRESENT LAND USE FEATURES

The present land use features in the immediate vicinity of the Lake Mzingazi study area are shown in Figure 97. There are large commercial forest to the north of Richards Bay. There are extensive areas with subsistence / informal settlements all round the northern parts of the lake. In the southern sections, the recent harbour developments cover a large part of the catchment area of the lake. Interspersed in these land use types are significant areas with swamps, swamp forests, dune forest and remnant grasslands.

8.4.1.2 HISTORICAL (PRISTINE) LAND USE FEATURES

Studies on various regions of the Zululand Coastal Plain have identified the indigenous vegetation types for many areas. Recent photographs in the Zululand Observer showed the main harbour area in 1902 was covered almost entirely with natural grassland (Figure 98). It has been assumed that similar conditions prevailed around the coastal lakes at Richards Bay before there were any significant developments. Consequently, the natural land use types for the region would follow similar patterns and the estimated spatial distribution of vegetation types are shown in Figure 99.

The swamp forests along the rivers and lake shores are assumed to have remained undisturbed in the riparian zone while the dune forest are assumed to be distributed in a similar pattern as the present conditions. The urban, industrial and commercial sectors, as well as the commercial forests, are assumed to have been natural grasslands. The areas surrounding rivers are assumed to have been indigenous forests.

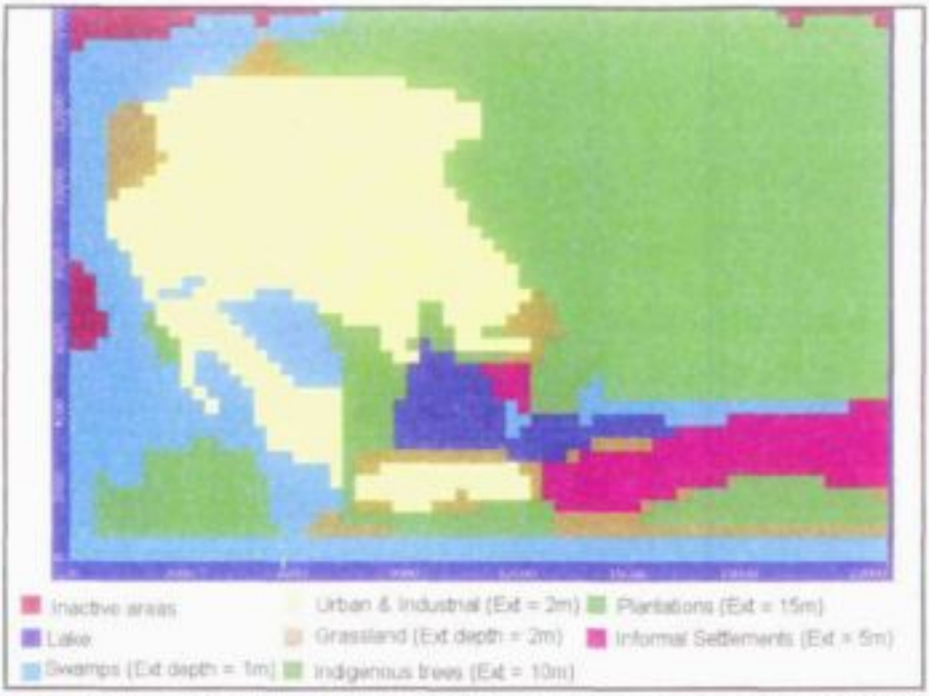


Figure 97 Present Land Use features in the Richards Bay Area assumed to influence the primary aquifer.

Figure 98 1902 Photograph of Richards Bay overlooking the Harbour (Zululand Observer, 1998)

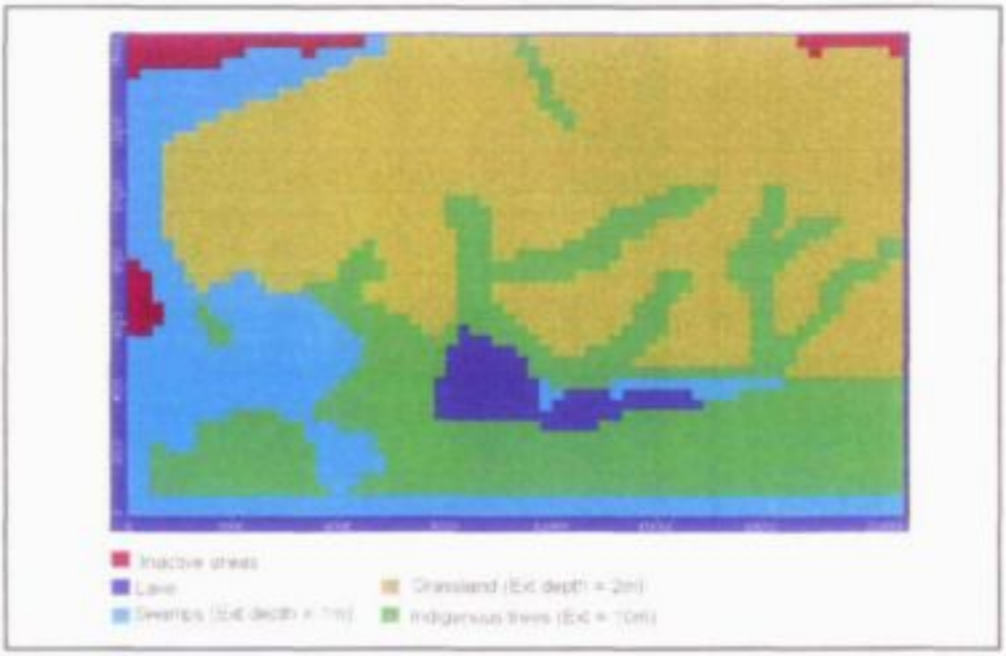


Figure 99 Assumed Pristine Land Use features in the Richards Bay Area.

8.4.2 MODEL PARAMETERIZATION

The model domain for this study has been described in Section 8.3. Only the features pertinent to land use studies are described.

8.4.2.1 HYDRAULIC PARAMETERS

It has been assumed that there is a rapid (exponential) decrease in lake recharge with distance from the shoreline from the groundwater system (see literature review in section 8.3.1). This would restrict the influence on lake recharge through the lower stratigraphic units. Consequently, it has been assumed that a **one layer model** would suffice for this study and the model features chosen are the same as those presented in the regional flow dynamic study and the lake water balance study presented in previous sections.

8.4.2.2 EVAPORATION PARAMETERS

The principle land use types included in the model simulations are listed in Table 33 together with their estimated parameter values for describing the evapotranspiration rates in an unconfined aquifer. For a description of the parameters refer to section 6.5.

Table 33 Estimated parameter values for the different land use types.

Parameter	Emax (% of gross)	Rooting depth (m)	Recharge
Urban	31	1.4	Urban recharge is 31% Remaining 69% runoff to lakes
Settlements	58	3.2	
Commercial forest	110	10.0	
Grasslands	60	2.0	
Dune forest	80	10.0	
Swamp forest	100	1.0	

The parameters for the **urban environment** have been based on a modified coastal grassland system. The parameter estimates have assumed an impermeable surface comprising buildings, roads and pavements which cover approximately 50% of the land surface area. This impermeable surface drains directly from the area into a water body through the articulated drainage system. The remaining surface acts as a coastal grassland with assumed natural parameter values.

The rooting depth of **coastal grass lands** is not known and has been assumed to be approximately 2 m. This is less than sugar cane which is a similar C4 plant species that has a rooting depth of approximately 4 m (SA Sugar Association Experiment Station).

The **exotic plant** species of forest generally grown in the regions are *pinus elioti* and *eucalyptus grandus*. The rooting depth of these two species is also unknown but has been assumed to reach depths of 10 and 12m respectively in unconfined sandy soils with unlimited soil moisture.

Indigenous coastal forest growth features affecting recharge and evaporation are unknown and seldom mentioned in the literature. Consequently it has been necessary to make several assumptions about the recharge and evaporation features of these species in a coastal environment.

(A) Dune forest. These species have adapted through evolutionary processes to the harsh coastal environment with deep, fast draining soils. Hattingh (personal communications) has indicated that these trees which are felled in the mining operations along the coastal dunes in the Richards Bay area have a very shallow rooting depth. It has been assumed that the average rooting depth of the indigenous dune forests is 10 m. While the canopy structure in the indigenous tress is different to the exotics, it is assumed that the leaf area of the canopy expressed as a fraction of the horizontal land area (leaf area index) is similar for all tree species. Consequently the interception of rainfall is likely to be similar. However, the difference in the rooting depth differentiates the available moisture storage capacity available for evaporation in the unsaturated zone. This is likely to influence the groundwater recharge mechanism. Consequently, the recharge rate for the exotic trees is assumed to be approximately 80% of that of the

indigenous trees.

(B) Swamp Forests. The swamp forests are usually located in regions with very shallow water tables and consequently the rooting depth of these trees is likely to be extremely shallow. It has been assumed that the rooting depth of swamp forests is about 73% of exotic trees. However, the rainfall interception is likely to remain the same as the exotics. Because the swamp forests are located in very wet conditions, the rainfall is likely to fall directly onto the saturated areas and contribute immediately to the groundwater system. Consequently, the recharge in the swamp areas is assumed to be equivalent to the natural rainfall (100% rain).

8.4.3 CALIBRATIONS AND SENSITIVITY

The evaporation parameters used to simulate the groundwater land use interaction are the maximum loss of vapour from the capillary zone (water table) and the representative rooting depth. Neither of these two parameters are known and there is little in the literature to describe their possible range of values. Consequently, these parameters should be calibrated against field observations. Unfortunately there is no information available for these calibrations. This study has highlighted the need for research on the surface groundwater interaction. In this study the values presented in Table 33 are assumed to be representative for comparative studies.

8.4.4 RESULTS

The simulated groundwater conditions for pristine conditions described above were compared to the simulated groundwater conditions for the present land use types. Figure 100 shows the seepage rate (m^3/day) for both land use scenarios. There is very little difference in seepage rates during the periods when the conditions were near or above mean hydrological state. However, there is a significant reduction in the seepage into the lake during extended drought periods when the groundwater interaction becomes increasingly important in sustaining the water balance of the lake. The difference in seepage rates reached 1000m^3/day during drought periods when water supply becomes critical.

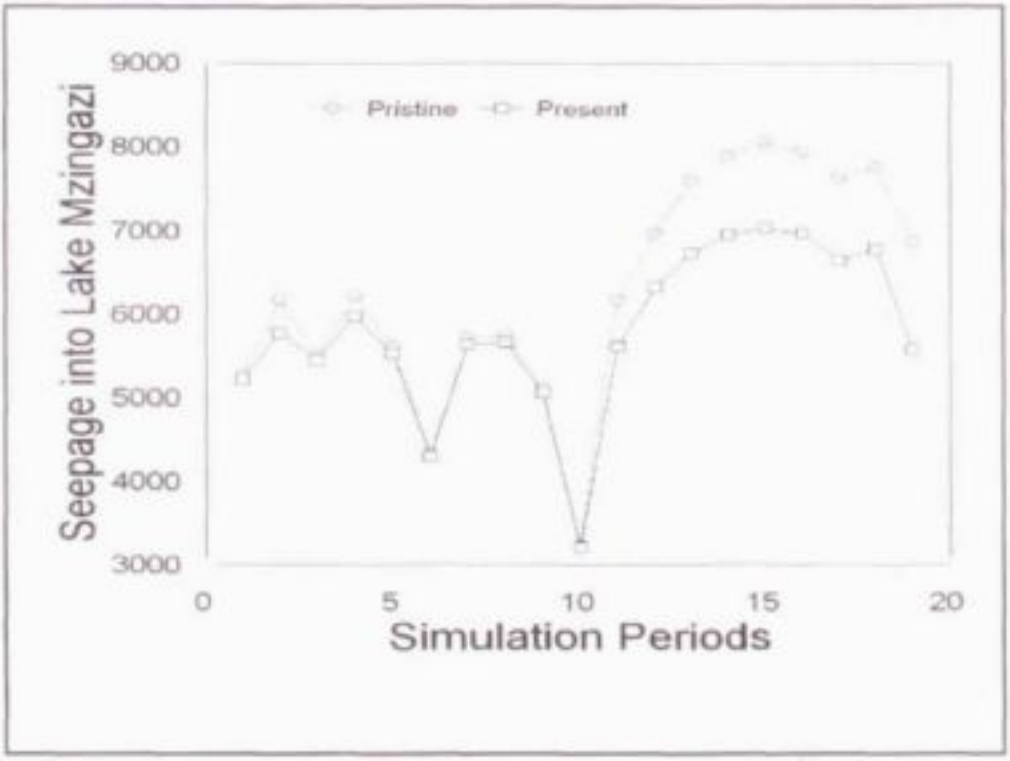


Figure 100 Simulated groundwater seepage rates (m^3/day) into lake Mzingazi under two land use scenarios.

