PREFERENTIAL FLOW MODELLING IN A VADOSE ZONE USING MACRO 5.0 – CAPE FLATS POROUS SANDS AND MPUMALANGA HIGHVELD CLAYS CASE STUDIES

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KEYWORDS

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ABSTRACT

Preferential flow modelling in a vadose zone using MACRO 5.0 – Cape Flats porous sands and Mpumalanga Highveld clays case studies

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Understanding fluid flow and solute transport within the vadose (unsaturated) zone is an essential prerequisite for protection of groundwater from contaminant sources occurring overland. Preferential flow paths in the vadose zone pose a significant problem because they are potential avenues for rapid transport of chemicals from contamination sources to the water table. The objectives of this study were:

i) To review and understand flow and transport processes in unsaturated zones. In this study, particular emphasis is placed on understanding mechanisms that cause non-uniform (preferential) flow for two case studies, namely the Cape Flats sandy environment and the Mpumalanga Highveld fractured rock environment.

ii) To evaluate the adequacy of models, in particular MACRO 5.0, in simulating flow and transport in the vadose zone, by making use of two case study sites (Cape Flats and Mpumalanga Highveld). Of particular importance is the evaluation of transfer coefficients to represent fluid and solute exchange between macropores and matrix.

iii) To run a sensitivity analysis with MACRO 5.0 in order determine which input model parameters are the most relevant in describing the effects of preferential flow in water and solute transport.

Two case studies were investigated, the first at a landfill site overlying sandy unconfined aquifer (Coastal Park, Cape Town), and the second at an industrial site overlying cracking clayey soil and fractured rocks (Mpumalanga Highveld - Secunda, Mpumalanga Province). For the Coastal Park site, simulations of soil water content and leaching of a generic mobile contaminant were compared to monitored soil water contents and chloride concentrations in groundwater. For the Mpumalanga Highveld site, simulations of soil water content and concentrations of boron and fluoride originating from effluent irrigation were compared to soil profile measurements. In both cases, the MACRO 5.0 model predictions agreed with measurements well, provided appropriate input calibration data were used. The sensitivity analysis indicated that soil water properties related to preferential flow (hydraulic conductivity at the boundary between macropores and matrix, soil water content and tension, and diffusion) have influence on simulation results. Similarly, the solute balance is mostly influenced by degradation rate coefficients (both in solid and liquid phases), sorption distribution coefficients and solute concentrations.

DECLARATION

I declare that, *Preferential flow modelling in a vadose zone using MACRO 5.0 – Cape Flats porous sands and Mpumalanga Highveld clays case studies* is my own work, that it has not been submitted for any degree or examination in any other university and that all the sources I have used have been acknowledged by complete references.

Kwazikwakhe Majola

18 August 2008

Signed: …………………………..

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CHAPTER 1

INTRODUCTION

1.1 Background to the study

Fluid flow and solute transport within the vadose zone (the unsaturated zone between the land surface and the water table) is the cause of expanded plumes arising from localized contaminant sources. Therefore, an understanding of vadose zone processes is an essential prerequisite for cost-effective contaminant remediation efforts. Contamination of the vadose zone can result from many causes, including chemical spills, leaky underground storage tanks, leachates from waste disposal sites and mine tailings, and application of agricultural chemicals. Another major environmental concern is the potential for long-term migration of radionuclides from low-level and high-level nuclear waste disposal facilities (U. S. National Committee for Rock Mechanics, 2001). The main requirement for designing remediation and long-term strategies is the development of flow and transport models for the vadose zone. The presence of fractures and other channel-like openings in the vadose zone poses a significant problem, because they are potential avenues for rapid transport of chemicals from contamination sources to the water table (U. S. National Committee for Rock Mechanics, 2001).

According to the U.S. National Committee for Rock Mechanics (2001), structured soils and fractured rocks exhibit many similarities in flow and transport processes. Macropores and aggregates in structured soils are respectively analogous to fractures and matrix blocks in rock, and therefore communication between researchers in both soil science and fractured rock fields will be mutually beneficial. The interaction between fracture and matrix exerts a strong control on fluid and solute movement. Solute transport in the fractured vadose zone can exhibit complex behavior due to the large variations in fluid velocity and the interplay of advective and diffusive transport between fractures and matrix. Solute transport models are more complex than flow models, and can involve multiple regions to represent the diversity of macropore and micropore sizes.

1.2 Research Problem/ Hypothesis

The unsaturated zone is regarded as a line of defense to prevent contaminants from reaching the aquifer (saturated zone). However, if preferential flow mechanism/system within a vadose zone is not understood, it becomes difficult to understand the transport process of contaminants since they use water as transport mode. Preferential flow in the macropore is coupled with the flow in the soil matrix. Flow in the soil matrix is simulated by the Richards equation. Modelling would help in simulating preferential flow in the vadose zone and thus assist in an attempt to manage contaminants before they reach the aquifer. Various modelling softwares are used to model such conditions. In this study we investigate the capability of MACRO 5.0 to modelling preferential flow in unsaturated zones. Hence, we ask the following question: How is the preferential flow mechanism in the unsaturated zones (vadose zones) of the Cape Flats and Mpumalanga Highveld study areas. Moreover, how is MACRO 5.0 handling such simulations?

The hypothesis of this study was that a dedicated soil water balance model like MACRO 5.0 would be able to reasonably predict preferential flow and the contamination of groundwater from sources occurring at the surface at two sites that have fundamentally different environmental conditions such as climate, soil and geological properties.

1.3 Aims and Objectives

Normally it is either impossible or very costly to decontaminate an already contaminated aquifer. It is therefore crucial to come up with preventative measures that will guide against potential polluting factors in order to ensure the sustainability of usable groundwater resources. This could be achieved by assessing, continuously monitoring and properly managing these available resources. Thus, a complete understanding of hydraulic properties of a given groundwater resource is inevitable for effective protection of such resources as aquifers. As a central aim, this project is trying to understand the preferential flow mechanism of water (and therefore contaminants) in unsaturated zones of the Cape Flats and Mpumalanga Highveld using a relevant modelling method.

The main objectives are:

- To review and understand flow and transport processes in unsaturated zones. Particular emphasis is placed on understanding mechanisms that cause non-uniform (preferential) flow for two case studies, namely the Cape Flats sandy environment and the Mpumalanga Highveld fractured rock environment.
- To evaluate the adequacy of models, in particular MACRO 5.0, in simulating flow and transport in the vadose zone, by making use of two case study sites (Cape Flats and Mpumalanga Highveld). Of particular importance is the evaluation of transfer coefficients that will represent fluid and solute exchange between macropores and matrix.
- To run a sensitivity analysis with MACRO 5.0 in order to determine which input model parameters are the most relevant in describing the effects of preferential flow in water and solute transport.

CHAPTER 2

LITERATURE REVIEW (PREVIOUS WORK)

This chapter aims to review the previous work on preferential flow in the vadose zone, including the modelling methods available. In this case, only two possible modelling methods that have been used worldwide are briefly reviewed. They are MACRO 5.0 and SWAP. Thereafter, one of them will be selected for use based on the objectives of this project and its applicability regarding various conditions of the case study areas, that is, porous sands of the Cape Flats and the clays of Secunda.

2.1 Preferential Flow in a Vadose Zone

Preferential flow is generally described as the flow of fluids within fractures and joints or other existing channels, and in the case of a vadose zone, water and solutes by-pass large portions of soil matrix. This is a crucial phenomenon since there is a great prevalence of preferential flow channels in the shallow subsurface (Jarvis, 2002). Larsbo et al (2005) describe preferential flow as the generic term for non-uniform infiltration and recharge processes characterized by flow convergence and an increase in the effective velocity of water flow through a small fraction of the vadose zone. Micropore and macropore fluxes, including preferential flow, make it difficult to estimate travel times of contaminants through the vadose zone due to their complex nature. That way it becomes even more difficult to assess the vulnerability of groundwater to various impacts such as contaminants. A study done in Mpumalanga Highveld by Campbell (2000) indicated that the contaminant transport in the vadose zone depends on both the properties of the medium and the pollutant. Macropores represent microsites in the soil with larger clay and organic carbon contents, better nutrient supply and oxygen status, and larger microbiological activity (Jarvis, 2002). These factors generally contribute to a larger sorption and degradation capacity per unit mass of soil.

The vadose zone of South Africa varies in depth and composition. In many cases, the extent of preferential flow may diminish with depth since structural development generally becomes weaker in the absence of biotic macropores and physical processes, which generate structure, such as wetting and drying or freezing and thawing. However, in other widespread hydrogeological formations, such as glacial clayey tills, fracture flow has been demonstrated to be continuous to great depth during periods of seasonal saturation and is the dominant mechanism of contaminant transport towards underlying aquifers. Therefore, it is vital to understand what chemical and hydrologic processes occur at a given location in order to correctly predict the behaviour and impacts a contaminant may have on the environment. In some places soil cover forms the unsaturated zone due to either a result of in-situ weathering or the deposition of transported material whilst, in others, there is negligible soil cover whereby the vadose zone is mainly composed of fractured or intact bedrock with primary porosity. Geological setting of a vadose zone could be very complex and rarely homogeneous because this zone is subjected to weathering, erosion, pedogenic and other processes since it represents the top portion of the geological profile. Preferential flow can also occur in matrix of unstructured sandy soils.

The vadose zone is divided into three subzones, namely the *capillary fringe* - immediately above the groundwater surface, the *capillary zone* - with larger pores filled with air and smaller pores filled with water, and the *discontinuous zone* – where water is only retained as adsorbed water (Martin and Koerner, 1984). However, areas above the capillary fringe may be temporarily saturated due to surface ponding of water or because of the development of perched water tables above relatively low permeability soil layers. According to Fetter (1999), there are three types of preferential flow in the vadose zone, namely: short circuiting, fingering, and tunneling. They take place due to various conditions of the media through which water and solute move as they percolate downwards (vertically or horizontally). Here is their brief description:

Short-circuiting (or macropore channeling) occurs when water and solute move through macropores (like plant roots, shrinkage cracks and animal burrows) at faster rate than they would in normal soil matrix hydraulic conductivity conditions. See Figure 2.1 below.

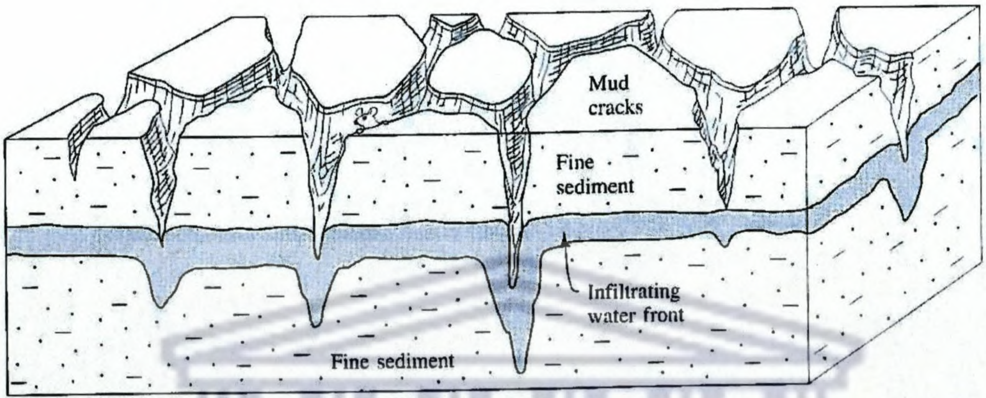


Figure 2.1: Preferential water movement in the vadose zone due to short circuiting (Fetter, 1999).

Fingering is caused by variations in pore-scale permeability. Here, a uniform solute front is split in a finger-like manner moving downwards. See Figure 2.2 below.

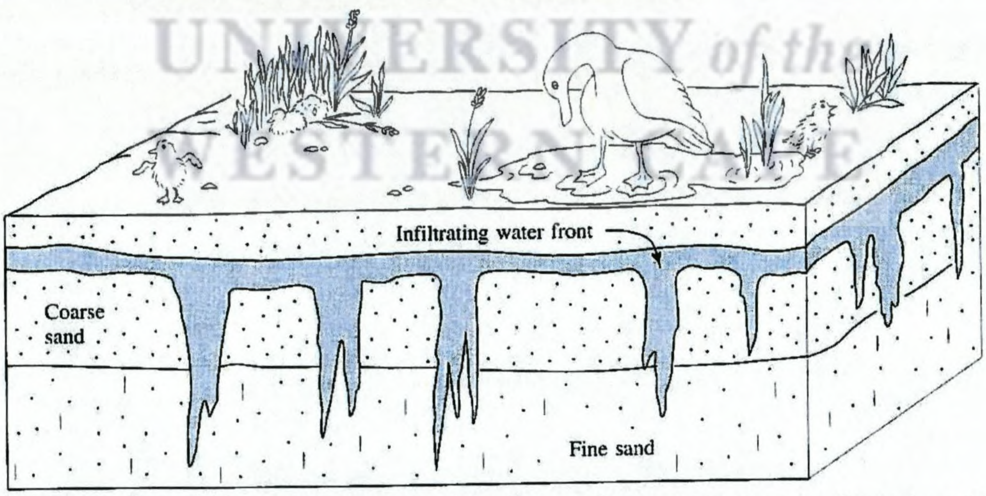


Figure 2.2: Preferential water movement in the vadose zone due to fingering (Fetter, 1999).

Funneling is governed by sloping beds or layers (normally stratified soils and sediment profiles) that are impermeable or with low permeability. The sloping layer collects water from the sides to the end of the layer where it can infiltrate vertically again in a concentrated volume. See Figure 2.3 below.

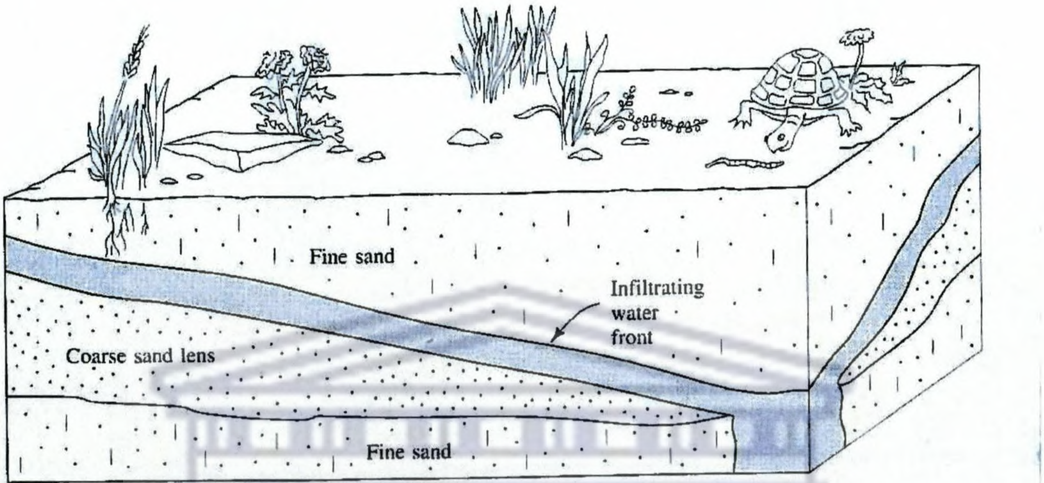


Figure 2.3: Preferential water movement in the vadose zone due to funneling (Fetter, 1999).

Climate also plays a role in the macropore flow system. Macropore flow is generated frequently in wet climates, whereas in dry climates it is better developed with shrinkage cracks contributing proportionally more to the flow. In Jarvis' (2002) view, the extent of leaching in the presence of macropore flow does not only depend on total rainfall, but perhaps more importantly on rainfall distribution and intensity. Experiments have shown that the higher rainfall intensity usually leads to greater bypass flow in macropores and enhanced leaching of tracers and agrochemicals (Jarvis, 2002).

2.2 <u>Preferential Flow Modelling</u>

There are many studies done on the subject of preferential flow modelling in the unsaturated zone. For instance, Ruan and Illangasekare (unknown date) in their study to model colloid (fine grained material with an electrostatic surface charge) transport in macroporous vadose zone, assumed that the colloid flux from the macropore is controlled mainly by the combination of five factors, namely;

i) Lateral infiltration rate through the macropore wall.

ii) The ratio of the pore size in the soil matrix to the colloid size. A small ratio will cause the colloid coagulation in the soil matrix near the macropore and decrease the further transport of colloids and the lateral infiltration rate.

iii) Degree of saturation of the soil matrix around the macropore. Water moves in larger pores when water content is higher.

iv) The flow velocity in the macropore. Higher velocity moves more colloids into a deeper part of the macropore.

v) The cumulative amount of colloids generated through a unit length of the macropore wall.

The U.S. National Committee for Rock Mechanics (2001) deems the following questions necessary for the development of appropriate conceptual models of fluid infiltration in fractured media:

1) Does the conceptual model provide an adequate characterization of the system?

2) How well does the model perform in comparison with competing models?

3) Is the data base adequate to estimate model parameters with sufficient reliability that the associated prediction uncertainties are acceptable in light of the intended application of the model?

4) What are the opportunities for field testing and verification of the model?

Model results, however, are always subject to some degree of uncertainty due to limitations in field data and incomplete knowledge of natural processes. A key consideration in any modelling process is whether the model has undergone sufficient development and testing to address the problem being analyzed in a sufficiently meaningful manner. Although model calibration does provide a certain level of model testing, a good fit to the calibration data does not necessarily prove that the model is adequate to address the issues in question.

Beven and Germann (1981) suggested that any model of a combined matrix/macropore system should be reduced to a Darcy type model in a soil containing no macropores, and they even introduced the domain concept in modelling where the matrix domain conforms to Darcian principles. However, that does not address the macropore flow phenomenon.

Vanderborght et al (2005) concluded that the differences among water flow simulations by different models can be attributed to the implementation of the soil surface boundary conditions in the models. Also, both the spatial discretization of pressure head profile close to the soil surface and the methods of averaging the hydraulic conductivities in the first grid layer influence the numerical solutions. An overestimation of solute dispersion would lead to an overestimation of leaching, especially when substance decay is considered, hence the importance of a correct simulation of solute dispersion.

Below is the review of two process models that have been used widely, evaluated and compared with other macropore soil models and studies.

2.2.1 A General Review of some Vulnerability Assessment Process Modelling Methods in Relation to Preferential Flow in the Vadose Zone.

This section takes a general look at two possible models, namely MACRO 5.0 and SWAP that can be used to simulate dual porosity and preferential flow. In the end one of them is selected (with the reasons for such selection) for use in this project. Detailed description of the selected model is given in Chapter 3.

2.2.1.1 MACRO 5.0

MACRO is a one-dimensional, dual-permeability model that considers transient fluxes of water, heat and solute in the vadose zone. The total porosity is partitioned into two separate flow regions (matrix and macropores), each with its own degree of saturation, conductivity, water flow rate, solute concentration, and solute flux density. The primary objectives of developing this model were to:

- Synthesize current understanding of flow and transport processes in structured soils, and

- To develop an easy to use physically based simulation model, which could be used as a management tool to evaluate the likely impacts of macropore flow on water flow and solute transport to surface and groundwaters. (Larsbo and Jarvis, 2003).

Convective–dispersive transport is calculated for solutes undergoing "two-site" (kinetic and instantaneous) sorption, passive plant uptake, and first-order degradation controlled by soil moisture and temperature.

MACRO employs Richards' equation to calculate vertical water fluxes in the matrix. In macroporous soils, hydraulic conductivity increases very rapidly across a small pressure head range as saturation is approached (Clothier and Smettem, 1990; Jarvis and Messing, 1995), thus a "cut and join" approach is used to define the matrix–macropore hydraulic functions (Jarvis et al., 1991). Soil water retention in the matrix is calculated using a modified form of van Genuchten's (1980) equation (Vogel et al., 2001). Richard's equation and van Genuchten's equation are described in detail in Chapter 3.

2.2.1.2 SWAP

SWAP is the successor of the agrohydrological model SWATR (Feddes et al, 1978) and some of its numerous derivatives. According to Kroes (2003), the core of the model exists for implementations of mathematical descriptions of soil water flow, solute transport and soil temperatures, with special emphasis on soil heterogeneity. SWAP focuses on the transport of salts, pesticides and other solutes that can be described with relatively simple kinetics and thus the following processes are not considered in SWAP (Kroes and van Dam, 2003):

- volatilization and gas transport,
- transport of Non-Aqueous Phase Liquids (NAPLs),
- chemical equilibrium of various solutes (e.g. between Na^+, Ca^{2+}, Mg^{2+}),
- chemical and biological chain reactions (e.g. mineralization, nitrification).

The description of SWAP given in this section is mostly abstracted from the Reference Manual by Kroes and van Dam (2003). SWAP 2.0 was developed for calculations with daily meteorological input data. In general, model results should be analysed on a daily base. SWAP also uses Richard's equation to describe water flow in variably saturated soils at a scale where soil can be considered to be a continuum of soil, air and water. Hydraulic functions $\theta(h)$ and $K(\theta)$ as analytical expressions have to be specified for each distinct soil layer. Among other advantages of using analytical functions, one is that they allow for calibration and estimation of soil hydraulic functions by inverse modelling. In situations of total saturation and ponding on soil surface, SWAP can adjust the following calculations:

- Richard's equation is solved for the soil profile, with prescribed head, $h = h_{pond}$ at the soil surface;
- then the next ponding depth h_{pond} is updated from the water balance of the total soil profile, including surface runoff.

To avoid instability of simulated surface water and groundwater levels, SWAP warns the user if large oscillations of surface or groundwater levels occur. Thence, reducing the time step is the solution. Transition takes place in the bottom boundary of the one-dimensional SWAP, which is either in the upper part of the saturated zone or in the unsaturated zone. Lower boundary condition can be prescribed for input and there are eight options to consider (see Table 2.1).

Table 2.1: Eight options for the lower boundary condition in SWAP (Kroes and van Dam, 2003).

Lower boundary condition	Description	Type of condition	Typical scale of application
1	Prescribe groundwater level	Dirichlet	Field
2	Prescribe bottom flux	Neumann	Region
3	Calculate bottom flux from hydraulic head of deep aquifer	Cauchy	Region
4	Calculate bottom flux as a function of groundwater level	Cauchy	Region
5	Prescribe soil water pressure head of bottom compartment	Cauchy	Field
6	Bottom flux equals zero	Neumann	Field
7	Free drainage of soil profile	Neumann	Field
8	Free outflow at soil-air interface	Neumann	Field

Assuming a steady state situation and equal distances between soil layers, the displacement of non-reactive solute through this system may be described by a set of linear differential equations (van Dam et al, 2003).

Transportation of solutes in the unsaturated zone is predominantly vertical. The residence time there is important because many activities, like decomposition of organic compounds, water and nutrients extraction by plants, and more others, take place in the unsaturated zone. Diffusion, convection and dispersion are the main solute transport mechanisms in soil water.

For simulation in SWAP, basic daily meteorological data are used to calculate daily potential evaporation but if basic meteorological data are not available, potential evaporation or reference evaporation can be inputs. Kroes and van Dam (2003) believe that the detailed simulation of physical transport processes in macropores is not feasible due to the fact that a dynamic morphology of each location would require a huge amount of data. They then suggest a search for a systematic behaviour on a larger scale. Shrinkage cracks are the sole macropores considered for a simple macropore flow model, whilst water flow and solute transport are described with basic physics using normal numerical procedures (van Dam, 2000). According to Bronswijk (1988), this shrinkage characteristic enables the calculation of the crack volume and depth, and it also describes the relation between the amount of pores (void ratio) and the amount of water (moisture ratio),

Stroosnijder (1976) and Bronswijk (1988) distinguished four stages of shrinkage, and they are outlined below:

- Structural shrinkage – saturated soils dry up and water filled pores may be emptied, thus the volume changes are negligible.
- Normal shrinkage – Volume decrease of clay aggregates is equal to moisture loss, and thus the aggregate remains fully saturated
- Residual shrinkage – Air enters the aggregate pores since the moisture loss is greater than the volume decrease upon drying of aggregates. In this stage, SWAP employs exponential relationship, $e = \alpha_{sh} e^{-\beta_{sh} v} + \gamma_{sh} v$, in order to facilitate input and data analysis (Kim, 1992). α_{sh}, β_{sh}, and γ_{sh} are dimensionless empirical parameters which are generated by SWAP from the user input values of e_o (the void ratio at zero water content), v_l (the moisture ratio at transition of residual to normal shrinkage), and v_s (the structural shrinkage). Then the $e(v)$ relationship is described.
- Zero shrinkage – Moisture loss is equal to air volume increase of the aggregates. Rigid soils, like sands, only show this stage.

Assumptions

There are limitations in the usage of SWAP due to many assumptions and schematizations of the flow pattern, therefore, van Dam et al (2003) alert the user of the following:

- assumption of steady state during the time increment;

- constant depth of the drainage base;
- assumption of perfect drains;
- uniform thickness of the hydrological profile

2.3 Case Study Sites Review

Study areas for this project are the Cape Flats and the Mpumalanga Highveld. This chapter investigates the geological, geochemical and geohydrological characteristics of the selected areas with emphasis on the vadose zone.

2.3.1 CAPE FLATS

2.3.1.1 Description

The choice of the Coastal Park Landfill site on the Cape Flats as one of the study areas, was based on the conditions suitable for the application of the selected modelling software and the availability of required data for a modelling process. The site is also prone to pollution due to the existence of various sources like landfill and waste water treatment sites, and more others. Most of these are close to residential areas and could pose a threat to the Cape Flats Aquifer.

The Cape Flats falls within a Mediterranean climate where rain falls mainly during winter between May and October. Its annual rainfall averages around 600 mm. It also experiences somewhat hot and dry summers, for which the temperature fluctuates between an average monthly minimum of 8°C and an average monthly maximum of 28°C.

The Cape Flats area falls in relatively low-lying planes. These are coastal planes of up to 300 m above mean sea level along the west coast covering about 600 km^2 in area. It is bounded by latitudes 33°45' E to 34°05' E and longitudes 18°20' S to 18°50' S. It is covered by urban development and most of Cape Metropolitan population lives within the area.

The case study site, Coastal Park, has a landfill site located on the northern coast of False Bay. The shallow Cape Flats Aquifer (CFA) supplies fresh water and its flow directions are southwards towards False Bay and southeast towards the Zeekoevlei outlet. Figure 2.4 shows the Coastal Park landfill site in the Cape Flats area.

Figure 2.4: The Coastal Park Landfill site (Saayman et al., 2007).

According to Usher et al. (2004), volatile organic compounds, pesticides, insecticides and herbicides are possible contaminants from a typical landfill site. From fertilizers applied in peri-urban areas, contaminants such as ammonia, sulphur, chloride, nitrates, potassium, phosphates, lead and arsenic are to be expected. Bacterial pathogens and organic nitrate in animal farms and abattoirs are common contaminants for that environment. Table 2.2 outlines some of the pollution sources and their resulting contaminants, especially in the Cape Flats area.

Table 2.2: Other contaminants reported in Cape Town – the urban catchment (extracted from Usher et al, 2004).

Source Type	Expected contaminants
On site sanitation	Nitrate, potassium, chloride, COD, faecal pathogens, phosphate, boron
Cemeteries	Ammonium, potassium, microbial pathogens
Wood processing and preserving	Ammonia, arsenic, chromium, copper, creosote, dioxins, polyaromatic hydrocarbons, pentachlorophenol, phenol, tri-n-butyltin oxide, PCB, PAHs, beryllium
Mechanical and electrical workshops	Polyaromatic hydrocarbons, diesel, benzene, alkanes, acids, aluminium, arsenic, beryllium, cadmium, lead, mercury, nickel, chlorinated solvents.
Automotive refinishing and repair	Paint, scrap metals, waste oils, toluene, acetone, perchloroethylene, xylene, gasoline and diesel fuel, carbon tetrachloride, hydrochloric and phosphoric acid.
Petrol service stations (Underground storage tanks)	Benzene, toluene, xylenes (BTEX), oxygenates (alcohol, MTBE), metals (lead, nickel), sulphur, alkanes, TPH, PAH.
Rubber and plastics Textile manufacture	Acrylonitrile, antimony, benzene, butadiene, cadmium, chloroform, chromium dichloroethylene, lead, phenols, phthalates, styrene, sulphur, nynil chloride, toluene, heptane, formaldehyde, ammonium, arsenic, nickel, hexane
Hazardous waste sites	Ammonium salinity, DOC, heavy metals, methane
Incinerators	Dioxin, various municipal and industrial waste.
Transport Research and educational institutions Printing industry Food and beverage manufacturing	Benzene, toluene, xylenes (BTEX), oxygenates (alcohol, MTBE), metals (lead, nickel), sulphur, alkanes, TPH, PAH, inorganic acids, organic solvents, metals and metal dust, photographic waste, waste oils, paint, heavy metal, pesticides, silver, Methyl-Ethyl Ketone (MEK), TCE, chlorine, chlorine dioxide, nitrate/nitrite, biogenic amines, methane, dioxins, bacteria

Source Type	Expected contaminants
Railroad yards Adhesives and sealants Pharmaceuticals and cosmetic manufacturing Paint/ink manufacturing and coatings	Petroleum hydrocarbons, VOC, BTEX, solvents, fuels, oil and grease, lead, PCB, benzenes, toluene, MEK, alcohols, benzoates, bismuth, dyes, glycols, mercury, mineral spirits, sulphur, methylene chloride, nitrate, acetates, acrylates, aluminium, cadmium, chromium, cyanides, glycol ethers, nickel, phthalates, styrene, terpenes, 1,4-dioxane, ammonia, anthraquinones, arsenic, benzidine, ethyl acetates, hexane, oxalic acid, phenol.
Hospitals and Health Care	Formaldehyde, radionuclides, photographic chemicals, solvents, mercury, ethylene oxide, chemotherapy chemicals
General and domestic waste sites	Ammonium, salinity (sodium, chloride, sulphate), DOC, methane, lead, mercury
Photographic manufacturing and uses	Silver bromide, methylene chloride, solvents, photographic products
Chlorinated solvents Non-chlorinated solvents Munitions manufacturing	Carbon tetrachloride, chlorofluoroethanes, dichloroethylene, methylene chloride PCE, TCE, vinyl chloride, 1,1,1-trichloethane, acetates, alcohols, benzene, ethylbenzene, ketones, toluene, xylene, nitrate, sulphate, chromium, copper, boron, lead, antimony and phosphate.
Leather manufacturing	Toluene, benzene, arsenic, chromium, cadmium, sulphate
Marine maintenance industry	Solvents, paints, cyanide, acids, VOC emissions, heavy metal sludge, degreasers
Electricity generation	Radioactive waste, salinity, PCBs

The landfill site is underlain by aeolian dune sands that are calcareous at depth. Seawater intrusion has been detected, especially in the deep Varswater Formation, the main water bearing formation (Traut and Stow, 1999). The Coastal Park site is receiving hazardous waste from domestic sources and small business, despite not being lined nor permitted to receive such waste. This landfill is only separated from groundwater by a 2 m unsaturated zone comprising Cape Flats sands, and it is believed that any pollution would be attenuated and migrate towards the sea. However, the monitoring process has detected leachate generation and pollution plume, and hence groundwater pollution (Ball and Novella, 2003). Leachate migration rate from the landfill is 6 to 7 m per year (Ball and Stow, 2000).

2.3.1.2 Soil characteristics

This section focuses in particular on soil hydraulic properties, which are the most important soil characteristics in the context of preferential flow. Due to lack of data on hydraulic properties of the soil in Coastal Park, data from iThemba Labs (Samuels, 2007) were used for modelling considering that they are exposed to similar environmental conditions.

The vadose zone of the Cape Flats Aquifer (CFA) occurs above the unconfined aquifer. Its thickness is a function of topography of the land surface and underlying bedrock, the seasonal water level, and the degree of interconnectivity with the underlying fractured rock aquifer. For unconsolidated material overlying an unconfined aquifer, the thickness of the vadose zone is defined as the distance from the surface to the water table (Adams and Jovanovic, 2005). Hence the thickness of the vadose zone of the CFA is averaged at 3 m (within a range of 1 – 5 m). Calcrete and clay layers tend to create perched aquifers within the system. The sand is generally well sorted with minor amounts of granules, and low silt and clay content. Grain sizes range from 0.75 to 3.25 phi (Adams, unpublished data). Freeze and Cherry (1979) estimated hydraulic conductivities for various aquifer material. They estimated hydraulic conductivities for both clean and silty sands within ranges of 10^{-4} to 1cm/s and 10^{-5} to 10^{-1} cm/s, respectively.

Figure 2.5 together with the soil profile logs of Figure 2.6 give clear description of the soil types found on the Cape Flats area, specifically at iThemba Labs . Topsoil comprises fine to medium loose sands up to shallow depths. With depth comes sandy clay loam and beyond 4 m, clay. Water retention capacities for these various soil types are different.

Sandy loam and sandy clay have higher water retention capacities whereas the opposite is true for loose sandy soils.

Since the Cape Flats Aquifer is very shallow the soils are well drained. Therefore the chemical properties of groundwater as explained in section 2.3.1.4 below also apply to the soils of this study site.

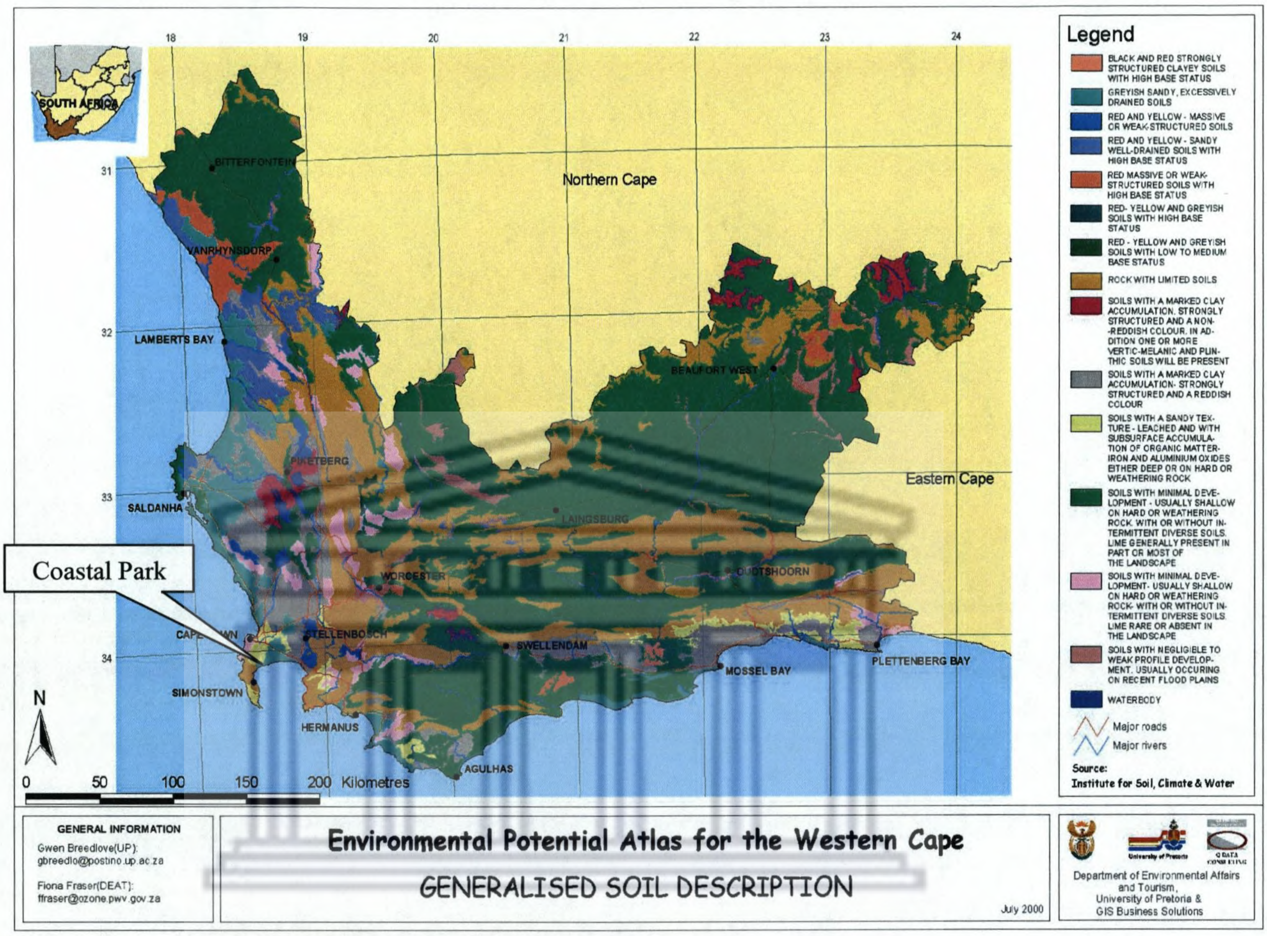


Figure 2.5: Generalised soil description for the Cape Flats where the Coastal Park Landfill site lies (source: Department of Environmental Affairs and Tourism).

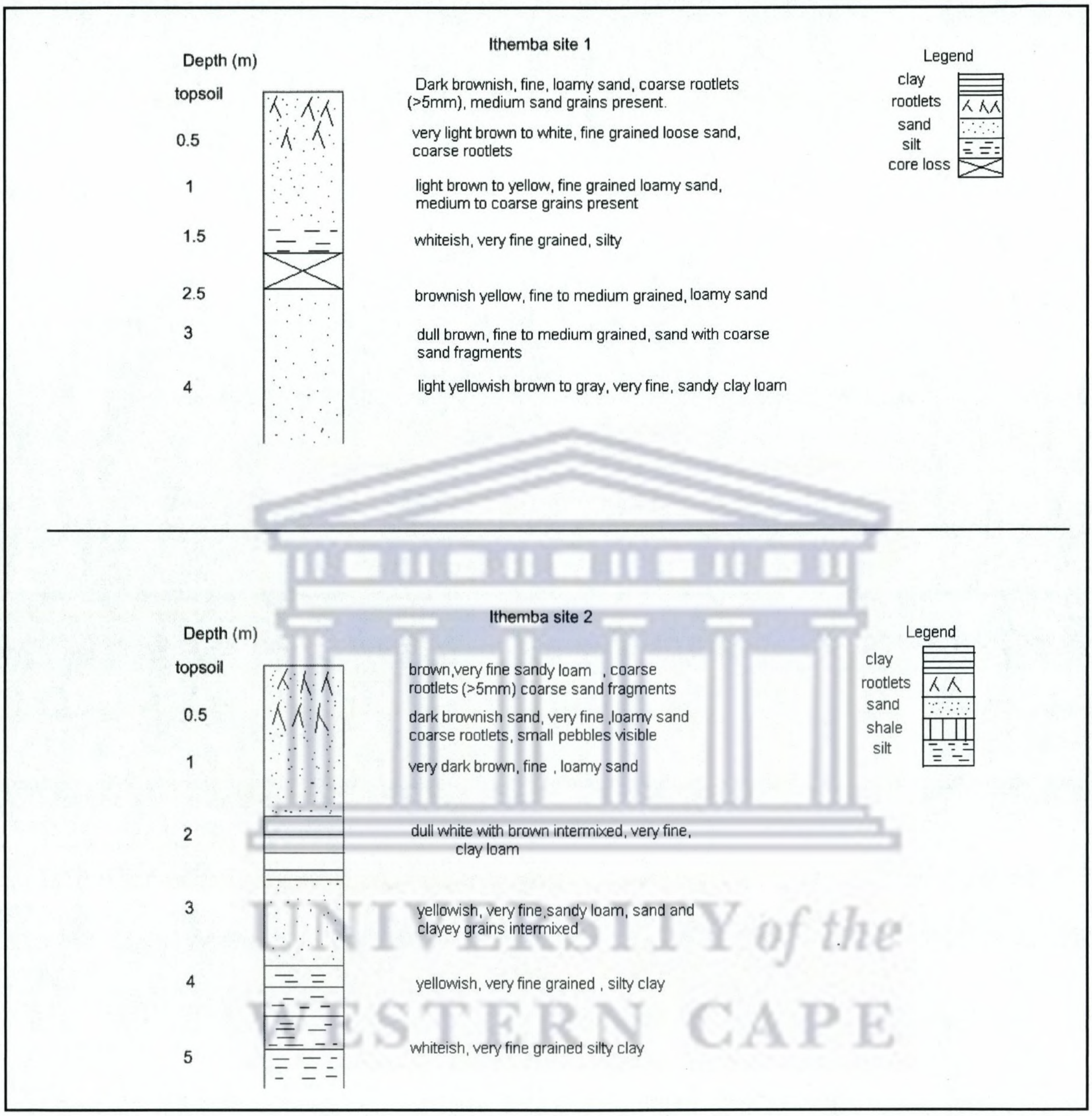


Figure 2.6: Borehole soil logs from iThemba Labs site (modified from Samuels, 2007).

2.3.1.3 Geology

Cape Flats is an area with low topography, which was created by the removal of Table Mountain Group between False Bay and Table Bay during Post-Palaeozoic erosion (See Figure 2.7).

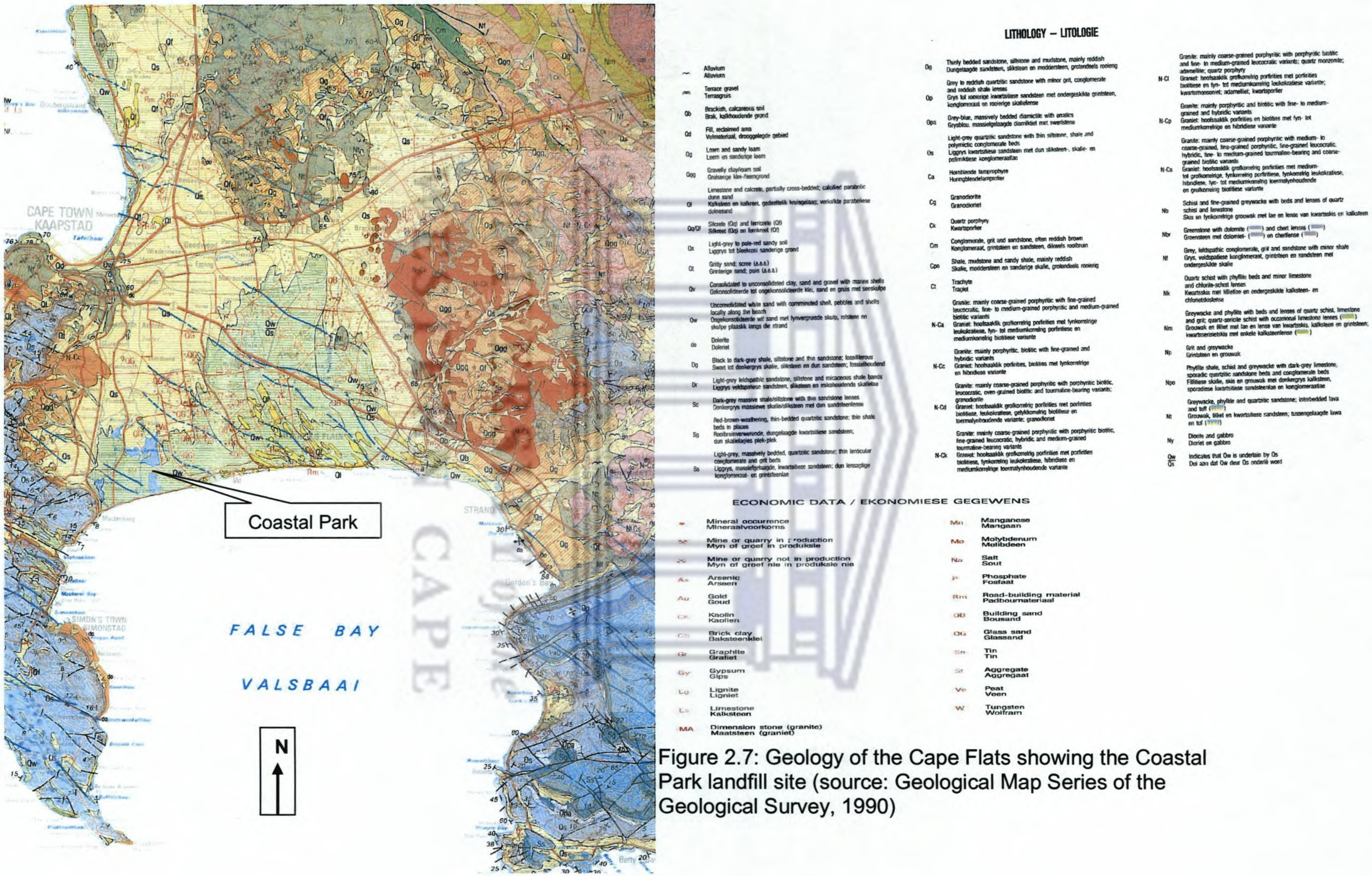


Figure 2.7: Geology of the Cape Flats showing the Coastal Park landfill site (source: Geological Map Series of the Geological Survey, 1990)

The oldest geological rock formation is the Malmesbury Group which is intruded by granite batholiths resulting in the deformation and metamorphism of the shales. The Cape Granite and the Malmesbury shales are in turn unconformably overlain by the sandstones of the Table Mountain Group as shown in Figure 2.7 above.

2.3.1.4 Groundwater Quality/Chemistry

The sandy substrate of the Cape Flats and Atlantis areas has a low filtering efficiency and, as groundwater is recharged by slow seepage from the surface, this water resource is particularly vulnerable to pollution from human activities. The Cape Flats aquifer is of variable water quality. Variable amounts of water are abstracted on an ad hoc basis. Illegal dumping of waste at industrial and building sites throughout the Cape Flats poses a threat to this aquifer.

Groundwater tends to be of sodium-chloride-calcium-alkaline nature (see Piper plot, Figure 2.8). Salinity values are high as a result of evaporation due to shallow water tables, vlei or marine deposits, agricultural practices, rapid urbanization, industrialization and many other potential pollution sources in the CFA (Fraser and Weaver, 2000). There are three natural environments according to Fraser and Weaver (2000): aquatic ecosystem, terrestrial ecosystem and the marine environment. These environments can be impacted if there is large-scale abstraction from the CFA. The CFA is extensively used for small-scale farming in the Philippi area and for water supply to the town of Atlantis.

Piper plot (Majola, 2006) in Figure 2.8 shows the abundance of sodium and chloride. This is to be expected from a coastal aquifer. This could also be explained as old groundwater with persistent chloride. It has been said that sulphate pollution occurs in some parts of the area, especially Philippi where agriculture is practiced. The Piper plot however indicates that the Cape Flats groundwater is of (Na, K)-Ca-Cl type. But the two groupings of points on the plot could indicate two water types which imply two different groundwater sources. Probable sources are seepage of sea water and groundwater that has reacted with calcrete which is perching the sands in the aquifer. The maximum recommended limits for salt concentration (TDS) and Electrical Conductivity (EC) in water fit for human consumption are abstracted from Meyer (2001) as 1200 mg/l and 70 mS/m, respectively. However, it was observed that some boreholes record excessively high TDS concentrations, and whilst EC is mostly beyond the recommended limit, it is within the maximum allowable limit of 300 mS/m. This proves high salinity of groundwater in the Cape Flats area.

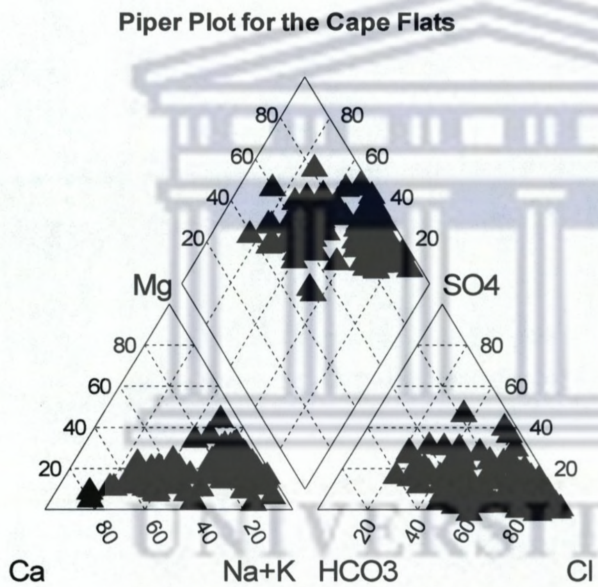


Figure 2.8: Piper diagram for the Cape Flats Aquifer (Majola, 2006).

2.3.1.5 Geohydrology Characteristics

The Cape Flats Aquifer (CFA) consists predominantly of Tertiary to Recent unconsolidated sand deposits. These sedimentary strata were deposited partly under fluvio-marine conditions and partly under aeolian conditions (Gerber, 1976). Its thickness ranges from 20 m to 30 m.

i) <u>Primary Aquifer</u>

The primary aquifer system is known as the Sandveld Group and various formations were deposited under shallow marine, lacustrine and aeolian conditions. The sands of the Witzand and Springfontyn Formations constitute the major groundwater target, with hydraulic conductivities ranging between 30 – 40 m/d in the central area and 15 – 50 m/d in the eastern portion (Vandoolaeghe, 1989). These are fine to coarse, generally well sorted and well rounded sands. There is, however, an occurrence of sandy clay and clayey sandy lenses due to grain size variation with depth and width. Therefore, heterogeneity is caused. In some parts, the underlying white clay layer of thickness ranging from 40 m to 60 m is a result of weathering of underlying Malmesbury Group rocks that consist mainly of shale.

ii) <u>Secondary Aquifer</u>

The Malmesbury metasediments are extensively weathered and pelitic, hence they are considered impervious. However, high yields were observed in the arenaceous brittle sandstones along the west coast. In the eastern Cape Flats, boreholes were seen by Wessels and Greeff (1980) to be yielding good quality water. Also, Philippi agriculture abstracts some of its water from the Malmesbury aquifer. This is a transmissive aquifer, characterized by brecciated zones associated with faults. The groundwater is generally of sodium-chloride-alkaline nature (Meyer, 2001).

iii) <u>Impermeable Layers</u>

These are Langebaan and Varswater Formations. The calcareous clay and calcrete layers of the Langebaan Formation act as an impermeable barrier and hinder the free flow of groundwater and hence are regarded as aquitard layers when present. The Varswater Formation has shelly gravel and calcareous sands. It is regarded as an aquitard as well when the Springfontyn and Witzand Formations are present. Hydraulic conductivity here ranges from 1 to 23 m/d. (Vandoolaeghe, 1989).

iv) **Regional Flow System**

The CFA is an unconfined aquifer, not linked hydrogeologically to any other aquifer and with no lateral hydraulic or geological boundaries internally. It pinches out against impermeable boundaries in the east, west and north, whilst it is defined by the coastline extending along False Bay in the south (Wright & Conrad, 1995). Groundwater flow is either west to Table Bay or south to False Bay, that is, flow directions in the main part of the aquifer are either westerly or southerly. Water levels indicate a lower hydraulic conductivity along the coast compared to that inland. The groundwater levels of the Zeekoevlei shallow pond are partly maintained by groundwater seepage, with possible exceptions of short periods after heavy rains.

According to studies done by Henzen (1973) and Gerber (1976), transmissivity values ranged from 50 to 650 m^2/d with effective porosity in the order of 0.10 to 0.12 although values of 0.25 were found in other areas. Storage coefficients, according to van Tonder and Botha (1985), range from 0.002 to 0.35.

2.3.2 MPUMALANGA HIGHVELD

2.3.2.1 Description

This choice of Mpumalanga Highveld as the second study area was based on the conditions suitable for the application of the selected modelling software and the availability of required data for a modelling process, more than other possible study areas. Sasol operates a large petrochemical facility at Secunda (Mpumalanga Highveld). Some surplus ammonia rich process effluent containing elevated concentrations of fluoride and boron have been disposed of by permitted irrigation, exploiting evaporation to get rid of the excess water. This was the method approved by the Department of Water Affairs and Forestry. Effluent has been irrigated onto land from 1991 to 2000 at the Goedehoop site. Moreover, it has been observed that the clays in some areas are cracked to great depths. This fractured environment makes Mpumalanga Highveld distinct from the Cape Flats thus allowing the run of the model for two different environments. Continuous soil and groundwater monitoring in the area has been conducted by Sasol. Such monitoring of soil properties and groundwater quality implies therefore that most of the required data for this study are available.

Mpumalanga Highveld falls within the temperate climate, therefore it experiences warm summers and cold winters with sharp frosts. Mean daily temperatures show a minimum range of 13.2 °C in January to 0.2 °C in July (but extremes can occur from time to time), whilst the maximum range is from 25.8 °C in January to 17.1 °C in July, even though it could rise up to 34.7 °C at times. Mean Annual Precipitation (MAP) for Mpumalanga Highveld is about 700 mm falling mainly in summer months, from October to April in the form of showers and thunderstorms. Wind speed is normally above 10 km/h (typical range: 10 – 30 km/h).

The Highveld is a gently undulating area, largely sloping northwards with altitude ranging between 1590 m and 1610 m (amsl), and covering about 600 km^2 area. The slope ranges from 1% to 5%. It is bounded by latitudes 26°30' S to 26°45' S and longitudes 29°00' E to 29°15' E. The area is drained by the Klipspruit River and its tributaries. However, Klipspruit is also a tributary to Waterval River in the Vaal Catchment.
The design of irrigation systems theoretically was such that irrigation volumes should not exceed Mean Annual Rainfall Deficit (MARD) which is estimated at 737 mm per annum.

Soil water quality following irrigation was observed to be constantly changing in character and concentration because of non-uniform disposal of sludge water, attenuation capacity of soils, and chemical processes occurring under aerobic/anaerobic conditions in the soil. High variability in laboratory results led to the conclusion that there is no definite trend in about 50% boreholes analyzed. Infiltration of irrigation water occurs into the underlying Shallow Weathered Zone Aquifer. Figure 2.9 shows the location of the study site.

Figure 2.9: The Goedehoop irrigation site with the Sasol Synfuels complex in the background.

2.3.2.2 Soil characteristics

The average thickness of the vadose zone is about 7 m (mostly within 1 – 13 m range). It is characterized by the Rensburg (black clay turf) and the Swartland (acid sandy clay loam) Forms of soil that experience high cation exchange capacity due to high clay content. Rensburg has strong expansive properties like wide cracking. It is mainly found in low-lying positions associated with dolerite sills (Soil Classification Working Group, 1991). Its clay content does not increase with depth. Swartland Form on the other hand is characterized by increased clay content down the profile. Here, the B horizon is located within 300 mm of the surface with clay content of about 50 %. Also, very dark sandy loam (about 100 mm thick) overlies clay loam within 400 mm of the surface.

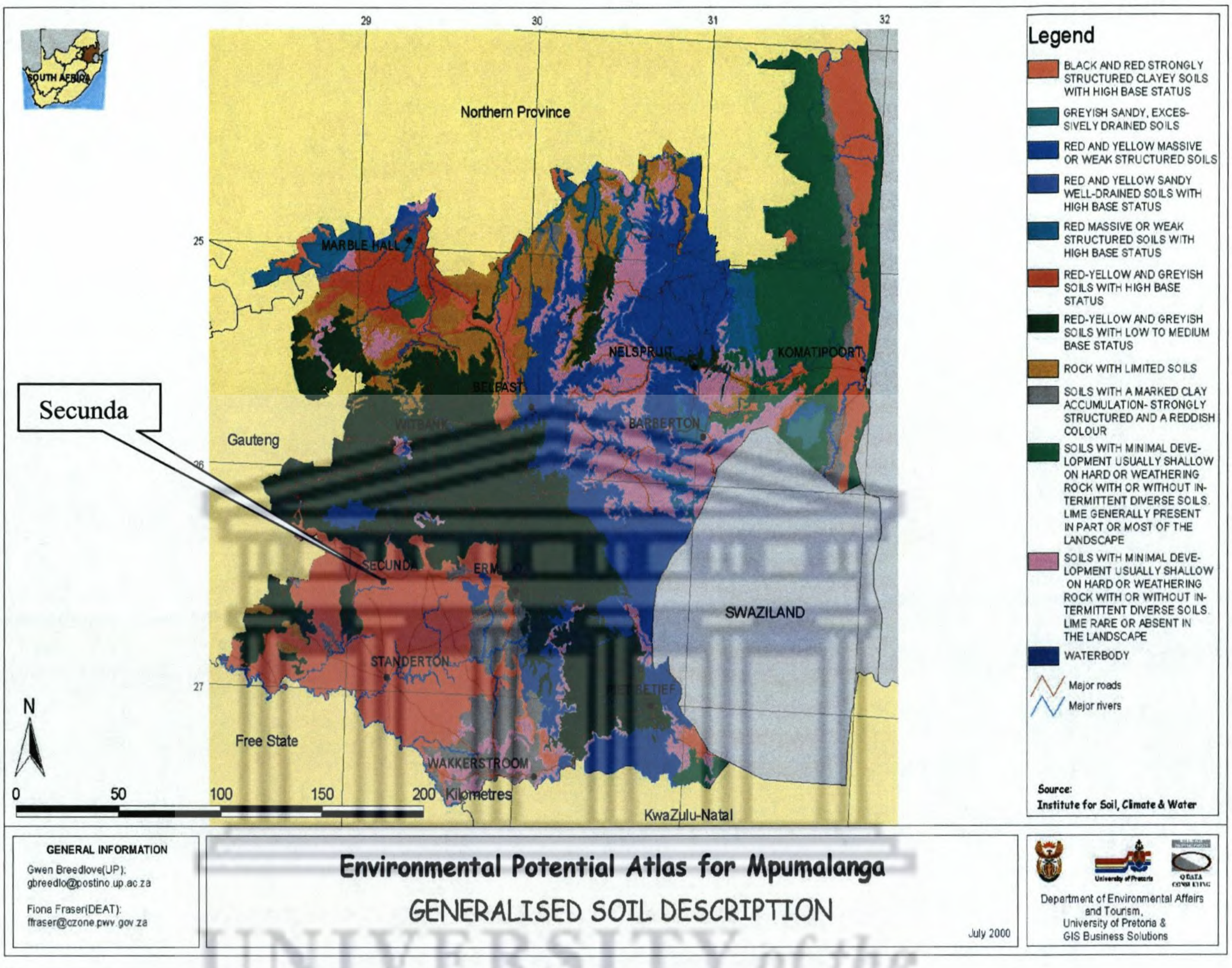


Figure 2.10: Generalised soil description for Mpumalanga province showing the position of Secunda where the Goedehoop study site lies (source: Department of Environmental Affairs and Tourism).

The topsoil in the area remains wet for long periods after heavy rainfall and, additionally, water logging is common due to slow infiltration. Figure 2.11 shows soil sampling site positions and Table 2.3 gives descriptions to some of the soil profiles from the Goedehoop irrigation site. It is clear from Table 2.3 that the clay content increases with depth promoting cracking due to shrinking and swelling. That results in preferential flow and pollutant flux. The S-value and pH do not give thorough conclusions as to their effect on sorption (Saayman, 2007). However, the study observed that some strong sorption rates occur in highly weathered soils.

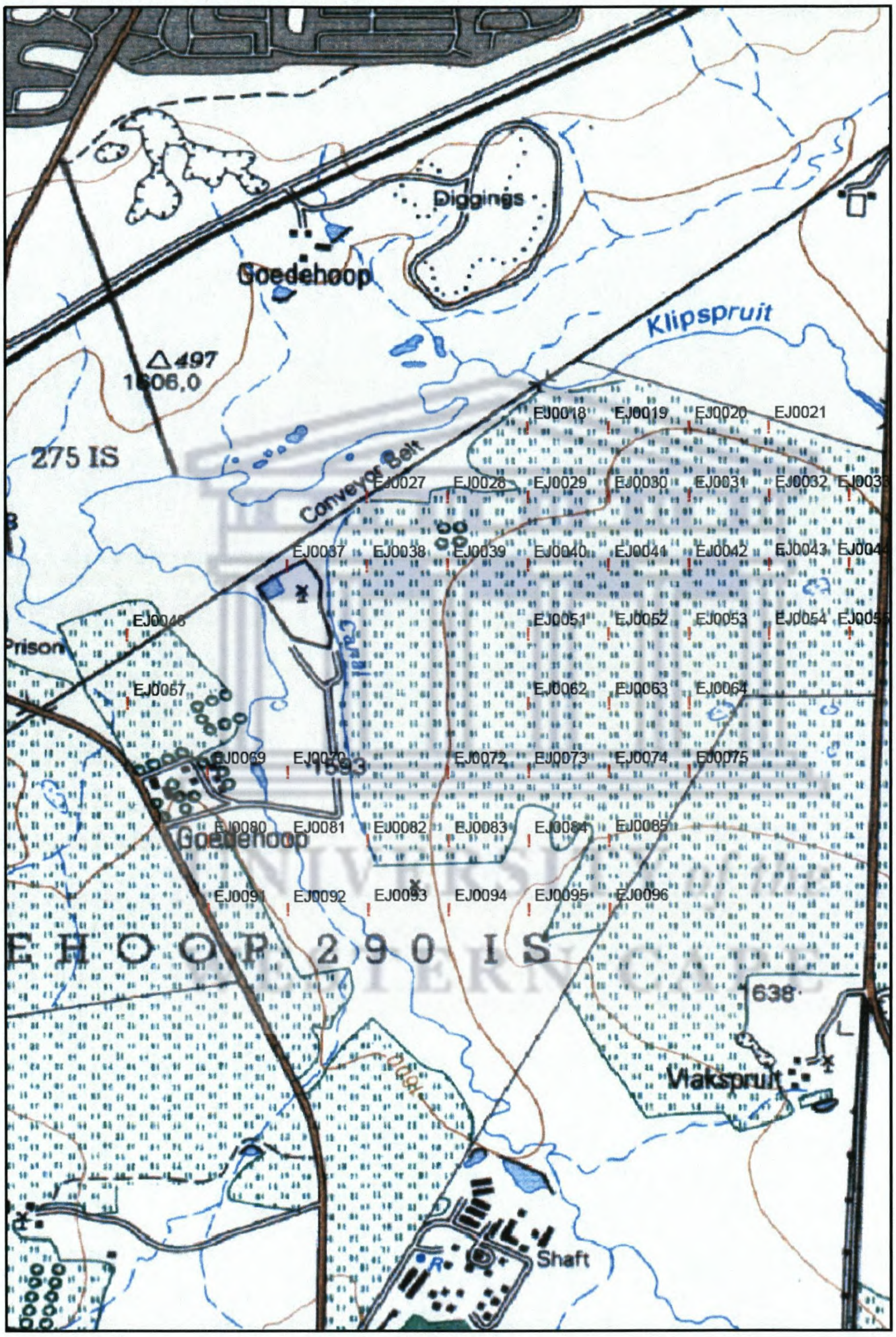


Figure 2.11: Map showing position of sampling sites on the Goedehoop irrigation lands (Saayman et. al., 2007).

Table 2.3: Analysis of some of the soil profiles from the Goedehoop irrigation site (Extracted from Saayman et al., 2007).

Soils Profiles			Average compositions						Saturated water extract	Hot water	Comments
Field Location	Soil Form	Sample depth (cm)	Clay		Sand		Silt		Average F	Average B	
			%	Std Dev	%	Std Dev	%	Std Dev	(mg/kg)	(mg/kg)	
EJ57	Rg2000	1000	38.8	7.56	42.5	7.51	18.7	0.65	0.67	0.19	No cracks at surface but full of slickensides
EJ92	Rg2000	1000	45.6	7.92	20.7	3.99	33.7	4.01	0.79	0.23	Cracks at surface
EJ82	Rg2006	1000	37.2	6.42	39.88	2.22	22.92	4.25	0.13	0.59	No comment
EJ84	Rg2006	1000	46	9.06	27.96	7.22	26.04	2.57	2.16	0.23	No comment
EJ75	Rg1000	1000	43.6	6.69	32.24	5.16	24.16	2.04	0.95	0.15	Surface heavily cracked
EJ62	Rg2000	1000	42.4	10.43	36.42	8.53	21.18	2.09	0.76	0.13	Surface cracked - next to abandoned weather station
EJ38	Rg2000	1000	36	6.78	41.3	6.37	22.7	0.85	4.11	0.37	Surface cracked
EJ29	Va1122	800	39	8.86	39.3	8.84	21.7	0.61	0.89	0.02	No comment
EJ19	Va1122	1000	42.4	8.17	35.72	8.42	63.02	1.06	0.4	0.11	No comment
EJ41	Va1122	1000	46	9.27	34.9	6.35	19.1	3.1	1.44	0.17	No comment
EJ54	Va1121	1000	42.4	6.54	35.88	3.34	21.72	3.51	0.18	0.22	No comment
EJ32	Va1121	1000	44	6.32	34.76	5.67	21.24	1.59	0.69	0.24	No comment

*Effective depth on all profiles is 200 cm

2.3.2.3 Geology

The geology of the Mpumalanga Highveld comprises of sandstones, shales, sub-ordinate gravels and mudrocks of the Vryheid Formation of the Ecca Group of the Karoo Supergroup. The dominant clay in the sandstones is kaolinite with lesser amounts of illite. Dolerite sills and dykes also form part of the geology and they mostly intrude horizontally. However, others do intrude gently and are unevenly inclined (Brink, 1983). The Karoo Supergroup is about 200 m thick (including about 9 m thick Dwyka Formation at its base), and it directly overlies Archean granite. Table 2.4 below briefly outlines the lithostratigraphy of the Highveld as per the 2628 East Rand Geological Map Series of 1986.

Table 2.4: Lithostratigraphy of Mpumalanga Highveld (created from Geological Map Series of the Geological Survey, 1986).

PERIOD	SUPERGROUP	GROUP	LITHOLOGY
QUATERNARY/TERTIARY	___	Kalahari	Alluvium
JURASSIC	Karoo	Karoo Dolerites	Dolerite intrusions
PERMIAN	Karoo	Ecca	Sandstone, shale, coalbeds.

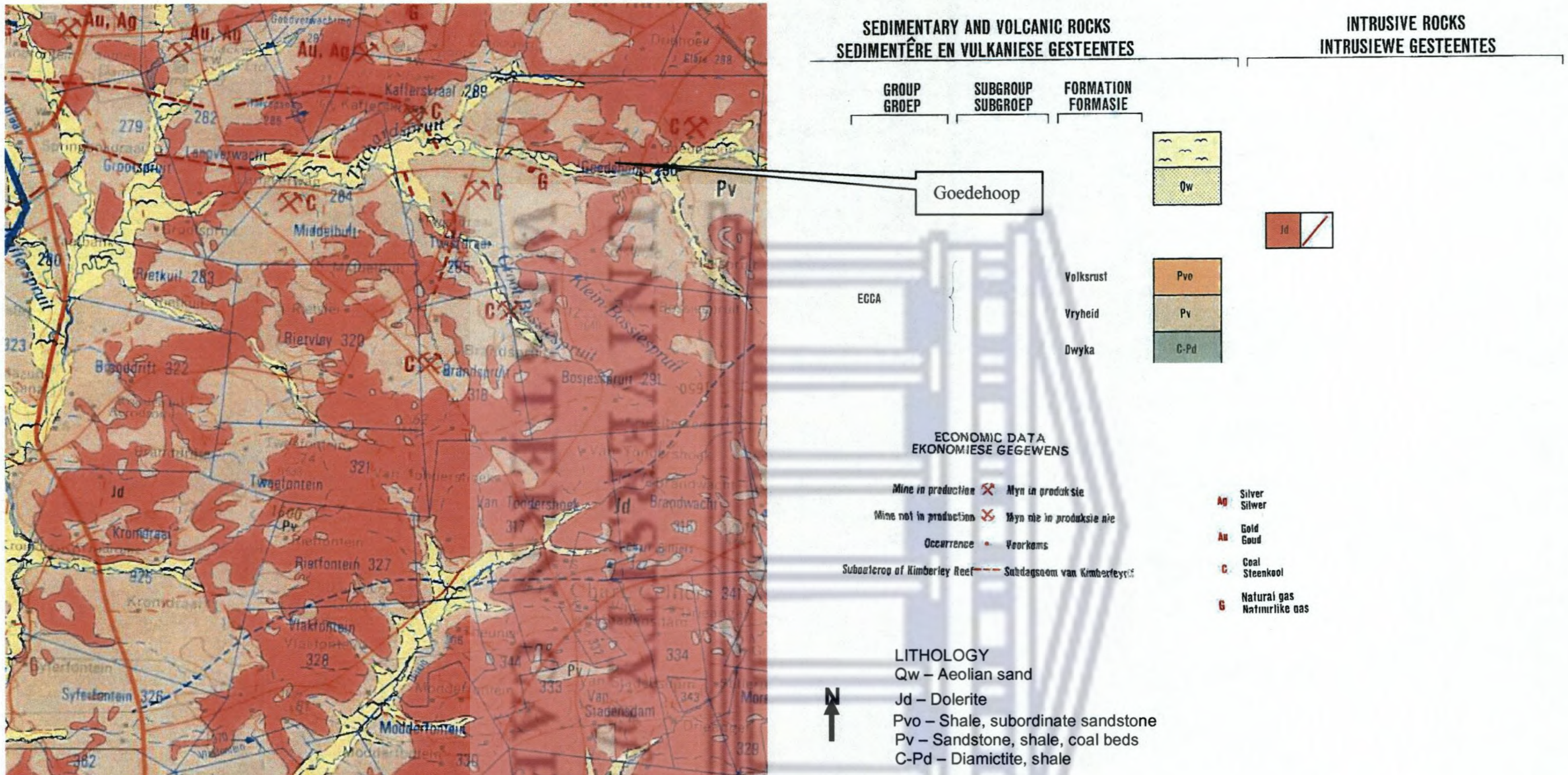


Figure 2.12: Geological description of Secunda showing the geology of the Goedehoop study site (source: Geological Map Series of the Geological Survey, 1986).

2.3.2.4 Groundwater Quality/Chemistry

An ongoing programme of soil and groundwater monitoring began in 1991 (Ginster, 2002). Figure 2.13 shows monitoring borehole positions and Table 2.5 shows the average borehole water quality for the Goedehoop irrigation site for the period 1991 to 2002.

Figure 2.13: Aerial photograph showing monitoring borehole positions in the Goedehoop irrigation site (Ginster, 2002).

Table 2.5: Average borehole water quality for the Goedehoop irrigation site (Ginster, 2002).

	Borehole Number/Identity					
Ions (*units*)	**REGM-27**	**REGM-28**	**REGM-29**	**REGM-111**	**REGM-30**	**REGM-110**
pH	7.7	7.6	7.8	7.9	7.6	7.6
EC (*μS/cm*)	804	1522	950	717	1377	1097
TDS (*mg/l*)	528	897	613	353	963	684
Ca (*mg/l*)	72	85	68	49	150	63
Mg (*mg/l*)	35	48	43	29	44	34
Na (*mg/l*)	87	174	62	67	67	121
K (*mg/l*)	3	3	7	6	2	2
Si (*mg/l*)	21	21	33	20	32	12
Cl (*mg/l*)	26	294	25	16	286	75
SO_4 (*mg/l*)	14	29	63	34	40	62
NO_3 (*mg/l*)	1.7	5.1	9.2	6.1	5.7	4.5
F (*mg/l*)	0.8	1.7	0.7	0.7	0.8	0.8
CO_3 (*mg/l*)	1.9	1.4	1.5	-	1.0	-
HCO_3 (*mg/l*)	189	188	170	-	365	-
Al (*mg/l*)	0.1	0.1	-	0.1	0.1	0.1
Fe (*mg/l*)	2.4	3.1	4.2	0.1	3.8	6.9
Mn (*mg/l*)	0.1	0.1	0.1	0.0	0.1	0.1
NH_4 (*mg/l*)	0.7	2.2	1.0	0.2	0.9	0.2
PO_4 (*mg/l*)	0.3	0.3	0.2	0.2	0.3	0.2
B (*mg/l*)	0.6	0.6	0.8	0.0	0.4	0.0

It is observed from the table above (Table 2.5) that there is relatively high concentration of dissolved salts; hence electrical conductivity is very high. More so, on boreholes such as REGM-28 and REGM-30 that additionally show a significant amount of Chloride (Cl) and fluoride (F). This could be attributed to the positioning of the borehole relative to the gradient. The groundwater level in borehole REGM-28 is much deeper than for the other observation holes. The groundwater quality in upstream borehole REGM-30 may be influenced by a nearby depression in the topography (subsidence above high extraction mining panel). However, when compared to the South African drinking water standards, these elements are mostly within the recommended limits. These concentrations are presented on stiff diagrams in Figure 2.14.

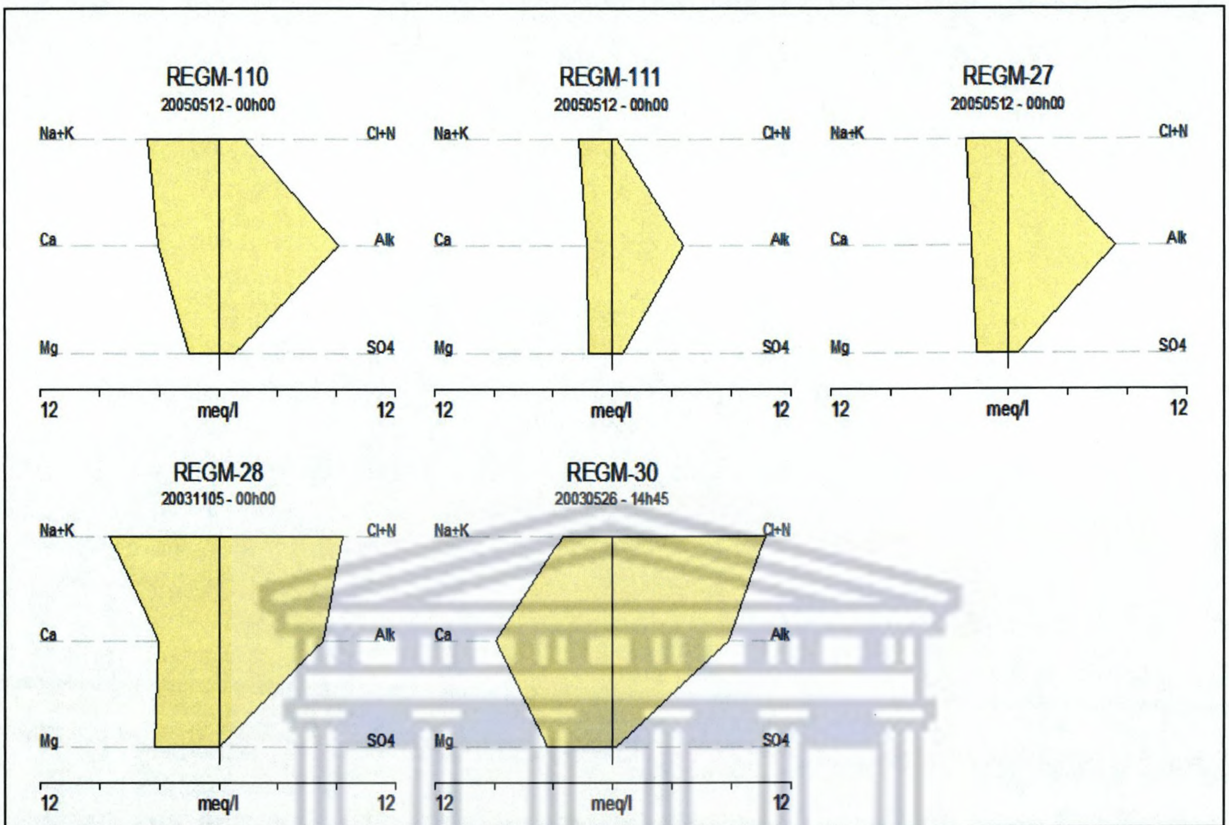


Figure 2.14: Stiff Diagrams for Borehole Samples from Goedehoop Irrigation Site (Campbell et al, 2005).

Azzie (2002) found that the cation exchange capacity (CEC) of the Vryheid Formation sediments is between 60 and 320 meq/kg. At a porosity of 20%, this is equivalent to between 300 and 1600 meq/litre of groundwater.

2.3.2.5 Geohydrology Characteristics

Mpumalanga Highveld has three superimposed groundwater systems. These are the Shallow Weathered Zone Aquifer, the Deep Fractured Aquifer, and the Deep Non-Fractured Aquifer.

i) <u>The Shallow Weathered Zone Aquifer</u>

This is the upper, unconfined and typically perched aquifer associated with weathered zone for which the water is often found within a few metres below surface. The Ecca sediments are weathered to depths between 5 and 12 m below surface throughout the area. According to Kirchner *et al.* (1991) and Bredenkamp (1978), recharge is mainly by rainfall and is estimated in the order of 1 - 3% of the annual rainfall. However, due to variations in the composition of the weathered sediments (which range from coarse-grained sand to fine clays), highly variable recharge values can be found from one area to the next and such isolated occurrences as high as 15% of the annual rainfall have been observed. This aquifer is generally low yielding (range 100 - 2000 litres/hour), because of its insignificant thickness. Few farmers therefore tap this aquifer by borehole.

The north-western portion of the coal-field is characterized by coarser grained sandstone and therefore higher recharge values are expected there, whilst dolerite sills often occur at surface further south where rain water recharges with ease since they are weathered or fractured. The movement of groundwater is lateral and in the direction of the surface slope.

ii) <u>The Deep Fractured Aquifer</u>

All groundwater movement here is along secondary structures, such as fractures, cracks and joints because the pores within the sediments are well cemented. These structures are better developed in competent rocks such as sandstone and this implies better water-yielding properties. However, not all secondary structures are water yielding. It has been observed that the chances of intersecting a water bearing fracture by drilling generally decrease rapidly with depth although some open cast coal mines were producing significant yields at depths greater than 30 m.

Underlying the coal is the impermeable Dwyka tillite, forming a hydraulic barrier between the Non-Fractured Aquifer and those high up in the succession due to its massive nature and fine matrix. In terms of water quality, the fractured aquifer always contains higher salt loads than the upper weathered aquifer. This is ascribed to the longer residence time of the water in the fractured aquifer.

iii) <u>Deep Non-Fractured Aquifer</u>

This is a low yielding aquifer at great depth. Its water quality is poor because of high fluoride levels associated with granitic rocks. It experiences low recharge due to the overlying impermeable tillite. Hence, drilling has intersected basement rocks underneath the Karoo Supergroup in very few instances.

In the southern portion of the catchment, dewatering of this aquifer has occurred, to some extent, because of the pumping during mining activities. However, the fractured aquifer was not impacted on due to the presence of the Dwyka tillite.

CHAPTER 3

DETAILED DESCRIPTION OF MACRO 5.0

As the modelling method of choice, MACRO 5.0 is described in detail here. The chapter looks at how the model deals with different processes involved in the preferential flow mechanism in a vadose zone. These would include, among others, macropore-micropore water and solute exchange, hydraulic properties, drainage, evapotranspiration, precipitation, soil water content and solute transport in the vadose zone. In the equations used in this chapter, some parameters are regarded as constants and others as variables. Table 3.1 below lists those parameters accordingly.

Table 3.1: Parameters considered in the MACRO program.

Constant parameters	Variable parameters
K_s – total saturated hydraulic conductivity	z – depth
θ_s – saturated water content	t – time
θ_b – boundary water content	d – effective diffusion pathlength
θ_r – residual water content	S_i – source-sink term
N – van Genuchten's n value	S – effective water content
α - mobile/immobile transfer rate exchange	θ_{mi} – micropore water content
l – tortuosity factor	θ_{ma} – macropore water content
n^* - kinematic exponent reflecting macropore size distribution.	M_{vg}, n_{vg}, α_{vg} – pore shape parameters
	K_b – boundary hydraulic conductivity
G – geometry factor (set to 3 for rectangular slab)	K_{ma} – hydraulic conductivity function in macropores
D – dispersion coefficient	K_{mi} – hydraulic conductivity function in micropores
K^*_s – fictitious saturated hydraulic conductivity	
ψ - pressure head	D_w – effective water diffusivity
β - geometry coefficient (= 3 for parallel fractures)	$D_{\theta mi}$ – water diffusivity at the current matrix water content
D^*_m – effective diffusion coefficient in micropore region	U_e – source-sink term for solute mass transfer between micro-/macropores
s – sorption coefficient	S_{ma} – macropore degree of saturation
D_e – effective diffusion coefficient	

3.1 Model Description

MACRO is a one-dimensional, dual-permeability model that considers transient fluxes of water, heat and solute in the variably saturated layered soil profile. The total porosity is partitioned into two separate flow regions (matrix and macropores), each with its own degree of saturation, conductivity, water flow rate, solute concentration, and solute flux density.

Full water balance is simulated taking into consideration occurrences such as precipitation, evapotranspiration, root water uptake, deep seepage and horizontal fluxes to tile drains. Convective–dispersive transport is calculated for solutes undergoing "two-site" (kinetic and instantaneous) sorption, passive plant uptake, and first-order degradation controlled by soil moisture and temperature. Table 3.2 below outlines the treatment of flow and transport processes in the MACRO model.

Table 3.2: Treatment of flow and transport processes in the MACRO model (Larsbo & Jarvis, 2003).

Process	Treatment
Unsaturated water flow	Richards' equation in micropores, gravity flow in macropores
Root water uptake	Empirical sink term, water preferentially extracted from macropores
Seepage to drains and groundwater	Seepage potential theory. Sink term in vertical water flow equations
Solute transport	Convection/dispersion equation in the micropores, mass flow only in the macropores
Mass exchange	Approximate first-order rate equations for mass exchange of both solute and water
Sorption	Instantaneous equilibrium/kinetic sorption according to the 'two-site' model, Freundlich isotherm, sorption partitioned between micro- and macropores.
Degradation	first-order kinetics, separate rate coefficients for four pools (solid and liquid, micro- and macropores)
Soil temperature	Heat conduction equation

3.2 Soil Water Flow

Richards' equation (equation 3.1) is used to calculate vertical water fluxes in the matrix:

$$C\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial z}\left[K\left(\frac{\partial \psi}{\partial z}+1\right)\right] \pm \sum S_i \qquad [3.1]$$

where C = $\partial\theta/\partial\psi$ (m^{-1}) is the differential water capacity, θ (m^3 m^{-3}) is the volumetric water content, ψ (m) is the soil water pressure head, t (s) is time, z (m) is depth, K (m s^{-1}) is the unsaturated hydraulic conductivity, and S_i (s^{-1}) are source–sink terms accounting for water exchange with macropores, drainage, and root water uptake.

The use of Eq. [3.1] to calculate water flows in the macropore domain is problematic; a major reason for this is the lack of information concerning $\psi(\theta)$ close to saturation. Therefore capillarity is assumed to be negligible in the macropores, thus water flow is driven by gravity only (i.e., $\partial\psi/\partial z$ = 0). The governing equation for water flow in macropores is the kinematic wave equation (Germann, 1985):

$$\frac{\partial\theta_{ma}}{\partial t} = \frac{\partial K_{ma}}{\partial z} \pm \sum S_i \qquad [3.2]$$

where θ_{ma} (m^3 m^{-3}) and K_{ma}(m s^{-1}) are the macropore water content and hydraulic conductivity, respectively.

3.3 Hydraulic Properties

In macroporous soils, hydraulic conductivity increases very rapidly across a small pressure head range as saturation is approached (Clothier and Smettem, 1990; Jarvis and Messing, 1995). In MACRO, a "cut and join" approach is used to define the matrix–macropore hydraulic functions (Jarvis et al., 1991). Thus, a user-defined pressure head, ψ_b (m), partitions the total porosity into matrix pores and macropores, while a corresponding water content, θ_b (m^3 m^{-3}), and hydraulic conductivity, K_b (m s^{-1}), represent the saturated state of the soil matrix.

Soil water retention in the matrix is calculated using a modified form of van Genuchten's (1980) equation (Vogel et al., 2001):

$$S = \frac{\theta_{mi} - \theta_r}{\theta_s^* - \theta_r} = \left(1 + |\alpha_{vg}\psi|^{n_{vg}}\right)^{-m_{vg}} \tag{3.3}$$

where S is an effective water content; m_{vg}, n_{vg}, and α_{vg} (m $^{-1}$) are shape parameters (where m_{vg} is set equal to 1-1/n_{vg}); θ_{mi} (m^3 m^{-3}) is the micropore water content; θ_r (m^3 m^{-3}) is the residual water content; and θ_s* (m^3 m^{-3}) is a "fictitious" saturated water content, obtained by extrapolating the fitted water retention function to zero pressure head. Parameter θ_s* does not represent the actual saturated water content in the model, which is separately defined by the user to reflect macroporosity. It is only used internally in the program to extend the retention curve to pressure head values larger than ψ_b to allow for temporary over-saturation in the micropores when solving Richard's equation.

The van Genuchten–Mualem model in the form given by Luckner et al. (1989) is used to describe the unsaturated hydraulic conductivity function in the matrix, using K_b as the 'matching point' hydraulic conductivity:

$$K_{mi} = K_b \left(\frac{S}{S_{mi(\theta_b)}}\right)^l \left\{\frac{\left[1 - \left(1 - S^{1/m_{vg}}\right)^{m_{vg}}\right]}{\left[1 - \left(1 - S_{mi(\theta_b)}^{1/m_{vg}}\right)^{m_{vg}}\right]}\right\}^2 \tag{3.4}$$

where l is the tortuosity factor, and S_{mi} is the effective water content at micropore saturation given by replacing ψ with ψ_b in Eq. [3.3].

The hydraulic conductivity function in the macropores is given as a simple power law of the macropore degree of saturation, S_{ma}:

$$K_{ma} = K_{s(ma)} S_{ma}^{n^*} = (K_s - K_b) S_{ma}^{n^*} \tag{3.5}$$

where $K_{s(ma)}$ (m s^{-1}) is the saturated hydraulic conductivity of the macropores, K_s (m s^{-1}) is the total saturated hydraulic conductivity, and n* is a "kinematic" exponent reflecting macropore size distribution and tortuosity. The macropore degree of saturation is expressed as:

$$S_{ma} = \frac{\theta_{ma}}{e_{ma}} \quad [3.6]$$

where e_{ma} is the macroporosity equivalent to the total saturated water content θ_s minus θ_b. Since macroporosity and macropore hydraulic conductivity keep varying due to shrinkage and swelling, Messing and Jarvis (1990) came up with the relationships as follows:

$$e_{ma} = e_s + p(\theta_b - \theta_{mi}) \quad [3.7]$$

Thence $$K_{s(ma)} = (K_{s(\min)} - K_b)\left(\frac{e_{ma}}{e_s}\right)^{m*} \quad [3.8]$$

where, p is the slope of the shrinkage characteristic, e_s is the minimum value of macroporosity given by θ_s - θ_b, $K_{s(\min)}$ is the minimum saturated hydraulic conductivity of a swelling soil attained when $e_{ma} = e_s$, and m^* is an empirical exponent.