8.5 CASE 5 : COMPARISON OF CALIBRATION TECHNIQUES

In South Africa, Waste Disposal Sites (Slimes Dams) are regulated by the Minerals Act No 50 of 1991. These structures require environmental management programmes that form part of a site-specific legal obligations, on the part of the mine authorities, to establish the impact of the sites on the environment. The decommissioning of the waste site also requires the minimization of adverse environmental impacts after closure. Consequently, these sites are ideal for numerical studies because they are required to undertake a detailed monitoring programme which should be sufficient to provide the data needs for numerical model calibration and testing. The models would then provide a means for prognosis and prediction. The waste disposal site used in this study, has been in operation for ten years and is now due for closure. This case study examines calibration routines to determine the parameter values using common trial and error approach and the numerical techniques developed by Häfner *et al* (1996).

8.5.1 SITE DESCRIPTION AND DATA

The test site is located in a natural depression in coastal dunes approximately 1000 m from the beach and about 60 m above mean sea level (*AMSL*). Consequently there is very little surface runoff and most surface water will percolate to groundwater or evaporate to the atmosphere. The water leakage into the aquifer from the site has been estimated by Hattingh *et al* (1995) to be approximately 300 m^3/day. This leakage is over and above the natural recharge from rainfall which is estimated to be ~8170 m^3/day over the model area.

Several boreholes have been drilled in the vicinity of the site and some of them are monitored at regular intervals. The location of all the boreholes are shown in Figure 101. The prefix M in the borehole number identifies the monitoring boreholes. All the borehole logs were used in the development of a conceptual geological model of the area.

Figure 101 Map of Borehole locations. The waste site is indicated by the shaded area. The transects are labelled A-A' and B-B'.

8.5.2 GEOLOGY

The waste site is located in the recent (Holocene) unconsolidated sands which have very high infiltration rates, with permeability and porosity that induces rapid flow under saturated conditions. The general geology (Figures 102 and 103) conforms closely to the description presented in section 3.

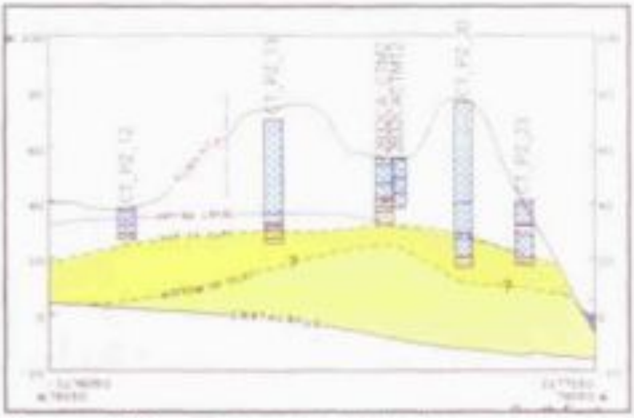


Figure 102 Transect A-A' shown in Figure 101

All the geological information provided have been used to create a conceptual geological model of the area for incorporation into a numerical model for simulation purposes. A geological transect perpendicular to the coast (A-A') is shown in Figure 102 and a transect parallel to the coastline (B-B') is shown in Figure 103.

The basement of the stratigraphy generally slopes toward the south-east (coastline) but is relatively flat along the axis perpendicular to the coastline. There is only a small change in the elevation of the water table parallel to the coast. Therefore, it could be assumed that the geohydrological system is essentially two dimensional with flow mainly toward the coast (south-east direction) from a groundwater divide near the north-western section of the study area (Hattingh *et al*, 1995). The approximate position of the water divide is indicated by the dashed line in transect A-A', shown in Figure 102. This divide runs parallel to and inland of the transect B-B' in Figure 103.

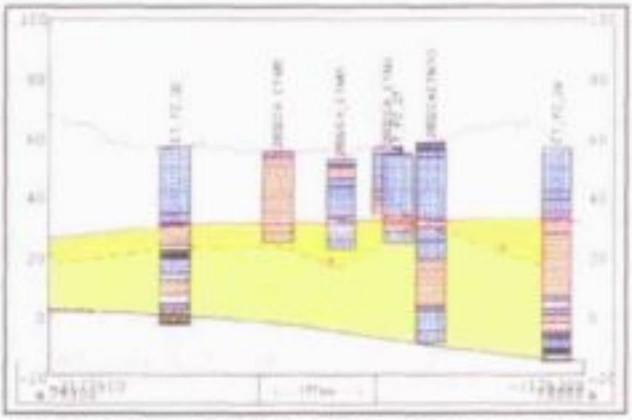


Figure 103 Transect B-B' shown in Figure 101.

The stratigraphic cross-sections show three main geological layers which are considered separate hydraulic units for geohydrological modelling in this study. The base of the system is assumed to be impermeable and is defined by the upper surface of Cretaceous Age siltstone. This surface was interpolated from the four boreholes which were deep enough to intercept the layer. These boreholes are indicated by circles in Figure 101. Overlying the siltstone is a layer composed of Miocene Age deposits which have been observed by several geologists in the Richards Bay area (Webb *et al*, 1972; Worthington, 1978). This layer has been associated with reef relics which formed along the coastal region several million years ago (Hattingh, 1998). It is absent in many places along the coast probably due to drainage erosion in later geological times. For this specific site very little information on the presence of this layer was available. Only in two of the borehole logs could the Miocene deposits be identified with relative certainty. In at least one log the absence of this member is recorded. The Miocene deposits are found in discontinuous units which are generally orientated in a NE-SW direction (Hattingh *et al*, 1995). Since these deposits are generally discontinuous, the groundwater flow in this formation is assumed to be controlled by the overlying Port Durnford layer of Holocene Age for the flow model simulation studies.

The Port Durnford Formation that is observed along the entire Zululand coast, overlies the Cretaceous and Miocene deposits. In this region it is a layer which is generally associated with a higher clay content than that of the overlying sands and has been described in detail in section 5.4. This layer was not easily identifiable from the borehole logs because of the subjectivity in geological classifications. However, the interpolated surface compared favourably with independent estimates provided by Hattingh (1996).

The borehole logs were used to define the layer overlying the Port Durnford, This layer is comprised of more recent cover sands that are generally associated with an aeolian origin. These have also been described in detail in section 5.5.

Limited information is available on the hydraulic properties of all these layers and consequently it has been necessary to infer conditions from other areas as described in Section 5. The hydraulic properties of the different layers presented by Davies Lynn & Partners (1992) for St Lucia (~200km NNE from the site) were assumed for the initial estimates of the model parameters (Table 13) before calibration.

8.5.3 NUMERICAL MODEL DOMAIN

The model domain assumed that the system was bounded by the ocean on the SE boundary and a river transecting the NE sector. The other two perpendicular boundaries are assumed to be no-flow boundaries (Figure 102).

8.5.4 HYDRAULIC PARAMETERS

No measurement of hydraulic properties or their variability were available for this study. Consequently, it was assumed that the estimated permeability and porosity are uniform throughout each layer. This assumption was later discarded in the calibrations when an attempt was made to introduce some heterogeneity in the numerical calibration studies discussed later.

8.5.5 SURFACE ELEVATION OF LAYERS

The model layers were interpolated from the borehole logs using the SURFER© (refer note 1, p5) and GWW© software routines. It is assumed that the recent cover sands form a layer bounded by the topographical surface (not shown) and the Port Durnford. The upper surface elevation of the Port Durnford layer was not easily identifiable in the borehole logs. Nevertheless, all the borehole logs were used to plot the top elevation of this layer using the Universal Kriging surface fitting technique (Figure 104).

The lower surface (boundary) of this layer coincided with the Cretaceous siltstone. There were only 4 boreholes which specifically identified Cretaceous age deposits and they are circled in Figure 101. These were used to form an "initial surface". Boreholes that were drilled deeper than this "initial surface", were assumed to stop on the upper Cretaceous level and their depth were used as extra information to create the final lower surface boundary of the model domain (bottom of aquifer). The interpolated surface contours are shown in Figure 105.

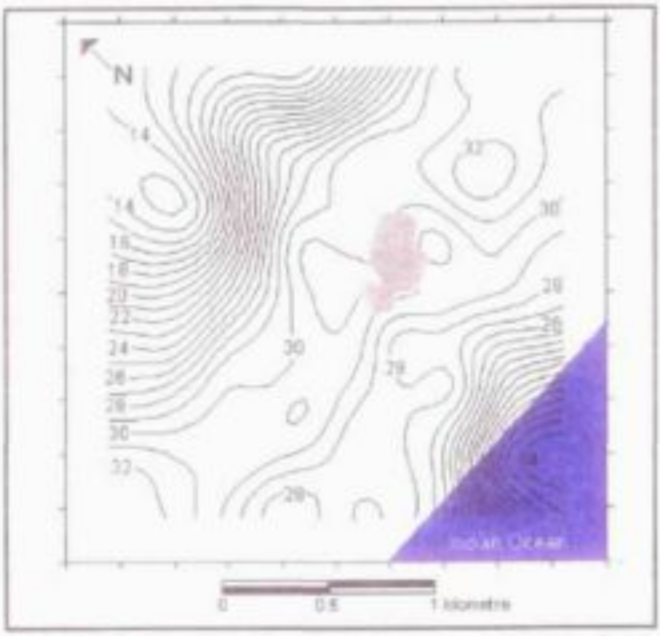


Figure 104 Interpolated upper surface of the Port Durnford.

For the five layer model, these two layers were further subdivided. The top (sand) layer was divided into 3 additional layers and the bottom (clay) layer was divided into a further 2 layers.

8.5.6 FLOW

All simulations were derived for average, steady state hydrological conditions. For the initial boundary conditions, the parameters were estimated from information derived from other areas. These were then adjusted **subjectively** during initial calibration to find the best agreement between

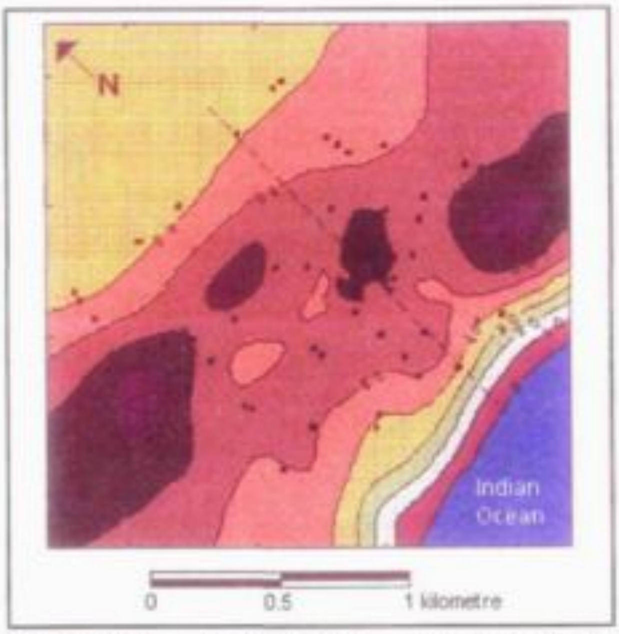


Figure 105 Interpolated upper surface elevation of the Cretaceous layer in the model domain.

observed and simulated water table elevations. Thereafter numerical calibration was done using CALIF in search of better parameter values for permeability.

The conditions given in Table 13 were used to derive the initial estimates for the model parameters. The first estimate of the recharge value was assumed to be 994 mm/year which is based on the model described in section 6.3.6.2. The initial parameter values for permeability were adjusted systematically to achieve a closer comparison between observed and simulated data according to the methods described in section 7.2. The correspondence between observations and predictions in the water table elevations, for steady state conditions, are shown in Figure 106.

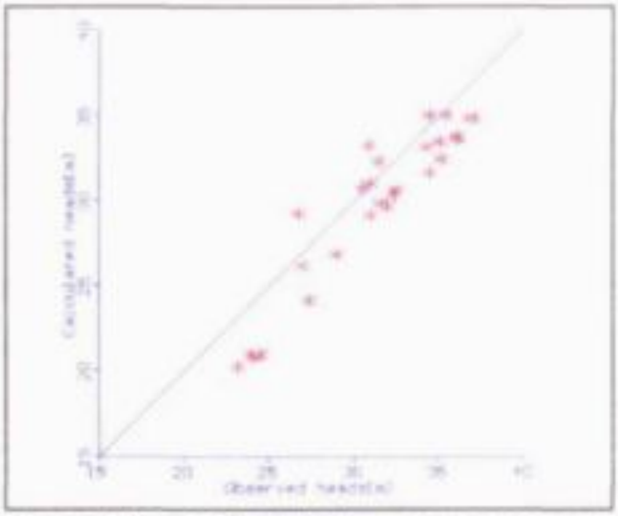


Figure 106 Calculated versus observed water table elevation (m AMSL).

8.5.7 CALIBRATION METHODOLOGY

Experience has shown that some of the automatic calibration procedures require large resources in time and hardware. Therefore one needs to set objective criteria for the calibration procedure to optimize the time required. In this study permeability was the chosen parameter to be optimized for flow simulations. The following general criteria were used for the two case studies presented in the next sections:

1) Scenario 1 *assumes that all layers are homogeneous and the numerical calibration program CALIF is used to identify the optimum parameter value throughout each layer.*

2) Scenario 2 *assumes some heterogeneity within layers by subdividing layers into zones. A zone may be part of a layer or it may stretch over several layers. CALIF is used to identify the optimum parameter in each zone.*

3) Scenario 3 *assumes heterogeneity in each layer, by subdividing one layer at a time into 4 zones for optimization of parameters.*

8.5.8 PERMEABILITY CALIBRATIONS

The initial estimates for permeability values were derived from other studies (Table 13) and then adjusted using the trial and error method of calibration to achieve the comparison between simulated and observed data shown in Figure 106. These calibrated values were used as initial estimates in the numerical calibration procedures and for comparison between the calibration techniques. However, the expected range of values for parameter identification was set according to the limits given in Figure 64.

The calibration of the permeabilities for flow simulations was conducted on both a two layer model and a five layer model. Different calibration techniques and different zonation structures were used in the two models. Permeability parameters identified for the different calibration efforts are compared to the initial estimates of permeabilities. The simulated water level surfaces using the parameters identified in the calibration cases are compared to the observed water table surface in the figures that follow those tables.

The criteria described in scenarios (1), (2) and (3) were used for different case studies labelled A, B, C *etcetera* in the following sections. Case A always refers to the observed conditions while all other cases refer to simulated conditions. Case B defines the simulations derived from the trial and error calibrated parameter estimates and is referred to as the initial data set. Cases C, D, E and F refer to the cases with different iterations and different zonation procedures.

8.5.8.1 TWO LAYER MODEL WITH NO CALIBRATION LIMITS IMPOSED

Numerical calibration was allowed to proceed with no upper or lower boundary to the permeability values. For the two layer model there were some large changes in the permeability values compared to the initial estimates using the different zonation procedures and iteration techniques. Initial (trial and error) parameter estimates for layers 1 and 2 are given in Table 34 under column (case) B. The simulated water table surfaces for these parameters are shown in Figure 107B and are compared to observed water table surfaces shown in Figure 107A.

Table 34 Permeability values (m/day) as a result of calibrating a two layer model

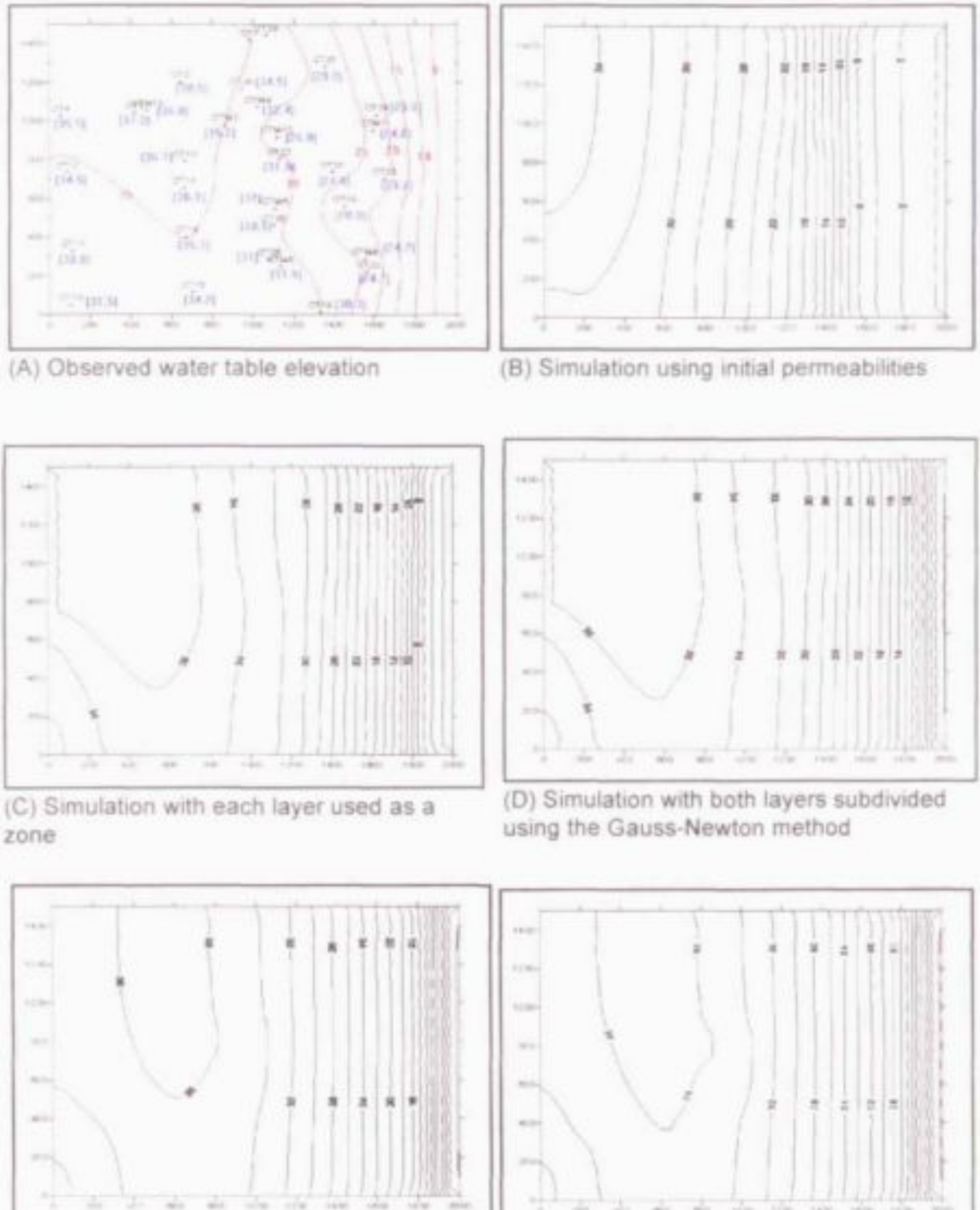
CASE		B	C	D	E	F
SCENARIO		Initial estimates	1. Layers	2. Subdivided into more zones		
ITERATION			Gauss-Newton		Powell	
Layer 1	Zone 1	25.0	40.0	25.0	1.0	0.3
	Zone 2			2.47	0.007	
Layer 2	Zone 3	2.5	1.8	2.5	13.0	10.0
	Zone 4			2.66	2.9	2.9

For case C (where the optimization used the full extent of each layer as a separate zone) the numerically calibrated permeabilities increased by 160% to 40 m/day in the first layer and decreased by 72% to 1.8 m/day in the second layer as indicated in Table 34 column C. Both these values are within the expected ranges given in Figure 64. Resulting water levels (Figure 107 (C)) compare well with observed water levels (Figure 107 (A)) and seem to be an improvement on the simulated water table elevations derived from the initial (trial and error) permeabilities (Figure 107 (B)).

For case D the layers were subdivided into zones. In this optimization the first layer was divided into two zones (demarcated by the area where the Port Durnford is exposed near the sea).

The second layer was divided into a zone consisting of the first three columns of the model domain (inland) and another zone accounting for the other seventeen columns. For this case, the derived permeabilities were very similar to the expected values for the sandy sections (zone 1 in layer 1) and they also approximated the Port Durnford values in zone 2 of layer 1 (Table 34, column D). The resulting water levels shown in Figure 107 (D) compared better with the observed water levels than the trial and error approach.

Case E used the same zonation as case D, but the Powell iteration technique was employed instead of the Gauss-Newton technique. Optimized permeabilities are shown in Table 34, column E. These appear to be very low for the cover sands. The resulting water levels shown in Figure 107 (E) appear to be better estimates than the initial calibration values.



(A) Observed water table elevation

(B) Simulation using initial permeabilities

(C) Simulation with each layer used as a zone

(D) Simulation with both layers subdivided using the Gauss-Newton method

(E) Same as (D) using Powell iteration method

(F) Same as (E) with layer one at initial permeability

Figure 107 Water table elevation simulations from different calibration techniques for optimizing permeability in a two layer model.

Case F used the Powell iteration technique for a zonation structure similar to cases D and E in layer 2, but there was no subdivision in layer 1. The results are similar to the simulation for case E (see Table 34, column F and Figure 107 (F)).

Some of the optimized permeabilities in the top layer are not in the accepted range for the Powell iteration method and are probably a result of dry cells, where permeability may "adopt" any value because there is no water in those cells. These dry cell permeabilities affect the average permeability of the zone because the program does not ignore dry cells. Häfner (1996) suggested keeping the top layer parameter values fixed, that is, not to use it as a zone for identification of parameters.

The similarity in simulated water table elevation for different permeability values indicates the difficulty in using calibration techniques to derive parameter values.

8.5.8.2 FIVE LAYER MODEL WITH NO CALIBRATION LIMITS

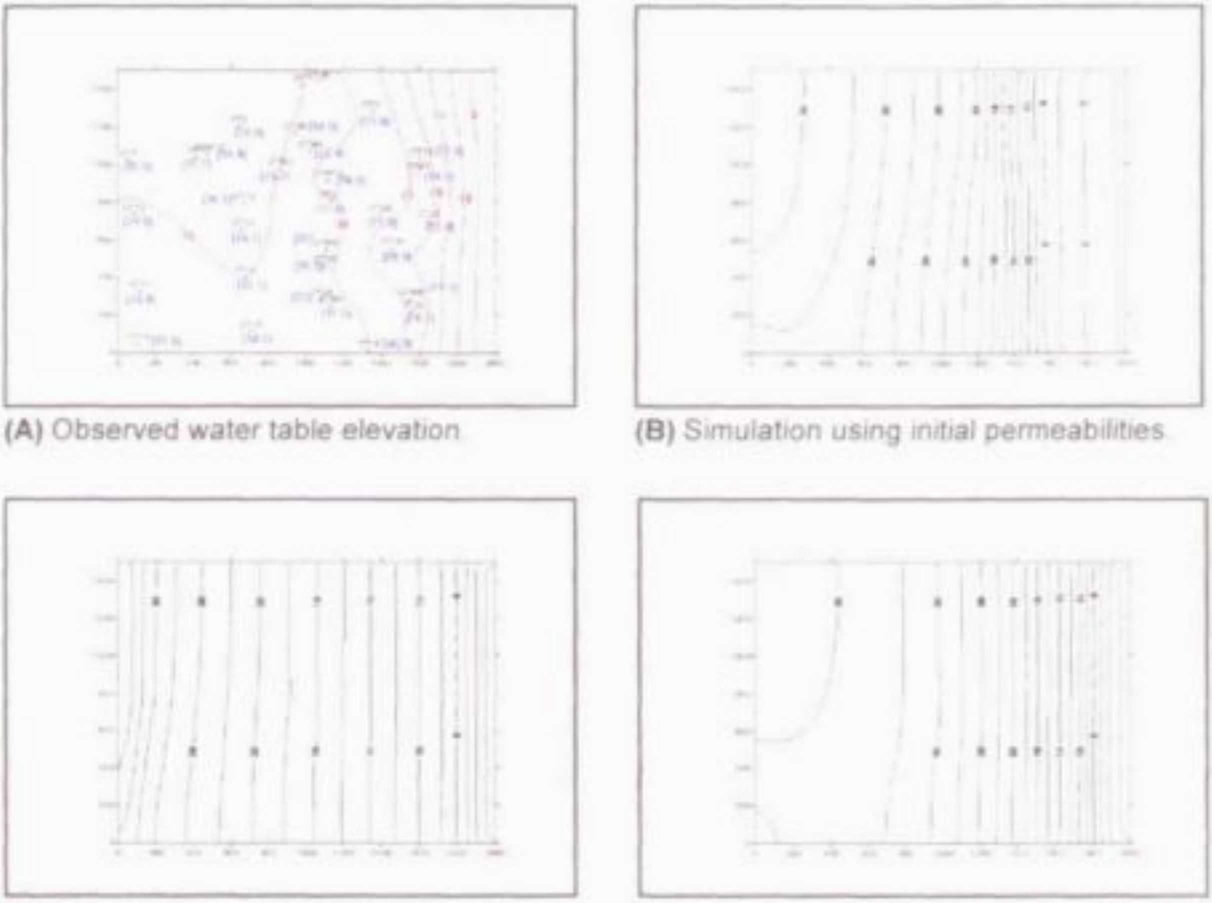
This case study was conceived because the observation data was available for several layers. Initial parameter values for the 5 layer model are given in Table 35, column B and the resulting simulated water table elevations using these values are shown in Figure 108 (B). There are some features which are common to the observed surfaces shown in Figure 108 (A).

The top layer in case C calibration was not used as a zone for identification; instead it was fixed at a permeability of 25 m/day. Layers 2 and 3 were grouped together as one zone, because there were no observations available in the third layer. The optimized permeabilities, indicated in Table 35, column C, were low in layers 2 and 3 and high in layers 4 and 5. This agrees with the idea of a highly permeable layer of Miocene age deposits. However, the water levels shown in Figure 108 (C) as a result of using these permeabilities, are up to 15 m lower than the observed levels (Figure 108 (A)).

Table 35 Permeability values (m/day) as a result of calibrating a 5 layer model.