3.4 Macropore – Micropore Water Exchange

In the absence of gravity, Richards' equation can be recast as a diffusion equation, with gradients in water content as the driving force. In MACRO, imbibition of water from macropores into an unsaturated matrix is treated as a first-order approximation to this water diffusion equation, assuming rectangular-slab geometry for the aggregates (van Genuchten and Dalton, 1986; Booltink et al., 1993):

$$S_w = \left(\frac{GD_w\gamma_w}{d^2}\right)(\theta_b - \theta_{mi}) \quad [3.9]$$

where d (m) is an effective diffusion pathlength calculated from $d = A/2L$ (Assuming parallel fractures in a unit area A, and L is the fracture length for each subclass). Gerke and van Genuchten (1993) also used the following relationship to calculate d:

$$d = \beta \theta_{mi} D_m^* / \alpha \qquad [3.10]$$

where, β is a geometry coefficient (equals 3 for parallel fractures); θ_{mi} is the micropore water content; D_m^* is an effective diffusion coefficient for the micropore region; and α is the mobile/immobile transfer rate exchange. The diffusion pathlength, d, is related to aggregate size and the influence of coatings on macropore and aggregate surfaces. In equation 3.9, D_w ($m^2\ s^{-1}$) is an effective water diffusivity, G is a geometry factor (*set internally to 3 for a rectangular slab geometry*; Gerke and van Genuchten, 1996), and γ_w is a scaling factor introduced to match the approximate and exact solutions to the diffusion problem (Gerke and van Genuchten, 1993). The scaling factor γ_w varies with the initial water content and hydraulic properties, but not strongly, so for simplicity γ_w is set within the program to an average value (Gerke and van Genuchten, 1993; Jarvis, 1994) The effective water diffusivity is given by

$$D_w = \left(\frac{D_{\theta_b} + D_{\theta_{mi}}}{2} \right) S_{ma} \qquad [3.11]$$

where $D_{\theta b}$ ($m^2\ s^{-1}$) and $D_{\theta mi}$ ($m^2\ s^{-1}$) are the water diffusivities at the saturated matrix water content and the current matrix water content, respectively, and where S_{ma} is introduced to account for incomplete wetted contact area between the two pore domains. In the Mualem–van Genuchten model, $D_{\theta mi}$ is given by (van Genuchten, 1980)

$$D_{\theta_{mi}} = \left[\frac{(1 - m_{vg}) K_s^*}{\alpha_{vg} m_{vg} (\theta_s^* - \theta_r)} \right] S^{1 - 1/m_{vg}} \left[\left(1 - S^{1/m_{vg}}\right)^{-m_{vg}} + \left(1 - S^{1/m_{vg}}\right)^{m_{vg}} - 2 \right] \qquad [3.12]$$

where K_s* (m s^{-1}) is a "fictitious" saturated hydraulic conductivity obtained by extrapolating the matrix conductivity function to zero pressure head. $D_{\theta b}$ is given by setting S in Eq. [3.12] to $S_{mi(\theta b)}$. It should be noted that the true saturated hydraulic conductivity of the soil (see Eq. [3.5]) will usually be larger than K_s* as a result of the effects of macropores.

Equation [3.9] is treated as a source term to Eq. [3.1] and a sink term to Eq. [3.2]. Water transfer in the reverse direction (from the matrix to macropores) occurs instantaneously when the pressure head in the matrix exceeds ψ_b following the fundamental physical principle governing the filling of pores when the water-entry pressure is exceeded.

In MACRO, flow to drains occurs if the macropores are saturated irrespective of the degree of saturation of micropores. Drainage is considered for lateral flow to seepage surfaces, that is, a source sink term in Richard's Equation (equation 3.1). Drainage scenarios could be flow to field drains (i.e. ditches or drains with highly permeable backfill) or groundwater seepage to a secondary drainage system (streams, canals, or perimeter field ditches). Assumptions are that the drains are overlain by fully penetrable seepage surfaces.

3.5 Solute Transport

Solute transport is calculated using the convection–dispersion equation with source–sink terms, U_i (kgm^{-3} s^{-1}), to represent a wide range of processes, including mass exchange between flow domains, kinetic sorption, solute uptake by plants, biodegradation, and lateral leaching losses to drains and/or regional groundwater:

$$\frac{\partial\left[c\theta_{mi(m)} + (1 - f - f_{ne})\gamma s\right]}{\partial t} = \frac{\partial}{\partial z}\left(D\theta_{mi(m)}\frac{\partial c}{\partial z} - qc\right) - \sum U_i \quad [3.13]$$

where s (kg kg^{-1}) is the sorbed concentration in the equilibrium pool, c (kg m^{-3}) is the concentration in solution, f is the mass fraction of the solid material in contact with water in the macropore domain, f_{ne} is the fraction of the solid material providing nonequilibrium (i.e., kinetic) sorption sites, $\theta_{mi(m)}$ (m^3 m^{-3}) is the accessible water content accounting for anion exclusion, q (m s^{-1}) is the water flow rate, and D (m^2 s^{-1}) is the dispersion coefficient calculated as the sum of an effective diffusion coefficient and a dispersion term. In the macropores, an equivalent approach is used to calculate transport, except that dispersion is assumed to be zero and only equilibrium sorption is considered. Equilibrium sorption partitioning is calculated using the Freundlich isotherm:

$$s = k_f c^m \qquad [3.14]$$

where, k_f is the sorption coefficient and m is the Freundlich exponent.

3.6 Solute Uptake by the Matrix

The source–sink term for mass transfer of solute between matrix and macropores, U_e (kgm^{-3} s^{-1}), is given by a combination of a diffusion component and a mass flow component:

$$U_e = \left(\frac{G_f D_e \theta_{mi(m)}}{d^2} \right) (c_{ma} - c_{mi}) + S_w c' \qquad [3.15]$$

where the prime notation indicates either the solute concentration in macropores or in "accessible water" in the matrix, depending on the direction of water flow, S_w, and D_e (m^2 s^{-1}) is an effective diffusion coefficient.

3.7 Macropore Flow in MACRO 5.0

A pressure head, ψ_b, and the corresponding water content, θ_b defines the division between flow domains (Refer to figure 3.1 below).

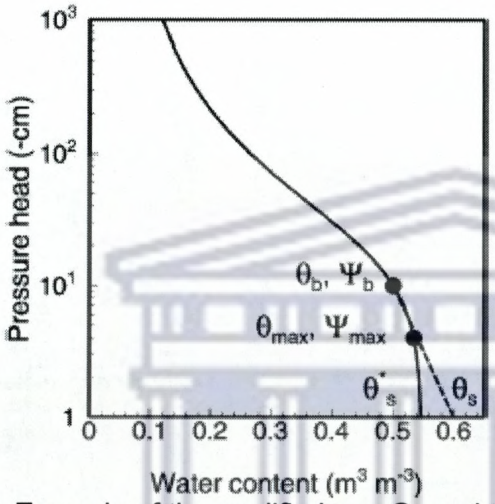


Figure 3.1: Example of the modified van Genuchten soil water retention function used in MACRO for a fictitious soil (α_{vg} = 0.03 cm^{-1}, n_{vg} = 1.5, θ_r = 0, θ_b = 0.5 $m^3\ m^{-3}$) (Larsbo et al, 2005)

If the water content in the matrix exceeds θ_b, the excess water will drain into the macropores. However, the macropores only have a finite storage capacity for water, C_{ma} ($m^3\ m^{-3}$), equal to:

$$C_{ma} = (1 - S_{ma})(\theta_s - \theta_b) \quad [3.16]$$

Therefore, an additional point on the modified van Genuchten retention curve (θ_{max} [$m^3\ m^{-3}$], ψ_{max} [m]) defines the maximum amount of water allowed in the matrix at each timestep ($\theta_{max} = \theta_b + C_{ma}$). When solving Richards' equation, the pressure heads are allowed to increase above ψ_{max} only if the macropores are also saturated. In this situation, the differential water capacity in the matrix is set to zero for pressures above ψ_{max}. For pressure heads above ψ_b, the hydraulic conductivity is set to K_b. Once Richards' equation has been solved, all water exceeding θ_b is instantly removed from the matrix and added to the macropores.

The local water balance in the macropores is solved implicitly for S_{ma} using a bisection method ("interval halving") for each layer, in turn, from the soil surface downward. If the flow capacity of both matrix and macropores is exceeded in any layer, then the local water balance cannot be solved (oversaturation develops in the macropores). In this case, the excess water is added to the macropore storage in the layer(s) above, and the water fluxes between layers are corrected accordingly.

3.8 Root Water Uptake

This phenomenon is calculated from evaporative demand, root distribution and soil water content (Jarvis, 1989). The ratio between the actual and potential root water uptake (E_a/E_r) is assumed to vary as a function of a dimensionless water index, and in addition to that, a threshold function is assumed before transpiration is reduced. The dimensionless water stress index is denoted as ω^* and the threshold function as ω^*_{c}. Feddes et al (1976) again assumes a threshold type of response for the reduction factor, ω, accounting for soil conditions that are either too wet or too dry. These threshold relations are displayed on figures 3.2 and 3.3 respectively.

Root water uptake is assumed to be reduced to zero both at the saturated water content θ_s and also at the extractable water content (wilting point) θ_w. Thus the calculated uptake is preferentially extracted from water in the macropores and then any excess demand is taken from water stored in the micropores.

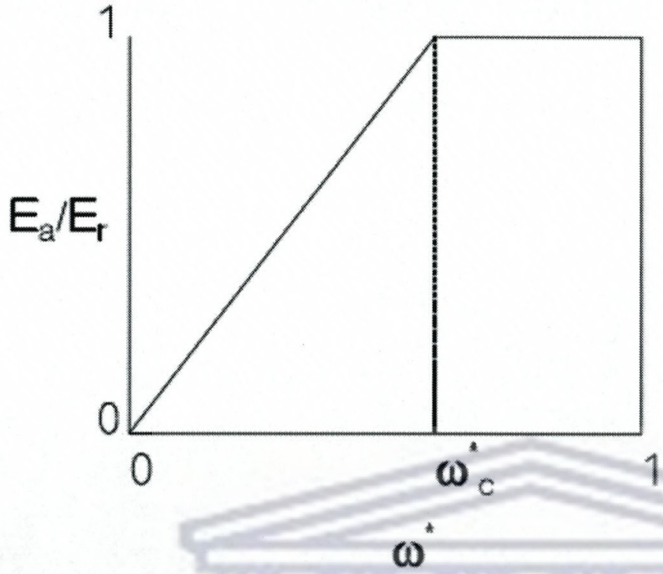


Figure 3.2: Ratio of actual to potential transpiration as a function of the stress index ω^*.

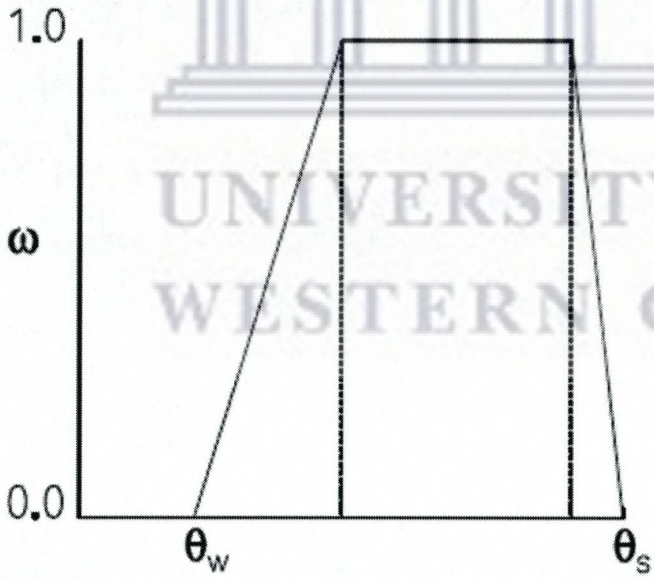


Figure 3.3: Soil water stress function for reduction of transpiration

3.9 Simulation output reading

After the simulation is complete, two files are created as resulting outputs; a binary (*.bin) file and a (*.sum) file. There are three different ways of reading and using them for further analysis. In this study, the (*.bin) file was used for further analysis. The first way to read a (*.bin) file is to convert it into ASCII from the program and create a text file which can then be imported into any graphics program like EXCEL. The second way would be to read the (*.bin) file directly using the auxiliary program PG supplied with MACRO. The output variables are limited to 400 in this case. The third way is to use built-in tools and functions to compare simulated with measured data by calculating goal functions, or by plotting such comparisons. Although all three ways were tested, only the first one was applied in this study. The process followed is covered in Chapter 5.

3.10 Motivation for selecting MACRO 5.0

For the purpose of this study, the software model MACRO 5.0 was selected among several other models that were reviewed. This Section outlines the reasons for this selection.

The main selection criterion was that MACRO can simulate in the unsaturated zone and it takes preferential (macropore) flow into account. Different types of contaminants are accommodated for simulation. It also takes into consideration the interaction of water and solutes with the solid phase.

MACRO is capable of simulating conditions encountered at the site. This is a one-dimensional model and therefore it could be used where field data show that vadose zone flow or ground water flow and transport processes are relatively simple. Also, it should be used primarily for sites where the degree of heterogeneity or anisotropy is low, known to be isotropic, or sites where a potential receptor is immediately down-gradient from contaminant source.

Shortage of data is to some extent accommodated in MACRO. For example, if minimum and maximum temperatures are not available, the daily mean temperature can be substituted for both variables. MACRO requires two data files to run a simulation. Those are precipitation data and meteorological data to calculate potential evaporation. However, temperatures and pre-calculated potential evaporation data can be used if meteorological data are not available or not adequate. In South Africa, not all the required data is readily available, so the flexibility of this model to allow the usage of alternative data files helps with simulations based on the representative enough data that could be acquired.

A model calibration consists of changing values of model input parameters in an attempt to match field conditions within some acceptable criteria. MACRO is capable of comparing model-simulated conditions and field conditions. These comparisons are presentable in tables and/or graphs. Generally, there are no universally accepted "goodness-of-fit" criteria that apply in all cases. However, it is important that the modeller makes every attempt to minimize the difference between model-simulated and field conditions. MACRO has been extensively used and hence tested in the field in different areas with research studies such as Lodgson (2002); Selim and Ma (1998); and Alaoui et al. (2003).

CHAPTER 4

MODELLING PROCESS DATA AND SET-UP FOR CASE STUDY SITES

This chapter describes how the simulation data were obtained for both areas. Moreover, it gives insight to the simulation set-up process that was followed in this study.

The climate data (i.e. temperature, relative humidity and rainfall) required for MACRO obtained from the South African Weather Bureau, also known as Weather SA. These data are vital as they are inputs in the modelling process. Soil data were obtained from various organizations like the Institute for Soil, Climate and Water (ARC - ISCW) and the Engineering Geology Unit of the Council for Geoscience (CGS). This information assisted in the description of soil properties/characteristics where needed in the model. Groundwater data, including chemistry data, were obtained from the National Groundwater Database (NGDB) administered by the Department of Water Affairs and Forestry (DWAF). Such data were used as input to eventually understand the extent of groundwater pollution in the study areas and to determine the depth of their vadose zones. Some land use information was abstracted from various reports in order to know the locations of different possible pollution sources and their expected contaminants. The Cape Flats aquifer with its vadose zone information was obtained from the Campus Test Site of the University of the Western Cape. That contributed to the understanding of the Cape Flats vadose zone. For the case study, soil hydraulic properties collected from iThemba Labs were used in the simulation process (Samuels, 2007). Monitoring data from Jarrod Ball and Associates assisted with the amounts of contaminants in the Coastal Park area covering the simulation period (Jarrod Ball & Associates, 2003). In addition to the other data sources for Mpumalanga Highveld, some data were acquired from SASOL and their previous reports. The website http://fred.csir.co.za/extra/project/avap/ is also referred to.

4.1 Climate data formatting for input process

In the case of MACRO, climate data such as relative humidity, and maximum and minimum temperatures were used to estimate reference evapotranspiration for the period 1993 to 2005. In order to achieve this, the ETo calculator software (developed by the University of Pretoria and NB Systems cc) was used (Annandale et al., 1999). The ETo calculator calculates reference evapotranspiration according to the procedure of Allen et al. (1998). Figure 4.1 displays the behavioural pattern of reference evapotranspiration over the period 1993 to 2005 for the Cape Flats and an example of the data used is attached in Appendix A. In the case of Mpumalanga Highveld, such data are available in Appendix B.

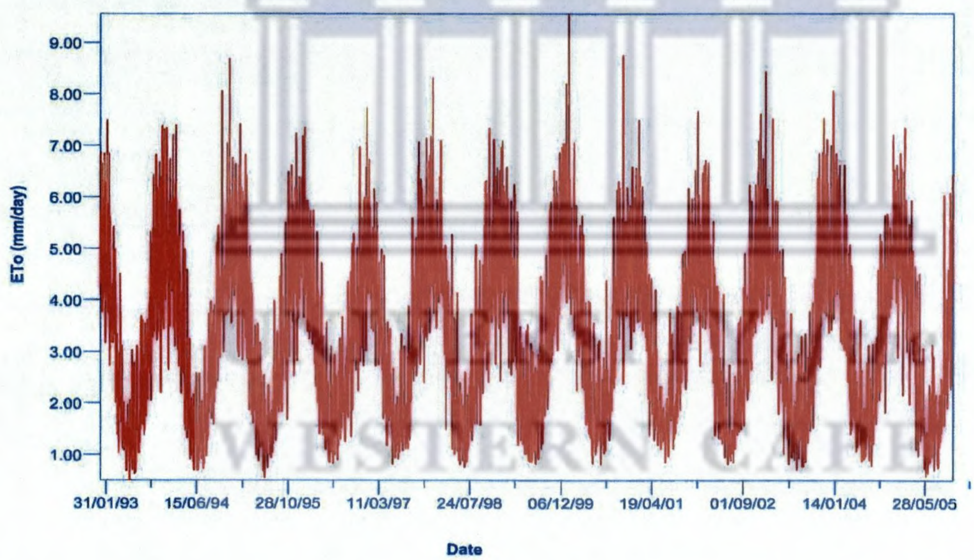


Figure 4.1: Evapotranspiration pattern for Cape Flats over a period from 1993 to 2005.

In the absence of measured data for the Cape Flats, the ETo calculator was used to calculate reference evapotranspiration from estimated solar radiation (Rs) and wind speed (U). For Mpumalanga Highveld, the measured relative humidity was not available and therefore the estimated vapour pressure (VP) was included in the calculation. The estimated reference evapotranspiration data, together with temperature data, were then converted from text format to binary format in order to be uploaded into the MACRO program under the *Simulation Set – Up* tab as explained in detail below.. The same procedure was followed for rainfall data. Examples of uploaded driving data for both Cape Flats (in 2004) and Secunda (in 2002) areas are attached in Appendices A and B, respectively. Weather SA provided rainfall and temperature data.

4.2 Input of data

MACRO 5.0 includes five tabs, namely Properties, Options, Parameters, Outputs, and Simulation Setup. Any input and data upload changes done prior the simulation should be saved otherwise they will not be detected and thus not included in the simulation process. That implies incorrect simulation results. The tabs are discussed below.

PROPERTIES – This is where various properties of a given soil profile are described, including the number of horizons and the numerical layers assigned for the simulation (between 60 and 200 numerical layers). In the simulations for this study, 60 numerical layers were used. The properties of the soil profiles used in the simulations are shown in Table 4.1.

Table 4.1: Properties of soil profiles used for the Cape Flats (Adams - unpublished data and Samuels, 2007) and the Mpumalanga Highveld (Saayman et. al., 2007) areas.

Horizon	Clay %	Silt %	Sand %	pH	Bulk Density (g/m^3)	Organic C %	Thickness (cm)	Texture	Shape
Cape Flats									
Ap	0	0	100	7.00	1.30	2.00	50	Sand	Granular
B	1	5	94	7.00	1.10	1.00	250	Sand	Granular
Mpumalanga Highveld									
Ap	26	22	52	4.20	1.20	1.28	200	Sandy clay loam	Granular
B	42	22	36	5.20	1.40	1.14	200	Clay	Granular
C	46	22	32	7.00	1.40	0.46	400	Clay	Granular

OPTIONS – This tab has four subdivisions, namely; Boundary conditions, Site Management, Crop and Solute. Here, the lower boundary conditions and initial conditions are defined, for instance one can use water table in the soil profile as the lower boundary condition. Site management option covers the tillage, irrigation and drainage conditions of the given area. The type of solute to simulate (including mass units), together with the sorption type are covered under the Solute option, whilst the crop type is defined under the Crop option. The program does not require characteristics of a given specific solute, but rather it requires the user to select a group type under which the solute falls. For example, one of the solute options is *pesticide* and not the name and specific characteristics of that pesticide the user is trying to simulate. However, the user is able to adjust some parameters in the program to suit solutes other than pesticides, for example in the case of boron, degradation rates can be set to zero since they are not applicable. The solute properties are selected in the PARAMETERS tab.

For the Cape Flats, water table at the bottom of the soil profile was selected as the lower boundary condition. Chloride (in mg/m^3), under the group type tritium (more comparable to chloride which does not sorb and degrade), was used as the solute to simulate because its concentrations in groundwater have been monitored in Coastal Park for a period within which the simulation period for this study lies. Under site management, tillage and irrigation were not considered since they are not applicable in the case of Coastal Park. According to Blight et al. (2005), chloride in groundwater was measured to be 4000 mg/l in 1999 and by 2004 it had increased to approximately 4500 mg/l since lithium and sodium chloride had been injected as tracers. Therefore 4000 mg/l was used as an initial concentration in the boundary since the boundary is set as the bottom of the soil profile, the water table depth. Field drains option was selected to simulate lateral flow. The Cape Flats area simulations resulted in rapid build-up of the water table when field drains were not selected. Crop type is perennial since there is no annual cultivation taking place but shrubs and grass are thriving.

In the case of Mpumalanga Highveld, pesticide (parent compound) was selected with degradation coefficients adjusted to zero to simulate boron and fluoride. Irrigation was also considered due to effluent application on the site for a period of more than ten years. According to the Sasol reports, the recommended amount of irrigation effluent was such that it is equal to net water deficit which was estimated at approximately 737 mm/annum for the area. However, the actual irrigation rate was lower. Bi-weekly amounts, based on the data given by Ginster (2002) as plots, were used and these data are attached in Appendix E for Indaba irrigation site and Appendix F for Goedehoop irrigation site. Data from the Indaba site had to be used for calibration since the solute concentration with respect to depth data were not available from the Goedehoop site. However, these two sites have similar environmental conditions.

PARAMETERS and OUTPUTS – These Input and Output parameters are selected according to what one wants to simulate, and not necessarily all of them at the same time. For instance, one could be interested in the response of water content output when hydraulic conductivity as an input is varied, hence only water content related parameters can be selected for the output file. The outputs to select at a given simulation time are limited in order to get readable output files. The program is not able to handle large chunks of data with regard to the output files. It can be mentioned, without disregarding other parameters, that the Physical Parameters and Solute sections are very crucial as inputs for the determination of preferential flow and the sensitivity analysis to changing input conditions. Input parameters used in this study are shown in Tables 4.2 and 4.3 for both case study areas, and Table 4.4 shows the list of outputs.

Table 4.2: Simulation input parameters for the Cape Flats area.

SUBDIVISION	PARAMETER	VALUE (units)
CROP	Root distribution - RPIN	Program default values applied
	Fraction of available water exhausted before reduction in transpiration occurred - FAWC	
	Critical soil air content for root water uptake - CRITAIR	
	Root adaptability factor - BETA	
	Canopy interception capacity - CANCAP	
	Correction factor for wet canopy evaporation - ZALP	
INITIAL/BOU-NDARY CONDITIONS	Solute concentration at bottom boundary - CONCIN	4000 (mg/l) for Chloride (Blight et al., 2005)
	Drainage basin area - AREA	1 (ha)
	Empirical parameter controlling percolation out of the bottom of the profile - BGRAD	0.00001 (h^{-1})
	Initial soil temperature - TEMPINI	10 (°C)
	Initial solute concentration in soil water - SOLINIT	1 (mg/m^3)
IRRIGATION	Not applicable	Not applicable
PHYSICAL PARAMETERS	Tortuosity/Pore size distribution factor in macropores - ZN	Default
	Tortuosity factor in micropores - ZM	Default
	Trapped air content - TRAP_AIR	Default
	Slope of shrinkage characteristic - ZP	0
	Exponent in the power function relating macropore hydraulic conductivity to macroporosity - ZA	0
	Bulk density - GAMMA	1.3 (g/cm^3) in A- horizon and 1.1 (g/cm^3) in B - horizon. (Samuels, 2007)
	Saturated water content - TPORV	A: 38 %, B: 28 % (Samuels, 2007)
	Boundary water content - XMPOR	A: 30 %, B: 20 %
	Boundary soil water tension - CTEN	Default
	Residual water content - RESID	A: 0.0006 %, B: 0.0362 % (Samuels, 2007)
	van Genuchten's n value - N	A: 1.68, B: 1.59 (Samuels, 2007)
	van Genuchten's alpha - ALPHA	A: 0.011(cm^{-1}), B: 0.33 (cm^{-1}) (Samuels, 2007)
	Saturated hydraulic conductivity - KSATMIN	300 (mm/h) (Samuels, 2007)
	Boundary hydraulic conductivity - KSM	0.1 (mm/h) by $^{+}$Pedotransfer function
	Effective diffusion pathlength - ASCALE	A: 3 mm, B: 6 mm by $^{+}$Pedotransfer function
SITE	Average annual temperature at the site - ANNTAV	18 (°C)
	Average annual amplitude in temperature - ANNAMP	10 (°C)
	Rainfall correction factor - RAINCO	1
	Snowfall correction factor - SNOWCO	1
	Snowmelt factor - SNOWMF	0 (mm/°C/day)
	Site latitude - PHI	34°
	Average rainfall intensity at the site - RINTEN	Default
	Ditch/Drainage depth for secondary drainage system - LAYERD	3 m
	Residence time for regional groundwater flow rate - RGWFLOW	1 day
	Drain depth (primary drainage system) - DRAINDEP	3 m

	Drain spacing - SPACE	10 m
SOLUTE	Excluded volumetric water content - AEXC	Default
	Sorption distribution coefficient - ZKD	Default
	Degradation rate coefficient, micropores, liquid phase - DEGMIL	Default, when applicable
	Degradation rate coefficient, macropores, liquid phase - DEGMAL	Default, when applicable
	Degradation rate coefficient, micropores, solid phase - DEGMIS	Default, when applicable
	Degradation rate coefficient, macropores, solid phase - DEGMAS	Default, when applicable
	Freundlich exponent - FREUND	Default (0 < FREUND <1)
	Other parameters	Default values applied
NUMERICAL LAYERS	Horizons thickness	A: 50 cm, B: 250 cm

[+]Pedotransfer on the table is an inbuilt default function used to estimate some parameters based on the available input parameters.

Table 4.3: Simulation input parameters for Mpumalanga Highveld area.

SUBDIVISION	PARAMETER	VALUE (units)
CROP	Root distribution - RPIN	Program default values applied
	Fraction of available water exhausted before reduction in transpiration occurred - FAWC	
	Critical soil air content for root water uptake - CRITAIR	
	Root adaptability factor - BETA	
	Canopy interception capacity - CANCAP	
	Correction factor for wet canopy evaporation - ZALP	
INITIAL/BOUNDARY CONDITIONS	Solute concentration at bottom boundary - CONCIN	B - 41.535, F - 1360 mg/m^3 (Saayman et al, 2007)
	Drainage basin area - AREA	205 ha, [96 ha - Goedehoop]. (Ginster, 2002)
	Empirical parameter controlling percolation out of the bottom of the profile - BGRAD	0.00001 (h^{-1})
	Initial soil temperature - TEMPINI	10 (°C)
	Initial solute concentration in soil water – SOLINIT[#]	1 (mg/m^3) initially[#]
PHYSICAL PARAMETERS	Tortuosity/Pore size distribution factor in macropores - ZN	Default
	Tortuosity factor in micropores - ZM	Default
	Trapped air content - TRAP_AIR	Default
	Slope of shrinkage characteristic - ZP	Default
	Exponent in the power function relating macropore hydraulic conductivity to macroporosity - ZA	Default
	Bulk density - GAMMA	1.2 (g/cm^3) in A, 1.4 (g/cm^3) in B & C horizons (Saayman et al, 2007)
	Saturated water content - TPORV	Default
	Boundary water content - XMPOR	Default
	Boundary soil water tension - CTEN	Default
	Residual water content - RESID	Default
	van Genuchten's n value - N	Default
	van Genuchten's alpha - ALPHA	Default
	Saturated hydraulic conductivity - KSATMIN	Default

	Boundary hydraulic conductivity - KSM	0.1 (mm/h) by +Pedotransfer function
	Effective diffusion pathlength - ASCALE	20 (mm) by +Pedotransfer function
SITE	Average annual temperature at the site - ANNTAV	19 (°C)
	Average annual amplitude in temperature - ANNAMP	7 (°C)
	Rainfall correction factor - RAINCO	1
	Snowfall correction factor - SNOWCO	1
	Snowmelt factor - SNOWMF	0 (mm/°C/day)
	Site latitude - PHI	26°
	Average rainfall intensity at the site - RINTEN	2 (mm/h)
	Ditch/Drainage depth for secondary drainage system - LAYERD	7 m
	Residence time for regional groundwater flow rate - RGWFLOW	1 day
	Drain depth (primary drainage system) - DRAINDEP	7 m
	Drain spacing - SPACE	10 m
IRRIGATION	Solute concentration in irrigation water - CONCI	47 mg/l for Fluoride and 10 mg/l for Boron (SASOL, 2002)
	Day of irrigation - IRRDAY	1 – 1461 days (approx. four years)
	Irrigation amount - AMIR	Bi-weekly amounts varying each year (see Appendix F)
	Start time of irrigation - IRRSTART	8 am
	End time of irrigation - IRREND	16 pm
	Fraction of irrigation intercepted by crop canopy - ZFINT	Default
SOLUTE	Excluded volumetric water content - AEXC	Default
	Sorption distribution coefficient - ZKD	Default
	Degradation rate coefficient, micropores, liquid phase - DEGMIL	0
	Degradation rate coefficient, macropores, liquid phase - DEGMAL	0
	Degradation rate coefficient, micropores, solid phase - DEGMIS	0
	Degradation rate coefficient, macropores, solid phase - DEGMAS	0
	Freundlich exponent - FREUND	Default (0 < FREUND <1)
	Other parameters	Default values applied
NUMERICAL LAYERS	Horizons thickness	A: 200 cm, B: 200 cm, C: 400 cm (Saayman et al, 2007)

+Pedotransfer on the table is an inbuilt default function used to estimate some parameters based on the available input parameters.

#SOLINIT values were determined from 4-year interval simulations (see paragraph below).

Small initial concentration (1 mg/m^3) was applied for the time of the beginning of effluent irrigation. Since MACRO cannot take more than 100 irrigation records, 4 – year interval simulation runs to estimate such solute concentrations in soil during irrigation period where effluent was applied twice every month were performed.

Table 4.4: Output parameters considered for both case study areas.

SELECTED OUTPUT PARAMETERS	MACRO 5.0 SYMBOL
Water content, micropores	THETA
Water content, macropores	THETI
Total water content	THETT
Water tension	CPSI
Water exchange rate (positive from macropores)	EXCHANGE
Degree of saturation in macropores	THETAMA
Root water uptake	ZUPTAKE
Accumulated precipitation	TTPRECIP
Net rainfall	RAIN
Accumulated net rainfall	RRNRAIN
Total accumulated tile drainage	TSEEP
Accumulated water flow to secondary flow drainage system	GSTOT
Actual evapotranspiration rate	CETA
Potential evapotranspiration rate	EPOT
Accumulated potential evapotranspiration rate	CCEPOT
Accumulated potential soil evaporation	CPSOIL
Potential soil evaporation rate	PSOIL
Accumulated potential transpiration	CUPT
Accumulated percolation	TFLOWOUT
Accumulated infiltration	CINFIL
Water storage (canopy)	CRES
Solute concentration in soil solution (micropores)	SOLMIC
Solute concentration in soil solution (macropore)	SOLMAC
Solute exchange rate, each layer (positive from macropores)	CEXCH
Total accumulated solute leaching	TSOUT
Accumulated amount of solute lost to regional groundwater	GSINK
Accumulated amount of solute lost to tile drains	DRAINLOS
Total solute flow to tile drains	DSOLTOS
Accumulated amount of solute degraded in soil	TDEG
Accumulated uptake of solute by crop	TUPT
Solute concentration in tile drainage water	DRAINCON
Solute concentration in groundwater flow	GRCON

A summary of baseline parameters, changed/varied parameters and output parameters that were looked at in these simulations are also listed in Table 5.1 of Chapter 5.

SIMULATION SETUP – This section allows for uploading of rainfall data, and evapotranspiration and temperature data. The period to simulate over is set here and it can be changed after a complete run. The simulation period from 1999 to 2004 was chosen for the Cape Flats and from 1998 to 2002 for Mpumalanga Highveld. The year 2006 was also simulated for the Cape Flats area in order to compare measured 2006 data with simulated data. The reason for selecting these periods is that the available measured data, especially for solute concentrations, fall within them. That is useful when comparing simulated data and measured data. Shorter periods also help in the detection of slight changes within the profile, for example hydraulic conductivity break-ups between soil layers of different properties. In this tab, the user also defines the folder into which the output results are to be stored.

CHAPTER 5

MODEL SIMULATIONS

Two sections are dealt with in this Chapter. Firstly, the MACRO 5.0 model is calibrated by comparing measured data and simulated data from both case study areas, with the aim of gaining confidence with the predictions of the model. This comparison is presented graphically and described in Section 5.1. Secondly, sensitivity analyses of model output are carried out for some inputs particularly relevant to preferential flow. The aim was to assess the effects of inputs relevant to preferential flow on the results of the model, in particular soil water and solute balance. The results of the sensitivity analyses were then plotted and described as seen in graphs of Section 5.2 for both case study areas areas.

The input and output parameters used for simulation and analysis are tabulated (see Table 5.1) and those parameters concerning irrigation are only applicable to the Mpumalanga Highveld. Additionally, the MACRO 5.0 symbols described in Table 5.1 for different parameters will be used in the legends of output plots/graphs in this Chapter. Thus, their descriptions as in the table will apply.

Table 5.1: Input and Output Parameters used for Simulation and Analyses.

BASELINE INPUT DATA	MACRO 5.0 SYMBOL	CHANGED INPUT DATA	MACRO 5.0 SYMBOL	SELECTED OUTPUT PARAMETERS	MACRO 5.0 SYMBOL
pH	pH	Clay, Silt, Sand percentages		Water content, micropores	THETA
Root distribution	RPIN	Bulk density	GAMMA	Water content, macropores	THETI
Fraction of available water exhausted before reduction in transpiration occurred	FAWC	Saturated water content	TPORV	Total water content	THETT
Critical soil air content for root water uptake	CRITAIR	Boundary water content	XMPOR	Water tension	CPSI
Root adaptability factor	BETA	Boundary soil water tension	CTEN	Water exchange rate (positive from macropores)	EXCHANGE
Canopy interception capacity	CANCAP	Residual water content	RESID	Degree of saturation in macropores	THETAMA
Correction factor for wet canopy evaporation	ZALP	van Genuchten's n value	N	Root water uptake	ZUPTAKE
Solute concentration at bottom boundary	CONCIN	van Genuchten's alpha	ALPHA	Accumulated precipitation	TTPRECIP
Drainage basin area	AREA	Saturated hydraulic conductivity	KSATMIN	Net rainfall	RAIN
Empirical parameter controlling percolation out of the bottom of the profile	BGRAD	Boundary hydraulic conductivity	KSM	Accumulated net rainfall	RRNRAIN
Initial soil temperature	TEMPINI	Slope of shrinkage characteristic	ZP	Total accumulated tile drainage	TSEEP
Initial solute concentration in soil water	SOLINIT	Exponent in the power function relating macropore hydraulic conductivity to macroporosity.	ZA	Accumulated water flow to secondary flow drainage system	GSTOT
Tortuosity/Pore size distribution factor in macropores	ZN	Effective diffusion pathlength	ASCALE	Actual evapotranspiration rate	CETA
Tortuosity factor in micropores	ZM	Excluded volumetric water content	AEXC	Potential evapotranspiration rate	EPOT
Trapped air content	TRAP_AIR	Sorption distribution coefficient	ZKD	Accumulated potential evapotranspiration rate	CCEPOT
Average annual temperature at the site	ANNTAV	Degradation rate coefficient, micropores, liquid phase	DEGMIL	Accumulated potential soil evaporation	CPSOIL

BASELINE INPUT DATA	MACRO 5.0 SYMBOL	CHANGED INPUT DATA	MACRO 5.0 SYMBOL	SELECTED OUTPUT PARAMETERS	MACRO 5.0 SYMBOL
Average annual amplitude in temperature	ANNAMP	Degradation rate coefficient, macropores, liquid phase	DEGMAL	Potential soil evaporation rate	PSOIL
Rainfall correction factor	RAINCO	Degradation rate coefficient, micropores, solid phase	DEGMIS	Accumulated potential transpiration	CUPT
Snowfall correction factor	SNOWCO	Degradation rate coefficient, macropores, solid phase	DEGMAS	Accumulated percolation	TFLOWOUT
Snowmelt factor	SNOWMF			Accumulated infiltration	CINFIL
Site latitude	PHI			Water storage (canopy)	CRES
Average rainfall intensity at the site	RINTEN			Solute concentration in soil solution (micropores)	SOLMIC
Ditch/Drainage depth for secondary drainage system	LAYERD			Solute concentration in soil solution (macropore)	SOLMAC
Residence time for regional groundwater flow rate	RGWFLOW			Solute exchange rate, each layer (positive from macropores)	CEXCH
Drain depth (primary drainage system)	DRAINDEP			Total accumulated solute leaching	TSOUT
Drain spacing	SPACE			Accumulated amount of solute lost to regional groundwater	GSINK
Freundlich exponent	FREUND			Accumulated amount of solute lost to tile drains	DRAINLOS
Solute concentration in irrigation water	CONCI			Total solute flow to tile drains	DSOLTOS
Day of irrigation	IRRDAY			Accumulated amount of solute degraded in soil	TDEG
Irrigation amount	AMIR			Accumulated uptake of solute by crop	TUPT
Start time of irrigation	IRRSTART			Solute concentration in tile drainage water	DRAINCON
End time of irrigation	IRREND			Solute concentration in groundwater flow	GRCON
Fraction of irrigation intercepted by crop canopy	ZFINT				
Horizons thickness					

5.1 MACRO 5.0 simulations for the case studies

5.1.1 Simulations for the Cape Flats area

Tables 5.2, 5.3 and 5.4 show the comparison between measurements and simulations. Concentration data are taken over a period from 1999 to 2004 whilst water content data is for July 2006. This is because measured data were available within this period for the Coastal Park area. In Table 5.2, measured data are presented in seasons as weighted averages for which their plots are available from Ball & Novella (2003) report. These are averages of records from a line of mini-wells and boreholes drilled in 1987 in the Coastal Park for experimental purposes. The dates from the simulation outputs were selected with the assumption that they correspond with the mentioned seasons of measured data.

Table 5.2: Measured and simulated chloride concentration data for Cape Flats area.

Season	Date	Measured average borehole concentration (mg/l)	Simulated concentration at 300 cm depth (mg/l)
1999 Wet	1999/06/05	649	37
1999 Dry	1999/12/15	642	34
2000 Wet	2000/06/05	274	113
2000 Dry	2000/12/15	370	27
2001 Wet	2001/06/05	317	57
2001 Dry	2001/12/15	573	750
2002 Wet	2002/06/05	904	1098
2002 Dry	2002/12/15	830	728
2003 Wet	2003/06/05	814	1110
2003 Dry	2003/12/15	555	761
2004 Wet	2004/06/05	737	1144
2004 Dry	2004/12/15	554	765

Ball & Novella (2003) report the existence of seawater intrusion in boreholes, which causes an increase in chloride concentration. According to Blight et al. (2005), during the period 1998/1999 the landfill height was raised by about 5 m and lithium and sodium chloride were injected as tracers. That also contributed to an increase in chloride concentration. Further, raising of the landfill height followed during the 1999/2000 period, and a lot of obstructions to the process were reportedly experienced. That could have resulted in distorted records. Again, the fact that the soil profiles used for simulation were not from the chloride sampling site could be the cause of visible differences between some measured and simulated data displayed in Table 5.2. These data are presented graphically in Figure 5.1, where definite trends are consistent for measured and simulated data.

The graphical trends of data in Tables 5.3 and 5.4 are displayed in Figure 5.2.

Table 5.3: Simulated water content (m^3/m^3) data for Cape Flats area.

Depth (cm)	2006/06/28	2006/07/06	2006/07/18	2006/07/20	2006/07/25	2006/07/27	2006/07/29
0	0.278	0.261	0.260	0.294	0.277	0.277	0.267
50	0.298	0.295	0.291	0.311	0.299	0.297	0.294
100	0.189	0.177	0.165	0.163	0.163	0.179	0.194
150	0.199	0.190	0.178	0.176	0.172	0.171	0.170
250	0.153	0.172	0.194	0.193	0.189	0.188	0.186
300	0.280	0.280	0.280	0.280	0.280	0.280	0.280

Table 5.4: Measured water content (m^3/m^3) data for Cape Flats area.

Depth (cm)	2006/06/28	2006/07/06	2006/07/18	2006/07/20	2006/07/25	2006/07/27	2006/07/29
0	0.383	0.380	0.354	0.349	0.254	0.217	0.207
50	0.381	0.377	0.348	0.343	0.200	0.157	0.140
100	0.210	0.201	0.165	0.160	0.177	0.136	0.134
150	0.282	0.281	0.244	0.236	0.239	0.220	0.214
250	0.301	0.250	0.155	0.141	0.132	0.125	0.113
300	0.357	0.333	0.295	0.269	0.167	0.148	0.136

Graphical trends are comparable. However, it is noted that the water content is higher in the topsoil than in deeper layers. This could imply probable heavy rainfall around the early days of the month of July since the data show a decreasing pattern as the month nears its end. With simulated data, water content is also higher at 300 cm depth. This depth is set as a water table level for the simulation process, so the aquifer could be acting as a source of additional water to the infiltration from the surface. Another noticeable difference is that the measured water content is higher at 150 cm depth compared to simulated data. This could be attributed to differences in soil properties of locations from which data were acquired.

The following figures (5.1 and 5.2) show the comparison of measured and simulated data in graphical format.

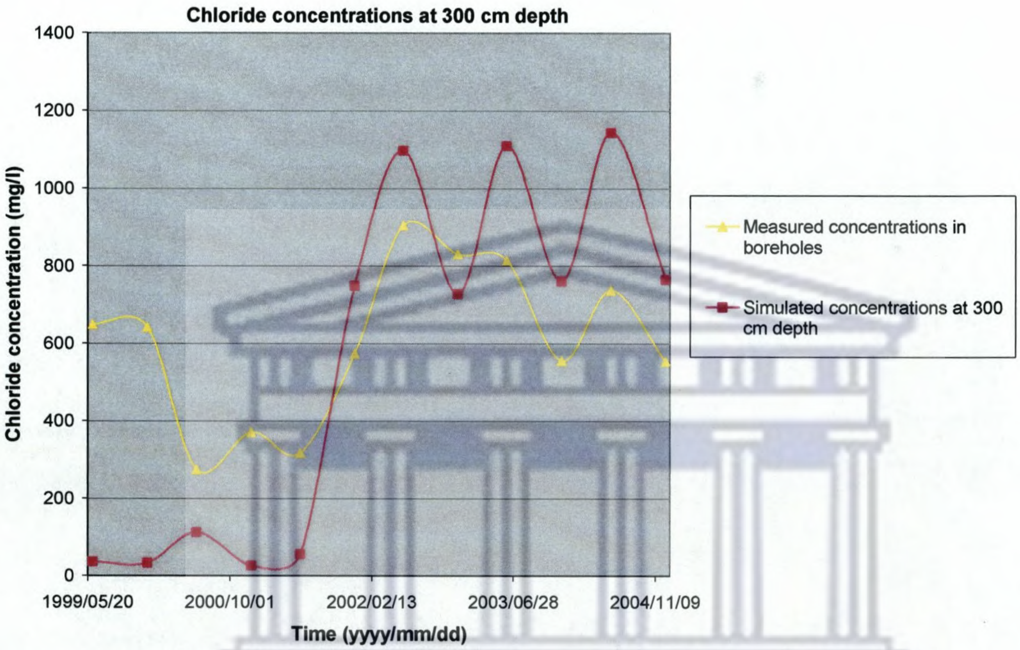


Figure 5.1: Measured (yellow line) and simulated (purple line) chloride concentration trends as a function of time at water level depth for the Cape Flats area. Simulated data run from 1999 to 2004.