<table>
<tr><td>CASE</td><td>B</td><td>C</td><td colspan="2">D</td></tr>
<tr><td>SCENARIO</td><td rowspan="2">Initial estimate</td><td>1. Layer zones</td><td colspan="2">2. Subdivision into three more zones across layers 2 to 5</td></tr>
<tr><td>ITERATION</td><td>Powell</td><td colspan="2">Gauss-Newton</td></tr>
<tr><td>Layer 1</td><td>25.0</td><td>25.0</td><td colspan="2">28.9 for layer 1</td></tr>
<tr><td>Layer 2</td><td>2.5</td><td rowspan="2">0.33</td><td rowspan="4">2.9 for zone 2 over layers 2 to 5</td><td rowspan="2">4.7 for zone 3, layers 2 and 3</td></tr>
<tr><td>Layer 3</td><td>2.5</td></tr>
<tr><td>Layer 4</td><td>2.5</td><td>62.2</td><td rowspan="2">4.7 for zone 4, layers 4 and 5</td></tr>
<tr><td>Layer 5</td><td>2.5</td><td>50.1</td></tr>
</table>

In case D the zonation stretched over more than one layer. The first layer formed one zone, the second zone was an area that stretched over all the other layers below the top layer and covered the first three rows from the western boundary, compare section 8.1 D. The remaining area below the top layer and to the south-east of the second zone, was further subdivided into two zones between layers three and four. The optimized permeabilities for the four zones can be compared to the initial estimates given in Table 35, column C. When these permeabilities were used for the flow simulations, the water levels (shown in Figure 108(D)) again were lower than the observed elevations (Figure 108 (A)).



(A) Observed water table elevation.

(B) Simulation using initial permeabilities.

(C) Simulation with each layer used as a zone with the Powell method.

(D) Simulation with 4 zones and Gauss-Newton method.

Figure 108 Observed and simulated water table elevation (m *AMSL*) for different calibration techniques used to optimize permeability in a 5 layer model.

8.5.8.3 FIVE LAYER MODEL WITH CALIBRATION LIMITS

To determine the effect of calibration method on the 5 layer model a sequential procedure for zoning individual layers, was compared to the reverse sequential order. In all cases the optimized values for each zone were constrained within an upper and lower limit estimated while all other permeability values were fixed at a constant value for the calibration simulation.

A systematic zonation procedure (Figure 109) was followed to reduce computing time and to make the process a little more objective. The procedure started with values in all layers fixed with initial parameter values (adjusted from Figure 64) and then subdivide one layer at a time into four zones for optimization of permeabilities in these zones. The "optimized" values for each zone were used as the starting values

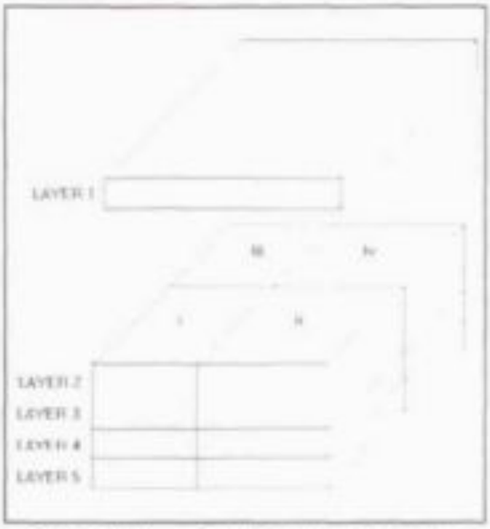


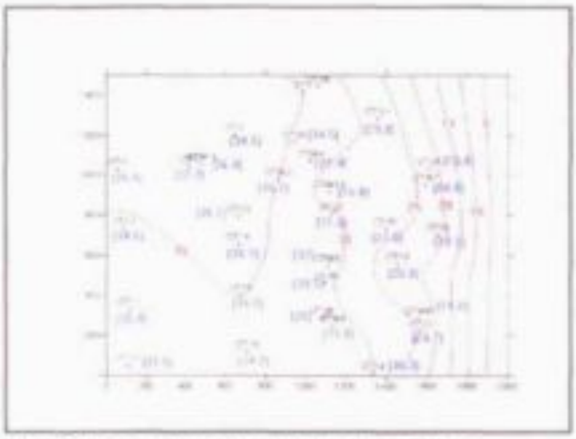
Figure 109 Systematic zonation procedure

for the next optimization sequence when the next layer was subdivided into four zones. This process was repeated for every layer. The top layer was not included as part of the optimization procedures, because the water table did not extend into this layer in many areas. In the first sequence, changes started from the bottom layer and proceeded to the higher layers. In the second sequence the process was reversed starting with changes in the second layer and proceeding downwards to the bottom. The two procedures resulted in very different permeability estimates (see Table 36). The optimized permeabilities for the sequence stating with layer two is shown as case D in Table 36 while the reverse sequence is given as case C. Three zones showed optimized values which were two orders of magnitude different between the two sequences (shown by * in Table 36). For all the layers given in Table 36, the optimized permeabilities were close to the expected minimum for zone (i), close to the expected maximum for two layers in zone (iv) and approximately the same for both runs in zone (iii). Consequently, a field study of the conditions in zone (ii) may help to explain the large differences in optimized values.

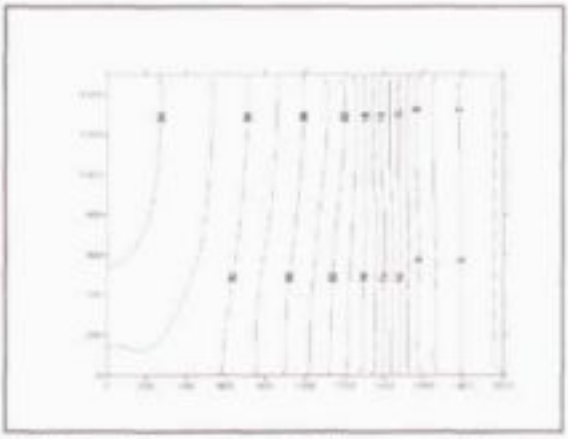
Table 36 Permeability values (in m/day) as a result of a calibration experiment using a reverse sequence of zonation in each layer.

CASE		B	C	D
SCENARIO		Initial estimates	3. Each layer optimised separately using Powell	
DIRECTION			Up	Down
	Layer 1	25	25 (fixed)	25 (fixed)
zone i	Layers 2 and 3	2.5	0.25	0.25
zone ii			**0.35**	**25***
zone iii			0.25	7.2
zone iv			**0.65**	**25***
zone i	Layer 4	2.5	0.25	0.25
zone ii			14.8	25
zone iii			25	19.5
zone iv			25	25
zone i	Layer 5	2.5	0.25	0.25
zone ii			**25**	**0.25***
zone iii			11.5	16.7
zone iv			25	25

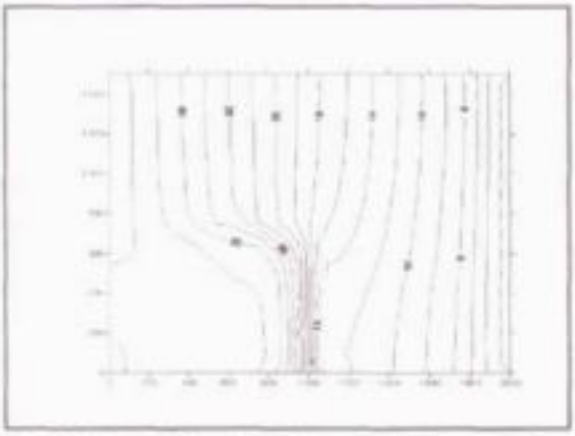
The simulated surface contours of the groundwater head looked similar to each other for the two cases (Figure 110. (C) & (D)). Unfortunately these simulated water table elevations do not look similar to the observed. A possible cause is that the zones should not be adjusted while the values in other zones are fixed. Another possible problem is that the range of values set in the program, was not allowed to reach a limit of optimization, but was constraint within defined limits. A third problem may be the choice of four zones per layer, which cannot be justified in terms of geology. The next step in this comparison should be to identify all these



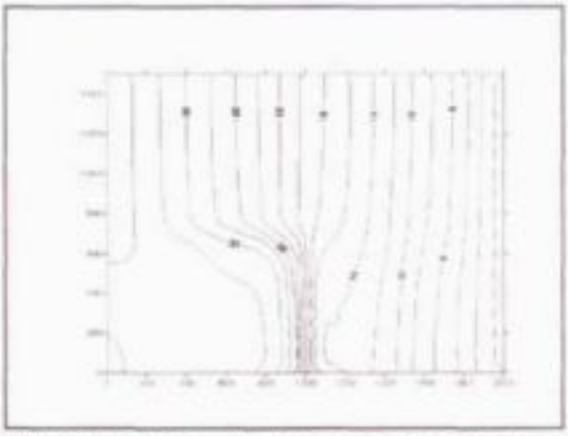
(A) Observed water table elevations.



(B) Simulation using initial permeabilities.



(C) Water table elevations as a result of bottom to top identification procedure.



(D) Water table elevations as a result of top to bottom identification procedure.

Figure 110 Water table elevation simulations from different calibration techniques for the five layer model.

zones at the same time and repeat the optimization until a true minimum is reached. However, this will probably take weeks of calculations on a desktop PC and was not done as part of this study, because run time was 40-50 hours per layer (a week to identify one sequence) on a 486 computer with 16 MB of RAM.

8.5.9 SUMMARY AND CONCLUSION

The numerical technique used in this study for optimizing the parameter estimation procedure through the minimization of comparative differences (errors) is still not sufficiently advanced to use on a regular basis without considerable effort. The effort used in automating the calibration was more beneficially used in the trial and error methods because this method also required a great deal of thought on the model concepts and parameter values that led to a greater understanding of the system. The temptation to use the numerical values without question is always present.

PART 4

SOLUTE TRANSPORT MODELLING

SECTION 9 SOLUTE TRANSPORT MODELS

SECTION 10 CALIBRATION

SECTION 11 CASE STUDIES

Section 9 NUMERICAL MODELS

There is increased concern by regulatory agencies and researchers about subsurface contamination. This can be attributed to the increase in waste disposal by means of landfills, sludge lagoons and deep injection wells (Anderson, 1979). To prevent the deterioration of the groundwater quality there is a need to develop methodologies for monitoring, analysing, and predicting the movement of contaminants in the groundwater. The predominantly light textured, sandy soils of the Coastal Plains as well as their poor nutrient and water retention characteristics generally have been recognized as important contributing factors to contamination of the shallow, unconfined groundwater (Townley *et al* 1995). The use of predictive tools, such as numerical models, can play an important role in the management of the groundwater systems.

There are several ways that contaminant transport models play a role in groundwater management. The most effective application is probably in assessing the impact of subsurface contamination at a specific site in advance of developments ("what-if" scenarios). However, these models are effective in assessing the long-term consequences of remedial action where contamination has occurred. The models can also be used to simulate the flow dynamics of the system and to develop the most effective monitoring program for these systems. The application of models in the Richards Bay area for prediction of existing contamination is discussed. Proposals for more detailed studies of a surface-groundwater interaction and waste disposal sites are covered in the final sections on future research.

In this project two models have been used in different ways to acquire an understanding of their behaviour and application in a primary coastal aquifer. These are:

-MT3D developed by Zheng (1990).

-CALIF developed by Häfner *et al* (1996).

Both these models have similar parameter requirements and consequently the main emphasis in this project has been on establishing the models and estimating representative values of their relevant parameters. The application covers two phases that involve

1. the establishment of conceptual and numerical models which are suitably calibrated for the flow dynamics of the study area (covered in Parts 2 and 3 of this report).
2. the extension of the flow models to include the contaminant transport that run in conjunction with the flow model (Part 4 of this report).

The application of transport models is generally more difficult than the flow model applications presented in the previous sections. Firstly, the errors in the flow model are carried forward to the transport models, and secondly but more importantly, the dispersion equation is dependent to a much greater degree on the composition of the porous media than the flow model. Anderson (1979) has pointed out the difficulties involved in obtaining descriptions of groundwater systems which are sufficiently detailed to allow accurate predictions of contaminant migration. These problems have been repeatedly encountered in this study and are considered in this report.

9.1 TRANSPORT MODELLING CONCEPTS

The model of solute transport is based on the following conceptual equation from Zheng (1990):

Concentration flux = advection + dispersion + sources and sinks + chemical reactions + radioactive decay (or biodegradation).

This can be described in numerical terms for saturated flow dynamics by the transport equation:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}\left(v_i C\right) + \frac{q_s}{\theta}C_s + \sum_{k=1}^{N} R_k \quad \text{.......... Eq 9-1}$$

where

$C = C(x,y,z,t)$ is the concentration of contaminants dissolved in groundwater $[ML^{-3}]$

t is time $[T]$

x_i is the distance along the respective Cartesian coordinate axis $[L]$

D_{ij} is the hydrodynamic dispersion coefficient in the "ij" plane $[L^2T^{-1}]$

$v_i(x,y,z,t)$ is the pore water velocity $[LT^{-1}]$

q_s is the volumetric flux of water per unit volume of aquifer representing sources (positive) and sinks (negative) $[T^{-1}]$

$C_s = K_sC$ is the concentration of contaminant sources and sinks $[ML^{-3}]$ where

K_s is a distribution coefficient

θ is the dimensionless porosity factor for porous medium

R_k is the chemical reaction term $[ML^{-3}T^{-1}]$

The transport equation is linked to the flow equation through the relationship

$$v_i = \frac{K_{ii}}{\theta}\frac{\partial h}{\partial t} \qquad \text{Eq 9-2}$$

where

K_{ii} is the principle component of hydraulic conductivity tensor and h is the head

Note that the hydraulic conductivity tensor (K_{ij}) has nine components. However, it is generally assumed that the principle components of the hydraulic conductivity tensor (K_{ii} or K_{xx}, K_{yy}, K_{zz}) are aligned with the x, y and z coordinate axes so that non-principal components become zero. This assumption is incorporated in most commonly used flow models, including Modflow (Zheng, 1992).

Three techniques have been used regularly to solve these equations. These include finite difference approximations, method of characteristics (MOC), and finite element techniques (Anderson, 1979). The finite difference approach to flow modelling has been described in section 6. This method has numerical dispersion problems related to the solution of a parabolic dispersion term and a hyperbolic advection term (with a ratio called the Peclet number). With low

Peclet numbers (<2) numerical dispersion can be the same order of magnitude as the physical dispersion. This led to the proposed MOC where the differential equation is first replaced by its characteristic equation (a set of ordinary differential equations), and then these are approximated using finite difference. This reduced numerical problems but was cumbersome to programme. Anderson (1979) gives a detailed review of the different approaches.

The application of these equations in numerical models depends on many assumptions of the system under investigation and the various methods of iterative solutions for the differential equations. Due to the large number of unknown numerical parameters in transport modelling, simplified methods are required to achieve solution in the fastest most efficient manner.

The main assumptions employed by the common models for solving these equations are summarised by Anderson (1979), Anderson and Woessner (1991) and Zheng (1992). The assumptions relevant to this study are summarized below.

Equilibrium models

The models which are applied in this project, assume that the rate of sorption of chemical species or organic compounds is much greater than the rate of change in their concentration due to other processes and that the flow rate is slow enough that equilibrium can be obtained.

Organic compounds are adsorbed on solid surfaces by the hydrophobic effect which is dependent on the polarity of the organic molecule. The dissolved molecules are attracted to surfaces that are less polar than water, primarily to the organic carbon fraction (f_{oc}).

Non-equilibrium models

The kinetic sorption models are not considered in this project because of the complete lack of information for calibrating them. These are non-linear models that include:

- the irreversible first-order kinetic sorption model,
- the reversible linear kinetic sorption model,
- the reversible nonlinear kinetic sorption model and
- the bilinear adsorption model

9.1.1 The Advection term

This term describes the transport of miscible contaminants that are transported at the same velocity as groundwater. It is generally the dominating term in equilibrium models and the degree of dominance is indicated by the Peclet number. When advection is the only process involved in transport, the Peclet number is infinitely large. In such cases the physical dispersion becomes negligible, but often problematic numerical dispersion occurs.

9.1.2 The Dispersion term

Hydrodynamic dispersion is the sum of mechanical dispersion and molecular diffusion. It has the effect of spreading contaminants over a greater region than would be expected from advection only. The mechanical dispersion is a complicated process dependent on scale factor (Luckner and Schestakov, 1991) ranging from molecular to regional scales. Molecular diffusion is usually negligible compared to mechanical dispersion and generally ignored in contaminant transport modelling.

9.1.3 Sinks and Sources

The sinks and sources term represent solute mass dissolved in water entering or leaving the simulated domain.

9.1.4 Other terms

Neither the chemical reactions nor the decay terms were considered in this study.

9.2 MODEL AVAILABILITY AND SUITABILITY FOR RICHARDS BAY

The models chosen for investigation in this project were the CALIF model developed by Häfner *et al* (1996) and the MT3D model developed by Zheng (1992). Many other models are available but have not been examined in this study.

9.2.1 MT3D (ZHENG, 1992)

The numerical solution implemented in MT3D is a mixed Eulerian-Lagrangian solution. In MT3D the user chooses one of 3 options to solve the advective term, namely

- the forward-tracking method of characteristics (MOC)
- the backward-tracking modified method of characteristics (MMOC)
- a hybrid of the above two methods (HMOC)

The MT3D transport model follows the same spatial discretization convention used by Modflow that is described in section 6. MT3D incorporates the simulated velocity profiles directly from Modflow in order to solve the dispersion equations. Based on a similar concept to Modflow, MT3D is modular in its development. The main program is supported by a large number of independent modules which are grouped into packages (Table 37). Each of these packages deals with a single aspect of the transport simulation.

The total simulation time is divided into "stress periods" during which time all the parameters are assumed to be constant. These stress periods are subdivided further into "transport periods" or "time steps" during which time the hydraulic heads and fluxes derived directly from Modflow are assumed to be constant. The specification of the time steps have a very profound impact on the initial convergence and stability of the numerical solvers and they need careful selection in all applications.

Table 37 Main packages included in MT3D transport model

PACKAGE	DESCRIPTION
Basic	Specify boundaries and initial conditions, step size, and prepare mass balance information. Presents the output
Flow interface	Interface to Modflow using for and flow terms
Advection	Solves the concentration changes due to advection with one of the three Eulerian-Lagrangian schemes (MOC, MMOC, HMOC)
Dispersion	Solves the concentration changes due to dispersion with the explicit finite difference method
Sink & source mixing	Solves the concentration changes due to fluid sink/source mixing with the explicit finite difference method. Sink/source terms include wells, drains, rivers, recharge and evapotranspiration. The constant head boundary and general head-dependent boundary are also handled as sink/source terms in the transport model
Chemical reactions	Solves for concentration change due to chemical reactions. Currently, the chemical reactions include linear or nonlinear sorption and first order irreversible rate reactions (radioactive decay or biodegradation).
Utility	General tasks such as I/O functions

9.2.2 CALIF (HäFNER *et al*, 1996)

Häfner *et al* (1996) presented a new approach to solving the advection-dispersion equation by using a Front Limitation algorithm. All standard finite-difference algorithms are faster than the MOC but suffer from numerical dispersion. MMOC does not have the same numerical constraints, but suffer from excessive simulation times. However, Häfner *et al* (1996) have developed a finite difference algorithm in the CALIF programme for solute transport modelling which is not limited by the same constraints. Their model has been applied in the first case study of contaminant plume migration in a coastal dune system.

Section 10 CALIBRATION

The solute transport models discussed in the previous section all require estimates and calibration of their respective parameters. The choice of model and the selection of parameter values depends on the problem under investigation. This project has applied both MT3D and CALIF under different conditions to gain experience in their application with limited data sets. This project has concentrated on common solutes which are likely to be found in sufficient concentrations to be detectable in the groundwater of the Richards Bay region.

One of the most serious atmospheric pollutants is sulphates which has prompted the development of the Clean Air Association of Richards Bay. Since there is a lot of sulphate in most waste products and in many fuels, it has been chosen as the initial solute for investigation in this project. The literature has many examples of sulphate studies (Luckner and Schestakow, 1991; Häfner *et al*, 1992), particularly those associated with coal handling facilities which abound in the Richards Bay region.

10.1 PARAMETER ESTIMATES

The parameters requiring estimation in sulphate modelling are :

10.1.1 HYDRODYNAMIC DISPERSION (D)

Hydrodynamic dispersion is a function of molecular Diffusion (D')and mechanical dispersion (D"). The ratio of these two is the Peclet number and it should be less than 2 if numerical dispersion can be neglected. The Peclet number can be written as:

$$P_e = \frac{|v| L}{D}$$

where:

$|v|$ is the magnitude of the seepage velocity vector $[LT^{-1}]$
L is a characteristic length, usually taken as the grid cell width [L]
D is the dispersion coefficient (=D' + D") $[L^2T^{-1}]$

Because the Peclet number is dependent on the cell length (L), it is important that transport time steps should be small enough to avoid solute particles moving more than the length of a cell in one time-step.

10.1.2 MOLECULAR DIFFUSION (D')

D' is a function of the solute involved, but is generally very small (negligible) compared to mechanical dispersion and only becomes important at very low water velocities. In this study it is assumed that this parameter is negligible and only the mechanical dispersion is considered in the modelling.

10.1.3 MECHANICAL DISPERSION (D")

According to Zheng (1992), D" describes the deviation from the actual particle velocity on a microscale (in three directions), and is a function of the porous media. It is complicated by the scale of observation. Luckner and Schestakow (1991) distinguish four levels of observation namely the molecular, microscopic, local and regional levels. At the <u>local</u> scale of investigation the causes of dispersion, as adapted from Luckner & Schestakov (1991) and Fetter (1994), are

- Differences in flow velocity between fluid at the edge of the pore and fluid in the centre of the pore.
- Variation in the cross-sectional area of different flow channels.
- Different path lengths.
- Transverse propagation.

To account for all these causes, mechanical dispersion is calculated statistically. When this value is very small, the Peclet number becomes large and numerical dispersivity may become a problem. Values of mechanical dispersivity used in this study were taken from Häfner (1996):

10^{1} m for longitudinal dispersivity (D^*_L),
10^{2} m for horizontal transversal dispersivity (D^*_{TH}), and
10^{-1} m for vertical transversal dispersivity (D^*_{TV}).

10.1.4 SINKS & SOURCES

The source/sink parameter which needs specification is the concentration of the sources which enter the groundwater (C_s in equation 9-1) or the concentration of the receiving water for sinks. These parameters are derived from specific site investigations.

10.1.5 RADIOACTIVE DECAY / BIODEGRADATION

Since the decay rate for sulphate was assumed to be negligible, this term was not included in the simulations.

10.1.6 RETARDATION

Retardation is either due to adsorbtion to the soil particles or it is due to reactions during its transportation. Retardation causes the solute front to advance slower (retarded) than the water velocity. The retardation factor can be described in different ways to model equilibrium-controlled linear or non-linear sorption and first order irreversible rate reactions. The linear sorption isotherm is assumed to be directly proportional to the sulphate concentration (C) according to $R = 1 + \rho_b/_\theta K_d$

where the distribution coefficient is $K_d = \partial \bar{C}/\partial C$,

ρ_b is the soil bulk density and
θ is the soil porosity.

In the case of sulphates the linear first sorption constant (R) was assumed to be 0.003 m^3/kg (Häfner, 1996) while the bulk density was assumed to be 1500 kg/m^3 at a porosity 0.4.

10.2 CALIBRATION

The calibration procedures that were described in section 7 are also applicable to the calibration of the transport model parameters. The trial and error method is generally the preferred approach. Anderson (1979) has indicates that the attempts to solve the inverse problem (numerical calibration) for dispersivities in the mass transport model are limited and still very much in the development stages. However, an attempt has been made to calibrate a model using the inverse procedures and this is presented as the first case study in Section 11.1 for a monitored site just to the north of Richards Bay.

Section 11 CASE STUDIES

Groundwater simulation models have been developed for general application to simulate groundwater flow and they have been applied in many situations. Because the local groundwater system in the Richards Bay area is overlain by urban, commercial and industrial developments and is close to the sea, it is prone to surface and saline pollution which could ultimately impinge on the local surface water resources that are considered to be an extension of the local groundwater system. In an effort to determine the flow and pollution potential of the local aquifers, groundwater flow and transport models are being applied in the region. The application of these models requires an understanding of the models and the systems in which they are being applied. This section presents a case study that has investigated situations were there is some information for evaluation and a second case study which is used to evaluate the methods for monitoring purposes and for management and planning of the water resources of a region.

1 The first case study (WASTE SITE INVESTIGATION) investigates the use of the CALIF numerical models in numerical calibration studies of a small waste site in the dunes to the north of Richards Bay which is leaching some sulphate into the groundwater. This is an example that illustrate the information requirements for numerical calibration techniques and the limit to which it can be applied.

2 The second case study (HYPOTHETICAL TRANSPORT OF HYDROCARBONS - LAKE MZINGAZI AREA) presents the use of Modpath and Modflow in a "what-if" situation arising from a hypothetical fuel spillage in Richards Bay.

11.1 CASE 1 : WASTE SITE INVESTIGATION

In this section, the application of the numerical calibration technique in sulphate transport simulation studies is described for a study site (dam) just to the north of Richards Bay where there was good groundwater quality information. The calibration of the retardation parameter was done using the trial and error methods and then compared to the numerical methods described in section 8.5.

In the coastal dunes just to the north of Richards Bay, a clarifier dam was monitored since initiation over ten years ago for groundwater contamination. This information provided an ideal opportunity to apply the solute transport models described in previous sections. The solutes are transported in a solution which behaves as a normal fluid that can be modelled in the manner described in part 2 of this report. Consequently, the solute transport models are linked to dynamic flow models such as Modflow. The flow and transport model CALIF (Häfner *et al*, 1996) was used in this case study.

The models have been described in section 9. The parameter requirements and their estimates have also been described in section 10. The flow model parameters were calibrated in accordance with the concepts presented in Section 7.2. The borehole network of data observations used in the calibrations is shown in Figure 111. The flow model calibration is based on comparisons with 32 measured water levels to optimize the permeability parameters.

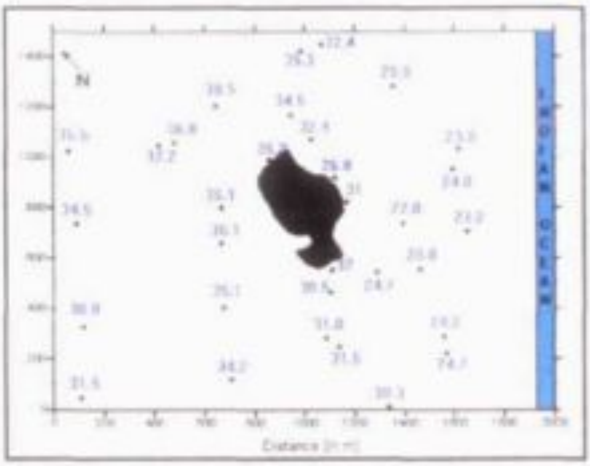


Figure 111 Averaged observations of water level elevations (m AMSL) used for calibration.