Measured data in Figure 5.1 are from Coastal Park boreholes that have been monitored since 1986. For the simulated plot, chloride concentrations used are from Coastal Park (Ball and Novella, 2003) but the soil profile hydraulic data are from iThemba Labs (Samuels, 2007) due to the shortage of available data from Coastal Park. These sites have similar geohydrological characteristics since they both fall within the Cape Flats environment.

Looking at Figure 5.1, it is seen that simulation trends are fitting measurements well, considering such a long period over which they are compared, even though the simulation is over-estimating in the high range of concentrations. The plots in Figure 5.2 indicate good correspondence between measurements and simulations. Minor differences could be attributed to the difference in soil properties of sampling locations.

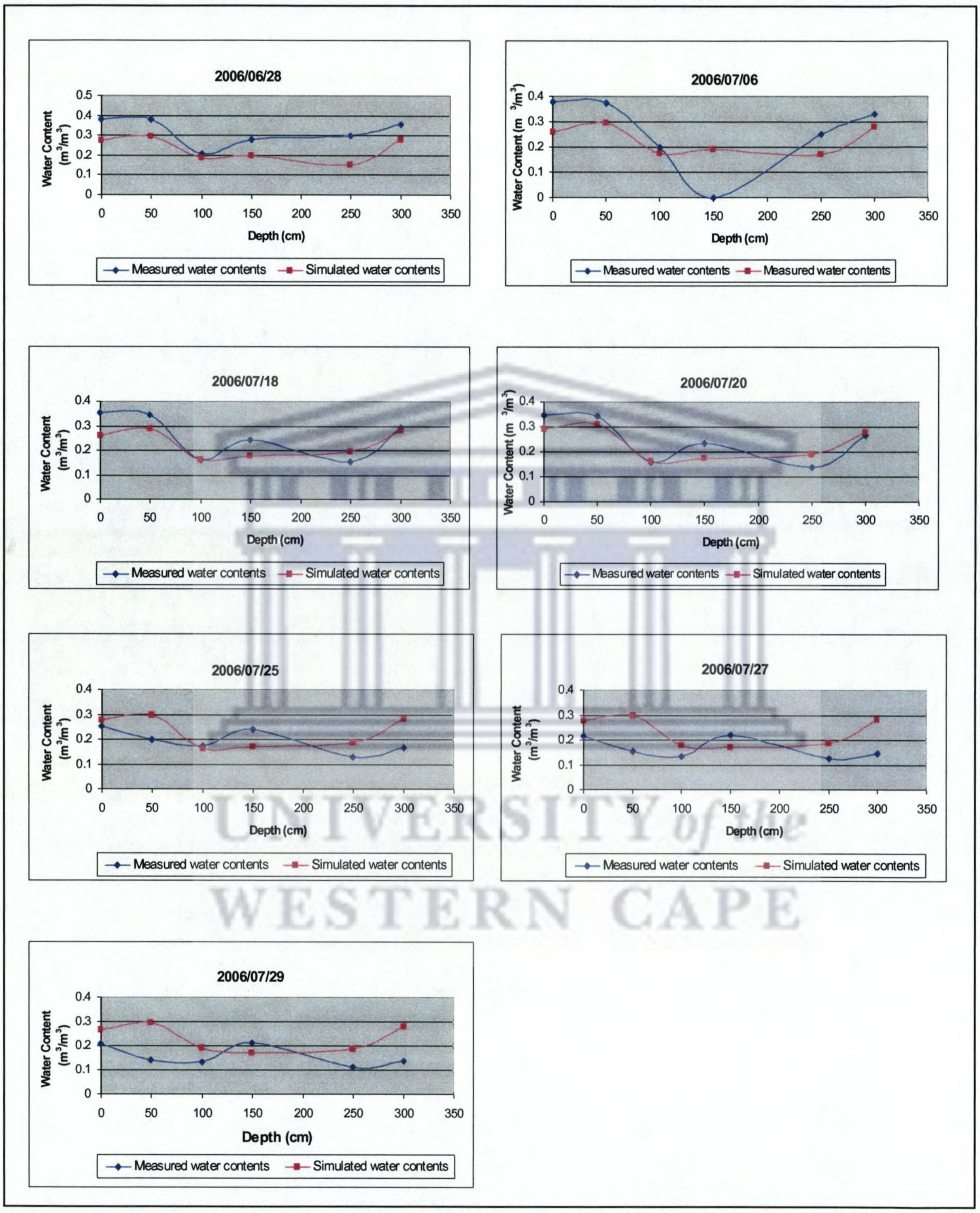


Figure 5.2: Measured and simulated soil water content graphs as a function of profile depth on selected days in July 2006 in the Cape Flats area.

5.1.2 Simulations for the Mpumalanga Highveld area

Calibration plots of solute (boron and fluoride) concentration for the Indaba irrigation site are presented in Figures 5.3 and 5.4. Three 4-year interval simulations were run. The first simulation was from 1991 to 1994, the second one from 1995 to 1998 and the third one from 1999 to 2002. These simulations were run separately because MACRO can only take up to 100 irrigation records. Hence, for bi-monthly applications (as was the case), more than 100 records had to be loaded. For estimation of the initial solute concentrations in the profile (SOLINIT) during effluent application period, the concentration output from the last day of each simulation was used as input to the next simulation. Appendices E and F show measured irrigation rates (applied every two weeks) for Indaba and Goedehoop irrigation sites from 1991 to 2001, respectively. These were calculated from monthly irrigation volumes as plotted and reported by Ginster (2002). Simulated boron and fluoride concentration output data for August 1991 and December 2002 are presented in Appendices D1 and D2, respectively. It proved very difficult to obtain raw measured data for solute concentrations in the soils of the Highveld area; instead the blue graphs (see Figure 5.3 and Figure 5.4) from Pit 3 and Pit 4 of the Indaba irrigation site were transferred from already plotted data from the Secunda reports by Ginster (2002) to this one. The reason for using data from the Indaba irrigation site was the fact that there were no soil depth profile data available for the Goedehoop irrigation site.

Both Figure 5.3 and Figure 5.4 show similar trends in measured data from the Indaba irrigation site and simulated data for the years 1991 and 2002. The slight differences between measurements and simulations could be due to the fact that the average concentration values were input for simulations, whilst the measured concentrations distribution was highly variable (i.e. at some instances or time frames there would be more data collected and at others, sparse data. Moreover, the differences between low and high concentration values were occasionally large) from 1991 to 2002.

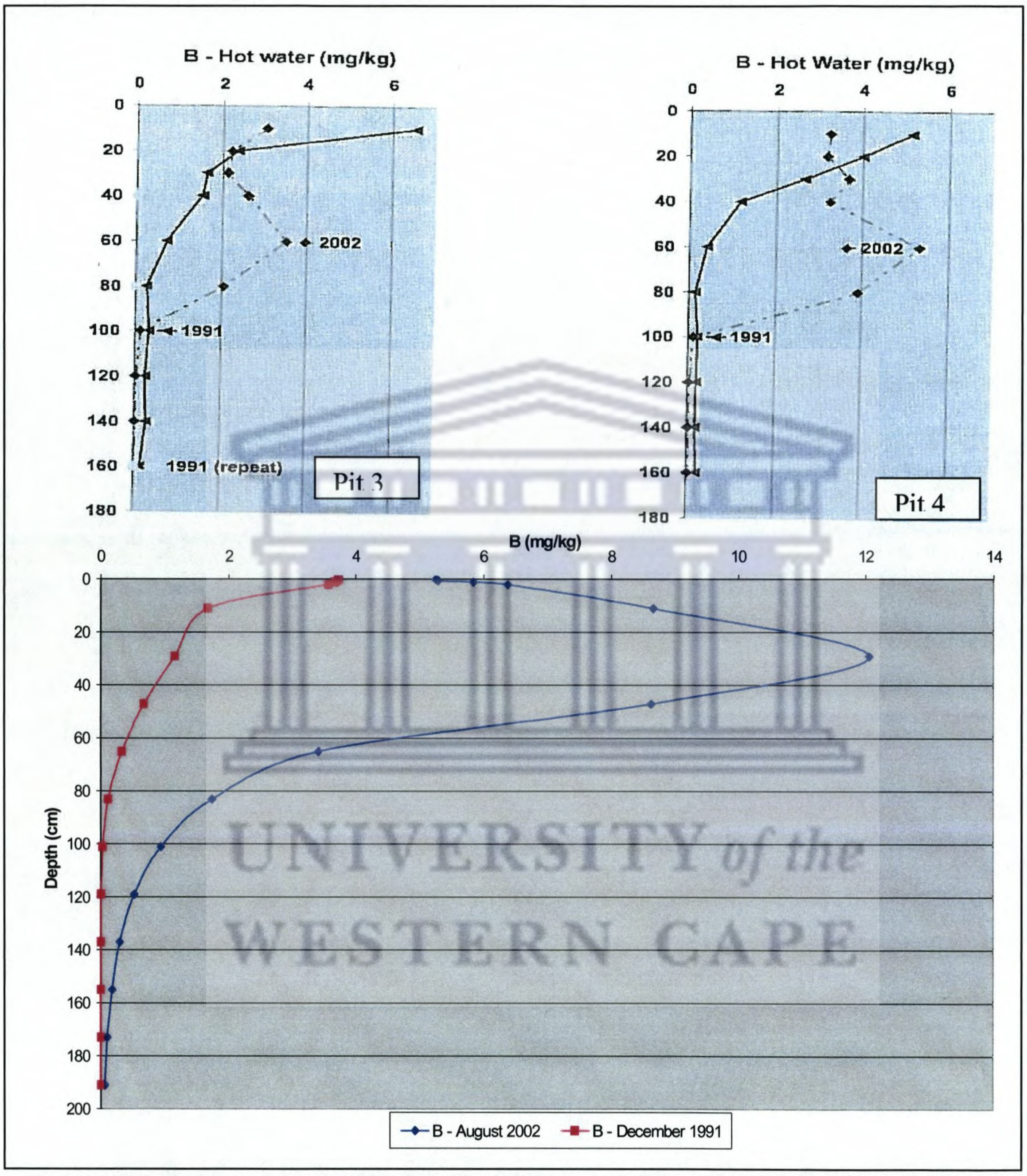


Figure 5.3: Boron concentration measured (two top blue graphs) and simulated data (bottom graph) for the years 1991 and 2002 as a function of depth for Indaba irrigation site of Mpumalanga Highveld.

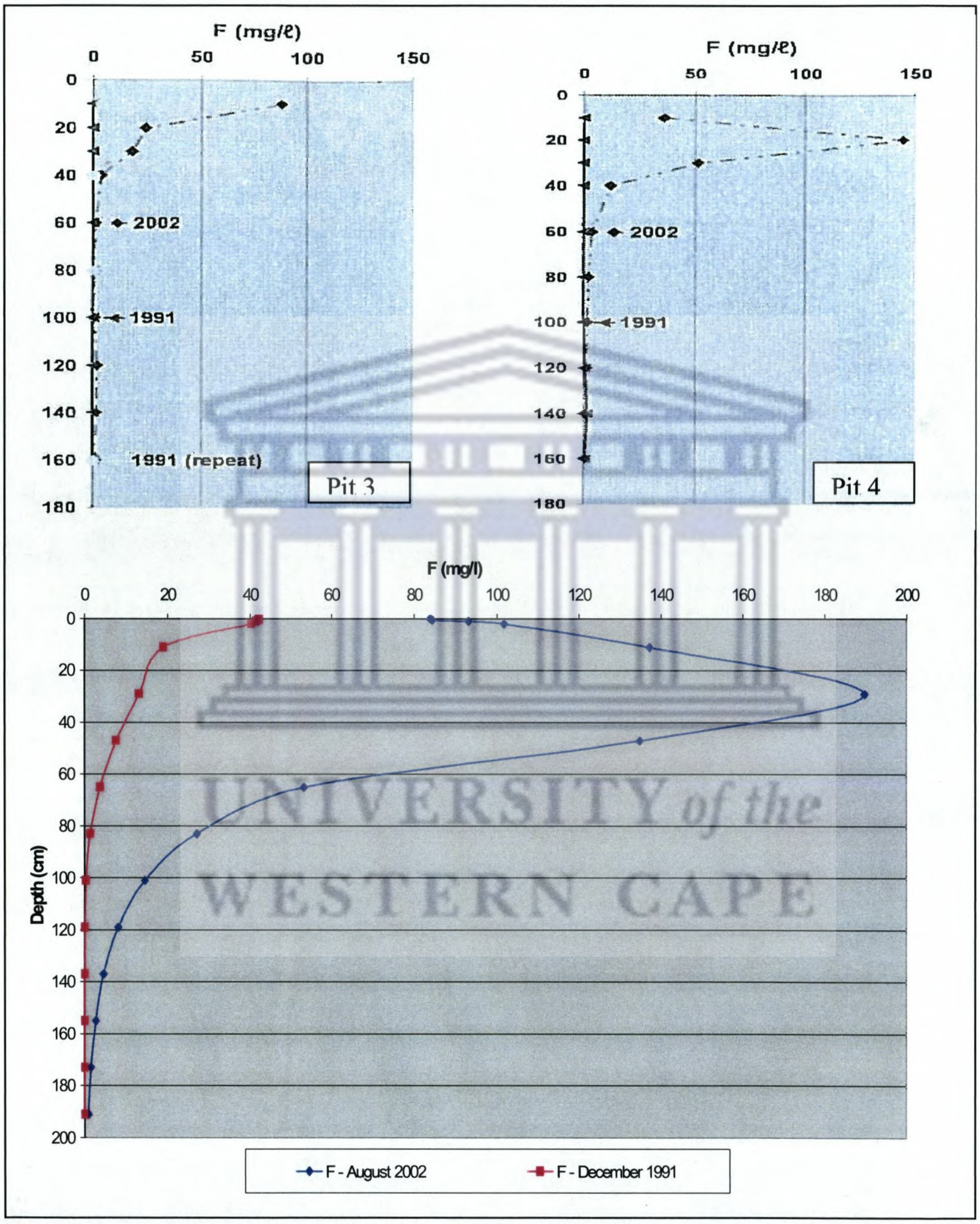


Figure 5.4: Fluoride concentration measured (two top blue graphs) and simulated data (bottom graph) for the years 1991 and 2002 as a function of depth for Indaba irrigation site of Mpumalanga Highveld area.

Only boundary initial concentrations and concentrations in irrigation water in this case differentiate boron from fluoride. Such data as the solute concentration factor (FSTAR) and diffusion coefficient in free water (DIFF) could also assist in differentiating among solutes in the simulation set-up. However, these parameters were not determined for this study and hence default values were applied. Fluoride boundary initial concentration was 1.36 mg/l (= 1360 mg/m^3) and its concentration in irrigation water was 47 mg/l. For boron, boundary initial concentration was 0.42 mg/l and its concentration in irrigation effluent was 10 mg/l.

Mpumalanga Highveld simulation data used for calibration of soil water content in October 1993 are presented in Appendix C. There were no measured depth profile data for soil water contents except for 1993, hence only this period is shown in the water content comparison plots of Figure 5.5. It represents average water content for the month of October in 1993.

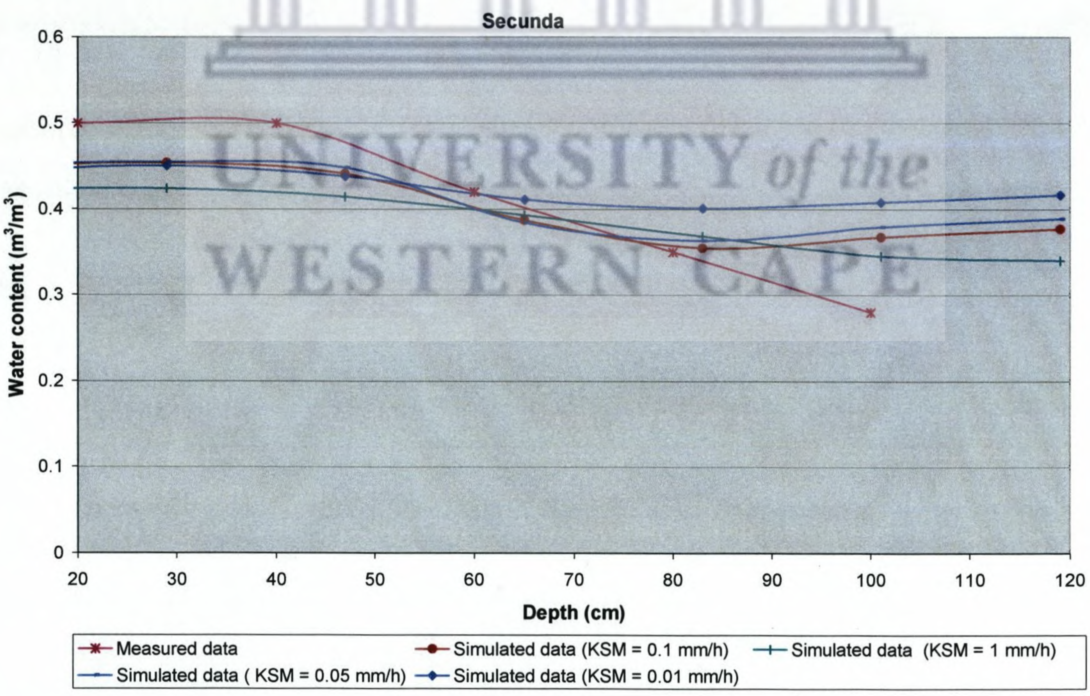


Figure 5.5: Measured and simulated (see legend) water contents as a function of depth simulated for October 1993 for the Mpumalanga Highveld area, with different boundary hydraulic conductivity (KSM) values.

Figure 5.5 shows a good correlation between the simulated and measured data, even with different boundary hydraulic conductivities. These simulations represent average water content for October 1993 after heavy rainfall at specific given depths. Figure 5.5 shows lower water content deeper in the profile whilst the topsoil contains more water. This is attributed to the fact that the topsoil becomes saturated for long periods, with high clay content forming an effective seal causing surface runoff, and slow migration and leaching.

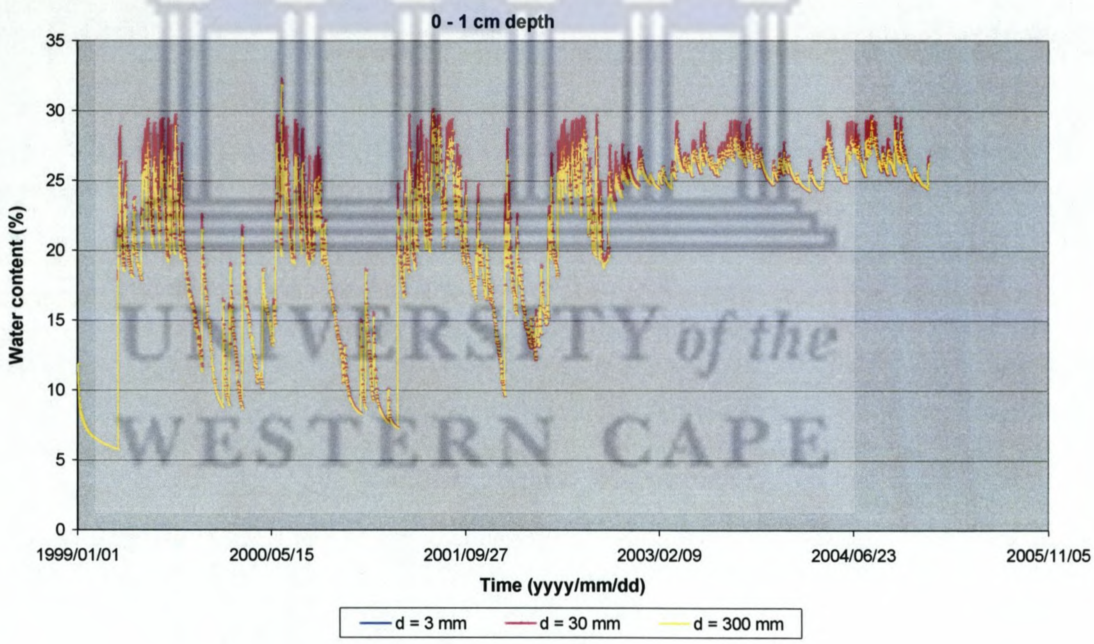
5.2 Sensitivity Analyses

Given the generally positive response of the MACRO model in terms of comparisons between measurements and simulation outputs, it was decided to run sensitivity analyses of model outputs to inputs related to preferential flow for different scenarios both for the Cape Flats and the Mpumalanga Highveld environments. The aim was to identify important inputs related to preferential flow that cause large variations in output results. Baseline parameters, varied input parameters, and output parameters will be discussed for each graph in this Chapter. Section 5.2.1 concentrates on the Cape Flats area scenarios and 5.2.2 deals with the Mpumalanga Highveld.

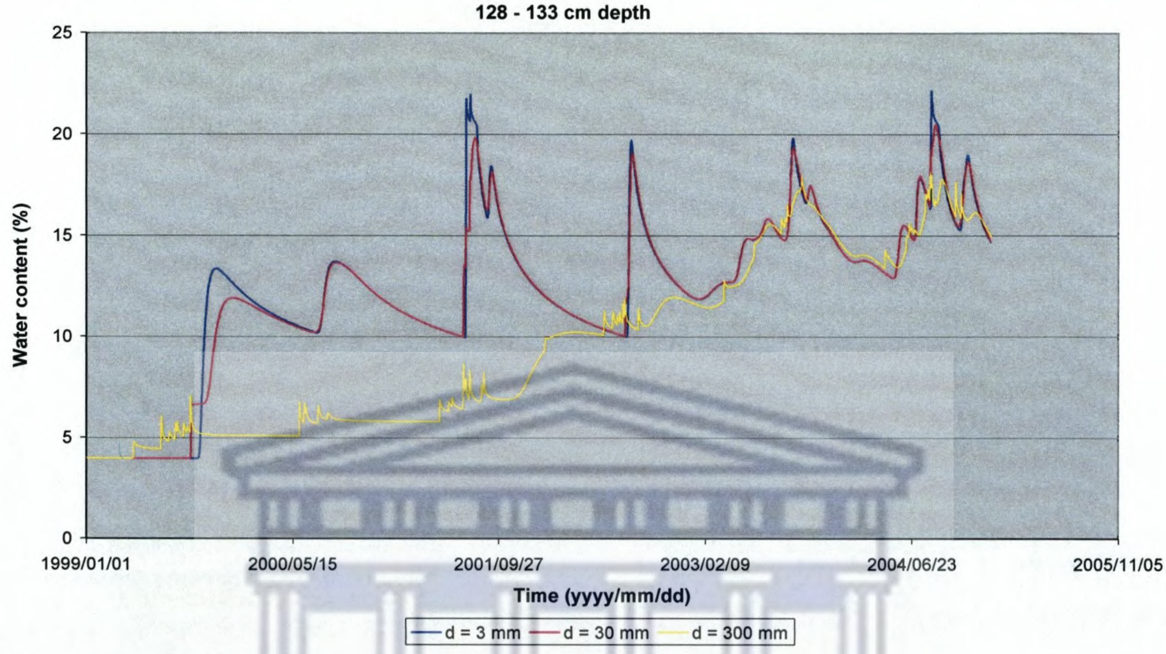
For all graphs in this Chapter, the criteria used in selecting parameters to vary, were trial and error. Various input values were substituted in order to see which one resulted in the visible effect on the pattern or trend of plots. The ones that show conspicuous or meaningful effects were then selected for plots to include in this document. Some parameters showed subtle or no difference, no matter how much the input values were varied. At least three values of each parameter were plotted in order to obtain reliable, adequate and comprehensible comparison.

5.2.1 Cape Flats

Diffusion pathlength is the half-width between two assumed parallel fractures. It is the parameter varied in Figure 5.6 in order to assess its effect on total water content as an output. From Figures 5.6 (a) and (b) it is clear that the soil water content mostly decreases as the diffusion pathlength increases, signifying physical non-equilibrium and thus preferential flow. Fluctuations decrease and water content evens out after 2002 as is evident on the graphs. This could be attributed to rainfall distribution around that time, that is, there was frequent but low rainfall during this period compared to the years prior.



(a)

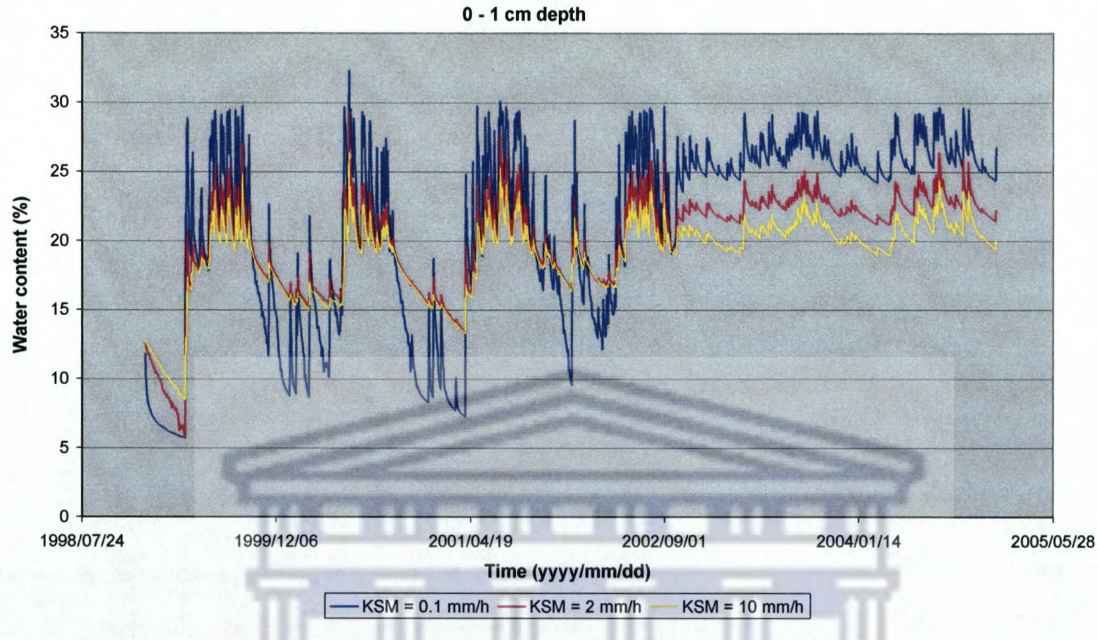


(b)

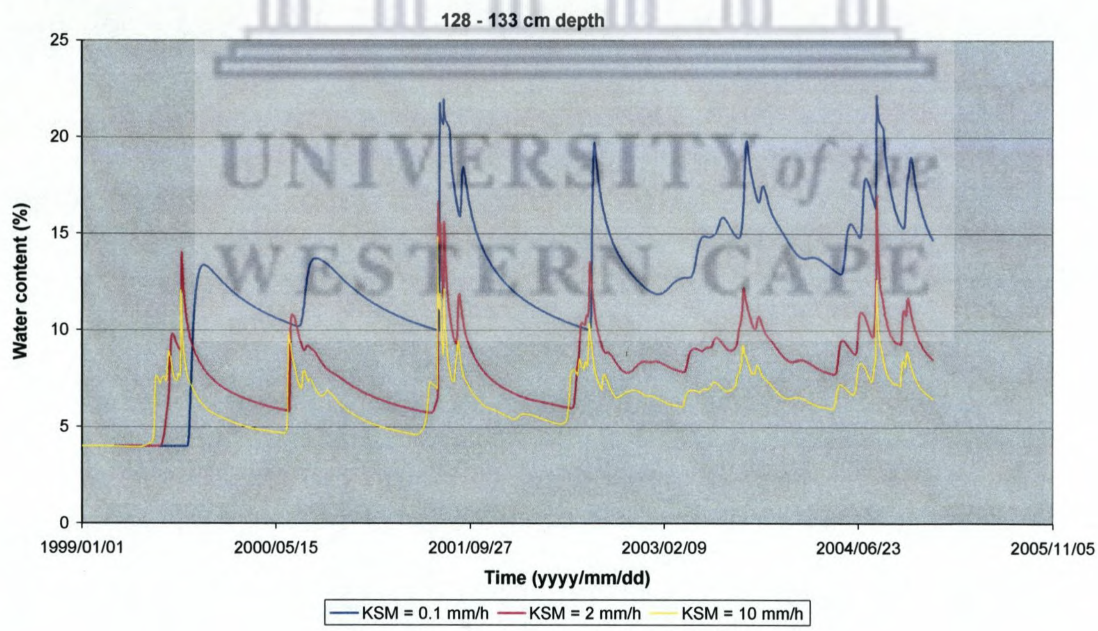
Figure 5.6: Simulated soil water contents as a function of the effective diffusion pathlength, d (mm) at (a): 0 – 1 cm, (b): 128 – 133 cm profile depths – Cape Flats area.

Although not shown here, it was also observed that the decrease in alpha (van Genuchten's alpha which determines the shape of the water retention function and related to a characteristic pore size distribution in the soil) causes an increase in water content. This is expected because capillary fringe thickness increases with decreasing alpha, thus slowing the gravity drainage, and therefore storing more water in the unsaturated zone due to capillary forces (Prasad et al, 2001).

For Figure 5.7, hydraulic conductivity at the boundary between micropores and macropores was varied and the total water content output was analysed. As this hydraulic conductivity increases, water exchange rate between these domains also increases, and thus soil water content decreases as depicted in Figures 5.7 (a) and (b). This is probably because water drains faster due to high hydraulic conductivity in the macropores. At shallow depths the variation in water content peaks evens out, whilst they show an even but gradual increase with time deeper in the profile.



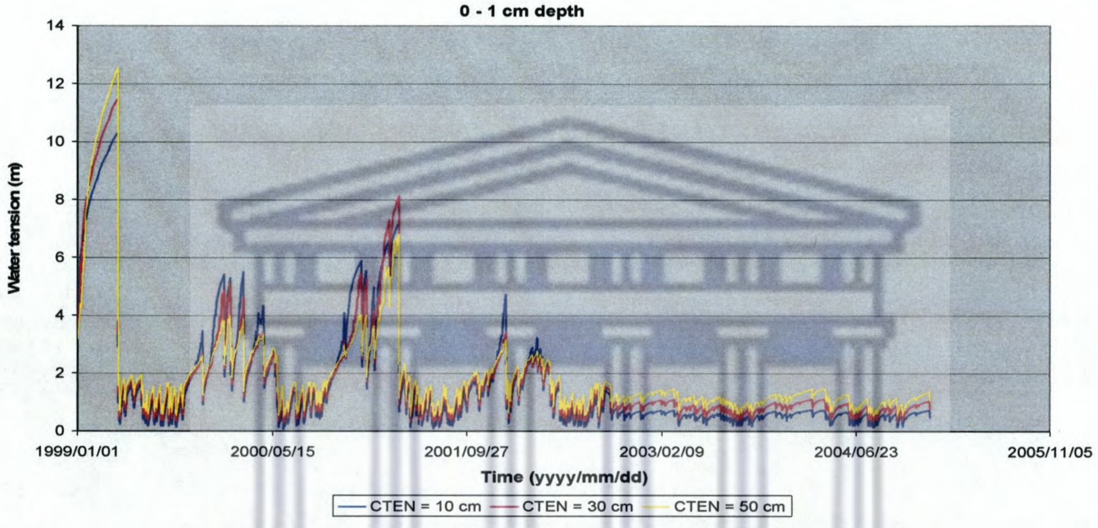
(a)



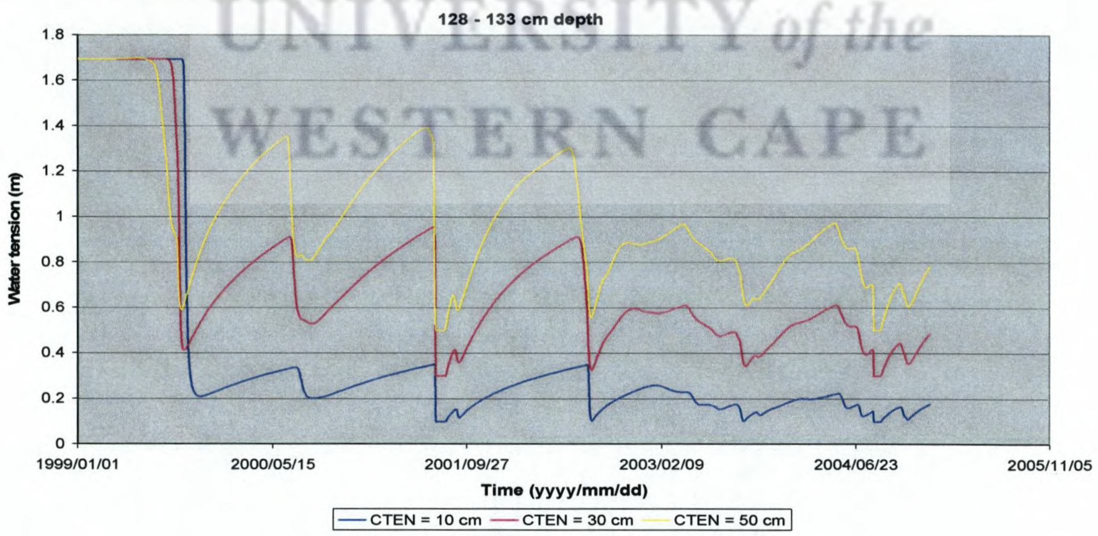
(b)

Figure 5.7: Simulated soil water contents as a function of boundary hydraulic conductivity, K_b at (a): 0 – 1 cm, (b): 128 – 133 cm profile depths – Cape Flats area.

As expected, Figure 5.8 shows an increase in soil water tension as water contents in Figures 5.7 and 5.6 above decrease. Additionally, the sharp peaks and leveling out are evident in the water tension plots too.



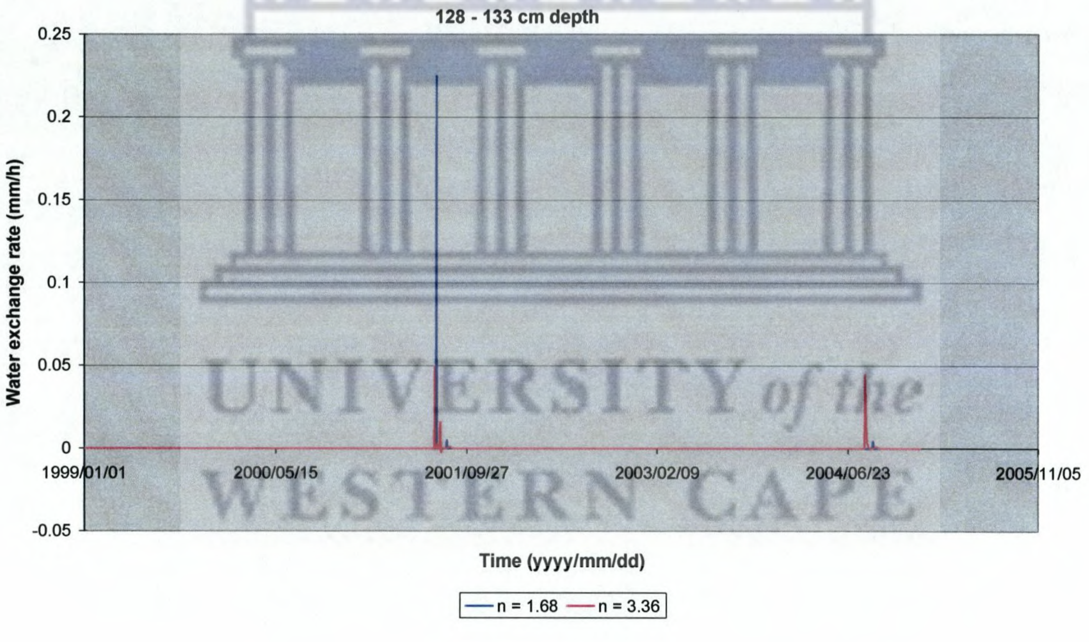
(a)



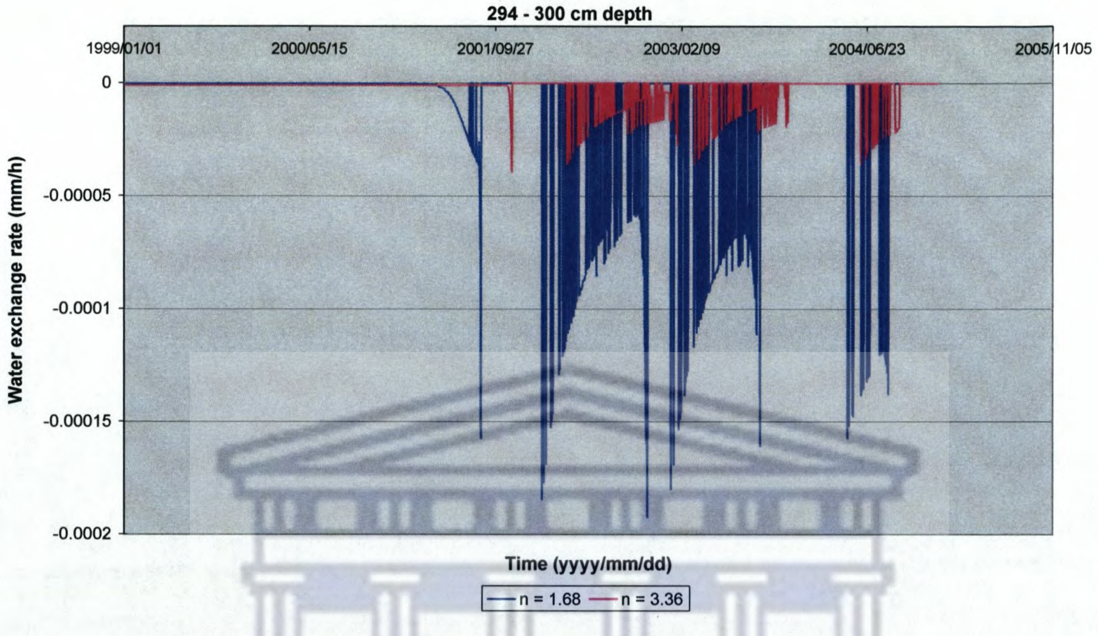
(b)

Figure 5.8: Sensitivity of simulated soil water tension to different values of the boundary soil water tension at depths 0 -1 cm and 128 – 133 cm, respectively – Cape Flats area.

For Figure 5.9, the varied input was *n* (van Genuchten's n value which defines the shape of the water release characteristic in the micropore domain) with the water exchange rate as output. From these plots, it is unclear whether a change in *n* has a significant effect on the water exchange rate between micropores and macropores. In the middle of the graph (Figure 5.9 a), the exchange from macro- to micropores (positive values) is dominant over the exchange rate from micro- to macropores (negative values). In contrast, the reverse is true at water table level (Figure 5.9 b), irrespective of *n* values. The sharp increases of the water exchange rates signify the existence of preferential flow and/or a source of water (heavy rainfall period or vicinity of the water table).



(a)



(b)

Figure 5.9: Simulated water exchange rates as a function of van Genuchten's n value at depths (a) 128 – 133 cm and (b) 294 – 300 cm – Cape Flats area.

Diffusion pathlength and boundary hydraulic conductivity were the respective parameters selected to vary in order to determine their effect on solute concentration. In this case, chloride is represented under the group type tritium in the MACRO simulation set-up. This is shown in Figures 5.10 to 5.12.

Compared to the concentration values of Figures 5.13 to 5.15 further down, the concentration values in Figures 5.10 to 5.12 are higher. This is to be expected because chloride does not sorb and degrade and hence it leaches rapidly, whilst generic pesticides undergo sorption and degradation during infiltration. Selaolo (1998) suggested that tritium is transported in both liquid and vapour phases (in the model tritium is set to be lost as water evaporates from the soil surface), whilst other solutes are transported in liquid phase only. That could explain higher concentration for tritium group type solutes.

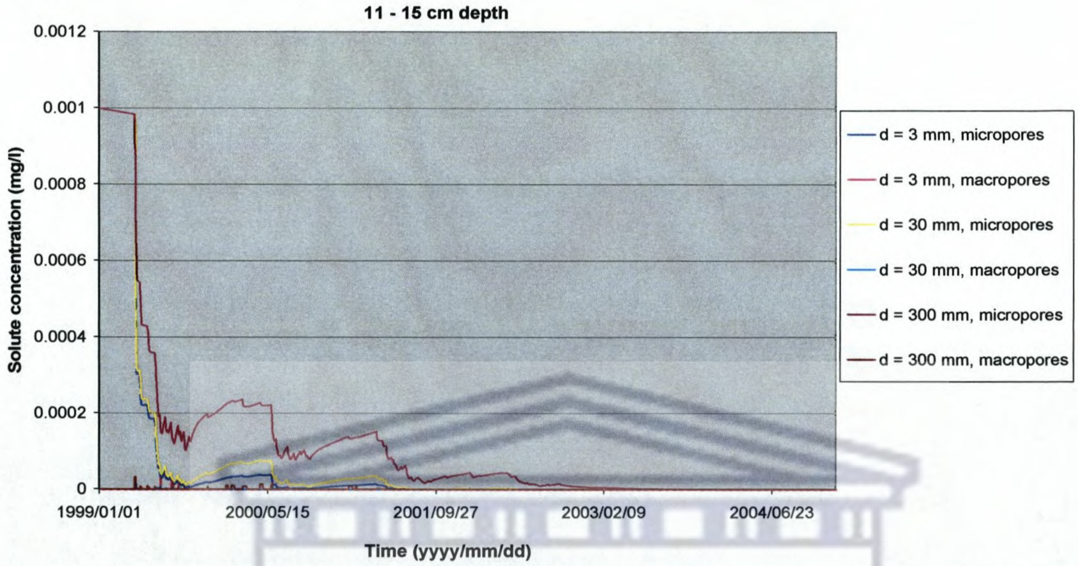


Figure 5.10: Simulated solute concentration with respect to the diffusion pathlength at 11 to 15 cm depth over a period 1999 to 2004 – Cape Flats area.

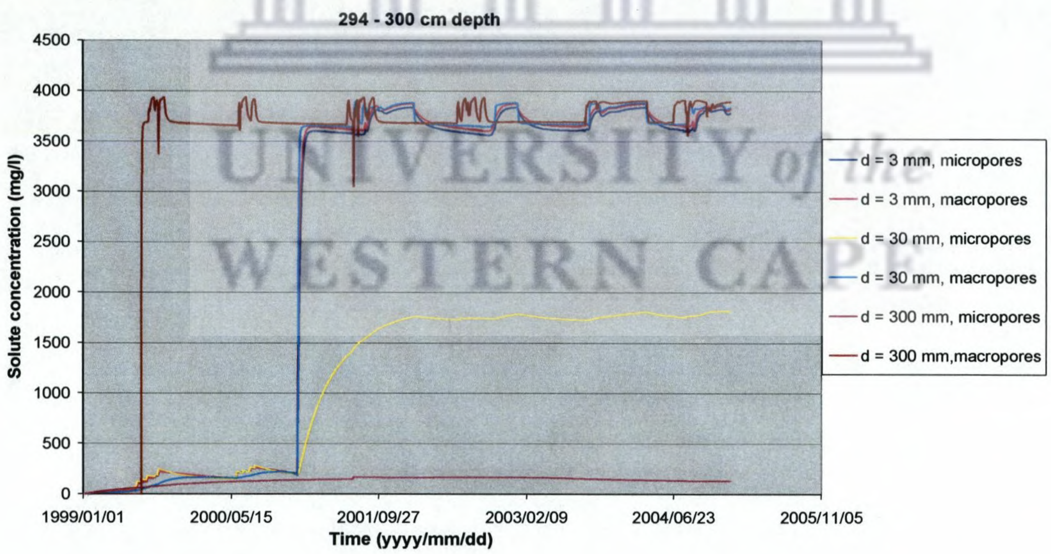


Figure 5.11: Simulated solute concentration with respect to the diffusion pathlength at 294 – 300 cm depth over a period 1999 to 2004 – Cape Flats area.