For this study the movement of a single species of SO_4^{2-} ions was modelled using the CALIF model developed by Häfner *et al* (1996). The transport modelling method requires many more complex parameters than the flow modelling and is generally based on inadequate data for the region. The parameter values used in this case study are described below.

11.1.1 INITIAL PARAMETER ESTIMATES

Molecular diffusion: According to Fetter (1994) the diffusion coefficient for SO_4^{2-} is generally between $1x10^{-9}$ and $2x10^{-9}$ m^2/s while Domenico and Schwartz (1990) suggested $1.07x10^{-9}$ m^2/s for SO_4^{2-} in water at 25°C. A value of $1.07x10^{-9}$ m^2/s was assumed as an initial value for use in these model simulations.

Retardation: Fetter (1994) mentioned that SO_4^{2-} ions are generally too big to be effectively adsorbed. This agrees with Carageeg *et al* (1987) who suggest that "dissolved sulphate probably moves though the unsaturated zone as a non-reactive solute (particularly in sand)". However, the retardation has been set to a value of 10 as a first estimate.

11.1.2 TRAIL AND ERROR CALIBRATION

Solute transport modelling requires a much greater level of understanding of the system than flow modelling. Ideally the conceptual model should be revised to create a more detailed description of the stratigraphy, particularly clay lenses which have a big influence on the movement of solutes. A lack of data and uncertainty in specifying the parameter values, made it inappropriate to change the initial conceptual model for this study.

The test site has been operational for about ten years and consequently, the solute transport model was run for a simulation period of ten years using an estimated groundwater leakage of 300 m^3/day (Hattingh, 1997) from the site. Both the two and five layer models were applied to simulating solute transport under average rainfall / recharge conditions during the ten year simulation period using the trial and error calibration and numerical methods.

11.1.2.1 TWO LAYER MODEL

The initial parameter values for molecular diffusion and retardation were adjusted by trial and error for the two layer model. Observed concentration of SO_4^{2-} at five observation points were used to calibrate the steady state model.

Simulated concentrations were comparable to observed values (Table 38) at most boreholes. However, there is a large difference between the simulated and observed concentrations for borehole CTM15. This could be due to a difference in the simulation and observation depths (Figure 112).

Table 38 Comparison between observed and simulated concentrations of SO_4 for a two layer model.

BORE HOLE	Observed (ppm)	10 year simulation
CTM3	~3	7
CTM5	~300	242
CTM8	~30	0
CTM10	~5	29
CTM15	~5	215

The observation depth for this borehole (CTM15) is at the bottom of the second layer, while the calculated value is an average concentration for a point in the middle of the second layer (see point of calculation in Figure 112).

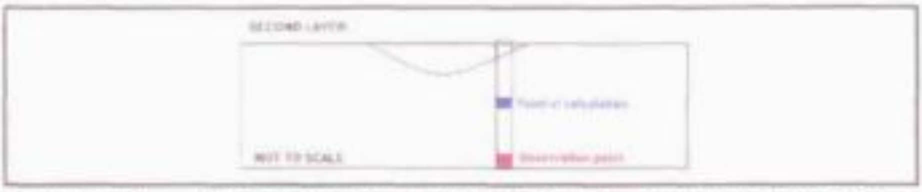


Figure 112 Vertical profile of solutes for the second layer in relation to observation borehole CTM15.

The spatial distribution of simulated concentrations for the top layer is shown in Figure 113. Similar distributions for the lower (second) layer are shown in Figure 114. These simulated distributions represent the SO_4^{2-} distribution at the present time, ten years after the commissioning of the site.

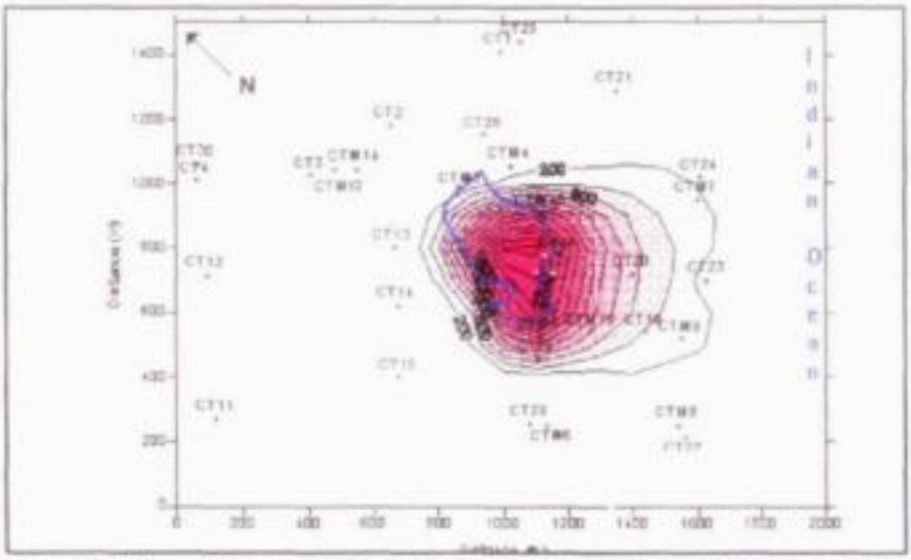


Figure 113 Solute concentration in the top layer after ten years. The shaded area have concentrations of >400 ppm.

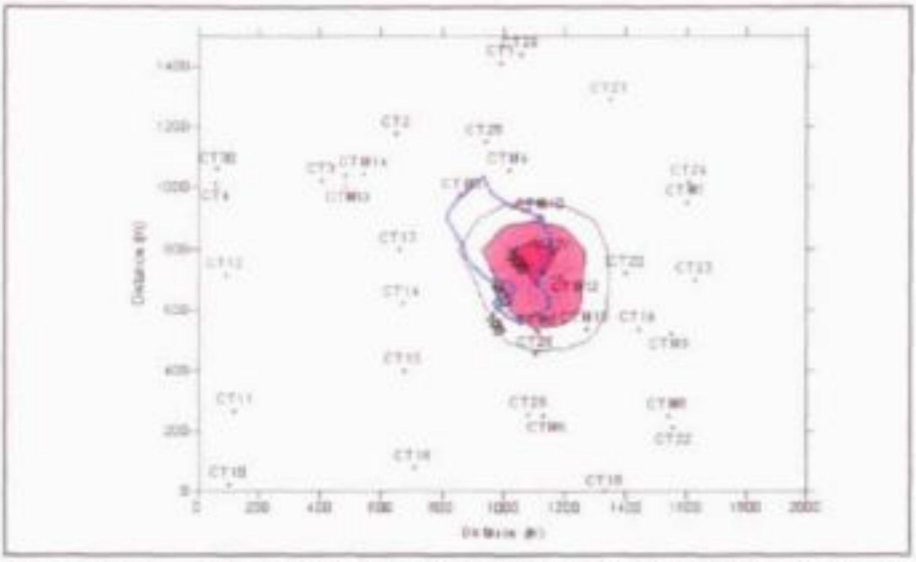


Figure 114 Solute concentration in the bottom layer after ten years. Blue indicating the location of the test site. Shaded areas have concentrations of >200 ppm.

11.1.2.2 FIVE LAYER MODEL

To refine the vertical partitioning in the model, the second layer was divided into 4 layers of equal thickness and assigned with the hydraulic permeabilities given in Table 39 . The results of the simulation studies were again comparable to the observed concentrations also shown in Table 39. The simulation of the second layer after a simulation period of ten years, agreed more closely with the observed than the two layer model, with the exception of CTM5 where the simulation were not as good as the two layer model. In view of the subjective stratigraphy and uncertainty in hydraulic parameters, these comparisons are considered adequate for this case study.

Table 39 Comparison between observed and simulated concentrations of SO_4 (in ppm) from a five layered modelling effort.

BOREHOLE	Observed SO_4	10 year simulation	20 year simulation
CTM3	~3	0.5	3.5
CTM5	~300	855.0	450.0
CTM8	~30	0	0
CTM10	~5	9.0	56.7
CTM15	~5	6.2	81.2

11.1.3 AUTOMATIC CALIBRATION

Several calibration approaches were used to optimize the transport parameter for retardation. The different scenarios have been labelled A, B, C and D. Case A always refers to initial estimates for the retardation factor. Simulated concentrations after ten years were compared with the concentrations after ten years of observations in this calibration exercise.

11.1.3.1 TWO LAYER MODEL WITH NO CALIBRATION LIMITS

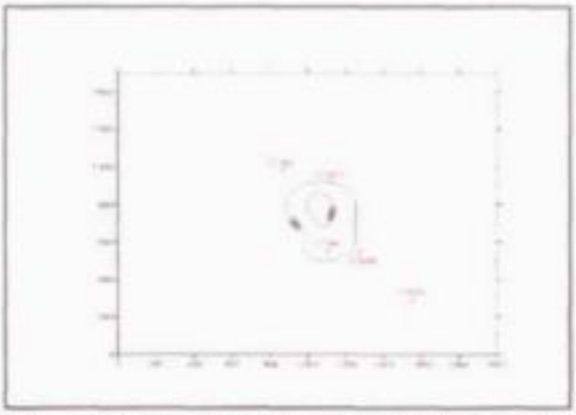
All the calibrations discussed in this section were done by optimising the retardation factor for each zone which occupied a complete layer.

The initial retardation factors used for case A, were 1 and 10 for the first and second layers respectively. Using these values, the simulated concentrations after ten years are listed in Table 40, column A and are shown as concentration contours for the second layer is shown in Figure 115 (A) together with the locations of observation boreholes.

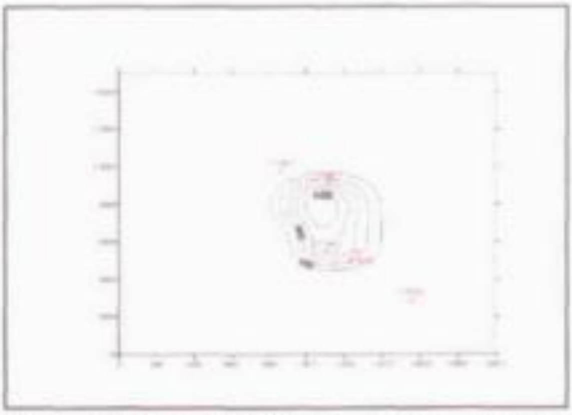
Table 40 Simulated versus observed concentrations (ppm) for different zonation and iteration procedures using the two layer model.

	OBSERVED	SIMULATED			
CASE		A	B	C	D
ITERATION		Initial estimates	Gauss-	Newton	Powell
CTM3	~3	7.0	31.9	8.5	1.5
CTM5	~300	242.0	846.0	232.0	68.0
CTM8	~30	0.0	0.0	0.0	0.0
CTM10	~5	29.0	246.0	41.0	4.6
CTM15	~5	215.0	589.0	114.0	10.7

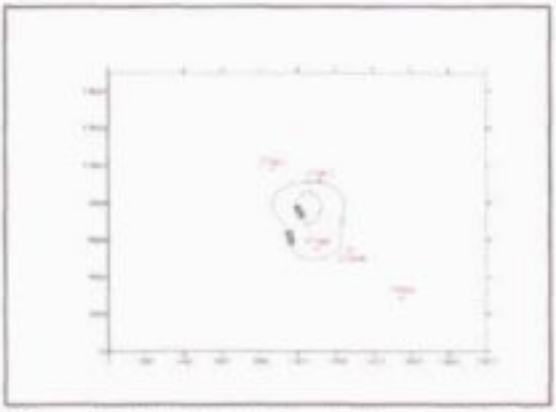
For case B, this calibration effort produced retardation factors of 1.2 and 5.9 for the first and second layers respectively. These retardation factors gave much higher concentrations than observed values (see Table 40, column B). A contoured map of solute concentrations after ten years for the second layer is shown in Figure 115 (B).



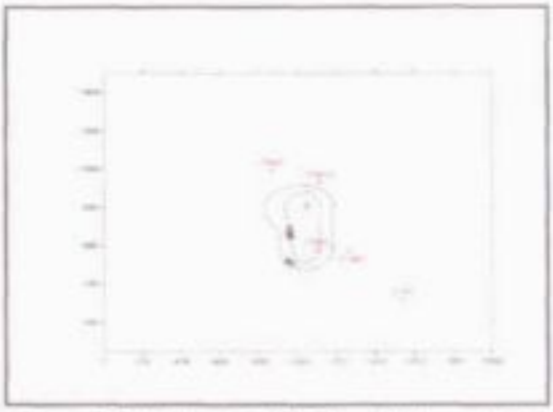
(A) Initial retardation factors and permeabilities used.



(B) Gauss-Newton with initial permeabilities.



(C) Gauss-Newton with calibrated permeability values.



(D) Powell method with initial permeabilities.

Figure 115 Simulated concentrations after ten years in the bottom layer from different calibration procedures using a two layer model.

Case C was similar to case B, but different flow parameters (permeabilities) were used. For case B the initial permeability values were used (Table 40 (B)), but for case C the permeability results of calibration 8.1 (D) were used (Table 40 (D)). The retardation factors identified for this calibration were 1.0 for layer 1 and 1.3 for layer 2. The optimized value for layer 2 is an order of magnitude lower than the initial estimates assumed for the second layer. However, this means that there is very little retardation, which is in agreement with Fetter (1994) and

Table 41 Retardation factors from calibrating with different techniques

<table>
<tr><td>CASE</td><td>A</td><td colspan="2">B</td><td>C</td></tr>
<tr><td>PERMEABILITIES</td><td>Initial</td><td colspan="2">Results from 8.2 (D)</td><td>Initial</td></tr>
<tr><td>SCENARIO</td><td>1. Layer zones</td><td colspan="2">2.Subdivision into more zones</td><td>1. Layer zones</td></tr>
<tr><td>ITERATION</td><td>-</td><td colspan="2">Gauss-Newton</td><td>Powell</td></tr>
<tr><td>Layer 1</td><td>1.0</td><td colspan="2">1.0 (fixed)</td><td>1.0 (fixed)</td></tr>
<tr><td>Layer 2</td><td>10.0</td><td rowspan="4">30.0 for columns 1-3 over layers 2-5</td><td rowspan="2">18.0 for columns 4-20 layers 2 &3</td><td rowspan="2">6.0</td></tr>
<tr><td>Layer 3</td><td>10.0</td></tr>
<tr><td>Layer 4</td><td>10.0</td><td>22.0 for columns 4-20</td><td>19.0</td></tr>
<tr><td>Layer 5</td><td>10.0</td><td>30.0 for columns 4-20</td><td>9.3</td></tr>
</table>

Carageeg *et al* (1987) who suggested that sulphate is non-reactive. Concentration distributions shown in Table 40, column C compare favourable with observations while the spatial distribution in Figure 115 (C) were similar to the initial estimates shown in Figure 115 (A). These results confirm that a good output from calibration needs good input for all parameters.

In case D the initial permeabilities (Table 40 (D)) were used again in conjunction with the Powell iteration method. The optimized retardation factor for layer 1 was much higher than expected, namely 41.6. The retardation factor for layer 2 was 7.4. Table 40, column D and Figure 110 (D) show much lower concentrations in the bottom layer as a result of the high retardation factors.

11.1.3.2 FIVE LAYER MODEL WITH NO CALIBRATION LIMITS

In a similar fashion to the calibrations done for permeability, several methods using the Gauss-Newton and Powell iterations were done for retardation with the five layer model. Some layers had no observations, so these were usually combined with others in creating the zones for calibration.

For the five layer model it is important to identify in which layer observations were made. Observations were available for the second layer at CTM5, the fourth layer at CTM3, CTM8 and CTM10 and for the fifth layer at CTM15. Calibrated values of retardation factor for the five layer model are shown in Table 41. The simulated concentrations using these retardation factors are shown in Table 42 and interpolated contour maps for some of the layers are shown in Figure 116.

Case A represents initial estimates for the retardation factors and permeabilities. Simulated concentrations of SO_4^{2-} compare reasonably with observed values except for CTM5 where the simulated concentration is very high and CTM8 where the simulated concentration is too low (see Table 42, case A).

In case B the permeability results of section 8.5.8.2 (D) were used. Layer 1 was fixed in the calibration because the water table did not extend into this layer in some areas. Simulated concentrations compared well to observed concentrations (Table 42, column B and Figures 116 (B) and (B')) with the exception of CTM8 which indicates no sulphates.

For case C, initial estimates of permeability was used in conjunction with the Powell iteration method. Here the retardation was assumed constant throughout each layer with the value for retardation given in Table 42, column A. The resulting concentrations were very low (Table 42, column C). Only the first two layers are shown in Figures 116 (C) and (C') because the concentrations in the other layers were too low.

Table 42 Observed and simulated concentrations in ppm for the five layer model, using different calibrated values of the retardation factor.

CASE	Observed concentration	A	B	C
CTM3	~3	0.5	0.2	0.002
CTM5	~300	855	202	0.4
CTM8	~30	0.0	0.0	0.0
CTM10	~5	9.0	3.0	0.04
CTM15	~5	6.2	5.0	0.02

11.1.4 SUMMARY

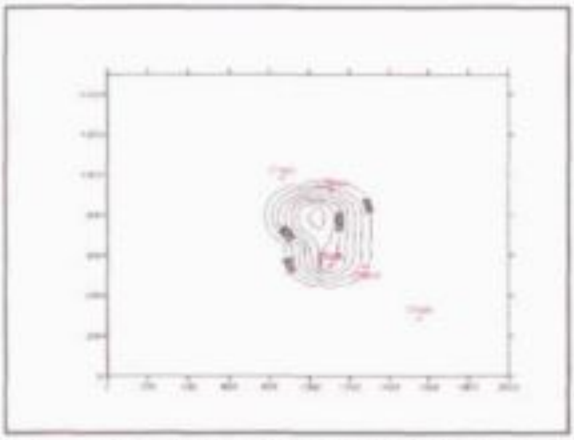
A conceptual geological model was created from available data at a site near Richards Bay. This conceptual model was incorporated into two and five layer numerical models. These two numerical models were used in calibration studies of permeability and retardation factors. Model simulation times are fast but the calibration procedure was very demanding of computer facilities and requires careful planning.

For initial calibration studies of the permeability factor, first estimates of values for each layer were derived from literature and then adjusted subjectively to achieve the best comparison with the observed water table elevation for 32 boreholes. Subsequent calibration used numerical methods incorporated in the CALIF program of Häfner *et al* (1996).

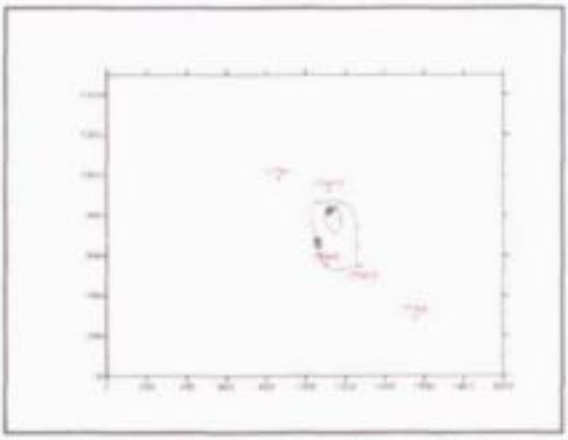
The numerical calibration results indicate that the process is sensitive to zonation procedures. Calibration worked well for the simple two layer model. However for the five layer model it is still not clear whether the lack of information, the zonation procedure or both, are the cause of inconclusive results. It became apparent that all flow simulations should have been conducted before any transport simulations were attempted.

The test site was chosen because of the availability of information. This information is generally not as complete in most other instances of model application in this region. However, for more accurate results, the information could still be improved. This is particularly true for calibration procedures where greater and more appropriate zonation could be employed.

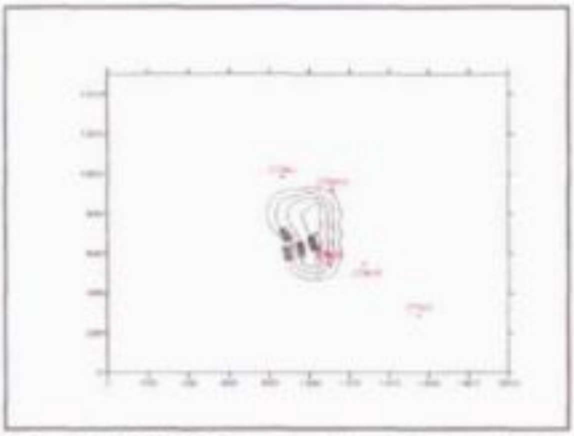
In the numerical program, CALIF, post simulation analysis could be enhanced by the presentation of more than the 5 simulated observation points which is currently the limit.



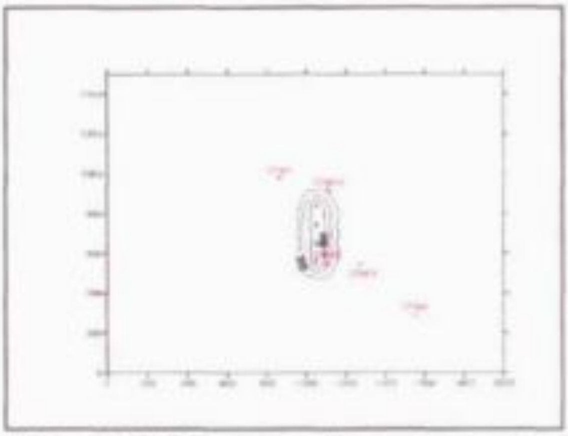
(A) LAYER 2 using initial estimates of retardation factors.



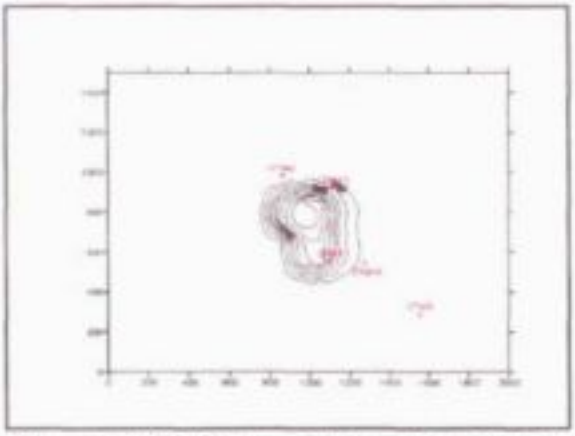
(A') LAYER 4 using initial estimates of retardation factors.



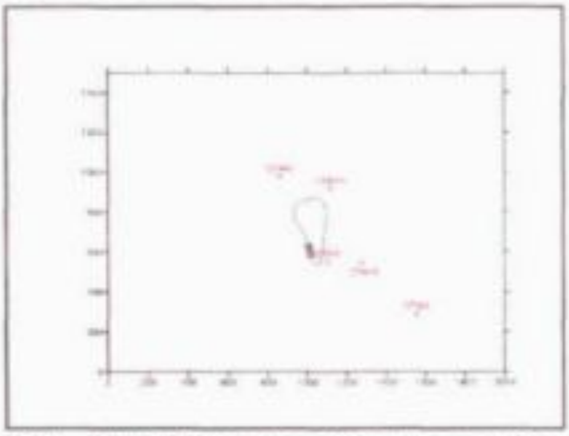
(B) LAYER 2 using calibrated retardation factors for different zones.



(B') LAYER 4 using calibrated retardation factors for different zones.



(C) LAYER 1 using calibrated retardation factors and the Powell method.



(C') LAYER 2 using calibrated retardation factors and the Powell method.

Figure 116 Simulated concentrations (ppm) from different calibrations of a five layer model.

11.2 CASE 2 HYPOTHETICAL TRANSPORT OF HYDROCARBONS - LAKE MZINGAZI AREA

This case has been extracted from a hypothetical study by Krikken and van Nieuwkerk (1997). The values are not derived from measurements, but have been extracted from published ranges in other studies. Consequently, the results are **highly speculative** and are only presented to demonstrate the potential use of the technology and to suggest monitoring sites.

Lake Mzingazi is used mainly for drinking water supply and consequently it is essential that severe pollution of the lake should be prevented. An example will be given of the use of the groundwater model for estimating the spreading of **possible** pollutants through the subsurface (solute transport) in order to identify the areas effected by pollution sources. In order to investigate the **risk** of pollution of Lake Mzingazi and its surroundings, this study uses two methods of investigating the transport characteristics of solutes through the surrounding aquifer with the use of a groundwater model. This case study presents the application of groundwater models as a tool to assist in water resources management and the design of groundwater monitoring networks for resource protection.

Several factors might form a threat to the water quality of the lake. For this investigation a distinction is made between point source pollution and non-point source pollution. One **potential** source of pollution to the groundwater in the vicinity of Lake Mzingazi is the Richards Bay airport. Possible leakage from fuel tanks could infiltrate into the groundwater and eventually enter the lake. The use of numerical models to predict the pathways of pollutants and to identify suitable monitoring points is examined for this case study.

11.2.1 SOLUTE TRANSPORT MODELLING USING PARTICLE TRACKING

The particle tracking program Modpath (Polluck, 1989), which uses the results of Modflow to simulate flow lines, can give an estimate of the travel time and direction of solutes travelling through an aquifer. This method assumes that solutes will be transported at the same velocity and in the same direction as flowing water (i.e. only advection is considered). The effects of dispersion and retardation, which influence the spreading of solutes, are not incorporated.

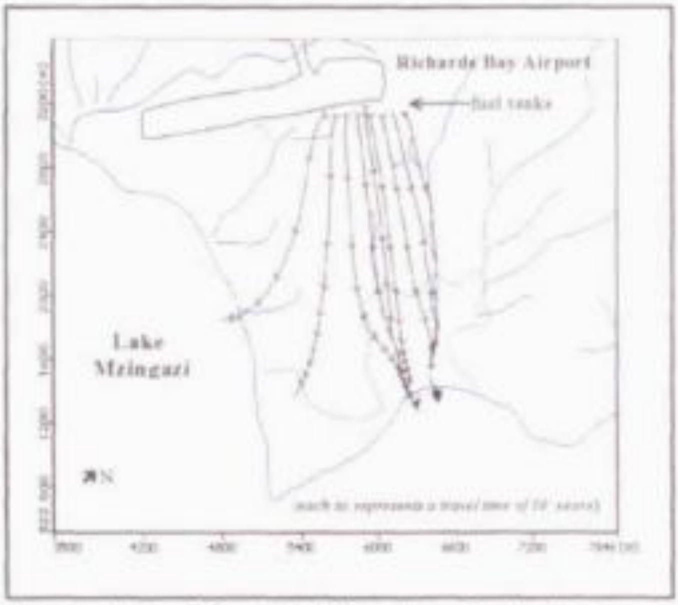


Figure 117 Simulated flow lines for the Lake Mzingazi area.