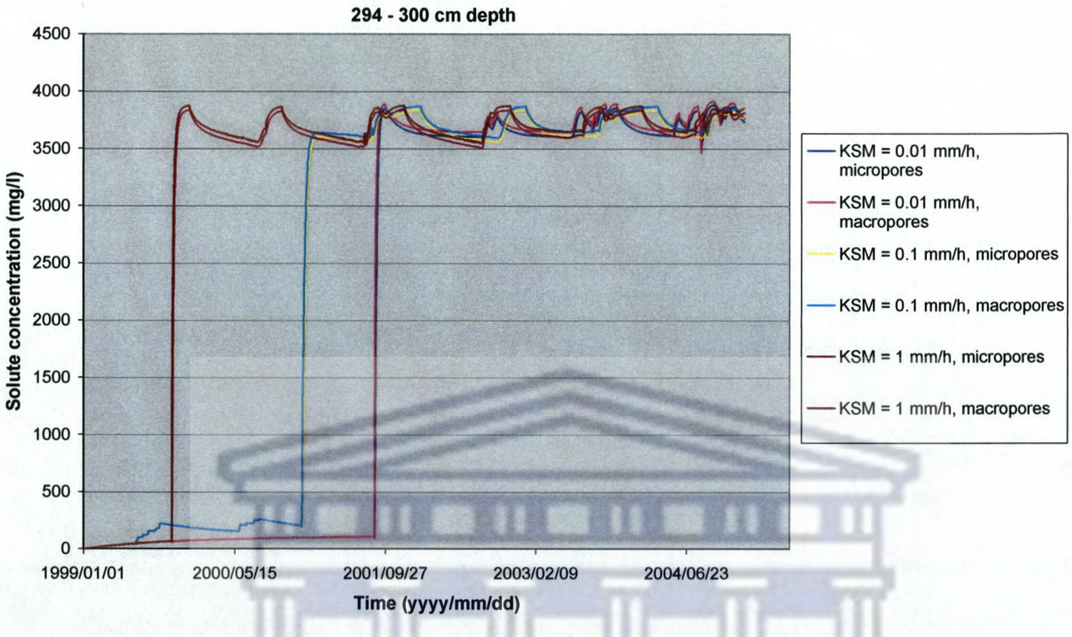


Figure 5.12: Simulated solute concentration with respect to boundary hydraulic conductivity (KSM) at 294 – 300 cm depth over a period 1999 to 2004 – Cape Flats area.

Scenario simulations were run for a generic pesticide in order to test model output to variations in sorption distribution coefficient, degradation rate coefficient in macropore solid phase and excluded volumetric water content. These plots are displayed in Figures 5.13, 5.14 and 5.15, respectively. In MACRO, there is an input parameter option for the initial solute concentration in soil water (SOLINIT) and in this case 1 mg/m^3 was the selected input. The input solute concentration at the lower boundary level (CONCIN - which in this case is the water table level at 300 cm depth) was 4000 mg/l.

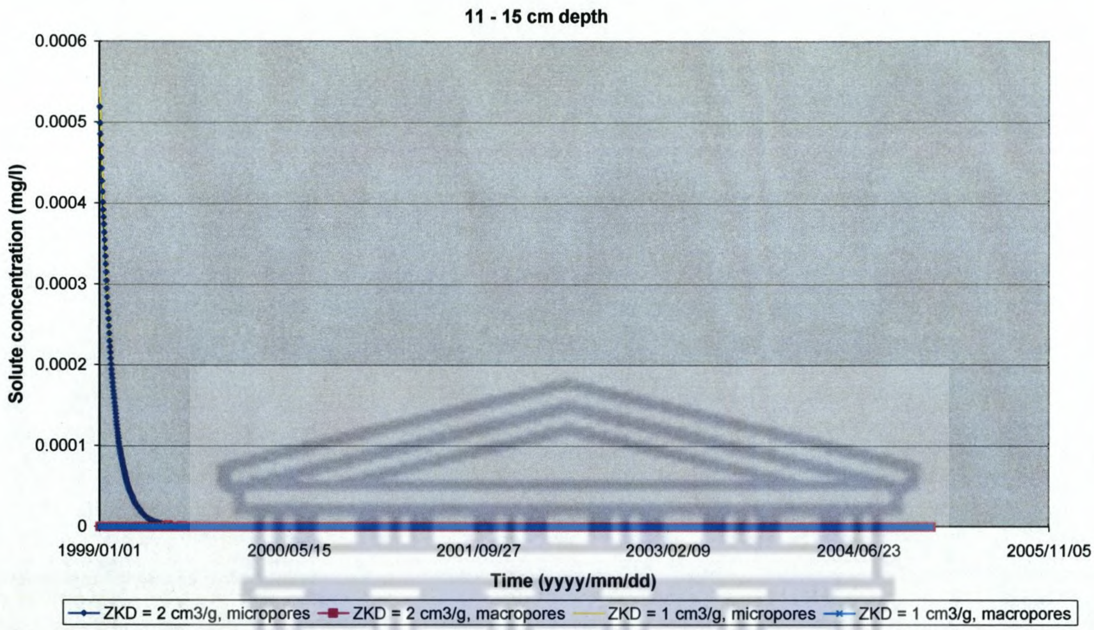


Figure 5.13: Simulated solute concentration with respect to sorption distribution coefficient at 11 – 15 cm depth over 1999 to 2004 period – Cape Flats area.

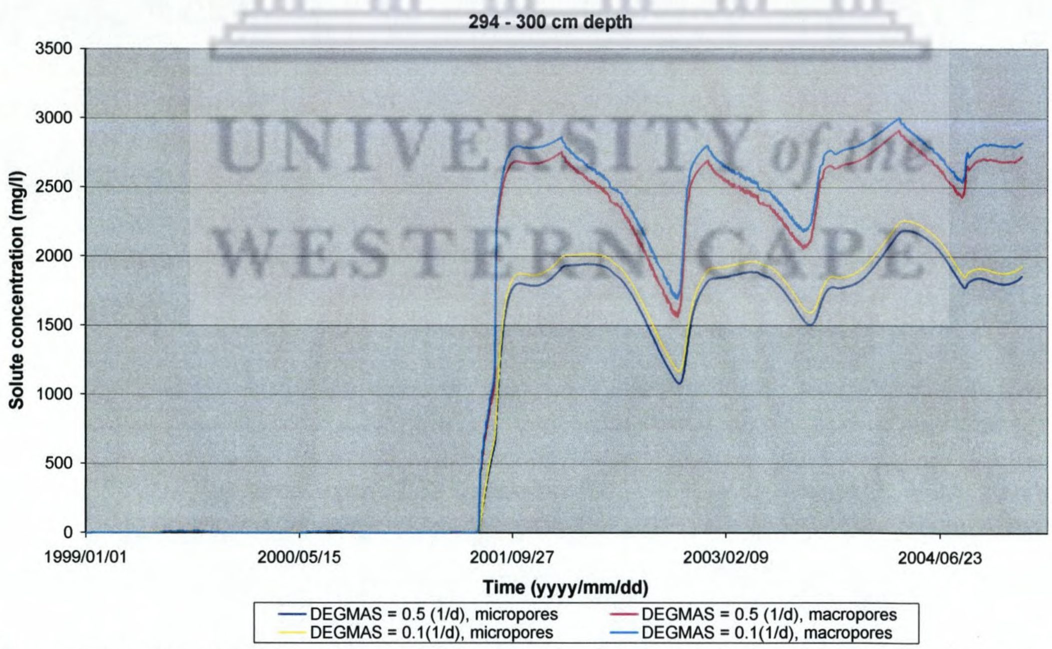


Figure 5.14: Simulated solute concentrations as a function of degradation rate coefficient in macropores solid phase at 294 – 300 cm depth over a period from 1999 to 2004 – Cape Flats area.

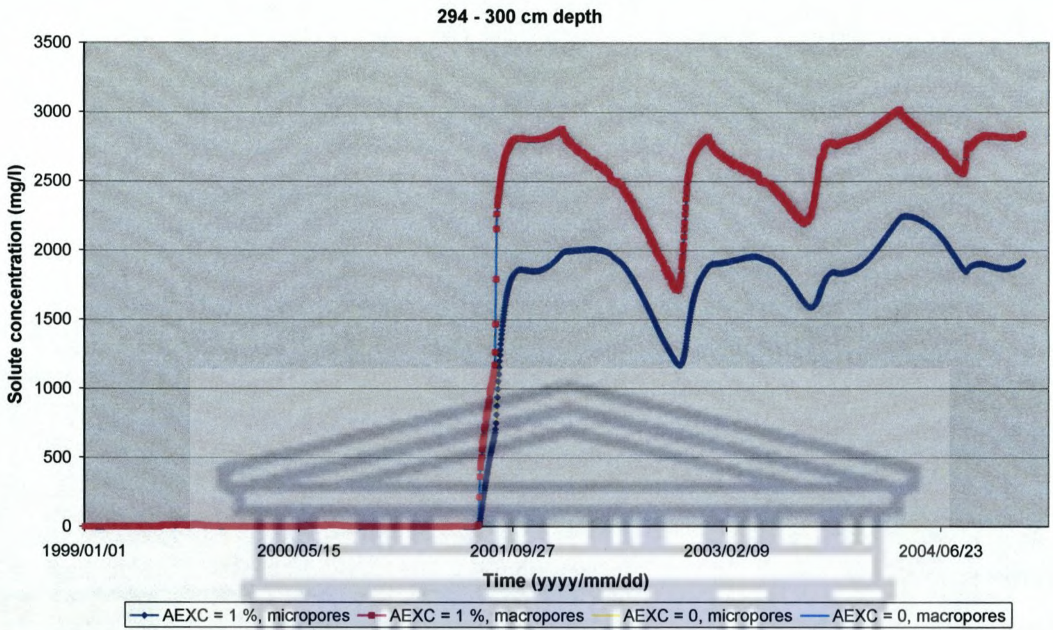
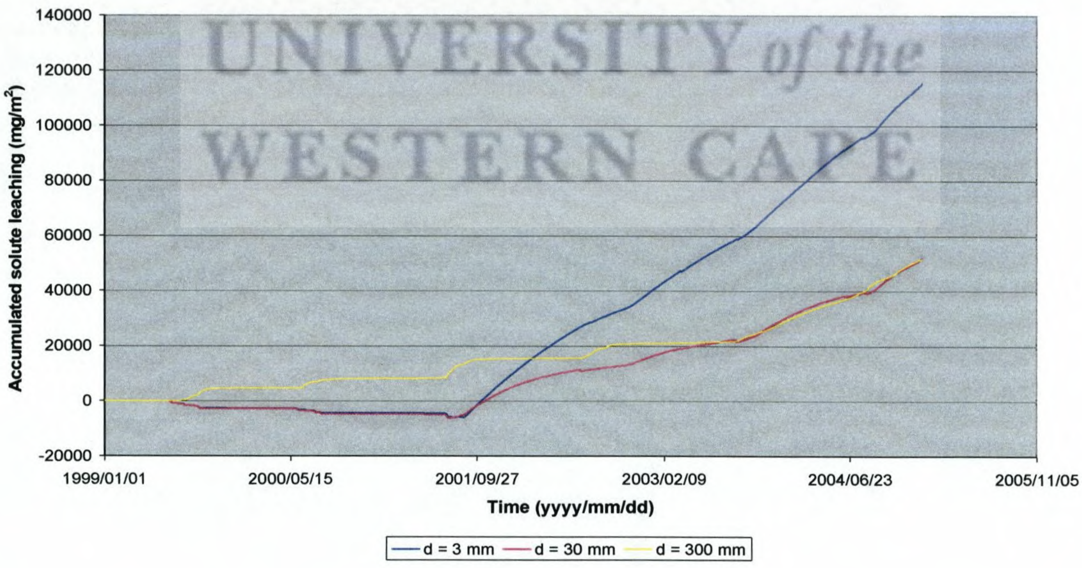


Figure 5.15: Simulated solute concentration as a function of excluded volumetric water content at 294 – 300 cm depth over a period from 1999 to 2004.

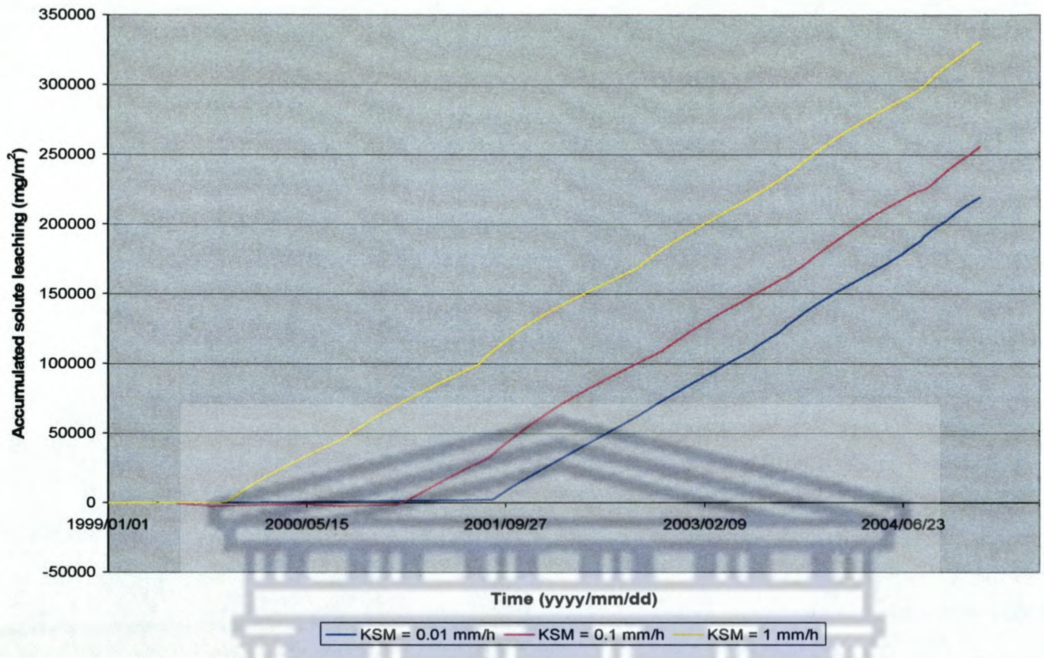
Figures 5.13 to 5.15 show that there is a higher solute concentration in macropores than in micropores over long simulation times and nearly equal over short time irrespective of any variable parameter. Although not shown here, similar patterns were observed with parameters like degradation rate coefficient in micropores (both liquid and solid phases) and macropores liquid phase. It is also noted that there is a sudden increase in solute concentration in 2001 for profile depth 294 – 300 cm. This could imply that the water table started to act as the source of the solute for layer 294-300 mm since this depth is set at water table level (lower boundary conditions). The simulation set-up is such that water table fluctuations are accommodated. Besides the bottom boundary being set at 300 cm depth, the Field drainage option was included to cater for a rising water table. Another explanation could be that the solute was transported rapidly through macropores after it took some time to leach. This could be promoted by heavy rain in the area. Furthermore, it could also be influenced by differences in soil properties of different soil horizons (B Horizon in this case).

The big difference between solute concentrations in soil water (SOLINIT) and at the lower boundary (CONCIN) results in output differences that are visible such as Figure 5.13 (the near surface plot) compared to Figures 5.14 and 5.15 plotted for depths 294 to 300 cm.

To see their effect on solute leaching, the diffusion pathlength (Figure 5.16a) and the boundary hydraulic conductivity (Figure 5.16b) parameters were varied. Figure 5.16 (a) represents the generic pesticide leaching scenario, whilst Figure 5.16 (b) represents the tritium type (chloride) leaching simulation results. Breakthrough in solute leaching is seen at the time around 2001 of simulation (see figure 5.16 (a)). Figure 5.17 suggests that this could be due to the increasing amount of percolation generated around this time. Again the theory by Selaolo (1998) of tritium being transported in both liquid and vapour phases, whilst other solutes are transported in liquid phase only, could explain the higher leaching in Figure 5.16(b) when compared to Figure 5.16 (a) since in the model, it is set to be lost as water evaporates from the soil surface . It could also be the fact that chloride does not sorb and degrade compared to pesticides.



(a)



(b)

Figure 5.16: Simulated solute leaching in response to different values of (a) diffusion pathlength and (b) boundary hydraulic conductivity – Cape Flats area.

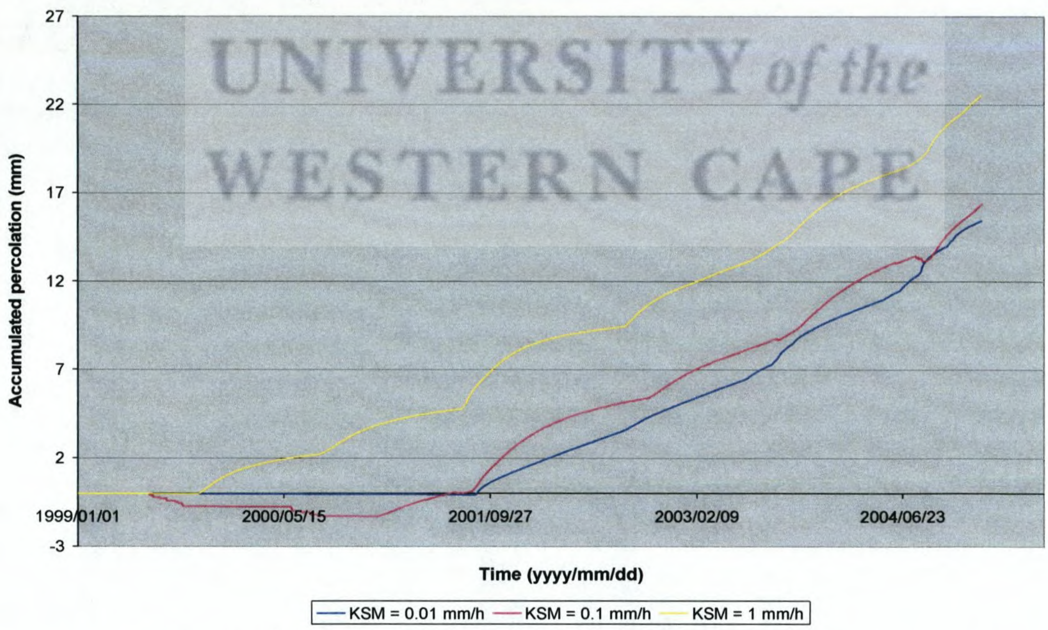


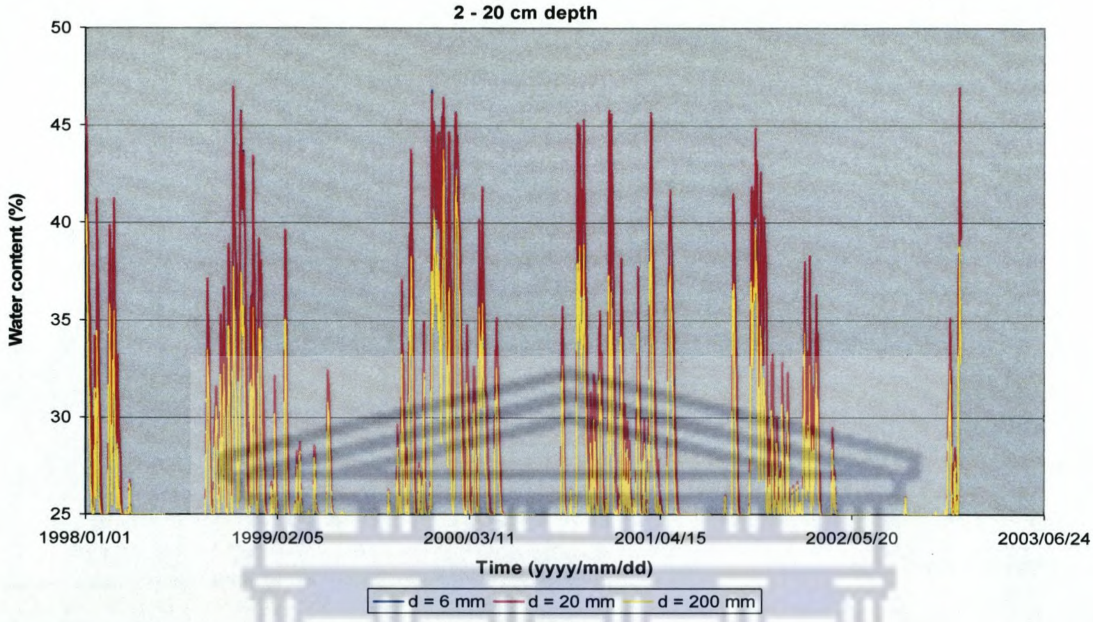
Figure 5.17: Simulated percolation in response to changing boundary hydraulic conductivity – Cape Flats area.

It is noted that percolation is low in the Cape Flats area (see Figure 5.17). Blight et al. (2005) observed reduced water content in Coastal Park which might be due to reduced rainfall. They concluded that the rain water was absorbed and mostly held by the landfilled general wastes, subsequently being drawn back to surface by capillary action, where it evaporated during the course of each year. However, the model was not set to do that, but it simulated reduced percolation in drier years. Vandoolaeghe (1989) found that the net groundwater recharge through Cape Flats sandy soils varies between 15% and 37% of annual precipitation which ranges between 300 mm and 500 mm, depending on climatological factors and soil conditions. On top of that, the losses through evapotranspiration are extremely high and exceed 80% of annual precipitation. Adams (unpublished data) estimated between 10% and 13% of annual precipitation recharge for the Campus Test site at the University of the Western Cape. Also, Henzen (1973) and Gerber (1976) concluded that vertical permeability in the Cape Flats is smaller than the horizontal permeability, and this plays a role in the amount of vertical recharge (percolation). Cape Flats is also a very shallow aquifer with less preferential flow paths and no irrigation taking place at Coastal Park.

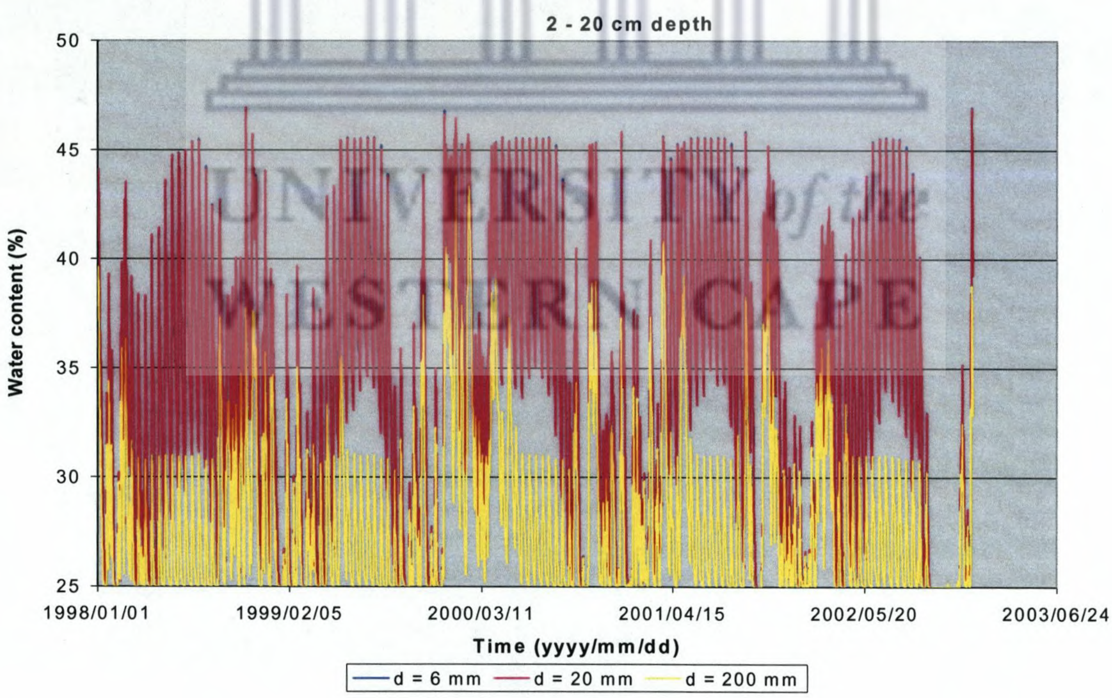
5.2.2 Mpumalanga Highveld

In the Mpumalanga Highveld, solutes considered were fluoride and boron. The boundary initial concentration for fluoride and boron was 1.36 mg/l (= 1360 mg/m^3) and 0.42 mg/l, respectively. The concentration values in irrigation water were 47 mg/l for fluoride and 10 mg/l for boron. Irrigation was applied twice in a month for a simulation and the data used are attached in Appendices E and F. These data are for Indaba and Goedehoop irrigation sites, respectively for the period 1991 to 2001.

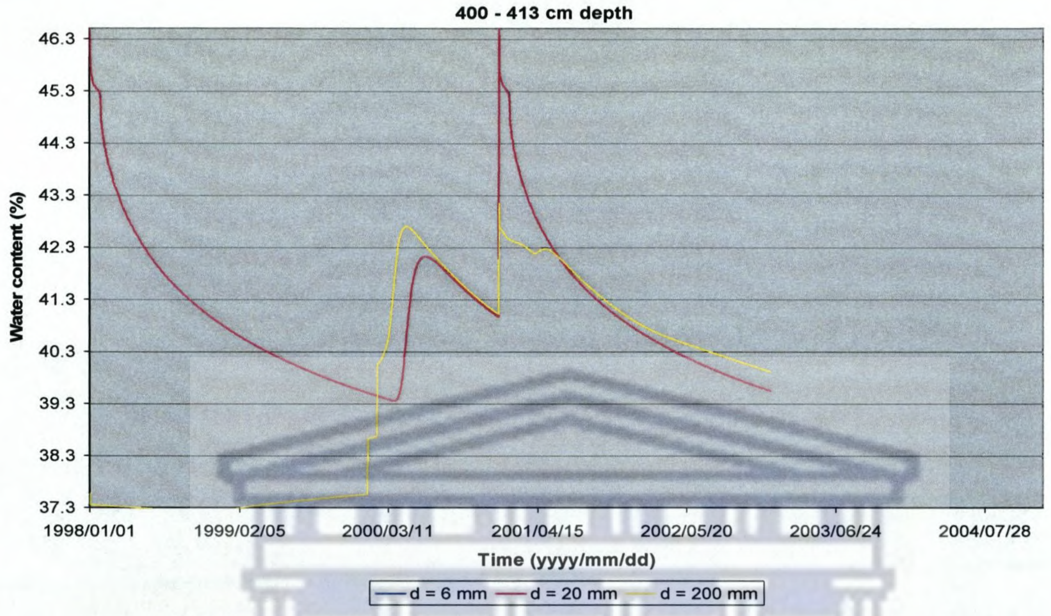
In order to determine their effect on the soil water content diffusion pathlength and boundary hydraulic conductivity are respective inputs that were varied. This is shown in Figures 5.18 and 5.19. Figures 5.18 (a) and (c) are for non-irrigated conditions, whilst Figures 5.18 (b) and (d) represent irrigated conditions. The same applies for Figure 5.19. These graphs indicate that the soil water content decreases with the widening of the diffusion pathlength and with an increase in boundary hydraulic conductivity. Sharp peaks on all the plots, especially in the year 2001, are a proof of existence of preferential flow. There is not much difference in water content between the simulation plots of Figures 5.18 and 5.19. Soil water content remains at approximately the same levels even in dry periods due to effluent irrigation applied. Boundary hydraulic conductivity and diffusion pathlength have the same effect for both irrigated and non-irrigated cases.


2 - 20 cm depth
Water content (%)
50
45
40
35
30
25
1998/01/01
1999/02/05
2000/03/11
2001/04/15
2002/05/20
2003/06/24
Time (yyyy/mm/dd)
d = 6 mm
d = 20 mm
d = 200 mm

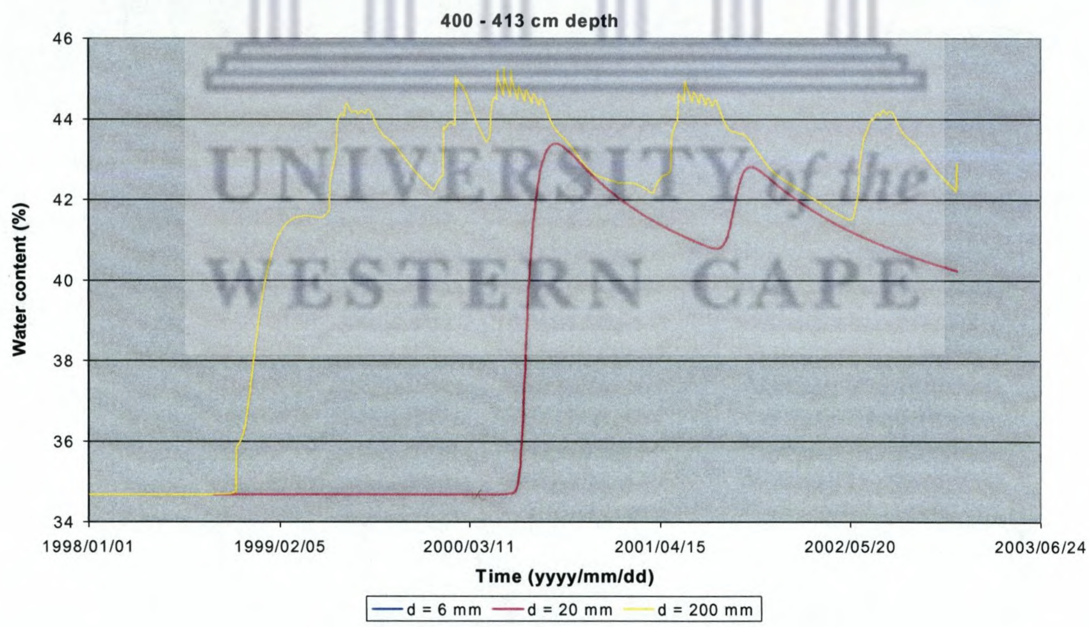
(a)


2 - 20 cm depth
Water content (%)
50
45
40
35
30
25
1998/01/01
1999/02/05
2000/03/11
2001/04/15
2002/05/20
2003/06/24
Time (yyyy/mm/dd)
d = 6 mm
d = 20 mm
d = 200 mm

(b)

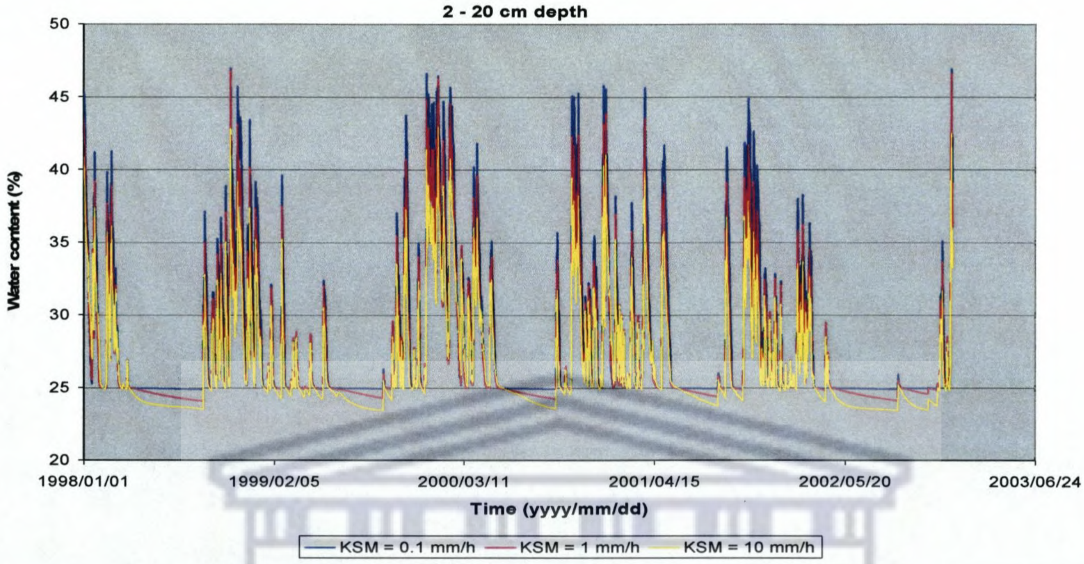


(c)

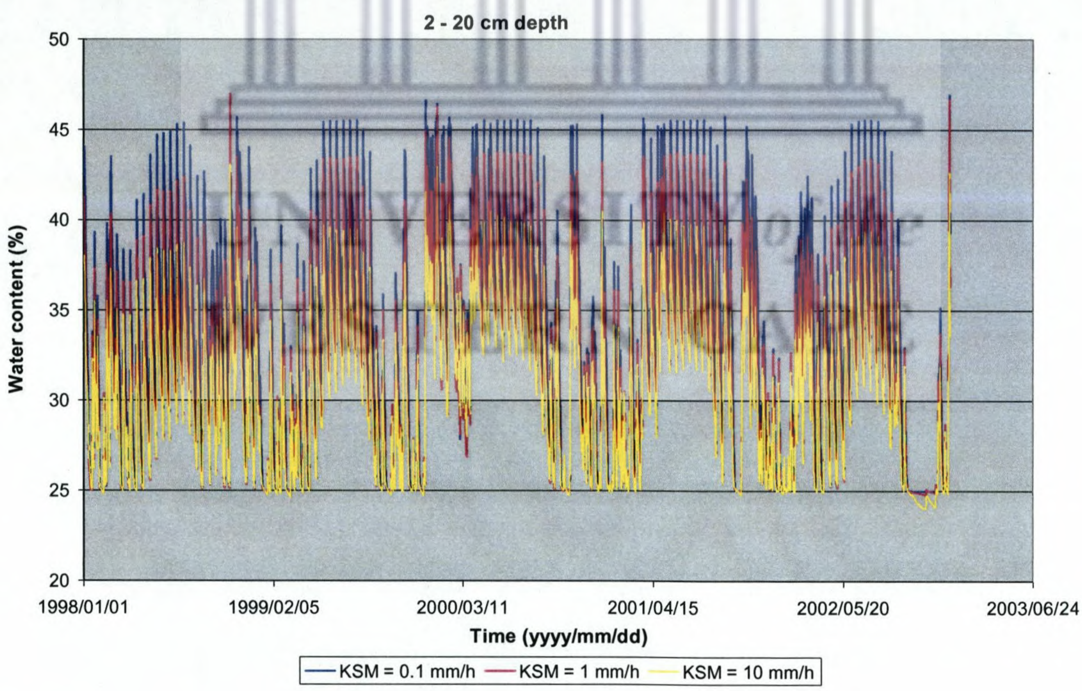


(d)

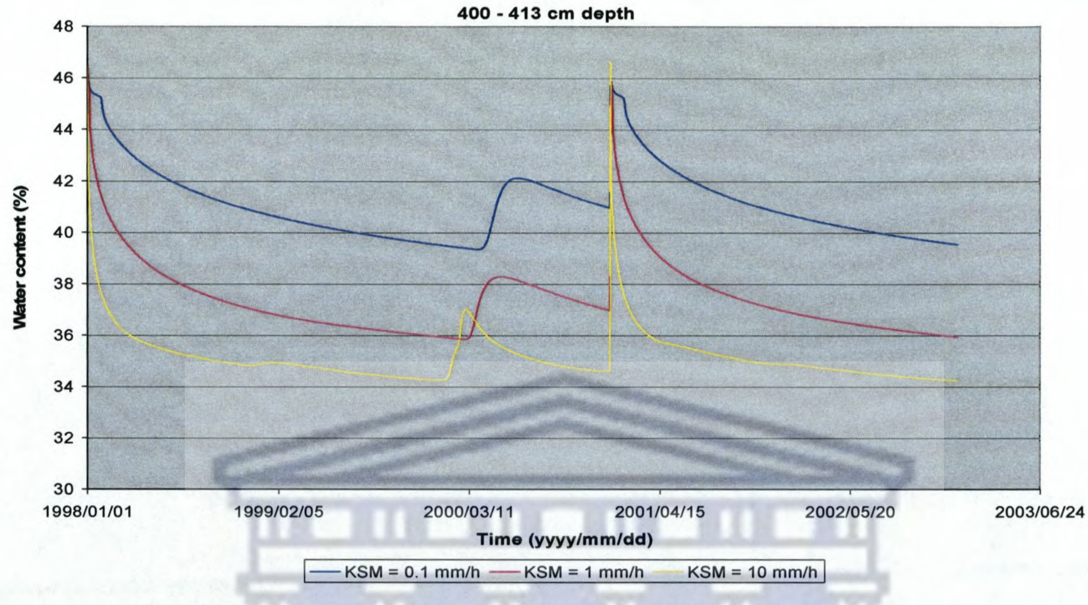
Figure 5.18: Simulated water content as a function of diffusion pathlength at depths 2 – 20 cm for (a) non-irrigated, (b) irrigated; and 400 – 413 cm for (c) non-irrigated, (d) irrigated case in Mpumalanga Highveld.


2 - 20 cm depth
Water content (%)
50
45
40
35
30
25
20
1998/01/01
1999/02/05
2000/03/11
2001/04/15
2002/05/20
2003/06/24
Time (yyyy/mm/dd)
KSM = 0.1 mm/h
KSM = 1 mm/h
KSM = 10 mm/h

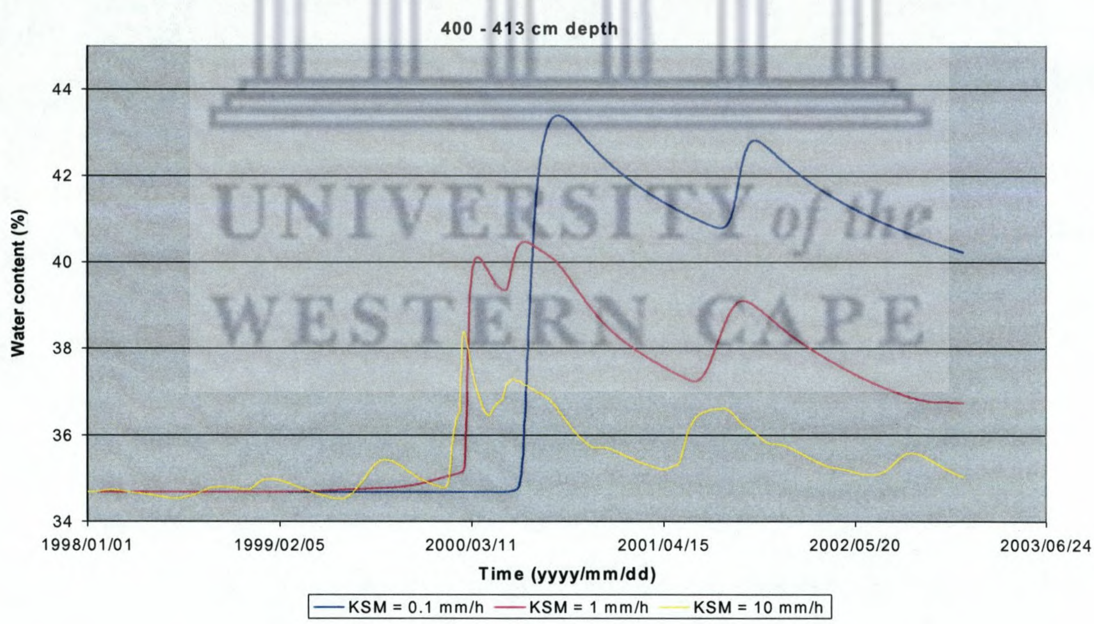
(a)


2 - 20 cm depth
Water content (%)
50
45
40
35
30
25
20
1998/01/01
1999/02/05
2000/03/11
2001/04/15
2002/05/20
2003/06/24
Time (yyyy/mm/dd)
KSM = 0.1 mm/h
KSM = 1 mm/h
KSM = 10 mm/h

(b)



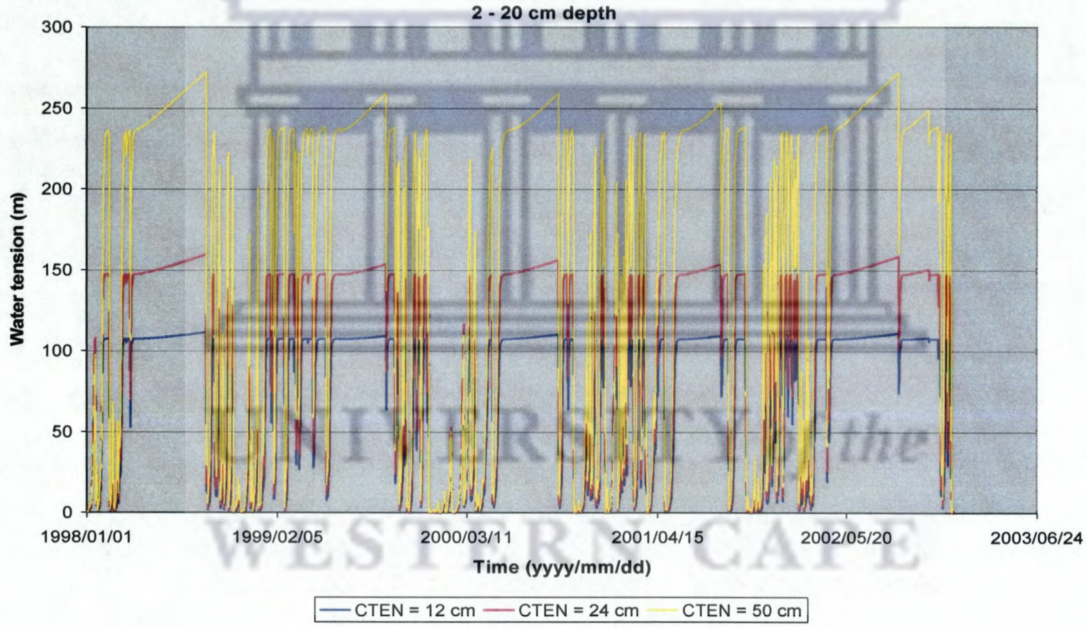
(c)



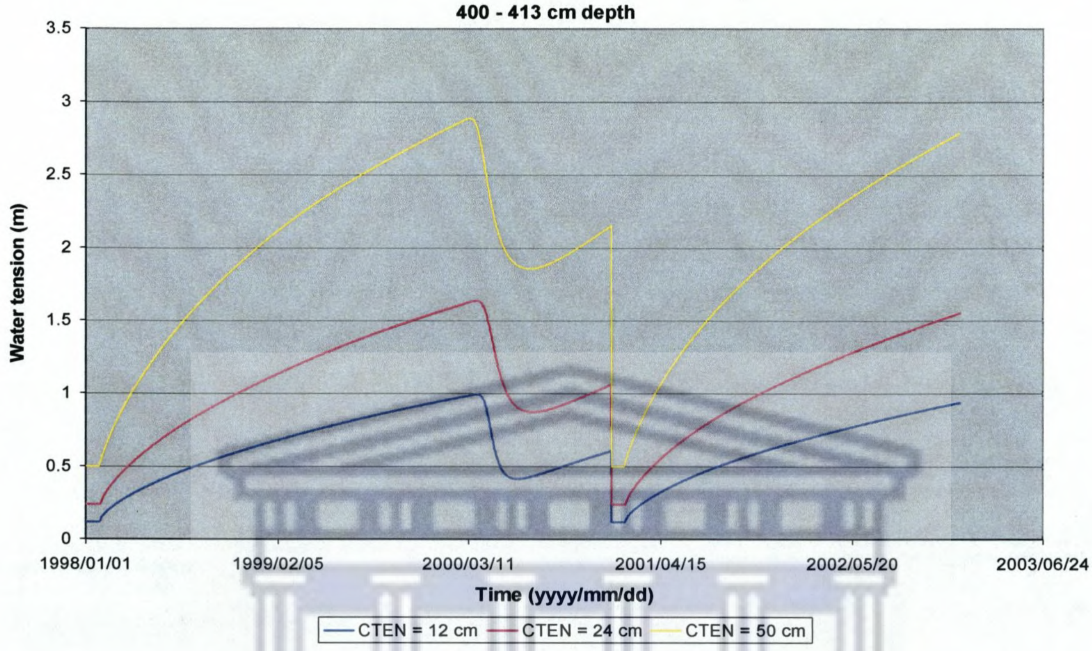
(d)

Figure 5.19: Simulated soil water content as a function of boundary hydraulic conductivity K_b at 2 - 20 cm for (a) non-irrigated, (b) irrigated; and 400 – 413 cm for (c) non-irrigated, (d) irrigated case in Mpumalanga Highveld.