This investigation uses the particle tracking method to examine a hypothetical scenario of leakage from the fuel tanks at Richards Bay Airport directly into the groundwater. Three tanks are situated near the airport below the surface in the second layer (Arenaceous unit) of the model. Each of these tanks contain 14000 dm^3 of aviation fuel. Figure 117 displays the simulated flow lines.

The simulated travel time from the fuel tanks to the lake is estimated to take between 50 to 100 years when only the advection is considered. The wetlands on the north-western shore of the lake are reached after 30 to 35 years by flowing water from the tanks and from both sides of them. Figure 118 shows the simulated flow paths, with each tic representing a 10 year travel time.

Modpath can also be used to determine the origin of groundwater at a certain location. The flow lines represent groundwater flow. Possible pollution at a certain location can be traced back to a source using the simulated flow lines. Figure 118 shows the flow lines for the groundwater in the second layer (Arenaceous unit) and emerging along the shoreline. The western part of the wetlands surrounding the lake receives groundwater and surface water (streams) inflow from the urban areas of Richards Bay. The rivers and particle tracking in Figure 118 provide a means for determining the origin of water flowing into sections of the lake. Much of the industrial area of Richards Bay will impact on the surface and groundwater flowing into the western part of the main lake compartment. The area between the lake and the main river network in Richards Bay contribute to the immediate shoreline. In particular the zone around the airport is

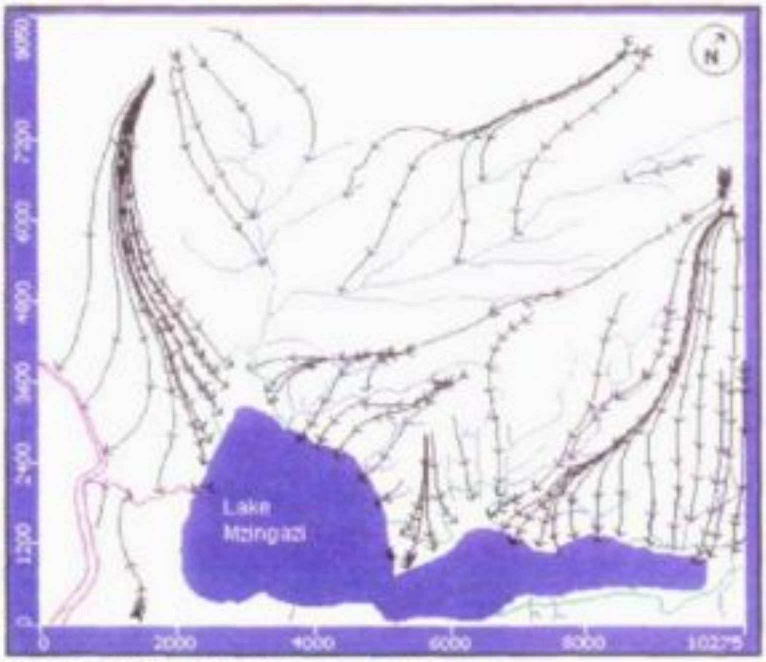


Figure 118 Flow lines in layer 2

expected to flow toward the headland between the two compartments of the lake. The zone to the North of Richards Bay which comprises mainly forestry will impact on the western shoreline of the northern compartment. Very little flow in the lake is estimated to originate from the eastern shores area.

11.2.2 SOLUTE TRANSPORT MODELLING USING THE MT3D MODEL

A second method of simulating the transport of solutes through the aquifer using the MT3D (Zheng, 1992) solute transport model is discussed. The MT3D model includes additional reaction dynamics for simulating the advection, dispersion as well as chemical reactions of contaminants in three dimensional space. The model uses the finite difference scheme of Modflow for the simulations.

This hypothetical case of aviation fuel transport dynamics is simulated using MT3D. Aviation fuel is a mixture of different hydrocarbons. For this study only the compound of 1,1,1-trichloroethane is considered. It is assumed that the recharge rate of soluble 1,1,1-trichloroethane is 965 mg/l (Domenico and Schwartz, 1990) in a geological setting similar to the model describe in section 8.1.

The longitudinal dispersivity (a_L) and the transversal dispersivity (a_T) values are unknown for Richards Bay, therefore published setimates were used (Table 43) as initial estimates for the three main aquifers. A value for the diffusion coefficient (D_i) would also be incorporated, but is only considered to be important when flow velocities are very low. Table 43 shows the dispersion parameter values used for this simulation.

1,1,1-trichloroethane is a hydrophobic organic pollutant. These substances have a low affinity for solution in water, but are easily sorbed by organic matter in aquifer sediments (Appelo and Postma, 1994). The compound is generally strongly influenced by retardation (K_d). The retardation (distribution coefficient) requires estimates of the bulk density (r_b) of the sediment (Appelo and Postma, 1994). Table 44 gives the estimated input parameter values for the retardation. A recharge rate of 965 mg/l was maintained at the site, where the fuel tanks are assumed to be situated, over an area of about 200 m^2.

Table 43 MT3D layer dependent input parameter values (dispersion)

Layer	a_L [m]	a_T [m]	e^*D_r [m^2/d]
Holocene	250	25	3.28*10^[illegible]
Arenaceous	250	25	3.63*10^[illegible]
Argillaceous	250	25	3.89*10^[illegible]
Miocene	250	25	3.50*10^[illegible]

Table 44 MT3D input parameter values (retardation)

Layer	% or. mat. in sediment	Bulk density, r_b [kg/m^3]	resulting K_d [m^3/kg]
Holocene	0.2	2023	$3.10*10^{-4}$
Arenaceous	0.2	1693	$3.10*10^{-4}$
Argillaceous	50	2500	0.0775
Miocene	0.1	2000	$1.55*10^{-4}$

This model was run to an assumed steady state. The simulated spread of the concentration plume after 100 years is shown in Figure 119.

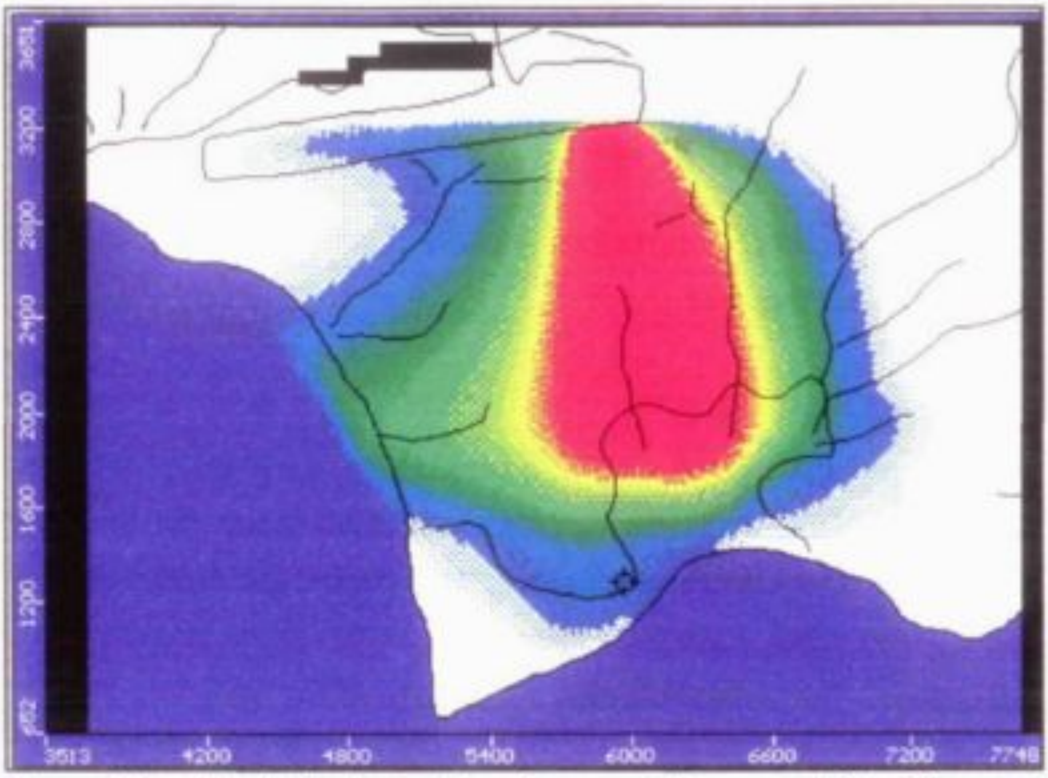


Figure 119 Hypothetical simulation of concentration spread after 100 years from Richards Bay airport towards Lake Mzingazi using MT3D solute transport model.

11.2.3 CONCLUSIONS AND RESULTS

This example of the possible use of a solute transport model is not based on actual measurements so it presents a hypothetical case that can only be used to demonstrate the method and indicate its use.

The model technique can be used to highlight deficiencies in observations and suggest monitoring sites. Despite the deficiencies in knowledge and measurement for calibration, the model does suggest that monitoring should be considered at the centre line of the simulated plume in Figure 119.

Section 12 DISCUSSION and RECOMMENDATIONS

This study has produced several products that have contributed to the geohyrological knowledge of the Richards Bay area.

1) Geological surfaces

Through a detailed analysis of the available borehole data that have been acquired, captured and analysed, a map of the upper surface of the Cretaceous siltstone deposits has been constructed. This map was discussed with geologists who have worked in the region (Rheeder, 1996, Maud, 1996, Hattingh, 1996, Meyer 1996). All of them agreed that this surface was acceptable. This surface defines the principle lower boundary of the primary aquifer in the region.

Overlying the Cretaceous sediments are discontinuous layers of the Miocene deposits (Davies Lynn and Partners, 1992, Simmonds, 1990, Maud and Orr, 1975, Worthington, 1978 and Hatting, Meyer and Barnes, 1995). The lower surface is described by the Cretaceous sediments and the upper surface has been estimated from the limited available data.

An attempt has been made to map the upper surfaces of other sedimentary layers. However, there is very low confidence in the accuracy of these surfaces because the borehole information was insufficient to allow a reasonable delineation.

2) Conceptual Models

Apart from the conceptual model of the geological features, conceptual models for recharge and evapotranspiration were refined and applied in the numerical model. Many groundwater modelers use a net recharge for groundwater studies (Bredenkamp *et al*, 1995). However, in this study a gross recharge is used together with evapotranspiration. Model results showed that the net recharge varies between 15% and 31% of rainfall depending on the land-use type. This is in the same range as the net recharge described by (Bredenkamp *et al*, 1995).

3) Numerical Model

The defined stratigraphy has been used to configure a numerical model of the area for regional groundwater studies. Calibration studies have been done and the resulting model was used too derive the regional flow patterns which indicate that most of the groundwater that originate in the industrial area of Richards Bay flows towards the harbour with a small portion flowing towards Lake Nsezi.

This model as well as the derived geological surfaces have subsequently been used for other studies of the coastal Lakes (Kelbe and Germishuyse, 1998, Germishuyse and Kelbe, 1999). The knowledge gained from this model has also been applied in the hydrological investigation of specific sites in the Richards Bay area (Kelbe and Germishuyse, 1999b).

12.1 RECOMMENDATIONS

The models examined in this project are mathematically and theoretically sound but their applications suffer from a lack of sufficient information. The lack of information in the region is a serious constraint to the use of the numerical models for other purposes such as solute transport modelling. In many cases this can be overcome through calibrations, but once again, only if there is sufficient field data. Clearly, the biggest limiting factor in numerical modelling is the availability of data and information about the system. However, one of the greatest assets of numerical modelling is that it identifies gaps in the information and the need for additional monitoring. This study has led to the establishment of a long term monitoring point in the centre of the industrial area of Richards Bay.

Groundwater flow models are critically dependent on hydrogeological data. The present extensive data base of borehole logs was conducted for geological or engineering surveys and very seldom contains specific information on the geohydrology or hydraulic properties of the aquifers. This information is even more important when solute transport modelling is considered because of the interaction between soils and particle movement. Consequently, it is strongly recommended that geological and soil surveys attempt to determine more hydraulic features of the profiles when logging the boreholes.

The rapid improvement in mass transport simulation tools needs to be matched by increased awareness in data requirements. There is a need to determine a common and reliable tracer in the regional groundwater system and establish a regular network of monitoring observation points in conjunction with other needs. In coastal regions such as Richards Bay, the potential for groundwater pollution and its potential impact on regional and local water resources needs to be carefully managed and this involves the establishment of a suitable monitoring programme.

There is a potential for contamination of the groundwater recharge areas for both Lakes Mzingazi and Nsezi and this may have serious long term detrimental impact on the water quality of the lakes. It is recommended that the local water authorities implement a programme for regional groundwater monitoring in the coastal primary aquifer.

Stream flow measurements at the inflow of lakes will provide better information on the lake water budget. This is crucial for management of water supply.

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