Soil water tension at the boundary between macropores and micropores is an input varied in order to determine its effect on the total soil water tension (Figure 5.20). Soil water tension in Figure 5.20 (b) corresponds inversely to the water content graph of Figure 5.19 (b) in the sense that it decreases with an increase in water content and vice versa. Additionally, it is observed that tension at the boundary is relatively proportional to the total soil water tension, in other words it increases with an increase in total soil water tension. Again, differences in changing boundary tension as a function of time are prominent both at depth and near the surface in the profile (see Figures 5.20 (a) and (b)).



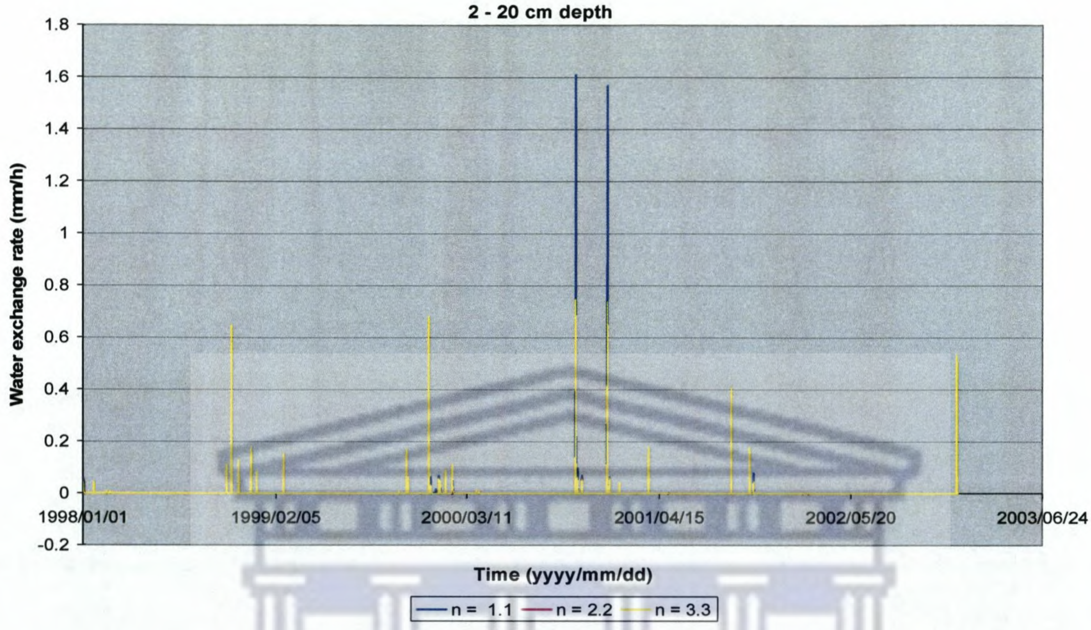
(a)



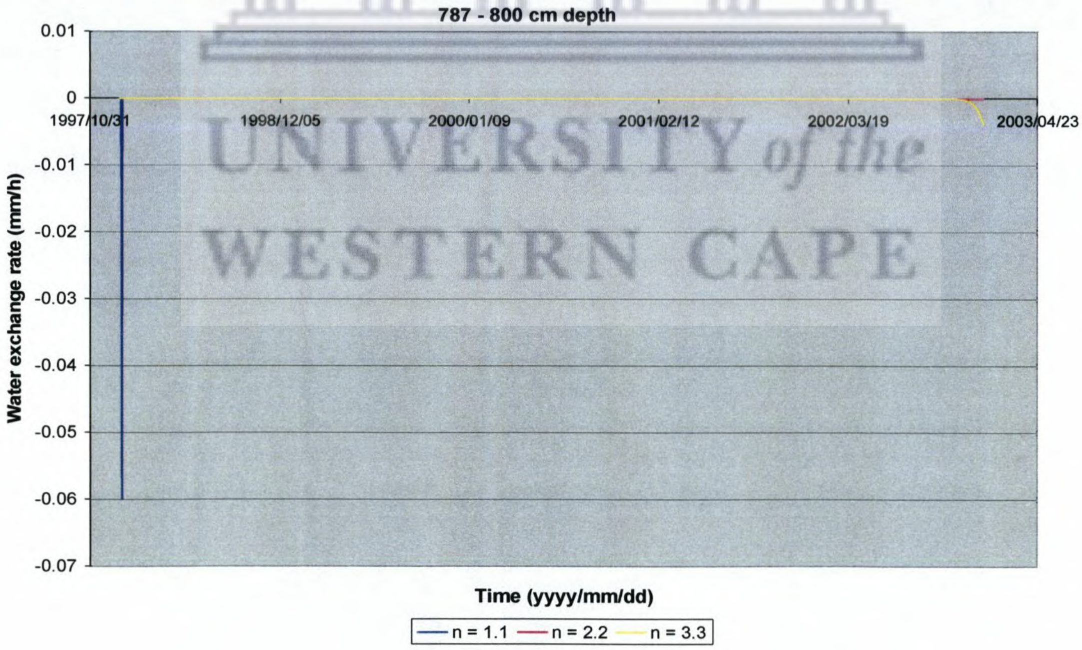
(b)

Figure 5.20: Sensitivity of simulated soil water tension to different values of the boundary soil water tension at (a) 2 – 20 cm and (b) 400 - 413 cm profile depth over a period from 1998 to 2002 – Mpumalanga Highveld area.

For Figures 5.21 (a) and (b), n (van Genuchten's value) is an input that was varied in order to determine its effect on water exchange rate output. Figure 5.21 represents non-irrigated conditions. At low rates, a higher n value results in a higher water exchange rate, but when one looks at the simulation period between 2000 and 2002 in Figure 5.21, the smaller n value renders the highest rate. The effect of the n value on the water exchange rate can therefore not be concluded with certainty in this case.



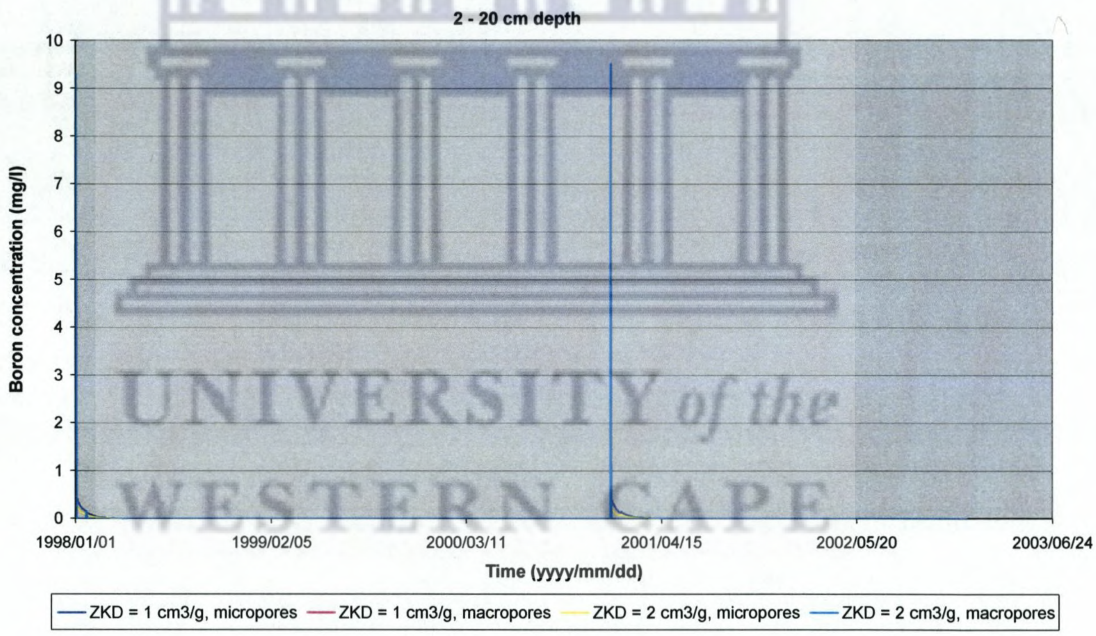
(a)



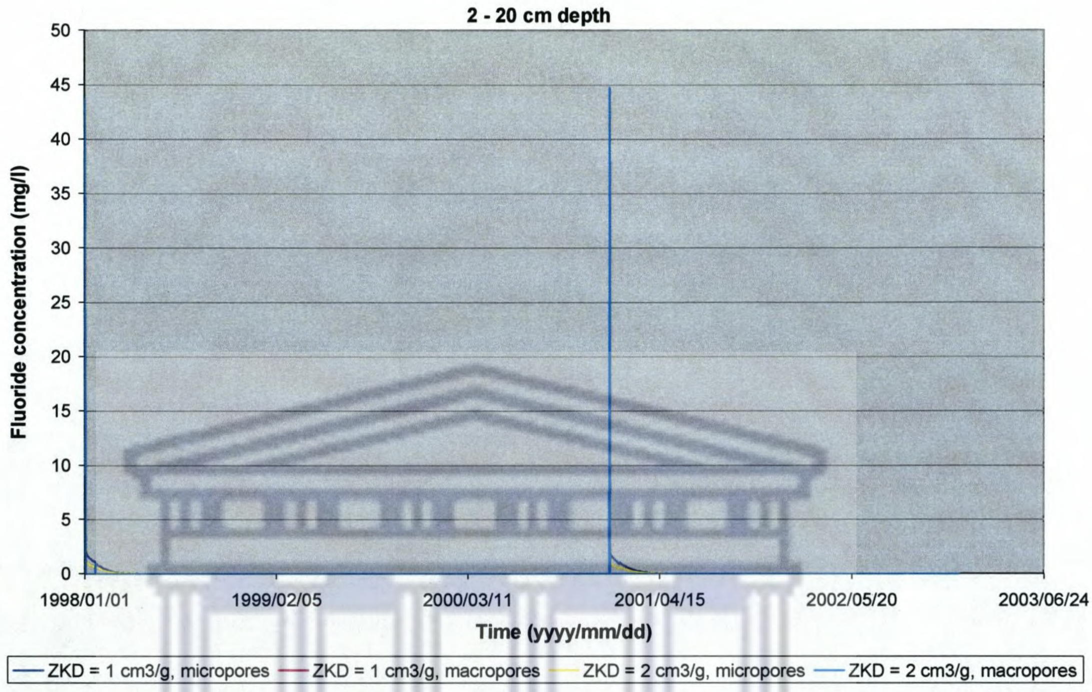
(b)

Figure 5.21: Simulated water exchange rate as a function of the van Genuchten n value at (a) 2 – 20 cm and (b) 787 – 800 cm depths.

Figures 5.22 (a to f) show how variation in the input parameters of the sorption distribution coefficient (ZKD), the excluded volumetric water content (AEXC), and the degradation rate coefficient (DEGMAS) affect the solute concentration at different depths. These are non-irrigated cases. In this case, we looked at the behaviour of generic chemicals at different depths that are prone to sorption and degradation, where the initial soil concentration inputs used in the simulation set-up were the same as for boron and fluoride. Therefore, the y-axes on the graphs are labeled accordingly. Concentration peaks are visible in all these graphs, particularly in macropores. This suggests the existence of preferential flow and possible flushing following heavy rainfalls.

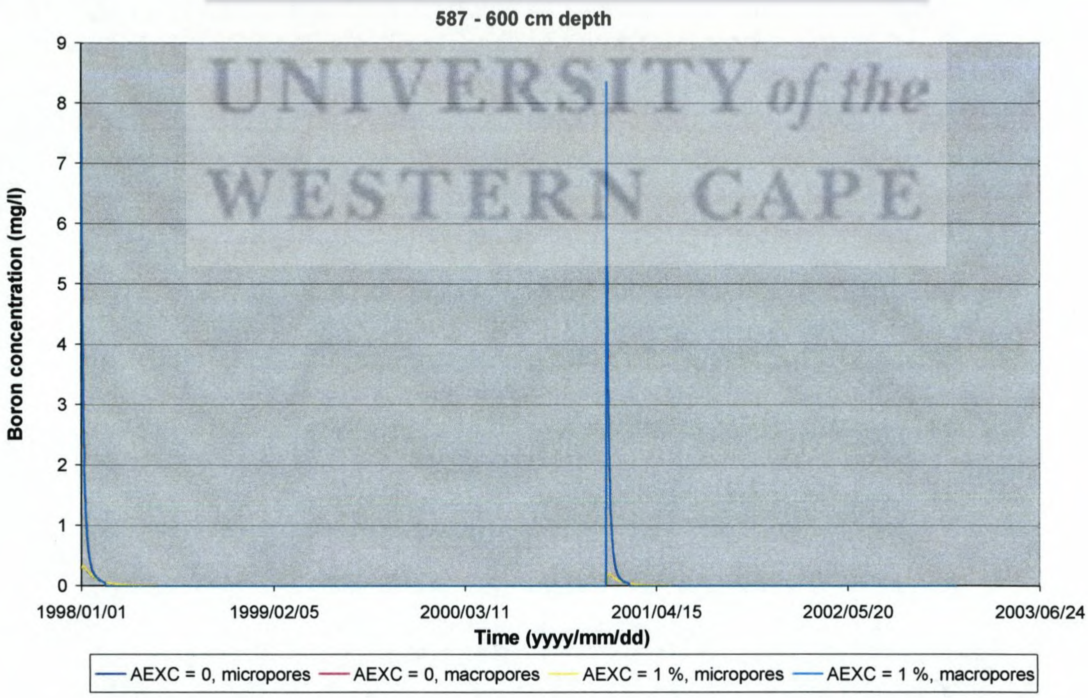


(a)



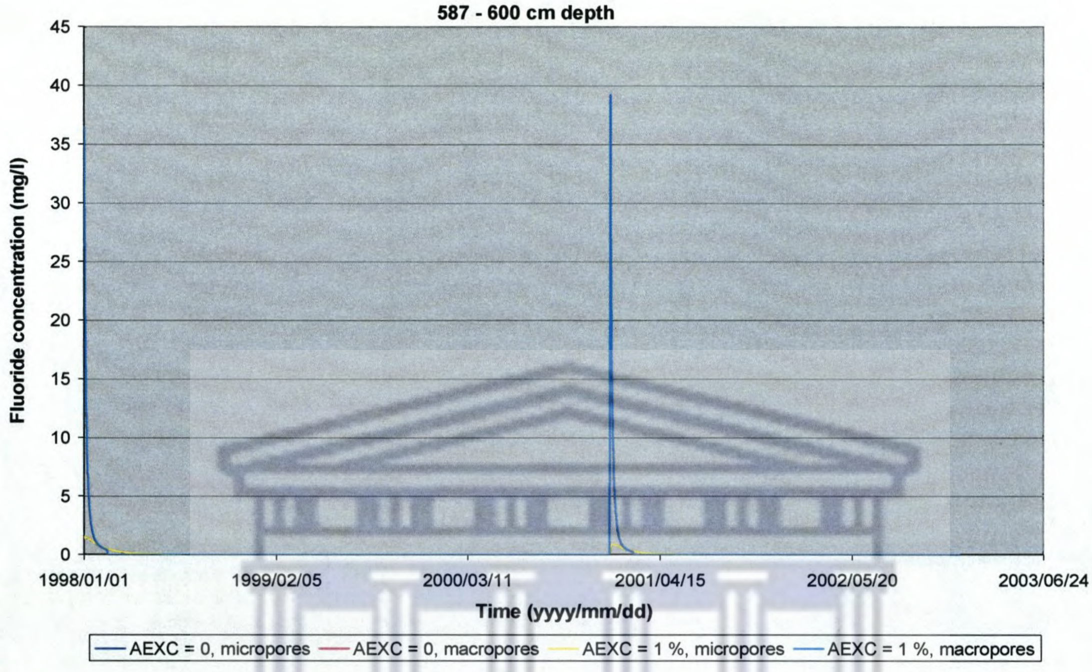
2 - 20 cm depth
Fluoride concentration (mg/l)
50
45
40
35
30
25
20
15
10
5
0
1998/01/01
1999/02/05
2000/03/11
2001/04/15
2002/05/20
2003/06/24
Time (yyyy/mm/dd)
ZKD = 1 cm3/g, micropores
ZKD = 1 cm3/g, macropores
ZKD = 2 cm3/g, micropores
ZKD = 2 cm3/g, macropores

(b)



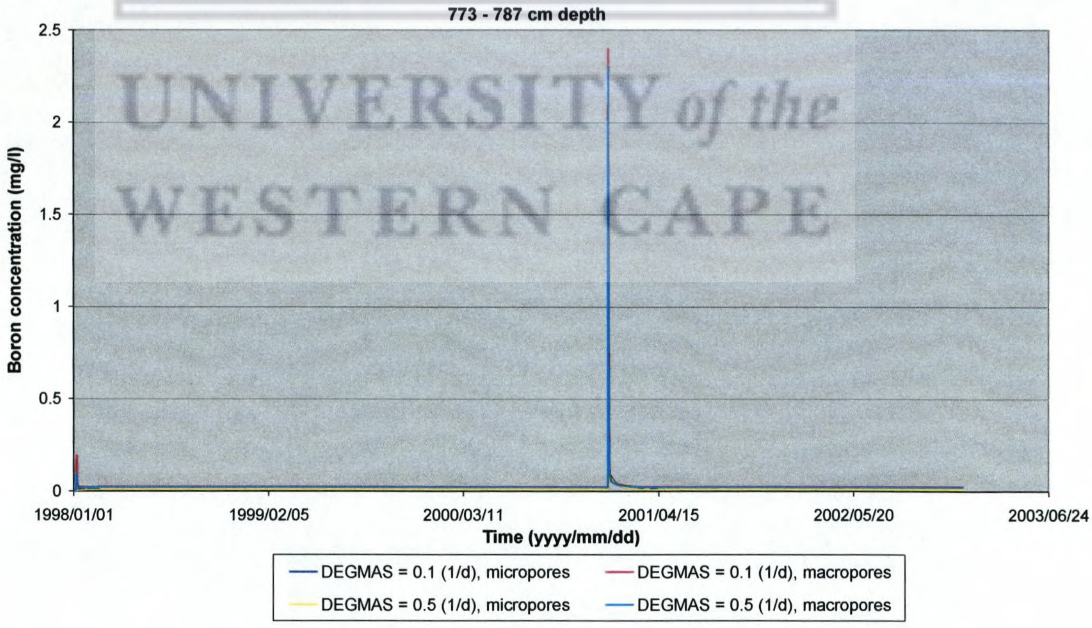
587 - 600 cm depth
Boron concentration (mg/l)
9
8
7
6
5
4
3
2
1
0
1998/01/01
1999/02/05
2000/03/11
2001/04/15
2002/05/20
2003/06/24
Time (yyyy/mm/dd)
AEXC = 0, micropores
AEXC = 0, macropores
AEXC = 1 %, micropores
AEXC = 1 %, macropores

(c)



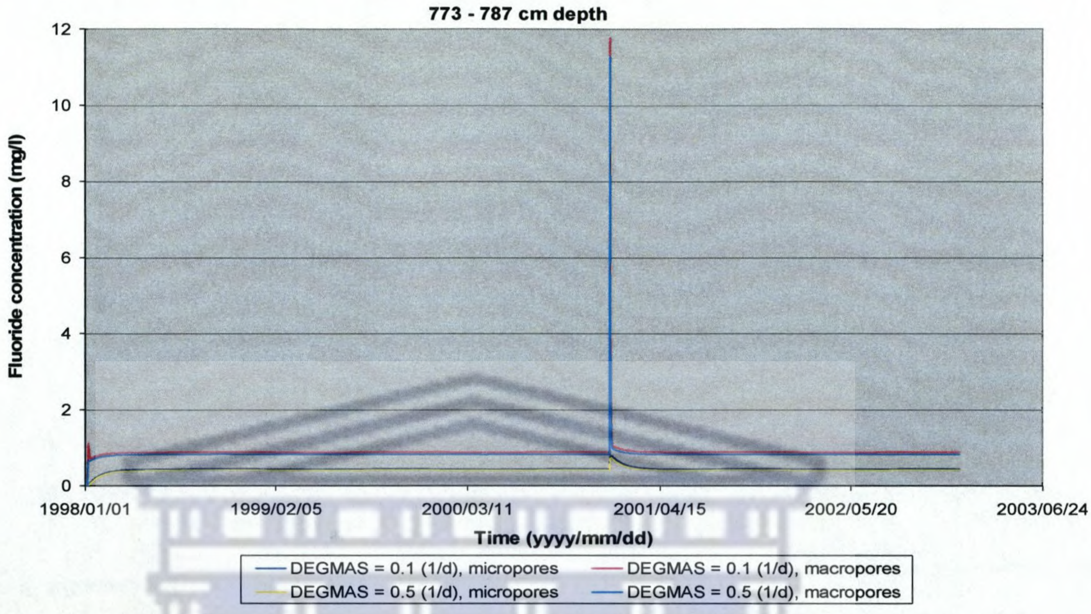
587 - 600 cm depth
Fluoride concentration (mg/l)
45
40
35
30
25
20
15
10
5
0
1998/01/01
1999/02/05
2000/03/11
2001/04/15
2002/05/20
2003/06/24
Time (yyyy/mm/dd)
AEXC = 0, micropores
AEXC = 0, macropores
AEXC = 1 %, micropores
AEXC = 1 %, macropores

(d)



773 - 787 cm depth
Boron concentration (mg/l)
2.5
2
1.5
1
0.5
0
1998/01/01
1999/02/05
2000/03/11
2001/04/15
2002/05/20
2003/06/24
Time (yyyy/mm/dd)
DEGMAS = 0.1 (1/d), micropores
DEGMAS = 0.1 (1/d), macropores
DEGMAS = 0.5 (1/d), micropores
DEGMAS = 0.5 (1/d), macropores

(e)



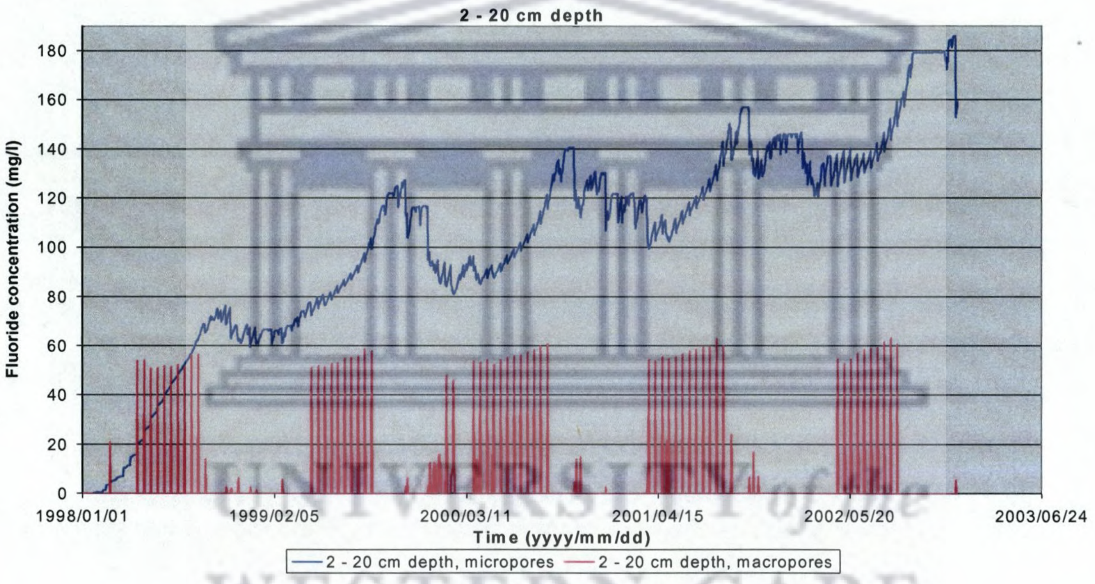
(f)

Figure 5.22: Simulated fluoride and boron concentrations as functions of sorption distribution coefficient (ZKD), excluded volumetric water content (AEXC) and degradation rate coefficient (DEGMAS) over a period 1998 to 2002 – Mpumalanga Highveld area.

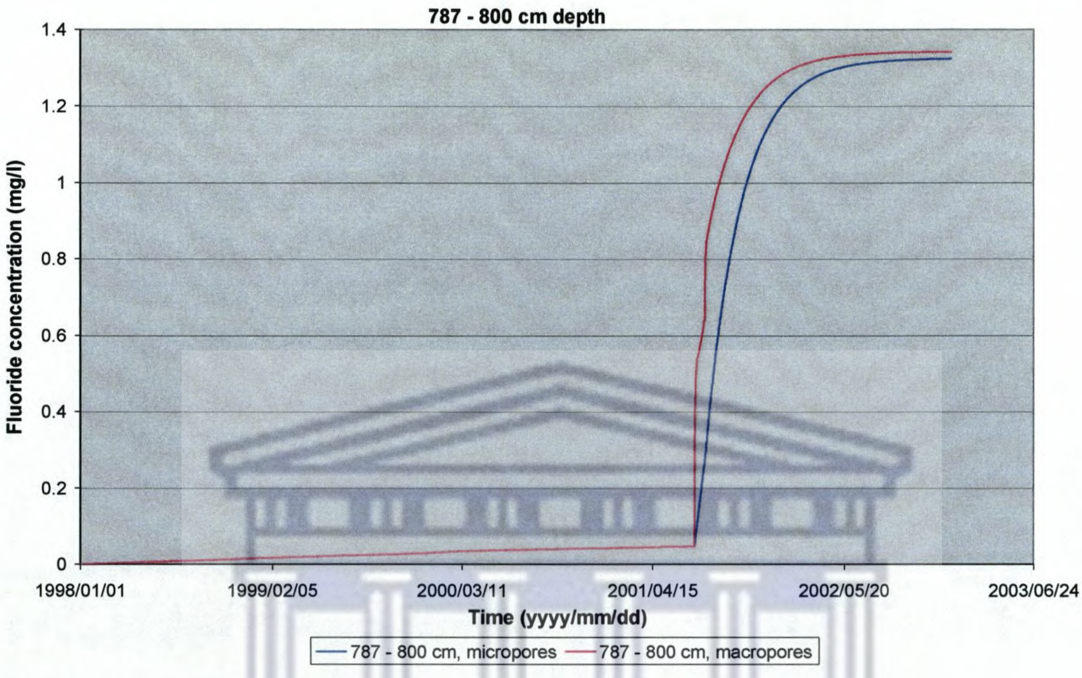
The graphs in Figure 5.22 show similar concentration patterns as other parameters such as solute concentration in soil water and solute concentration in irrigation water, when plotted. Concentration in bottom boundary when exposed to different distribution coefficient values follow the same trend (these graphs are not included here). It can be mentioned that soil properties like structure and shape did not affect the infiltration pattern.

Irrigated cases are now considered in Figures 5.23 (a) and (b). These graphs are used to determine the trends of fluoride concentration at certain depths in the profile with time. Also they compare the concentrations between micropores and macropores. Fluoride concentration is higher near surface whilst it is low at depth. Different rainfall events cause flushing and migration of solutes, after persisting on surface due to lack of mobilizing water, and that is observed in Figure 5.23. The solute concentration in irrigation water that fills the topsoil acts as the source to deeper layers during leaching over time. That is observed when comparing the graphs in Figure 5.23 (a) and (b).

It is also visible from the graph in Figure 5.23 (a) that the concentration of fluoride in macropores is similar to the concentration in irrigation water (47 mg/l) immediately after an irrigation event. Due to exchange in the bimodal flow system, the fluoride diffuses into micropores thereafter. Therefore, the concentration of fluoride in micropores increases during irrigation season, whilst it tends to decrease during the rainfall season due to flushing by rainfall.



(a)



(b)

Figure 5.23: Simulated fluoride concentration as a function of time on an irrigated site, Goedehoop for the period 1998 to 2002 at depths (a) 2 – 20 cm and (b) 787 – 800 cm.

Irrigation in the Mpumalanga Highveld was applied mainly during dry conditions. Thus, leaching continues to occur during this period mainly due to infiltrating irrigation effluent other than rainwater. A breakthrough of fluoride into the 787 – 800 cm layer of the soil appears in the year 2001 (Figure 5.23 (b)).

Figures 5.24, 5.25, and 5.26 represent simulated accumulated solute leaching and percolation for a non-irrigated case. There is a gradual increasing trend in boron and fluoride cumulative leaching (see Figure 5.24 and 5.25), which is due to an increase in cumulative percolation as seen on Figure 5.26. The wider the diffusion pathlength, the lesser the percolation.

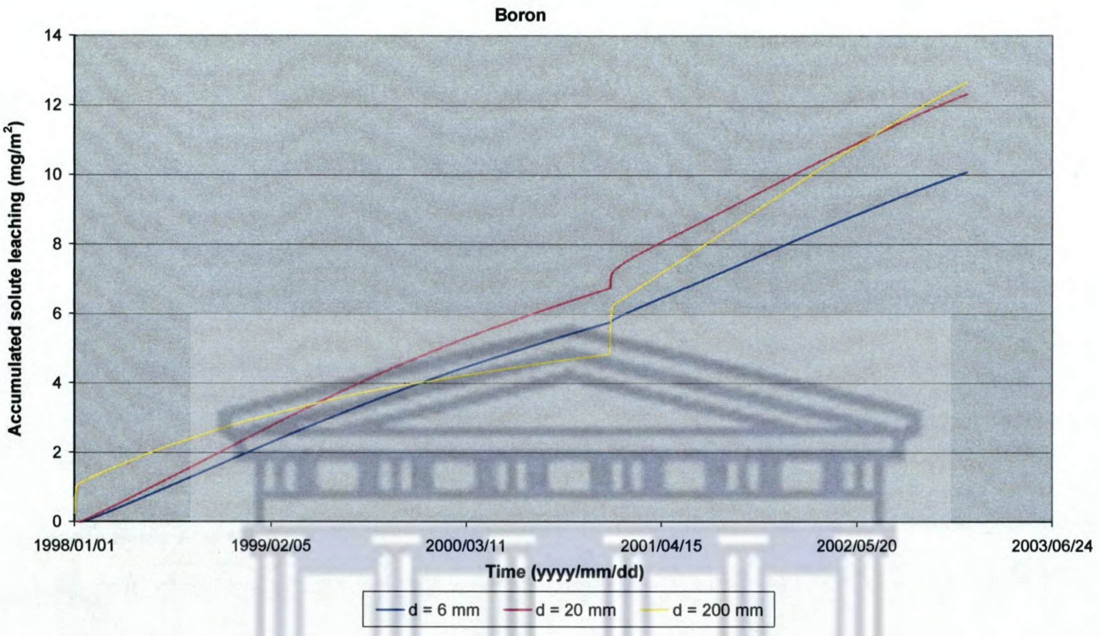


Figure 5.24: Simulated boron leaching with changing diffusion pathlength for a non-irrigated site.

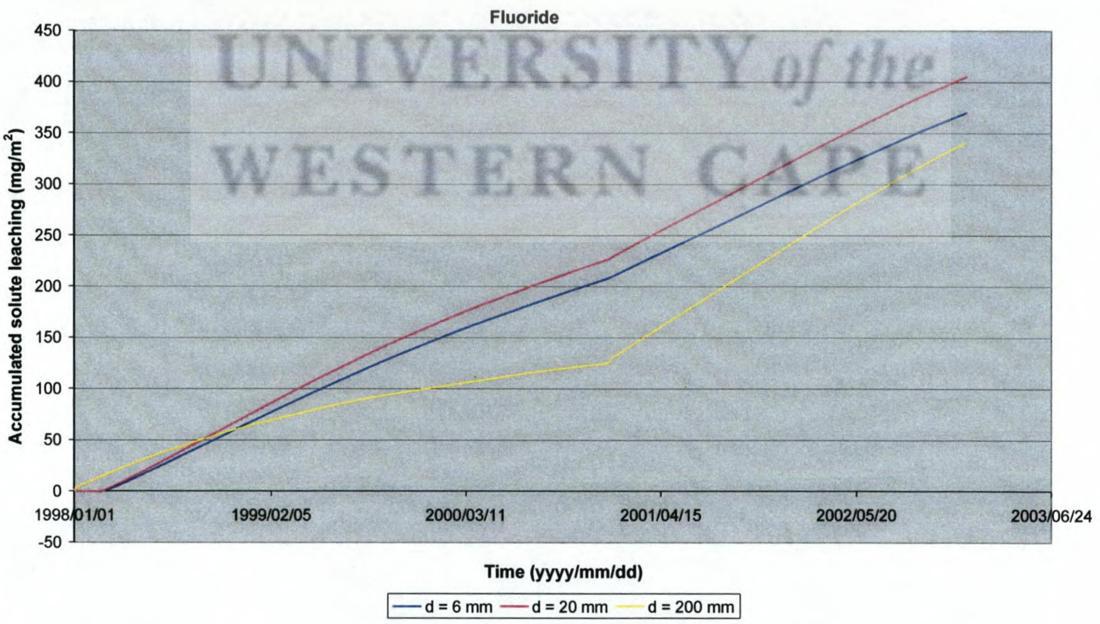


Figure 5.25: Simulated fluoride leaching with changing diffusion pathlength for a non-irrigated site.

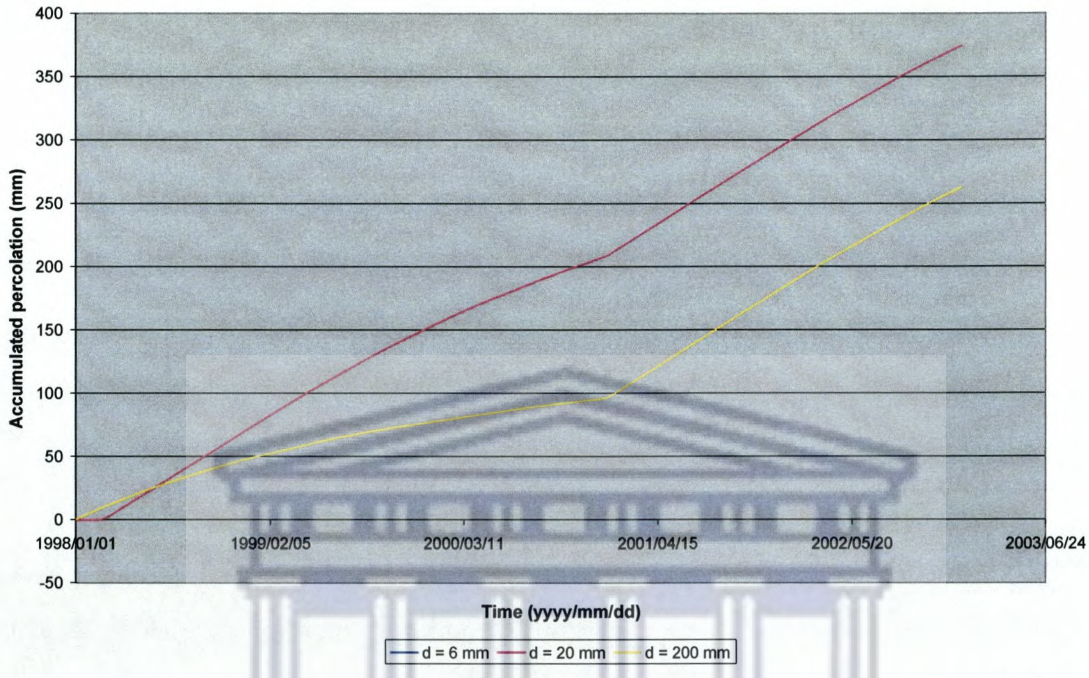


Figure 5.26: Simulated accumulated percolation with changing diffusion pathlength (blue line embedded in the purple line) for a non-irrigated site.

Figures 5.27 and 5.28 represent the irrigated case of the Goedehoop irrigation site. These two graphs display similar trends as those of non-irrigated conditions (Figures 5.25 and 5.26) in relation to the diffusion pathlength. However, it is not completely conclusive to say that leaching increases or decreases with increasing diffusion pathlength because leaching plots, especially for fluoride, display inter-crossing graphs for different diffusion pathlengths. Figures 5.27 and 5.28 show higher quantities of both leaching and percolation due to effluent irrigation applied. Furthermore, the percolation graph (Figure 5.28) indicates a proportional relationship with leaching and similar response to varying diffusion pathlength.

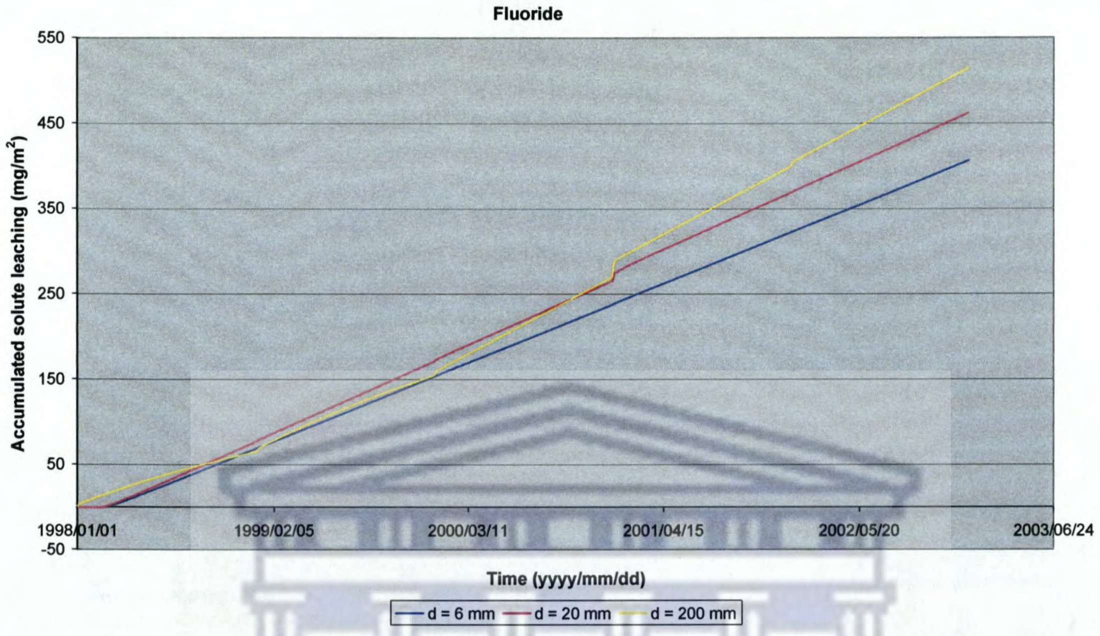


Figure 5.27: Simulated fluoride leaching with changing diffusion pathlength for irrigated site, Goedehoop.

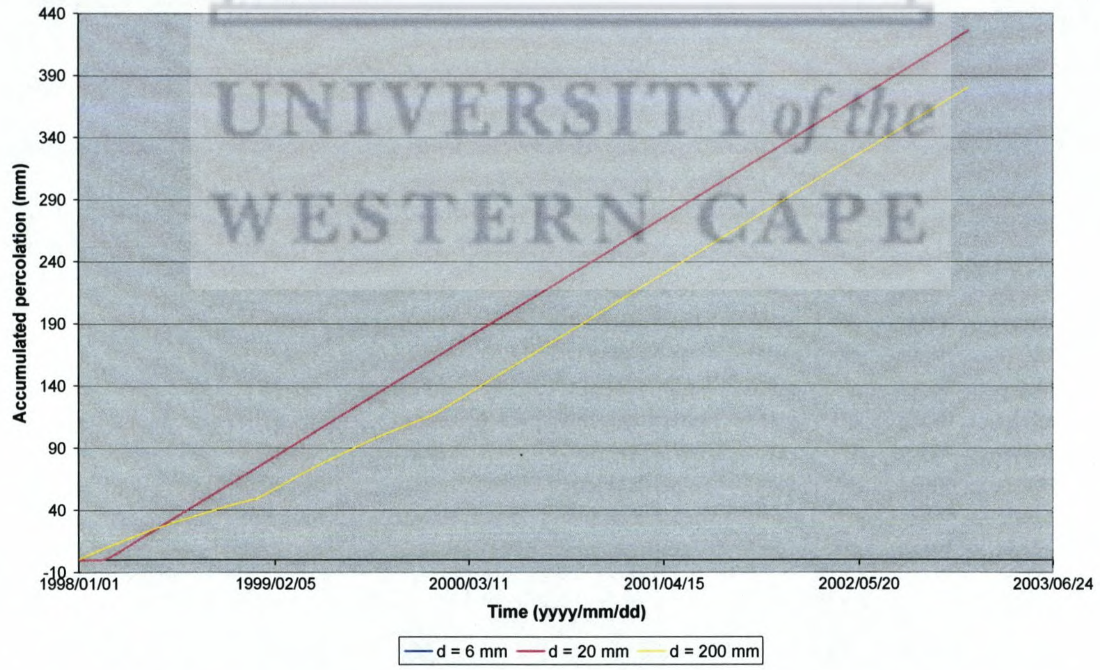


Figure 5.28: Simulated accumulated percolation with changing diffusion pathlength (blue line embedded in the purple line) for irrigated site, Goedehoop.

Percolation is higher in the Highveld than in the Cape Flats area (see Figures 5.26 and 5.28). Mpumalanga Highveld is a fractured environment, characterized by cracked clays, weathering and a thicker vadose zone of about 7 m. Irrigation was applied for which the rates were about 500 mm/annum in addition to annual precipitation of approximately 700 mm/annum. Some parts in the area are characterized by coarser grained sandstone and therefore higher recharge values are expected there, whilst dolerite sills often occur at surface where rain water recharges with ease since they are weathered or fractured. Table 4.5 also shows the shape, texture and composition of the soil profile as set up in MACRO for simulation process. Parameters ZP (slope of shrinkage characteristics) and ZA (shrinkage exponent) were set to zero for the Cape Flats area, whilst default values were used as input in the case of Mpumalanga Highveld. These properties promote preferential flow. Thus, higher percolation as seen in Figure 5.26 and 5.28 compared to Figure 5.17 is not unexpected. Climatic conditions of the area also favour the process since water logging is a common phenomenon causing soils to remain wet for longer periods.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

The MACRO 5.0 model was tested for preferential flow in the unsaturated zone of two different environments, namely the Cape Flats and the Mpumalanga Highveld. The Cape Flats are characterized by sandy soils and Mediterranean climate with winter rainfall, whilst the Highveld site is characterized by heavily cracked clay soils and summer rainfall in the form of thundershowers.

From the calibration process performed for the Cape Flats, it was evident that the MACRO 5.0 model predicted solute concentrations well. This indicated that the model is suitable to predict micropore flow, which is the dominant flow type in the unsaturated zone of the Cape Flats. The model was also able to predict macropore flow, which is dominant in Mpumalanga Highveld. Discrepancies between model predictions and measurements were however observed for some simulations. Environmental properties and the availability and adequacy of data, or lack thereof used in the simulation process for both case study sites could have had an influence on the results. It was therefore decided to run a sensitivity analysis of model output in order to indicate which input parameters are the most important to measure or accurately estimate.

Climate plays a role in solute transport since macropore flow is frequent in wet climates, whereas it occurs when shrinkage cracks are present in dry climates. Moreover, Jarvis (2002) realized that the extent of leaching in the presence of macropore flow does not only depend on total rainfall, but perhaps more importantly on rainfall distribution and intensity. Water content and concentration graphs for the Cape Flats area support that observation. Contaminant transport in the vadose zone depends on both the properties of the medium and the properties of the pollutant (Jarvis, 2002). Solute concentration graphs confirm this notion (see Figures 5.22 and 5.23). When it comes to the properties of the pollutant, the differences are clear when graphs of solutes set under tritium type in simulation set-up (Figures 5.10 to 5.12) are compared to generic solutes graphs (Figures 5.13 to 5.15) in the Cape Flats scenario. The same applies to Mpumalanga Highveld.

The unsaturated zone of the Cape Flats is not affected by preferential flow in the same way as the Mpumalanga Highveld. That is evident in the water content and solute concentration graph patterns. The concentration versus depth plots for Mpumalanga Highveld show sudden decreases in both micropore and macropore concentration with depth at certain points. This indicates the existence of significant preferential flow for the area. Nonetheless, these observations are expected since we are dealing with different environments. Unconsolidated porous sands of the Cape Flats, with some isolated calcrete, allow the flow to be mainly through matrix. Conversely, Highveld clays are susceptible to cracking especially due to climate. Weathering also plays a role at depth since the Ecca sediments are weathered to depths of between 5 - 12 m below surface throughout the area.

In relation to other soil hydraulic property parameters, the boundary hydraulic conductivity, the boundary water content, boundary soil water tension and the diffusion pathlength have significant influence on simulation results of the water balance. Other tested parameters that show subtle influence or had no significance, are: saturated water content, residual water content, excluded volumetric water content, bulk density, tortuosity or pore size distribution factors. Some parameters are only applicable if shrinkage is modelled, for example ZP (slope of shrinkage characteristics) and ZA (shrinkage exponent), which in this study is not applicable to the Cape Flats area conditions. The graphical representations of parameters, for which their outputs showed low sensitivity, were not included here.

The solute balance is mostly influenced by sorption distribution coefficients, initial solute concentration in soil water, solute concentration in bottom boundary, solute concentration in irrigation water, degradation rate coefficients (both in solid and liquid phases), and other specific chemical properties.

Clearly, further studies from different parts of the country are needed to build a database of soil hydraulic properties, with specific emphasis on the vadose zone. Such data is currently almost non-existent in South Africa.

As a modelling program, MACRO 5.0 is able to yield reliable results and the user is able to make various changes and perform numerous runs. Simulation runs may be too long at times, especially when the model is run over a long period and/or the number of numerical layers is high.

The program interface requires further development, especially when it comes to output files. In its current form, it allows the user to input all parameters and select all output parameters that need to be simulated. Unfortunately, sometimes the user cannot read all output results unless time consuming methods that are not part of the program are employed.

CHAPTER 7

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CHAPTER 8

APPENDICES

The Units of parameters given in Appendix A and Appendix B are as follows:

Maximum and Minimum Temperatures - °C

Potential Evapotranspiration – mm

Rainfall – mm

APPENDIX A:

Example of Potential Evapotranspiration, Temperatures, and Rainfall uploaded driving data of the Cape Flats area for 2004

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20040101	4.62	24.3	16.3	0
20040102	4.33	24.1	17.6	0
20040103	8.06	36.2	17.9	0
20040104	7.31	34.8	19.1	0
20040105	4.17	24.5	18	4.4
20040106	3.62	24.1	17.5	0
20040107	5.67	28.2	17	0
20040108	5.31	28.5	17.6	0
20040109	4.18	24.6	16.7	0
20040110	4.45	23.4	16.5	0
20040111	6.67	31.7	15.3	0
20040112	4.32	26.4	16.8	0
20040113	5.04	28.3	17.9	0
20040114	4.07	24.5	17	0
20040115	4.29	23.4	17.1	0
20040116	5.13	26.3	16.4	0
20040117	5.47	28	16.8	0
20040118	5.54	28.5	16.5	0
20040119	5.06	27.3	15.8	0
20040120	6.29	31.8	17.8	0
20040121	6.84	34.1	18.5	0
20040122	5.42	30.5	17.7	0
20040123	6.33	33.3	18.8	0
20040124	4.71	27.4	16.4	0
20040125	4.11	25.6	17	0
20040126	4.72	26	17.1	0
20040127	4.55	24.8	16.5	1.4
20040128	4.34	22.7	16.3	0
20040129	4.84	24.3	15.9	0
20040130	6.42	30.4	14.3	0
20040131	4.33	27.2	18.1	0
20040201	4.23	25.2	18.1	0

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20040202	5.75	29.4	16.2	0
20040203	4.4	25.8	16.9	0.2
20040204	4.27	24.4	15	0
20040205	5.62	28.1	12.3	0
20040206	5.76	30.4	16.9	0
20040207	6.16	32.2	18	0
20040208	6.41	33.8	18.9	0
20040209	6.62	34.3	18.7	0
20040210	5.63	32.4	16.7	0
20040211	4.03	26.1	17.8	0
20040212	4.62	27.4	17.5	0
20040213	4.13	26.3	16.4	0
20040214	3.18	24.6	18	0
20040215	4.29	24.6	14.5	0
20040216	4.27	25.4	15.8	0
20040217	3.74	23.8	17.7	0
20040218	4.8	27.9	17.8	0
20040219	5.11	29.3	18.3	0
20040220	4.87	29.5	17.6	0
20040221	3.69	26	17.1	0
20040222	3.84	24.7	17.6	0
20040223	4.66	28	17.5	0
20040224	3.15	23.2	16	0
20040225	4.09	24.9	15.6	0
20040226	4.08	26.5	15.3	0
20040227	3.91	26.8	17.6	0
20040228	3.89	26	17	0
20040229	4.26	24.9	14.7	0
20040301	3.77	23.2	12.9	6.8
20040302	3.56	20	12.7	0
20040303	3.9	22	11	0
20040304	3.04	20.1	10.8	1

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20040305	3.76	20.7	13.3	0
20040306	5.78	29.9	10.7	0
20040307	6.62	34.5	12.8	0
20040308	3.63	24.7	16.8	0.4
20040309	3.21	21	15.5	0
20040310	3.03	21.4	14.7	0
20040311	3.47	22.6	13.1	0
20040312	5.15	29	13.5	0
20040313	5.25	30.7	14.5	0
20040314	5.49	31.4	15.2	0
20040315	5.66	31.8	14.4	0
20040316	3.72	24.6	15.5	0
20040317	3.52	24.6	12.5	0
20040318	2.93	21.9	13.9	0
20040319	2.92	21.7	13.1	0
20040320	3.3	22.7	13.8	0
20040321	3.19	22.8	12.2	0
20040322	3.31	23.2	9.6	0
20040323	3.84	26.7	16.2	0
20040324	4.51	28.3	10.2	0
20040325	2.98	23.5	16	0
20040326	2.41	21.4	14.8	0
20040327	3.13	22.5	12.4	0
20040328	3.26	23.5	10.3	0
20040329	3.18	20.3	13.1	0
20040330	2.94	20.3	10.3	0
20040331	4.45	28	13	1
20040401	4.92	32	13.3	0
20040402	3.68	27.7	15.7	0
20040403	2.4	22.5	15.6	1
20040404	2.33	21.7	15.6	9.1
20040405	2.07	19.6	13.8	0.4

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall	Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall	Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20040406	2.91	23.1	9.2	0	20040508	2.63	25.6	10.7	0	20040609	1.39	17.6	7.1	0
20040407	5.08	33.6	11.5	0	20040509	1.63	24.2	14.5	0	20040610	1.94	20.4	5	0
20040408	2.35	21.8	14	3.7	20040510	1.86	20.6	13.4	0	20040611	2.64	23.4	3.9	0
20040409	2	19.2	13.6	2.8	20040511	1.28	17.8	13.3	0	20040612	1.29	17.9	7.2	2.4
20040410	1.39	18.4	13	3.2	20040512	1.05	17.5	13.6	1.8	20040613	0.87	16.1	13.4	13.7
20040411	2.46	21.9	12.6	0	20040513	1.87	20	9.6	0	20040614	1.34	19.1	12.5	14
20040412	2.87	24.7	14.9	0	20040514	1.98	20.9	5.9	0	20040615	0.93	17.1	13.4	1.8
20040413	4.67	31.3	13.1	0	20040515	1.65	21.5	9.8	0	20040616	1.36	19.6	12.2	0
20040414	2.12	21.6	14.3	0.2	20040516	2.42	23	8	0	20040617	1.62	22.7	6.8	0
20040415	1.81	20	14.4	18.6	20040517	1.14	16.9	13	0	20040618	1.28	18.8	11.2	9.5
20040416	1.48	16.9	12.7	11	20040518	1.4	19	9	0	20040619	1.24	17.6	8.1	0
20040417	2.24	18.9	9.2	0	20040519	1.15	19.7	14.5	0	20040620	1.6	19.4	5.4	0
20040418	2.21	20.6	12.2	0.5	20040520	1.55	21.5	10.3	0	20040621	1.85	21.5	7.4	0
20040419	2.24	18.3	11.3	0	20040521	1.58	21.1	11.7	0	20040622	1.9	21.1	9.2	6
20040420	2.14	18.6	6.8	8.2	20040522	1.68	21.6	9.7	0	20040623	0.9	16.8	11.5	0
20040421	1.85	19.2	12.2	3	20040523	1.43	18.8	13.3	0	20040624	1.41	18.4	6.7	0
20040422	2.14	19.8	13.3	0	20040524	1.67	21.6	10.4	0	20040625	1.07	16.9	4.5	1.4
20040423	2.86	24.7	9.9	0	20040525	1.73	22.1	11	0	20040626	0.93	14.9	7.2	10.4
20040424	1.72	20.5	13.2	1.4	20040526	2.11	23.6	7.5	0	20040627	1.28	14.4	3.5	0
20040425	2.14	17.8	10.4	0	20040527	1.96	20.4	11.4	0	20040628	1.89	17.2	1.4	0
20040426	3.16	23.2	11.1	0	20040528	1.54	17.2	13	1.6	20040629	1.07	14.5	2.8	0
20040427	2.54	23.5	8.1	0	20040529	1.57	17.8	9.5	0	20040630	1.5	17.2	4.7	0
20040428	3.7	29	10.6	0	20040530	2.16	20.4	3.1	0	20040701	1.45	16.2	5.8	0
20040429	3.44	28.9	10.4	0	20040531	2.43	21.3	4.7	0	20040702	0.96	15	8.3	7.2
20040430	2.86	24.7	13.7	0	20040601	3.19	27.8	3.6	0	20040703	0.99	16.6	9.1	1
20040501	1.67	19.9	15.6	0.4	20040602	3.61	29.5	10.9	0	20040704	1.1	15.3	6.7	0
20040502	2.75	24	13.5	0	20040603	3.55	30.1	12.6	0	20040705	1.56	16.5	1.8	0
20040503	2.93	25.4	10.3	0	20040604	1.48	20	13.4	19.2	20040706	1.87	19.8	2.6	0
20040504	2.48	24.1	7.1	0	20040605	1.19	16.4	12.1	8.4	20040707	1.92	20.6	3.2	0
20040505	2.58	25.4	10.4	0	20040606	1.18	15.7	10.3	0.9	20040708	2.39	23.5	3.3	0
20040506	2.1	26.5	11.2	0	20040607	1.54	15.9	10.2	3.2	20040709	2.79	24.7	5.8	0
20040507	1.77	21.1	11.5	0	20040608	1.23	16.6	8.8	0.2	20040710	1.68	18.8	9.8	0

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall	Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall	Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20040711	2.01	20.8	4.4	0	20040812	1.61	17.4	5.6	0	20040913	2.65	20.7	8.6	0
20040712	1.34	17.1	11.5	0	20040813	1.62	16.2	5.4	2	20040914	2.6	20.6	10.1	0
20040713	2.25	18.4	8.3	0	20040814	1.2	16.3	8.9	6.3	20040915	2.3	19.5	13.7	0
20040714	2.59	21.2	2.2	0	20040815	1.65	15.5	7.3	7.6	20040916	2.79	19.9	12.5	0
20040715	2.02	20.8	2	0	20040816	1.19	15.5	10.7	3.4	20040917	2.65	18.8	11.4	10.7
20040716	2.78	22.9	5.7	0	20040817	1.56	17.2	8.5	0.3	20040918	2.05	16.6	10	3.3
20040717	2.65	24.1	4.4	0	20040818	1.76	18	6.8	0	20040919	2.44	17.3	8.4	0
20040718	1.53	20.4	3.4	0	20040819	1.56	17.6	7.4	0	20040920	3.73	22.5	6.6	0
20040719	3.13	26.3	7.2	0	20040820	1.79	19.1	11.3	0	20040921	5.29	29.8	7.4	0
20040720	1.62	18.9	7.4	0	20040821	1.66	17.3	12.3	0	20040922	2.64	20.1	11.9	0
20040721	1.3	18.4	7.5	0	20040822	1.73	17.7	7.5	0	20040923	2.89	18.9	10.6	2
20040722	1.36	17.9	11.2	4.2	20040823	2.09	17.1	8.7	0	20040924	2.2	16.5	11	0
20040723	0.88	16	9.7	20.6	20040824	2.02	18	8.9	0	20040925	2.74	18.1	7.9	0
20040724	1.28	16.2	8.6	9	20040825	2.03	17.1	10.6	0	20040926	3.09	19.6	10.6	0
20040725	1.35	14.5	5.8	0.6	20040826	2.14	18.2	7	0	20040927	4.18	25	6.9	0
20040726	1.54	15.5	5.7	0	20040827	2.72	22.2	8.1	0	20040928	2.95	20.9	14.2	0
20040727	1.56	16.3	4.8	0	20040828	3.16	24.3	7.7	0	20040929	5.15	28.4	7.9	0
20040728	2.49	20.5	3.7	0	20040829	1.88	20.3	12.8	0	20040930	3.06	22.9	14.6	0
20040729	1.6	17.1	4.4	18.4	20040830	1.59	18.8	12.4	0	20041001	4.71	28.5	11.2	0
20040730	1.67	13.5	7.2	2.3	20040831	2.06	19.8	12.3	0	20041002	2.71	20.1	13.1	0
20040731	1.26	14.5	6.9	1.4	20040901	1.69	17.8	12	2.5	20041003	3.9	24.9	14.5	0
20040801	1.29	16.3	9.8	0	20040902	2.36	20.1	10	0	20041004	2.85	21.6	14.4	0
20040802	2.27	19.4	3.4	0	20040903	3.28	23.9	6.9	0	20041005	2.9	21	14.5	0
20040803	1.42	15.9	5.9	0	20040904	2.3	18.7	8.7	6.2	20041006	2.79	20.2	11.7	49
20040804	1.78	15.8	10.8	15.4	20040905	2.02	15.5	8	0.4	20041007	3.26	16.7	8.3	0.2
20040805	0.77	12	9.7	56	20040906	3.07	19.6	6.4	0	20041008	3.22	17.6	4.9	5
20040806	1.35	15	7.1	3.3	20040907	2.55	17.7	3.6	0	20041009	2.76	15.4	9	0.2
20040807	1.04	13.9	9.5	52.9	20040908	3	19.7	7.6	0	20041010	3.11	17.5	7.7	0
20040808	1.25	16.9	11.6	6.8	20040909	3.73	23	5.7	0	20041011	4.07	22.4	11.7	0
20040809	1.49	16.9	8	15.7	20040910	4.59	26.9	5.5	0	20041012	4.61	25.8	13.3	0
20040810	1.96	18.3	5.5	0	20040911	2.64	19.8	7.6	0	20041013	4.5	25.6	10.7	0
20040811	3.15	24.3	3.8	0	20040912	3.03	22.4	13	0	20041014	3.51	21.3	9.9	0

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20041015	3.13	20.7	13	0
20041016	3.4	20.4	13.7	1.3
20041017	3.43	20.5	13	0
20041018	5.64	27.3	6.9	0
20041019	4.58	25.4	13.9	0.2
20041020	1.8	17.2	14	39
20041021	2.72	19.1	13.4	1
20041022	3.44	20.4	11	0
20041023	4.08	24.6	14	0
20041024	3.05	21.2	14.9	0
20041025	3.47	21	13.1	0
20041026	3.71	19.7	13.2	0
20041027	3.7	19.3	11.8	0
20041028	4.33	21.4	7.8	0
20041029	3.42	19.6	13.7	3
20041030	5.67	26.4	8	0
20041031	3.55	21.1	12	0
20041101	5.21	27	14.3	0
20041102	3.71	22.3	16.8	0
20041103	5.51	27.6	12.9	0
20041104	3.8	23.7	16.6	0
20041105	4.11	21.8	14.5	0
20041106	4.41	23	11.1	0
20041107	4.57	25.3	15	0
20041108	4.86	24.8	14	0
20041109	4.54	24.9	14.8	0
20041110	3.68	23	17	0
20041111	3.67	23.8	17.3	0
20041112	4.65	26	16.5	0
20041113	4.58	26.9	18	0
20041114	4.22	25.8	17.2	0
20041115	3.97	23.6	17	0

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20041116	5.4	28.8	17.2	0
20041117	3.84	25.8	17.3	0.2
20041118	4.4	25.7	15.1	0
20041119	5.33	29.1	16.6	0
20041120	5.16	26	14.5	0
20041121	4.19	22.6	14.5	0.2
20041122	4.42	20.4	13.6	0
20041123	4.33	21.5	12.6	0
20041124	4.85	22.8	9.8	3
20041125	4.02	23.9	15.1	0
20041126	5.08	23.3	11.7	0
20041127	4.32	23	16.1	0
20041128	4.96	24.2	14.7	0
20041129	4.8	25.2	15.6	0
20041130	4.84	25.9	14.5	0
20041201	4.89	24.5	13.3	1
20041202	4.98	26.3	16.2	0
20041203	7.21	31.2	12.8	0
20041204	5.23	28.2	19.1	0
20041205	5.01	27.2	18	0
20041206	4.42	23.4	15.6	0
20041207	4.78	23.8	14.1	0
20041208	4.73	24.2	15.8	0
20041209	6.37	30.3	15.3	0
20041210	5.51	28.7	19.4	0
20041211	6.53	31	14.4	0
20041212	5.07	27.4	14.9	0
20041213	5.17	26.2	14.4	0
20041214	4.94	23.2	14.1	0
20041215	4.9	24.5	16.4	0
20041216	6.12	28.4	12.7	0
20041217	4.56	24.4	17.7	0.2

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20041218	4.66	24.1	17.4	0
20041219	4.95	25.7	17.3	0
20041220	6.02	28.6	15.6	0
20041221	3.94	24.9	19	0
20041222	5.01	27.1	19	0
20041223	6.03	30.8	19.5	0
20041224	6.63	32.4	18.6	0
20041225	4.92	27.1	16.1	0
20041226	4.5	26	18.3	0
20041227	4.72	25.3	15.7	0
20041228	5.05	27.5	18.8	0
20041229	4.86	26.7	17.3	1
20041230	2.87	21	16	7
20041231	4.36	22.7	13.1	0

APPENDIX B:

Example of Potential Evapotranspiration, Temperatures, and Rainfall uploaded driving data of Mpumalanga Highveld area for 2002

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall	Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall	Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20020101	6.55	30.5	12.8	0	20020202	5	26.7	14.5	0	20020306	4.42	26.2	14.2	0
20020102	5.37	28.7	17	1	20020203	5.08	27.3	15	0	20020307	3.66	24.5	16	9
20020103	4.78	25.7	15.2	1.5	20020204	5.48	29.3	16	0	20020308	3.11	20	12.3	0
20020104	4.63	25.7	16	20	20020205	6	30.8	15.3	0	20020309	4.3	25	12.5	0
20020105	5.56	26.6	12	0	20020206	6.32	32.1	15.5	1.5	20020310	4.89	26.5	10.5	0
20020106	5.37	27.3	14.5	0	20020207	2.51	19.3	15.5	25.5	20020311	4.07	24.5	13	0
20020107	6.15	30	14.5	0	20020208	4.25	22.4	11.4	14	20020312	3.94	25	14.6	3.5
20020108	4.3	25.5	17.2	3	20020209	4.64	22.4	8.5	0	20020313	3.71	23.8	14	0.1
20020109	5.65	27.5	13	0	20020210	5.34	25.3	8.6	0	20020314	4.61	25.7	10.5	0
20020110	5.64	28.5	14.9	0	20020211	5.73	28.3	11.6	0	20020315	4.42	25.5	11.5	0
20020111	5.9	29.3	14.7	0	20020212	5.96	30.5	14.2	1.5	20020316	4.6	26.5	11.8	0
20020112	5.3	28	16	0	20020213	2.49	20.6	17	1	20020317	4.84	27.5	11.5	0
20020113	5.79	28.5	13.8	0	20020214	1.73	17.7	15.9	13	20020318	4.99	28.5	12	0
20020114	5.33	27	14	4.5	20020215	3.82	23.1	14.6	0	20020319	4.81	28.2	12.8	0
20020115	5.95	28.7	13	8.5	20020216	4.53	26	15.1	0.7	20020320	4.93	28.8	12.7	0
20020116	5.73	29	15	0	20020217	3.55	22.2	14.5	1	20020321	4.94	29	12.8	0
20020117	5.83	29.9	16	0	20020218	3.41	22.1	15	23.5	20020322	5.03	29.3	12.4	0
20020118	5.61	29.3	16.2	0	20020219	4.12	22.8	12	0	20020323	4.21	26.5	13.6	0
20020119	5.12	27.3	15.6	3.5	20020220	4.81	25.5	12	0	20020324	4.03	25.5	13	0
20020120	5.44	27.8	14.5	0	20020221	4.9	27	14	0.4	20020325	4.31	26.8	13	0
20020121	6.2	31	15.5	0	20020222	4.35	24.3	12.8	0	20020326	4.34	26	11	0
20020122	5.77	29.3	15	3.5	20020223	4.88	26	12	0	20020327	4.48	27	11.5	0
20020123	5.4	29.2	17	0.5	20020224	5.12	27	12	0	20020328	4.15	26.7	13.5	0
20020124	4.56	26	16.3	8.5	20020225	5.8	30	12.5	17	20020329	4.83	26.8	6.8	0
20020125	4.73	24.9	13.5	0.2	20020226	4.28	25	14	0	20020330	3.96	25	11.5	0
20020126	4.24	22.9	13	0	20020227	4.37	26	15	0	20020331	4.59	27.3	10	0
20020127	4.14	23.5	14.5	0	20020228	4.78	28	15.7	1.5	20020401	4.45	26.8	10.1	0
20020128	5.06	27	15	2.5	20020301	4.55	28	17	10	20020402	4.64	28	10.5	0
20020129	5.64	28.8	14.5	6.5	20020302	4.29	27	16.8	5	20020403	4.77	28	8.8	0
20020130	4.86	27	16	1	20020303	4.1	26.5	17	9.5	20020404	4.68	27.6	8.5	0
20020131	4.59	26.1	16	0.2	20020304	3.15	21.8	15	12	20020405	4.48	27.4	10	0
20020201	4.96	27.1	15.5	6	20020305	4.38	25	12.5	0	20020406	4.31	27.2	11	0

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall	Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall	Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20020407	3.99	26.3	12	0	20020509	3.01	19.5	0.5	0	20020610	2.51	19	1.5	0
20020408	4.01	26	11	14	20020510	3.01	20	1.5	0	20020611	2.61	20	2	0
20020409	3.83	25.5	11.5	0	20020511	3.05	21	3	0	20020612	2.21	17	2	0
20020410	3.32	24	13	0	20020512	3.09	21.5	3.2	0	20020613	2.22	19	6	0
20020411	3.69	25.6	12.5	0.3	20020513	3.28	22.5	2.5	0	20020614	1.36	11	3.5	0
20020412	3.44	24.5	12.5	7.6	20020514	3.08	22	4	0	20020615	1.73	14	3.5	0
20020413	1.93	18	13.3	0	20020515	2.66	21	7.5	0	20020616	2.21	18	4	0
20020414	3.11	22	10.6	0	20020516	2.68	20.5	6	0	20020617	2.27	18.5	4	0
20020415	3.17	22.5	10.8	0	20020517	2.97	22	5	0	20020618	2.28	19	4.8	0
20020416	3.52	23.7	9.4	0	20020518	3.07	23	5.5	0	20020619	2.52	19.5	2	0
20020417	3.79	24.8	8.5	0	20020519	2.99	22	4.3	0	20020620	1.93	17	6	0
20020418	3.9	26.2	10	0	20020520	2.82	20	2	0	20020621	1.74	15.3	5.5	0
20020419	3.3	23.3	10.2	0	20020521	2.54	19.5	5	0	20020622	1.62	14	4.9	0
20020420	3.15	23	10.9	0	20020522	2.64	21.5	7.5	0	20020623	1.75	16.5	7.5	0
20020421	3.39	24	10.2	0	20020523	1.97	16.5	6.5	0	20020624	1.49	13	5	0
20020422	3.72	25.6	9.6	0	20020524	2.53	18.5	2.5	0	20020625	2.22	15.5	-2	0
20020423	3.59	25	9.6	0	20020525	2.79	21.5	4.9	0	20020626	2.1	16	1.5	0
20020424	3.45	23.6	8	0	20020526	2.8	21.5	4.5	0	20020627	2.32	17.5	1	0
20020425	3.67	25.5	9.2	0	20020527	2.62	21	6	0	20020628	2.27	18.5	4	0
20020426	3.47	26.2	12.5	0	20020528	2.68	22	7	0	20020629	2.44	19.5	3.5	0
20020427	3.6	26	10.5	0	20020529	3.08	24	5.5	0	20020630	2.13	15.5	0	0
20020428	3.7	26	9	0	20020530	2.78	23	7.5	0	20020701	2.08	15.5	1	0
20020429	3.62	26.5	10.8	0	20020531	1.27	14.4	10	0	20020702	2.17	16	0.5	0
20020430	3.21	25	12	0	20020601	1.35	13	7.2	0	20020703	2.36	17	-0.5	0
20020501	2.98	23.5	11.3	0	20020602	1.02	9	5	0	20020704	2.24	16	-0.5	0
20020502	3.35	25	10	0	20020603	1.75	14.1	4	0	20020705	2.18	15.5	-0.5	0
20020503	3.46	26	10.5	0	20020604	2.34	17	0.5	0	20020706	2.26	15.9	-1	0
20020504	3.08	24	10.6	0	20020605	2.33	17	0.5	0	20020707	2.29	16.5	0	0
20020505	3.25	24.8	10	0	20020606	2.02	15.5	2.5	0	20020708	2.49	18	0	0
20020506	2.33	19.5	10	0	20020607	2.2	16.5	1.5	0	20020709	2.63	20	2.5	0
20020507	2.09	12	-1.5	0	20020608	2.2	17.5	3.5	0	20020710	1.84	13	0.5	0
20020508	2.67	16.5	-0.9	0	20020609	2.32	18	2.6	0	20020711	2.37	15.5	-3.5	0

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall	Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall	Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20020712	2.31	16	-1	0	20020813	3.33	24	8.5	0	20020914	3.72	20	3.5	0
20020713	2.39	16.5	-1	0	20020814	3.47	24	7	0	20020915	4.27	22.5	3	0
20020714	2.63	19.5	2	0	20020815	3.02	22.5	9.5	0	20020916	4.47	24	4.5	0
20020715	2.65	20	3	0	20020816	3.61	25	8	0	20020917	4.53	25	6.5	0
20020716	1.82	12.5	0.5	0	20020817	1.71	16	11	0	20020918	4.68	26	7.5	0
20020717	1.84	11.5	-1.9	0	20020818	2.07	16.5	9	0	20020919	4.88	26	5.5	0
20020718	2.04	13.5	-1	0	20020819	2.8	20	8	0	20020920	5.01	26.5	5.5	0
20020719	1.72	11.5	0.5	0	20020820	3.17	21.5	7	0	20020921	4.77	25.5	6.2	0
20020720	1.54	10	0.5	0	20020821	3.23	22.5	8.5	0	20020922	4.86	27	9	0
20020721	1.05	6.5	1.5	0	20020822	3.69	24	6.5	0	20020923	4.9	27	8.8	0
20020722	2.5	17.5	1	0	20020823	3.5	23.5	8	0	20020924	5.12	29	11.3	0
20020723	2.94	22	4.5	0	20020824	3.47	24	9.6	0	20020925	5.02	29	12.5	0
20020724	3.51	24.5	1.6	0	20020825	3.42	24	10.4	0	20020926	5.2	28.5	10	0
20020725	2.68	17.7	-1.2	0	20020826	3.62	24.5	9.5	0	20020927	3.34	22	13	0
20020726	2.84	21	4.4	0	20020827	2.89	20.5	9.5	0	20020928	4.68	26	10	0
20020727	3.46	25	4.6	0	20020828	3.15	21.5	9	0	20020929	4.76	28	13.5	0
20020728	3.43	25	5.3	0	20020829	2.91	21	10.5	0	20020930	4.38	24.5	10	0
20020729	3.34	26	9	0	20020830	3	20.5	9	0	20021001	4.28	25	12	0
20020730	3.1	23	6	0	20020831	3.59	22.5	7	0	20021002	3.91	22	9.5	0
20020731	1.65	11.5	3	0	20020901	3.47	21.5	6.5	0	20021003	4.68	22.5	3	0
20020801	2.15	15.5	3.9	0	20020902	3.49	22.5	8.5	0	20021004	3.7	20.4	8.5	0
20020802	3.36	23	2.8	0	20020903	3.81	24	8.5	0	20021005	4.81	25.2	8.5	0
20020803	2.96	21	4.4	0	20020904	4.03	25	8.5	0	20021006	5.04	27	10.5	0
20020804	1.74	14	6.5	0	20020905	2.31	17	9.9	2	20021007	5.46	27	6.5	0
20020805	2.71	20	6.1	0	20020906	2.37	16	8	2.5	20021008	2.43	16	10.5	0
20020806	3.14	22	4.9	0	20020907	2.78	18	8	6	20021009	3.71	19.5	7.5	0
20020807	3.21	21.5	3	0	20020908	3.33	21	8.5	0	20021010	3.8	21.5	10.5	0
20020808	3.18	21	2.5	0	20020909	3.9	24.5	10	0	20021011	4.78	25	9.5	0
20020809	3.32	22	3	0	20020910	2.42	12.5	2	0.7	20021012	5.6	29	11	0
20020810	3.41	22	2	0	20020911	3.31	17	0.8	0	20021013	6.14	29.5	7	0
20020811	2.91	18.5	1.5	0	20020912	3.99	20.5	0.5	0	20021014	5.32	27	9.5	0
20020812	3.04	20.5	4.5	0	20020913	3.82	21.5	5.5	0	20021015	5.9	29.5	10	0

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20021016	6.31	31.5	11	0
20021017	5.92	32	15.5	0
20021018	6.07	32	14.5	0
20021019	6.17	33	16	0
20021020	5.01	26	11	0
20021021	6.25	31	11.4	0
20021022	5.74	30.5	14.6	0
20021023	5.3	29	15	0
20021024	5.72	29	12	0
20021025	6.1	29.5	10	0
20021026	5.95	29.5	11.5	0
20021027	4.57	27	16.5	0
20021028	5.46	29	14.5	0
20021029	4.73	26	14	0
20021030	1.93	14	11	0
20021031	4.49	21.5	7.5	0
20021101	4.5	23	10.5	0
20021102	3.89	21.5	12	0
20021103	5.22	27	13	0
20021104	5.27	28.5	15.5	0
20021105	4.74	22.5	8	0
20021106	3.19	15	6	0
20021107	5.09	22.5	5	1.6
20021108	5.65	26	8	2.5
20021109	5.84	29	13	4
20021110	4.02	22	12.5	0
20021111	4.49	22	9.5	0
20021112	5.2	24.5	9	0
20021113	5.62	28	13	0
20021114	5.62	28.5	14	0
20021115	5.17	25.5	11.5	0
20021116	6.06	30	14	0

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20021117	5.87	29	13.5	0
20021118	6.2	29	11	0
20021119	6.65	31.5	13	0
20021120	6.03	30	14.5	0
20021121	5.46	27	12.7	0
20021122	6.47	31	13.5	0
20021123	6.13	30	14	0
20021124	5.71	28.5	14	0
20021125	6.04	26	6	0
20021126	5.7	25.5	8	0
20021127	6.5	28.5	8	0
20021128	6.38	30	12.5	1.4
20021129	6.04	29	13	5.5
20021130	5.76	27.5	12	0
20021201	6.76	31	11.8	0
20021202	6.55	32	15.5	0
20021203	6.07	30.6	16	0.2
20021204	3.71	22.5	15.5	9.5
20021205	3.02	18.5	13	10
20021206	3.99	23	15	5
20021207	3.02	20	15	0.4
20021208	2.85	19.5	15	13.5
20021209	4.41	22.5	12	0
20021210	4.04	21.5	12.5	0
20021211	5.13	24.5	11	0
20021212	4.76	24	12.5	0
20021213	5.39	26.5	13	0
20021214	5.55	29	16.5	0
20021215	6.39	31	15	0
20021216	6.16	31	16.5	0
20021217	4.73	26	16	0
20021218	5.96	29.5	15	9.5

Date	Pot. Evapotrans	Max Temp	Min Temp	Rainfall
20021219	5.14	24.5	11	9
20021220	5.48	26.5	12.5	0
20021221	5.1	26	14	0
20021222	6.01	29	13.7	0
20021223	5.75	28.5	14.5	0
20021224	6.11	30	15	0
20021225	5.83	28	13	0
20021226	5.69	27	12	12.5
20021227	5.4	26.5	13	82.5
20021228	4.17	23.5	15	0
20021229	4.21	25	17	0
20021230	5.82	29	14.9	0
20021231	5.64	29	16	0

APPENDIX C: Simulation data of water content used for calibration plots for Secunda

Date	20 cm depth	40 cm depth	60 cm depth	80 cm depth	100 cm depth
1993/01/02	0.4565914	0.4576901	0.4584783	0.4591222	0.4596765
1993/01/03	0.4443051	0.4521911	0.4542354	0.4550185	0.4555284
1993/01/04	0.4333515	0.4449503	0.4515546	0.4535039	0.4541982
1993/01/05	0.4240276	0.4386414	0.4465788	0.4515436	0.4532119
1993/01/06	0.4154525	0.4333905	0.4421511	0.4477782	0.4517596
1993/01/07	0.4061916	0.4284461	0.4385357	0.4441948	0.4487913
1993/01/08	0.3969036	0.4237785	0.4353164	0.4413407	0.4456242
1993/01/09	0.3924832	0.4200228	0.4324449	0.4388649	0.4431569
1993/01/10	0.3893736	0.4169911	0.4299155	0.4366629	0.4410737
1993/01/11	0.3851574	0.4141143	0.4276491	0.4346828	0.4392296
1993/01/12	0.3792045	0.4110977	0.4255584	0.432879	0.4375639
1993/01/13	0.3715944	0.4077901	0.4235603	0.4312097	0.4360375
1993/01/14	0.3623622	0.4040187	0.4215893	0.4296391	0.4346217
1993/01/15	0.3508275	0.3994531	0.4195804	0.4281365	0.4332935
1993/01/16	0.3361273	0.3937018	0.4174557	0.4266728	0.4320338
1993/01/17	0.3172271	0.3862469	0.4151139	0.4252186	0.4308255
1993/01/18	0.300926	0.3779618	0.4124792	0.4237431	0.4296528
1993/01/19	0.2929518	0.3717291	0.4097424	0.4222358	0.4285021
1993/01/20	0.2827536	0.3643649	0.4068989	0.4207114	0.4273669
1993/01/21	0.2753334	0.3577494	0.403984	0.4191721	0.4262441
1993/01/22	0.3457092	0.3582623	0.4014585	0.4176419	0.4251338
1993/01/23	0.4237292	0.369148	0.3999501	0.4161986	0.4240427
1993/01/24	0.4171895	0.3775981	0.3994502	0.41493	0.4229883
1993/01/25	0.4098337	0.3815224	0.3992652	0.4138421	0.4219872
1993/01/26	0.4072986	0.3843822	0.3991943	0.4129042	0.4210472
1993/01/27	0.4029058	0.3859895	0.3991767	0.4120883	0.4201692
1993/01/28	0.3970166	0.3865982	0.3991564	0.4113699	0.4193511
1993/01/29	0.4081457	0.3880188	0.3991331	0.4107287	0.4185886
1993/01/30	0.4377206	0.4006763	0.399459	0.4101607	0.4178772
1993/01/31	0.4329054	0.4087304	0.4005882	0.4097101	0.4172164
1993/02/01	0.4249834	0.4114246	0.4020782	0.409407	0.4166105
1993/02/02	0.4168119	0.4114639	0.4034796	0.4092398	0.4160641
1993/02/03	0.4093173	0.4103946	0.4045874	0.4091735	0.4155778
1993/02/04	0.4015047	0.4086227	0.4053551	0.4091694	0.4151485
1993/02/05	0.4006049	0.4073524	0.4058409	0.409193	0.4147703
1993/02/06	0.3972099	0.4057285	0.406105	0.409222	0.4144359
1993/02/07	0.3944248	0.404414	0.4061956	0.4092394	0.4141376
1993/02/08	0.3891667	0.4026084	0.4061286	0.4092348	0.4138679
1993/02/09	0.3868305	0.4014454	0.4059466	0.4091999	0.41362
1993/02/10	0.3836014	0.4001187	0.4056881	0.4091332	0.4133877
1993/02/11	0.3782035	0.3983271	0.40534	0.4090338	0.413166
1993/02/12	0.3875452	0.3976594	0.4049414	0.4089004	0.4129505
1993/02/13	0.3918737	0.3969751	0.4045504	0.4087389	0.4127377
1993/02/14	0.4513093	0.4131222	0.404635	0.4085638	0.4125256
1993/02/15	0.4394609	0.4236081	0.4069828	0.4085231	0.4123202
1993/02/16	0.4316615	0.425226	0.4099759	0.4087605	0.4121446

Date	20 cm depth	40 cm depth	60 cm depth	80 cm depth	100 cm depth
1993/02/18	0.4315419	0.4251677	0.4144021	0.4099331	0.4119724
1993/02/19	0.4275452	0.4248746	0.4160162	0.4107341	0.411998
1993/02/20	0.4233648	0.4240207	0.4171891	0.4115981	0.4121014
1993/02/21	0.4165872	0.4220137	0.4178437	0.4124523	0.412277
1993/02/22	0.4095628	0.4195194	0.4179785	0.4132168	0.4125108
1993/02/23	0.4025768	0.4168085	0.4176999	0.4138348	0.4127822
1993/02/24	0.4003722	0.4148359	0.4171764	0.4142828	0.4130673
1993/02/25	0.3987592	0.4131061	0.4165443	0.4145715	0.4133447
1993/02/26	0.3950832	0.4110895	0.4158275	0.4147217	0.4135976
1993/02/27	0.3900771	0.4088666	0.4150186	0.4147494	0.4138147
1993/02/28	0.3846447	0.4065963	0.4141313	0.4146688	0.4139878
1993/03/01	0.3815235	0.4048427	0.4132151	0.4144953	0.4141125
1993/03/02	0.3827831	0.4036961	0.4123205	0.4142482	0.4141873
1993/03/03	0.4064649	0.4034016	0.411505	0.413949	0.4142135
1993/03/04	0.4114436	0.4042614	0.4108651	0.4136229	0.4141955
1993/03/05	0.4212446	0.4061451	0.4104402	0.4132964	0.4141401
1993/03/06	0.4183598	0.4076271	0.4102516	0.4129951	0.414056
1993/03/07	0.4128809	0.4080075	0.4101684	0.4127314	0.4139522
1993/03/08	0.4068751	0.4075409	0.4100739	0.4125012	0.4138366
1993/03/09	0.4005319	0.4064773	0.4099011	0.4122918	0.4137141
1993/03/10	0.3938678	0.4049917	0.409619	0.4120878	0.413587
1993/03/11	0.3876322	0.4033579	0.4092258	0.4118756	0.4134553
1993/03/12	0.3807248	0.4014125	0.4087275	0.4116454	0.4133179
1993/03/13	0.3748196	0.3995351	0.4081432	0.4113901	0.4131729
1993/03/14	0.3667673	0.3970335	0.4074621	0.4111059	0.4130182
1993/03/15	0.3588044	0.394336	0.4066802	0.410788	0.4128517
1993/03/16	0.3546633	0.3923253	0.4058434	0.4104351	0.4126715
1993/03/17	0.3490137	0.3898972	0.4049641	0.4100503	0.4124762
1993/03/18	0.3414497	0.3869199	0.4040252	0.4096356	0.4122651
1993/03/19	0.331542	0.3832062	0.4029983	0.4091902	0.4120377
1993/03/20	0.3285735	0.3809419	0.4019287	0.4087134	0.4117936
1993/03/21	0.3201903	0.3774467	0.4008215	0.4082101	0.4115328
1993/03/22	0.3078817	0.3724488	0.3996026	0.4076796	0.4112555
1993/03/23	0.3053574	0.3697817	0.3983235	0.4071187	0.4109618
1993/03/24	0.3041446	0.3677373	0.3970786	0.4065341	0.4106518
1993/03/25	0.2963957	0.3636861	0.3958073	0.4059325	0.4103267
1993/03/26	0.2883443	0.3590389	0.3944356	0.4053119	0.4099875
1993/03/27	0.2817755	0.354501	0.3929596	0.4046691	0.4096349
1993/03/28	0.2761564	0.3500193	0.3913963	0.4040025	0.409269
1993/03/29	0.2767988	0.3491215	0.3899029	0.403315	0.4088904
1993/03/30	0.2766858	0.3479333	0.3885572	0.40262	0.4085001
1993/03/31	0.273917	0.3452356	0.3872737	0.4019264	0.4081001
1993/04/01	0.2702745	0.3418099	0.3859588	0.4012344	0.4076923
1993/04/02	0.267118	0.3384679	0.3845992	0.4005414	0.4072782
1993/04/03	0.2645899	0.33541	0.3832137	0.3998459	0.4068588
1993/04/04	0.2628314	0.3329456	0.3818369	0.399148	0.4064348
1993/04/05	0.2633885	0.3331018	0.380588	0.3984516	0.4060071

Date	20 cm depth	40 cm depth	60 cm depth	80 cm depth	100 cm depth
1993/04/06	0.263538	0.3327256	0.3794928	0.3977658	0.4055767
1993/04/08	0.2609273	0.3284614	0.3774444	0.3964397	0.4047143
1993/04/09	0.2593894	0.3258336	0.3763598	0.3957941	0.4042845
1993/04/10	0.2579672	0.3231306	0.3752377	0.3951551	0.4038564
1993/04/11	0.2566824	0.32044	0.3740806	0.3945202	0.4034302
1993/04/12	0.2575904	0.3215625	0.3730282	0.3938898	0.4030059
1993/04/13	0.2582893	0.321998	0.3721468	0.3932716	0.4025839
1993/04/14	0.2586578	0.3221712	0.3713746	0.3926706	0.4021649
1993/04/15	0.2585401	0.3216614	0.3706656	0.3920885	0.4017498
1993/04/16	0.258039	0.3205571	0.3699763	0.3915246	0.4013393
1993/04/17	0.2570338	0.3184984	0.3692612	0.3909764	0.4009338
1993/04/18	0.256172	0.316639	0.3685044	0.3904401	0.4005335
1993/04/19	0.2554038	0.3148699	0.3677211	0.389913	0.4001384
1993/04/20	0.254683	0.3130693	0.3669165	0.3893929	0.3997484
1993/04/21	0.2541329	0.311595	0.3661023	0.3888786	0.3993632
1993/04/22	0.2536228	0.3100923	0.3652881	0.3883695	0.3989827
1993/04/23	0.2531668	0.308612	0.3644736	0.3878652	0.3986064
1993/04/24	0.2527966	0.3073022	0.3636648	0.3873653	0.3982344
1993/04/25	0.252501	0.3061669	0.3628705	0.3868699	0.3978663
1993/04/26	0.252236	0.3050399	0.3620937	0.3863795	0.397502
1993/04/27	0.2519709	0.3037693	0.361328	0.3858942	0.3971416
1993/04/28	0.2520476	0.3043216	0.3606268	0.3854146	0.3967848
1993/04/29	0.2518692	0.3033386	0.3599707	0.3849433	0.3964317
1993/04/30	0.2518014	0.302961	0.3593377	0.3844802	0.3960824
1993/05/01	0.2516576	0.302055	0.3587257	0.3840256	0.395737
1993/05/02	0.2515355	0.3012371	0.3581216	0.383579	0.3953954
1993/05/03	0.2514406	0.3005601	0.3575304	0.3831401	0.3950578
1993/05/04	0.2513284	0.2997047	0.3569496	0.3827086	0.3947242
1993/05/05	0.2512075	0.2987193	0.3563706	0.382284	0.3943945
1993/05/06	0.2510931	0.2977182	0.3557899	0.3818658	0.3940686
1993/05/07	0.2509922	0.2967687	0.3552089	0.3814532	0.3937466
1993/05/08	0.250923	0.2960714	0.3546357	0.381046	0.3934282
1993/05/09	0.2508599	0.2953869	0.3540756	0.3806441	0.3931135
1993/05/10	0.2509221	0.2960217	0.3535641	0.380248	0.3928024
1993/05/11	0.2508726	0.2954085	0.3530855	0.3798591	0.3924948
1993/05/12	0.2508254	0.294801	0.3526128	0.3794773	0.3921909
1993/05/13	0.2507749	0.294133	0.3521443	0.3791019	0.3918905
1993/05/14	0.2507189	0.2933692	0.3516763	0.3787327	0.3915936
1993/05/15	0.25071	0.2931789	0.3512229	0.3783692	0.3913002
1993/05/16	0.2506894	0.2928262	0.3507853	0.3780116	0.3910103
1993/05/17	0.2506728	0.292512	0.3503623	0.37766	0.3907239
1993/05/18	0.2506405	0.2919756	0.3499481	0.3773142	0.3904409
1993/05/19	0.2506051	0.2913812	0.3495362	0.3769739	0.3901611
1993/05/20	0.2505713	0.290792	0.3491256	0.3766388	0.3898847
1993/05/21	0.2505403	0.2902282	0.348717	0.3763086	0.3896116
1993/05/22	0.2505104	0.2896625	0.3483109	0.3759828	0.3893416
1993/05/23	0.2504834	0.2891253	0.3479078	0.3756614	0.3890748

Date	20 cm depth	40 cm depth	60 cm depth	80 cm depth	100 cm depth
1993/05/24	0.2504625	0.2886769	0.3475099	0.3753441	0.388811
1993/05/26	0.2504235	0.2877861	0.3467343	0.3747216	0.3882922
1993/05/27	0.2504099	0.2874344	0.3463569	0.3744163	0.3880371
1993/05/28	0.250399	0.2871261	0.3459893	0.3741148	0.3877848
1993/05/29	0.2503959	0.2869645	0.345634	0.3738174	0.3875353
1993/05/30	0.2503893	0.2867263	0.3452914	0.3735241	0.3872885
1993/05/31	0.250378	0.2863915	0.3449567	0.373235	0.3870443
1993/06/01	0.25037	0.2861187	0.3446288	0.3729499	0.3868027
1993/06/02	0.250358	0.2857593	0.3443065	0.3726688	0.3865637
1993/06/03	0.2503477	0.2854328	0.3439886	0.3723916	0.3863274
1993/06/04	0.2503446	0.2852604	0.3436781	0.3721181	0.3860935
1993/06/05	0.2503439	0.2851378	0.3433782	0.3718484	0.3858621
1993/06/06	0.2503411	0.2849653	0.3430879	0.3715826	0.3856331
1993/06/07	0.2503361	0.2847473	0.3428046	0.3713205	0.3854066
1993/06/08	0.2503268	0.2844315	0.3425252	0.3710622	0.3851825
1993/06/09	0.2503173	0.2841127	0.3422479	0.3708075	0.3849608
1993/06/10	0.2503082	0.2837997	0.3419726	0.3705562	0.3847413
1993/06/11	0.250303	0.2835768	0.3417009	0.3703082	0.3845242
1993/06/12	0.2503023	0.2834581	0.341436	0.3700633	0.3843094
1993/06/13	0.2503068	0.2834619	0.3411811	0.3698217	0.3840967
1993/06/14	0.2503068	0.2833583	0.3409356	0.3695834	0.3838862
1993/06/15	0.2503045	0.2832011	0.3406959	0.3693484	0.3836779
1993/06/16	0.2503001	0.2829987	0.3404602	0.3691167	0.3834718
1993/06/17	0.2502943	0.2827631	0.3402269	0.3688882	0.3832677
1993/06/18	0.2502861	0.2824723	0.3399945	0.3686626	0.3830657
1993/06/19	0.2502766	0.2821475	0.3397616	0.3684399	0.3828658
1993/06/20	0.2502702	0.281896	0.3395291	0.3682198	0.3826679
1993/06/21	0.250265	0.281676	0.3392987	0.3680023	0.3824719
1993/06/22	0.2502567	0.2813744	0.3390695	0.3677872	0.3822779
1993/06/23	0.2502468	0.2810256	0.3388394	0.3675745	0.3820858
1993/06/24	0.2502393	0.2807384	0.338609	0.367364	0.3818955
1993/06/25	0.2502325	0.2804655	0.3383794	0.3671556	0.3817071
1993/06/26	0.2502345	0.2804353	0.3381548	0.3669492	0.3815204
1993/06/27	0.2502353	0.280372	0.3379379	0.366745	0.3813355
1993/06/28	0.2502367	0.280324	0.3377278	0.366543	0.3811523
1993/06/29	0.2502337	0.2801573	0.3375224	0.3663432	0.3809707
1993/06/30	0.2502332	0.2800584	0.3373207	0.3661457	0.3807909
1993/07/01	0.2502347	0.2800155	0.3371242	0.3659503	0.3806127
1993/07/02	0.2502322	0.2798631	0.3369319	0.3657573	0.3804361
1993/07/03	0.2502293	0.2797025	0.3367417	0.3655664	0.380261
1993/07/04	0.250229	0.2796129	0.3365544	0.3653776	0.3800876
1993/07/05	0.2502272	0.2794818	0.3363703	0.365191	0.3799157
1993/07/06	0.2502225	0.2792751	0.3361877	0.3650064	0.3797453
1993/07/07	0.250223	0.2792118	0.3360073	0.3648238	0.3795764
1993/07/08	0.2502163	0.2789449	0.3358283	0.3646431	0.3794091
1993/07/09	0.2502103	0.2786966	0.335648	0.3644643	0.3792432
1993/07/10	0.250202	0.2783791	0.3354659	0.3642873	0.3790787

Date	20 cm depth	40 cm depth	60 cm depth	80 cm depth	100 cm depth
1993/07/11	0.2501947	0.2780836	0.3352816	0.3641118	0.3789156
1993/07/13	0.2501795	0.2774569	0.3349049	0.3637651	0.3785936
1993/07/14	0.25017	0.2770653	0.3347139	0.3635938	0.3784346
1993/07/15	0.2501583	0.2765831	0.3345179	0.3634235	0.3782769
1993/07/16	0.250149	0.2761718	0.3343171	0.3632543	0.3781205
1993/07/17	0.250147	0.2760182	0.3341163	0.3630859	0.3779653
1993/07/18	0.2501433	0.2758022	0.3339185	0.3629185	0.3778113
1993/07/19	0.2501412	0.275642	0.3337232	0.3627521	0.3776584
1993/07/20	0.2501414	0.2755726	0.3335322	0.3625866	0.3775067
1993/07/21	0.2501389	0.2754016	0.3333453	0.3624223	0.3773561
1993/07/22	0.25014	0.2753664	0.3331625	0.362259	0.3772065
1993/07/23	0.2501362	0.2751429	0.3329828	0.362097	0.3770581
1993/07/24	0.250133	0.2749406	0.3328039	0.3619361	0.3769107
1993/07/25	0.2501315	0.2748082	0.3326269	0.3617763	0.3767644
1993/07/26	0.250131	0.2747128	0.3324531	0.3616177	0.3766191
1993/07/27	0.2501304	0.2746119	0.3322828	0.3614604	0.3764748
1993/07/28	0.2501272	0.2744131	0.3321143	0.3613042	0.3763315
1993/07/29	0.2501218	0.2741147	0.331945	0.3611491	0.3761892
1993/07/30	0.2501169	0.2738278	0.3317739	0.3609952	0.3760479
1993/07/31	0.2501118	0.2735308	0.3316012	0.3608423	0.3759076
1993/08/01	0.2501058	0.2731778	0.3314261	0.3606902	0.3757682
1993/08/02	0.2501	0.2728206	0.331248	0.3605391	0.3756297
1993/08/03	0.2500941	0.2724487	0.331067	0.3603887	0.3754921
1993/08/04	0.2500907	0.2721896	0.3308845	0.360239	0.3753555
1993/08/05	0.2500882	0.27197	0.3307027	0.3600899	0.3752197
1993/08/06	0.2500854	0.2717398	0.3305218	0.3599415	0.3750847
1993/08/07	0.2500876	0.271773	0.3303463	0.3597939	0.3749506
1993/08/08	0.2500961	0.2721345	0.3301822	0.359647	0.3748173
1993/08/09	0.2500962	0.2720712	0.3300262	0.3595013	0.3746849
1993/08/10	0.2500961	0.272002	0.3298735	0.3593567	0.3745532
1993/08/11	0.2500924	0.2717505	0.3297216	0.3592132	0.3744224
1993/08/12	0.2500952	0.2718214	0.3295734	0.3590707	0.3742923
1993/08/13	0.2500947	0.2717303	0.3294282	0.3589295	0.3741631
1993/08/14	0.2500943	0.2716492	0.3292852	0.3587894	0.3740346
1993/08/15	0.2500897	0.2713573	0.3291418	0.3586504	0.373907
1993/08/16	0.2500835	0.2709691	0.3289945	0.3585124	0.3737801
1993/08/17	0.2500776	0.2705677	0.3288422	0.3583753	0.373654
1993/08/18	0.2500734	0.2702521	0.3286861	0.358239	0.3735287
1993/08/19	0.250069	0.2699035	0.3285272	0.3581034	0.3734041
1993/08/20	0.2500647	0.2695504	0.328365	0.3579684	0.3732803
1993/08/21	0.2500615	0.2692545	0.3282006	0.3578339	0.3731571
1993/08/22	0.2500602	0.2690754	0.3280361	0.3576999	0.3730347
1993/08/23	0.2500624	0.2691388	0.3278761	0.3575664	0.372913
1993/08/24	0.2500613	0.2689897	0.3277205	0.3574336	0.372792
1993/08/25	0.2500599	0.2688171	0.3275662	0.3573014	0.3726716
1993/08/26	0.2500582	0.2686209	0.3274126	0.3571698	0.3725519
1993/08/27	0.2500559	0.2683868	0.3272589	0.357039	0.3724329

Date	20 cm depth	40 cm depth	60 cm depth	80 cm depth	100 cm depth
1993/08/28	0.2500535	0.2681321	0.3271046	0.3569087	0.3723145
1993/08/30	0.250051	0.2677841	0.3267947	0.3566498	0.3720796
1993/08/31	0.2500508	0.2676873	0.3266435	0.3565213	0.3719631
1993/09/01	0.2500494	0.2675105	0.3264939	0.3563934	0.3718472
1993/09/02	0.2500469	0.2672409	0.326344	0.3562661	0.3717319
1993/09/03	0.2500538	0.2675406	0.3262003	0.3561394	0.3716173
1993/09/04	0.2500515	0.2672376	0.32606	0.3560135	0.3715031
1993/09/05	0.2500479	0.2668907	0.3259165	0.3558882	0.3713896
1993/09/06	0.2500444	0.2665555	0.3257697	0.3557636	0.3712767
1993/09/07	0.2500427	0.2663547	0.3256213	0.3556395	0.3711643
1993/09/08	0.2500399	0.2660499	0.325472	0.355516	0.3710525
1993/09/09	0.2500372	0.265742	0.3253205	0.3553929	0.3709413
1993/09/10	0.2500342	0.2653833	0.3251662	0.3552702	0.3708306
1993/09/11	0.2500319	0.2650663	0.3250094	0.3551479	0.3707204
1993/09/12	0.2500299	0.2647605	0.3248507	0.3550259	0.3706108
1993/09/13	0.2500283	0.2644855	0.3246909	0.3549041	0.3705017
1993/09/14	0.2500264	0.2641703	0.3245297	0.3547826	0.3703931
1993/09/15	0.2500248	0.2638624	0.324367	0.3546614	0.370285
1993/09/16	0.2500233	0.2635753	0.3242031	0.3545403	0.3701774
1993/09/17	0.2500218	0.2632654	0.3240382	0.3544195	0.3700702
1993/09/18	0.2500204	0.262956	0.3238719	0.3542988	0.3699635
1993/09/19	0.2500198	0.2627597	0.3237059	0.3541783	0.3698573
1993/09/20	0.2500191	0.2625409	0.323541	0.354058	0.3697515
1993/09/21	0.2500182	0.2622966	0.3233766	0.3539378	0.3696461
1993/09/22	0.2500175	0.2620804	0.3232128	0.3538179	0.3695412
1993/09/23	0.2500169	0.2618789	0.3230501	0.3536982	0.3694367
1993/09/24	0.2500168	0.2617704	0.3228896	0.3535788	0.3693326
1993/09/25	0.2500188	0.2619761	0.3227369	0.3534597	0.3692289
1993/09/26	0.2500191	0.2619599	0.3225912	0.353341	0.3691257
1993/09/27	0.2500179	0.2617313	0.3224467	0.3532229	0.3690228
1993/09/28	0.2500183	0.2617205	0.3223046	0.3531053	0.3689203
1993/09/29	0.2500173	0.26151	0.3221641	0.3529883	0.3688182
1993/09/30	0.2988075	0.2620368	0.3220314	0.3528719	0.3687166
1993/10/01	0.3333713	0.2632132	0.3219194	0.3527563	0.3686153
1993/10/02	0.3549989	0.2665407	0.3218508	0.3526421	0.3685145
1993/10/03	0.353976	0.2707652	0.3218564	0.3525302	0.368414
1993/10/04	0.3496789	0.2737058	0.3219124	0.3524216	0.3683141
1993/10/05	0.347603	0.2759516	0.3219966	0.3523168	0.3682148
1993/10/06	0.4291406	0.3142032	0.3221523	0.3522162	0.368116
1993/10/07	0.4393079	0.3853482	0.3240275	0.3521293	0.3680179
1993/10/08	0.4341377	0.3950809	0.3294399	0.3521033	0.3679212
1993/10/09	0.4267539	0.3969168	0.3354998	0.3521561	0.3678274
1993/10/10	0.4184763	0.3958004	0.3405359	0.3522715	0.3677377
1993/10/11	0.409996	0.3936542	0.3443892	0.3524312	0.3676528
1993/10/12	0.4538143	0.4112228	0.3487887	0.3526254	0.3675732
1993/10/13	0.4416039	0.4178567	0.3592054	0.3529175	0.3674998
1993/10/14	0.4348219	0.4172035	0.3677412	0.3533825	0.367435

Date	20 cm depth	40 cm depth	60 cm depth	80 cm depth	100 cm depth
1993/10/15	0.4539304	0.4408858	0.3869508	0.3542709	0.3673828
1993/10/17	0.4322156	0.4322972	0.4055545	0.3608588	0.3674088
1993/10/18	0.4269988	0.4288881	0.4075331	0.3651111	0.3675339
1993/10/19	0.4578586	0.4588645	0.4561656	0.3877114	0.3678229
1993/10/20	0.4492805	0.4535381	0.4484369	0.4142497	0.3710746
1993/10/21	0.438223	0.4478325	0.4455364	0.4229699	0.3780387
1993/10/22	0.4303178	0.4414758	0.4428118	0.4262971	0.3859176
1993/10/23	0.4221958	0.4360599	0.4396453	0.4273729	0.3928515
1993/10/24	0.4150039	0.4314048	0.4365591	0.4274585	0.3983568
1993/10/25	0.4080465	0.4271905	0.4336812	0.4270554	0.40252
1993/10/26	0.4151469	0.4247899	0.4311423	0.4263819	0.4055753
1993/10/27	0.4325	0.4258716	0.4293324	0.4256259	0.4077799
1993/10/28	0.4293253	0.4269336	0.428387	0.4249746	0.4093834
1993/10/29	0.4225983	0.4260457	0.4276915	0.4244719	0.4105912
1993/10/30	0.4149714	0.4239192	0.4268418	0.4240377	0.4115358
1993/10/31	0.4071039	0.421166	0.4257375	0.4235818	0.412287
1993/11/01	0.398771	0.4180267	0.4244073	0.4230507	0.4128776
1993/11/02	0.3906133	0.4147819	0.4229151	0.4224249	0.4133241
1993/11/03	0.3856082	0.4121507	0.4213757	0.421712	0.4136376
1993/11/04	0.3782627	0.409007	0.4198108	0.4209352	0.4138309
1993/11/05	0.3820643	0.4072671	0.4182875	0.4201104	0.413917
1993/11/06	0.3863592	0.4059939	0.4169104	0.4192693	0.4139114
1993/11/07	0.3863606	0.4047025	0.4156565	0.4184354	0.41383
1993/11/08	0.383707	0.4031962	0.414482	0.4176196	0.4136879
1993/11/09	0.3802904	0.4016316	0.4133547	0.4168238	0.4134975
1993/11/10	0.3758276	0.3998613	0.4122535	0.4160472	0.4132687
1993/11/11	0.3728592	0.398426	0.4111854	0.4152876	0.4130089
1993/11/12	0.3731527	0.3976412	0.4101768	0.4145459	0.4127242
1993/11/13	0.3727638	0.3967341	0.4092431	0.4138267	0.4124199
1993/11/14	0.3693569	0.3952224	0.4083363	0.4131305	0.412101
1993/11/15	0.3654105	0.3936085	0.4074286	0.412453	0.4117709
1993/11/16	0.3604156	0.3917713	0.4065113	0.4117899	0.4114323
1993/11/17	0.3533185	0.3894342	0.4055637	0.4111367	0.4110868
1993/11/18	0.3458319	0.386885	0.4045697	0.4104879	0.4107352
1993/11/19	0.4352336	0.3877199	0.4035947	0.4098406	0.410378
1993/11/20	0.4419011	0.4126103	0.4040259	0.4092481	0.4100174
1993/11/21	0.4313024	0.4175908	0.4057372	0.4088485	0.4096671
1993/11/22	0.4222468	0.4177924	0.4074803	0.4086661	0.4093471
1993/11/23	0.4566528	0.4563242	0.4217333	0.4089515	0.4090751
1993/11/24	0.4513821	0.4535926	0.4390085	0.4145064	0.4091502
1993/11/25	0.441986	0.4492525	0.4425341	0.4224748	0.4102845
1993/11/26	0.4412838	0.4452368	0.4431071	0.4288128	0.4127625
1993/11/27	0.4340812	0.4413158	0.4421412	0.4326783	0.4162
1993/11/28	0.4268209	0.4371142	0.4402469	0.4344843	0.419766
1993/11/29	0.4194139	0.4329177	0.4379433	0.4349322	0.4227804
1993/11/30	0.4123249	0.4289348	0.4355223	0.4345669	0.4249814
1993/12/01	0.404271	0.4248962	0.4331016	0.433734	0.426405

Date	20 cm depth	40 cm depth	60 cm depth	80 cm depth	100 cm depth
1993/12/02	0.3957162	0.4208623	0.4307088	0.4326304	0.4271998
1993/12/04	0.4003658	0.4154136	0.4263327	0.43007	0.4275051
1993/12/05	0.4072636	0.4146317	0.4246205	0.4287903	0.4272552
1993/12/06	0.4041978	0.4134701	0.4231792	0.427591	0.4268567
1993/12/07	0.3997244	0.4120959	0.4218752	0.4264744	0.4263691
1993/12/08	0.3962306	0.41074	0.4206633	0.4254289	0.4258296
1993/12/09	0.3916802	0.4090714	0.419492	0.4244419	0.4252615
1993/12/10	0.3866572	0.4072385	0.4183322	0.4234985	0.4246781
1993/12/11	0.3895455	0.4062729	0.4172234	0.4225889	0.4240867
1993/12/12	0.3903898	0.4052225	0.4162016	0.4217168	0.4234934
1993/12/13	0.3872478	0.4038219	0.4152158	0.420881	0.4229026
1993/12/14	0.3828019	0.402237	0.4142379	0.4200746	0.4223173
1993/12/15	0.3776393	0.4004745	0.4132522	0.4192908	0.4217388
1993/12/16	0.3731452	0.3988255	0.4122612	0.4185234	0.4211672
1993/12/17	0.3720339	0.3977412	0.4113014	0.4177709	0.4206022
1993/12/18	0.3680328	0.3960464	0.4103594	0.4170351	0.420044
1993/12/19	0.363162	0.3941761	0.4094053	0.4163125	0.4194927
1993/12/20	0.3573245	0.3920836	0.4084295	0.4155992	0.418948
1993/12/21	0.3500768	0.3896055	0.4074165	0.4148912	0.418409
1993/12/22	0.3421465	0.3868166	0.4063515	0.4141838	0.4178748
1993/12/23	0.3396891	0.3851081	0.4052792	0.4134741	0.4173442
1993/12/24	0.3334968	0.3825561	0.4042035	0.4127651	0.4168164
1993/12/25	0.321873	0.3785918	0.4030544	0.4120545	0.4162911
1993/12/26	0.3118399	0.3744692	0.401803	0.4113349	0.4157672
1993/12/27	0.309844	0.3721124	0.4005062	0.410602	0.4152435
1993/12/28	0.3072158	0.3697877	0.3992428	0.4098612	0.4147189
1993/12/29	0.4674833	0.4674568	0.4656745	0.4431783	0.4164249
1993/12/30	0.4514061	0.454507	0.4555507	0.456223	0.456743
1993/12/31	0.4407032	0.4496648	0.4532765	0.454247	0.4547711

APPENDIX D1: Simulated boron concentration data for December 1991 and August 2002 used for calibration plots for Secunda.

Date	Boron concentration (mg/m^3)														
	0 cm	*0.5 cm*	*1 cm*	*2 cm*	*11 cm*	*29 cm*	*47 cm*	*65 cm*	*83 cm*	*101 cm*	*119 cm*	*137 cm*	*155 cm*	*173 cm*	*191 cm*
1991/01/01	9205	9140	8952	8635	3962	2751	1577	761	259	65	13	3	1	1	1
1991/01/02	9188	9127	8946	8635	3963	2752	1579	763	260	66	13	3	1	1	1
1991/01/03	9172	9114	8941	8634	3964	2753	1581	764	261	66	14	3	1	1	1
1991/01/04	9265	9139	8951	8659	3981	2754	1582	766	263	67	14	3	1	1	1
1991/01/05	9225	9130	8946	8654	3982	2755	1583	767	264	67	14	3	1	1	1
1991/01/06	9201	9121	8941	8652	3983	2756	1585	768	265	68	14	3	1	1	1
1991/01/07	9182	9111	8937	8650	3984	2757	1586	770	266	68	14	3	1	1	1
1991/01/08	9164	9100	8932	8647	3985	2758	1587	771	267	69	14	3	1	1	1
1991/01/09	9148	9089	8927	8645	3986	2759	1589	772	268	69	15	3	1	1	1
1991/01/10	9134	9079	8922	8642	3987	2759	1590	773	269	70	15	3	1	1	1
1991/01/11	9120	9068	8916	8639	3987	2760	1591	774	269	70	15	3	1	1	1
1991/01/12	9107	9057	8911	8636	3988	2761	1592	775	270	71	15	3	1	1	1
1991/01/13	9095	9047	8905	8633	3989	2761	1593	776	271	71	15	3	1	1	1
1991/01/14	9083	9037	8898	8630	3990	2762	1594	777	272	71	15	3	1	1	1
1991/01/15	9072	9028	8892	8627	3991	2762	1595	778	273	72	15	3	1	1	1
1991/01/16	9061	9018	8886	8623	3991	2763	1596	779	273	72	15	3	1	1	1
1991/01/17	9050	9009	8880	8619	3992	2763	1596	780	274	72	16	3	1	1	1
1991/01/18	9170	9045	8886	8635	4008	2764	1597	781	275	73	16	3	1	1	1
1991/01/19	9129	9038	8882	8629	4010	2765	1598	781	275	73	16	3	1	1	1
1991/01/20	9108	9032	8878	8625	4011	2765	1599	782	276	73	16	3	1	1	1
1991/01/21	9090	9025	8874	8621	4012	2766	1600	783	277	74	16	3	1	1	1
1991/01/22	9075	9017	8870	8617	4012	2767	1601	784	277	74	16	3	1	1	1
1991/01/23	9061	9008	8865	8613	4013	2767	1602	784	278	74	16	3	1	1	1
1991/01/24	9049	8999	8860	8609	4014	2768	1602	785	278	75	16	3	1	1	1
1991/01/25	9037	8990	8855	8605	4015	2768	1603	786	279	75	16	3	1	1	1
1991/01/26	9026	8981	8850	8601	4016	2769	1604	787	279	75	17	3	1	1	1
1991/01/27	9015	8972	8845	8596	4016	2769	1605	787	280	75	17	3	1	1	1
1991/01/28	9005	8964	8839	8592	4017	2770	1605	788	281	76	17	3	1	1	1
1991/01/29	8995	8955	8833	8588	4018	2770	1606	789	281	76	17	3	1	1	1
1991/01/30	8985	8947	8827	8584	4018	2770	1607	789	282	76	17	4	1	1	1
1991/01/31	8976	8939	8821	8580	4019	2771	1607	790	282	76	17	4	1	1	1

Date	Boron concentration (mg/m^3)														
	0 cm	*0.5 cm*	*1 cm*	*2 cm*	*11 cm*	*29 cm*	*47 cm*	*65 cm*	*83 cm*	*101 cm*	*119 cm*	*137 cm*	*155 cm*	*173 cm*	*191 cm*
2002/08/01	17651	17481	18489	19690	28988	40500	28731	11622	5914	3176	1765	1005	609	351	205
2002/08/02	18005	17734	18745	19969	29016	40559	28754	11622	5913	3176	1765	1005	609	351	205
2002/08/03	18097	17821	18851	20094	29038	40639	28791	11622	5913	3176	1765	1005	609	351	205
2002/08/04	18168	17843	18860	20107	29046	40692	28819	11621	5913	3175	1765	1005	609	351	205
2002/08/05	18228	17874	18857	20104	29049	40717	28832	11621	5913	3175	1765	1005	609	351	205
2002/08/06	18279	17905	18856	20101	29052	40758	28858	11620	5913	3175	1765	1005	609	351	205
2002/08/07	18324	17936	18856	20096	29053	40796	28887	11620	5912	3175	1765	1005	609	351	205
2002/08/08	18364	17966	18857	20091	29054	40828	28914	11620	5912	3175	1765	1005	609	351	205
2002/08/09	18401	17995	18858	20086	29055	40853	28940	11619	5912	3175	1765	1005	609	351	205
2002/08/10	18435	18023	18859	20081	29055	40876	28966	11619	5912	3175	1765	1005	609	351	205
2002/08/11	18466	18051	18860	20076	29055	40895	28992	11619	5911	3175	1765	1005	609	351	205
2002/08/12	18496	18078	18862	20071	29055	40907	29012	11618	5911	3175	1765	1005	609	351	205
2002/08/13	18523	18104	18865	20066	29055	40919	29032	11618	5911	3175	1765	1005	609	351	205
2002/08/14	15929	16806	18464	19981	28991	40929	29053	11618	5911	3175	1765	1005	609	351	205
2002/08/15	17761	17804	19403	20910	29138	40938	29073	11617	5911	3175	1765	1005	609	351	205
2002/08/16	17821	17889	19500	21035	29187	40944	29091	11617	5911	3175	1765	1005	609	351	205
2002/08/17	17904	17918	19521	21066	29217	40951	29113	11616	5910	3175	1765	1005	609	351	205
2002/08/18	17976	17949	19514	21060	29222	40953	29118	11616	5910	3175	1765	1005	609	351	205
2002/08/19	18039	17982	19508	21055	29228	40956	29128	11616	5910	3175	1765	1005	609	351	205
2002/08/20	18096	18015	19503	21047	29233	40959	29143	11615	5910	3175	1765	1005	609	351	205
2002/08/21	18147	18048	19499	21039	29235	40963	29160	11615	5910	3175	1765	1005	609	351	205
2002/08/22	18194	18080	19496	21031	29236	40966	29176	11615	5909	3174	1765	1005	609	351	205
2002/08/23	18238	18112	19493	21023	29237	40968	29194	11614	5909	3174	1765	1005	609	351	205
2002/08/24	18279	18143	19491	21015	29237	40970	29210	11614	5909	3174	1765	1005	609	351	205
2002/08/25	18318	18173	19489	21007	29237	40972	29226	11614	5909	3174	1765	1005	609	351	205
2002/08/26	18355	18203	19488	20999	29237	40973	29240	11613	5909	3174	1765	1005	609	351	205
2002/08/27	18390	18232	19487	20992	29237	40974	29255	11613	5908	3174	1765	1005	609	351	205
2002/08/28	15794	16841	18741	20540	29170	40975	29264	11613	5908	3174	1765	1005	609	351	205
2002/08/29	17681	17829	19690	21493	29319	40975	29274	11612	5908	3174	1765	1005	609	351	205
2002/08/30	17771	17946	19822	21657	29379	40976	29284	11612	5908	3174	1765	1005	609	351	205
2002/08/31	17859	17981	19847	21692	29410	40976	29294	11612	5908	3174	1765	1005	609	351	205

APPENDIX D2: Simulated fluoride concentration data for December 1991 and August 2002 used for calibration plots for Secunda.

Date	Fluoride concentration (mg/m³)														
	0 cm	*0.5 cm*	*1 cm*	*2 cm*	*11 cm*	*29 cm*	*47 cm*	*65 cm*	*83 cm*	*101 cm*	*119 cm*	*137 cm*	*155 cm*	*173 cm*	*191 cm*
1991/12/01	43263	42959	42074	40587	18619	12930	7412	3575	1214	304	60	10	2	1	1
1991/12/02	43185	42896	42048	40583	18624	12934	7420	3582	1221	307	61	10	2	1	1
1991/12/03	43110	42836	42020	40578	18628	12937	7427	3590	1227	310	62	11	2	1	1
1991/12/04	43547	42954	42070	40695	18709	12942	7433	3596	1232	313	63	11	2	1	1
1991/12/05	43355	42910	42044	40675	18714	12948	7440	3603	1237	315	64	11	2	1	1
1991/12/06	43246	42868	42025	40665	18718	12953	7446	3609	1242	317	64	11	2	1	1
1991/12/07	43154	42821	42004	40654	18723	12957	7453	3615	1247	320	65	11	2	1	1
1991/12/08	43072	42771	41982	40642	18727	12961	7459	3620	1251	322	66	11	2	1	1
1991/12/09	42997	42720	41958	40630	18731	12965	7464	3626	1256	324	66	12	2	1	1
1991/12/10	42928	42669	41933	40618	18735	12968	7470	3631	1260	326	67	12	2	1	1
1991/12/11	42864	42619	41906	40604	18740	12971	7475	3636	1264	328	68	12	2	1	1
1991/12/12	42803	42570	41879	40590	18743	12973	7480	3641	1268	330	68	12	2	1	1
1991/12/13	42745	42522	41851	40576	18747	12976	7485	3645	1272	331	69	12	2	1	1
1991/12/14	42690	42475	41823	40561	18751	12978	7489	3650	1275	333	69	12	2	1	1
1991/12/15	42637	42429	41794	40545	18755	12981	7493	3654	1279	335	70	13	2	1	1
1991/12/16	42585	42385	41764	40528	18759	12983	7498	3658	1282	337	71	13	2	1	1
1991/12/17	42536	42341	41734	40511	18762	12985	7502	3662	1285	338	71	13	2	1	1
1991/12/18	43099	42510	41765	40583	18838	12988	7505	3666	1289	340	72	13	2	1	1
1991/12/19	42905	42479	41743	40556	18845	12992	7509	3670	1292	341	72	13	2	1	1
1991/12/20	42807	42451	41726	40536	18849	12996	7513	3674	1295	343	73	13	2	1	1
1991/12/21	42725	42417	41707	40517	18853	12999	7517	3677	1298	344	73	13	2	1	1
1991/12/22	42653	42378	41688	40498	18857	13002	7521	3681	1300	346	74	13	3	1	1
1991/12/23	42588	42336	41666	40479	18861	13005	7525	3684	1303	347	74	14	3	1	1
1991/12/24	42528	42295	41644	40460	18865	13007	7529	3688	1306	348	74	14	3	1	1
1991/12/25	42472	42253	41620	40441	18868	13009	7533	3691	1309	350	75	14	3	1	1
1991/12/26	42420	42211	41595	40422	18872	13011	7536	3695	1311	351	75	14	3	1	1
1991/12/27	42370	42170	41569	40403	18875	13013	7539	3698	1314	352	76	14	3	1	1
1991/12/28	42322	42129	41543	40383	18879	13015	7543	3701	1316	353	76	14	3	1	1
1991/12/29	42276	42089	41516	40364	18882	13017	7546	3704	1319	355	77	14	3	1	1
1991/12/30	42231	42050	41489	40344	18886	13019	7549	3707	1321	356	77	14	3	1	1
1991/12/31	42188	42012	41461	40323	18889	13021	7552	3710	1323	357	77	14	3	1	1

Date	Fluoride concentration (mg/m^3)														
	0 cm	*0.5 cm*	*1 cm*	*2 cm*	*11 cm*	*29 cm*	*47 cm*	*65 cm*	*83 cm*	*101 cm*	*119 cm*	*137 cm*	*155 cm*	*173 cm*	*191 cm*
2002/08/01	82857	82039	86728	92290	135222	187430	132175	53324	27048	14444	8023	4461	2625	1484	876
2002/08/02	84518	83226	87930	93598	135349	187704	132282	53322	27047	14444	8023	4461	2625	1484	876
2002/08/03	84947	83635	88426	94186	135454	188075	132451	53320	27046	14444	8023	4461	2625	1484	876
2002/08/04	85283	83740	88468	94246	135492	188323	132581	53319	27045	14444	8023	4461	2625	1484	876
2002/08/05	85561	83884	88456	94234	135503	188436	132643	53317	27044	14443	8023	4461	2625	1484	876
2002/08/06	85800	84029	88451	94220	135518	188624	132763	53315	27043	14443	8023	4461	2625	1484	876
2002/08/07	86009	84172	88450	94194	135526	188801	132894	53313	27042	14443	8023	4461	2625	1484	877
2002/08/08	86198	84312	88452	94170	135530	188948	133020	53311	27041	14443	8023	4461	2625	1484	877
2002/08/09	86369	84448	88456	94147	135531	189068	133139	53310	27041	14442	8023	4461	2625	1484	877
2002/08/10	86528	84581	88461	94124	135532	189171	133259	53308	27040	14442	8023	4461	2625	1484	877
2002/08/11	86676	84710	88469	94101	135532	189258	133377	53306	27039	14442	8023	4461	2625	1484	877
2002/08/12	86815	84836	88478	94078	135532	189318	133467	53305	27038	14442	8023	4461	2625	1484	877
2002/08/13	86941	84958	88488	94057	135532	189372	133562	53303	27037	14441	8023	4461	2625	1484	877
2002/08/14	74788	78884	86628	93688	135241	189418	133656	53302	27036	14441	8023	4461	2625	1484	877
2002/08/15	83382	83569	91033	98040	135923	189458	133750	53300	27035	14441	8023	4461	2625	1484	877
2002/08/16	83663	83966	91487	98624	136156	189488	133831	53298	27034	14441	8023	4461	2625	1484	877
2002/08/17	84050	84101	91587	98773	136293	189519	133931	53297	27033	14440	8023	4461	2626	1485	877
2002/08/18	84392	84246	91551	98742	136316	189528	133957	53295	27032	14440	8023	4462	2626	1485	877
2002/08/19	84687	84401	91523	98718	136344	189542	134003	53294	27032	14440	8023	4462	2626	1485	877
2002/08/20	84951	84557	91501	98680	136367	189558	134072	53292	27031	14440	8023	4462	2626	1485	877
2002/08/21	85190	84711	91482	98642	136379	189574	134149	53290	27030	14439	8023	4462	2626	1485	877
2002/08/22	85411	84862	91466	98605	136384	189586	134223	53289	27029	14439	8023	4462	2626	1485	877
2002/08/23	85616	85010	91453	98568	136387	189599	134308	53287	27028	14439	8023	4462	2626	1485	877
2002/08/24	85809	85155	91443	98531	136388	189608	134381	53286	27027	14439	8023	4462	2626	1485	877
2002/08/25	85991	85297	91434	98495	136388	189615	134451	53284	27026	14438	8023	4462	2626	1485	877
2002/08/26	86165	85435	91428	98459	136388	189621	134517	53282	27025	14438	8023	4462	2626	1485	877
2002/08/27	86330	85570	91424	98424	136388	189627	134587	53281	27025	14438	8022	4462	2626	1485	877
2002/08/28	74163	79056	87941	96331	136079	189629	134628	53279	27024	14438	8022	4462	2626	1485	877
2002/08/29	83015	83695	92391	100798	136776	189632	134675	53277	27023	14437	8022	4462	2626	1485	877
2002/08/30	83437	84241	93010	101567	137054	189634	134721	53276	27022	14437	8022	4462	2626	1485	877
2002/08/31	83852	84408	93130	101732	137199	189636	134768	53274	27021	14437	8022	4462	2626	1485	878

APPENDIX E: Indaba irrigation data for a period from 1991 to 2001 used in the simulation process for solute calibration plots, estimated from the plots in a report by Ginster (2002). Indaba irrigation site area is 40 ha.

Year	**Irrigation rates (m^3/month)**	**Irrigation rates (mm/month)**	**Irrigation rates (mm/two weeks)**	**Total irrigation in a year (mm/a)**
1991	2000	5	3	**305**
	1000	3	3	
	1000	3	2	
	7500	19	10	
	15000	38	19	
	20000	50	25	
	14000	35	18	
	15000	38	19	
	15000	38	19	
	10000	25	13	
	10000	25	13	
	11000	28	14	
1992	1000	3	1	**75**
	1000	3	1	
	10000	25	13	
	4000	10	5	
	5000	13	6	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
1993	1000	3	1	**36**
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
	1000	3	1	
1994	1000	3	1	**548**
	7500	19	9	
	14000	35	18	
	23000	58	29	
	35000	88	44	
	36000	90	45	
	25000	63	31	
	29000	73	36	
	32000	80	40	
	7000	18	9	
	7000	18	9	
	1000	3	1	

Year	Irrigation rates (m^3/month)	Irrigation rates (mm/month)	Irrigation rates (mm/two weeks)	Total irrigation in a year (mm/a)
1995	1000	3	1	**545**
	1000	3	1	
	24000	60	30	
	1000	3	1	
	11000	28	14	
	30000	75	38	
	36000	90	45	
	38000	95	48	
	29500	74	37	
	23000	58	29	
	21000	53	26	
	1000	3	1	
1996	1000	3	1	**168**
	1000	3	1	
	1000	3	1	
	1000	3	1	
	9000	23	11	
	33000	83	41	
	20000	50	25	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
1997	0	0	0	**78**
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	14500	36	18	
	7500	19	9	
	8000	20	10	
	1000	3	1	

Year	Irrigation rates (m^3/month)	Irrigation rates (mm/month)	Irrigation rates (mm/two weeks)	Total irrigation in a year (mm/a)
1998	1000	3	1	519
	10000	25	13	
	17000	43	21	
	30000	75	38	
	32000	80	40	
	36000	90	45	
	40000	100	50	
	30000	75	38	
	7500	19	10	
	1000	3	1	
	1000	3	1	
	1000	3	1	
1999	1000	3	1	377
	1000	3	1	
	7500	19	10	
	28000	70	35	
	25000	63	31	
	30000	75	38	
	30000	75	38	
	3000	8	4	
	5000	13	6	
	10000	25	13	
	8000	20	10	
	1000	3	1	
2000	1000	3	1	279
	1000	3	1	
	1000	3	1	
	1000	3	1	
	8000	20	10	
	17000	40	20	
	28000	70	35	
	28000	70	35	
	15000	38	19	
	9000	23	11	
	1000	3	1	
	1000	3	1	
2001	1000	3	1	537
	10000	25	13	
	15000	38	19	
	14800	37	19	
	15200	38	18	
	14900	37	19	
	15000	38	19	
	26000	65	33	
	29000	73	36	
	30000	75	38	
	22000	55	28	
	21000	53	26	

APPENDIX F: Goedehoop irrigation data for a period 1991 to 2001 used for the sensitivity analyses of the Mpumalanga Highveld estimated from the plots in a report by Ginster (2002). Goedehoop irrigation site area is 96 ha.

Year	**Irrigation rates (m^3/month)**	**Irrigation rates (mm/month)**	**Irrigation rates (mm/two weeks)**	**Total irrigation in a year (mm/a)**
1991	0	0	0	**163**
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	17000	18	9	
	38000	40	20	
	32000	33	17	
	20000	21	10	
	35000	15	8	
	14000	36	18	
1992	29000	30	15	**392**
	41000	43	21	
	39000	41	20	
	29000	30	15	
	44000	46	23	
	38000	40	20	
	38000	40	20	
	32000	33	16	
	38000	40	20	
	37000	39	19	
	8000	8	4	
	2000	2	1	
1993	1000	1	1	**112**
	1000	1	1	
	100	1	1	
	2000	2	1	
	20000	21	10	
	15000	16	8	
	29000	30	15	
	28000	29	15	
	8000	8	4	
	1000	1	1	
	1000	1	1	
	1000	1	1	
1994	1000	1	1	**307**
	1000	1	1	
	1000	1	1	
	7500	8	4	
	36000	38	19	
	44000	46	23	
	43000	45	22	
	60000	63	31	
	51000	53	27	
	43000	45	22	
	4000	4	2	
	2000	2	1	

Year	Irrigation rates (m^3/month)	Irrigation rates (mm/month)	Irrigation rates (mm/two weeks)	Total irrigation in a year (mm/a)
1995	1000	1	1	**283**
	14000	15	7	
	31000	32	16	
	1000	1	1	
	22000	23	11	
	40000	42	21	
	41000	43	21	
	45000	47	23	
	35000	37	18	
	26000	27	14	
	13000	14	7	
	1000	1	1	
1996	1000	1	1	**139**
	1000	1	1	
	1000	1	1	
	1000	1	1	
	10000	10	5	
	60000	63	31	
	59000	62	31	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
1997	0	0	0	**75**
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	0	0	0	
	29500	31	15	
	24000	25	13	
	18000	19	9	

Year	Irrigation rates (m^3/month)	Irrigation rates (mm/month)	Irrigation rates (mm/two weeks)	Total irrigation in a year (mm/a)
1998	1000	1	0.5	**632**
	28000	29	15	
	30000	31	16	
	60000	63	31	
	85000	89	44	
	95000	99	48	
	82500	86	43	
	82500	86	43	
	65000	68	34	
	37500	39	20	
	1000	39	0.5	
	1000	1	0.5	
1999	1000	1	0.5	**618**
	1000	1	0.5	
	45000	47	24	
	65000	68	34	
	58000	60	30	
	80000	83	42	
	85000	89	44	
	80000	83	42	
	80500	84	42	
	72000	75	38	
	25000	26	13	
	1000	1	0.5	
2000	1000	1	0.5	**283**
	75000	78	39	
	1000	1	0.5	
	1000	1	0.5	
	15000	16	8	
	40000	42	21	
	35000	37	18	
	60000	63	31	
	25000	26	13	
	15000	16	8	
	1000	1	0.5	
	1000	1	0.5	
2001	1000	1	0.5	**434**
	11000	12	6	
	30000	31	16	
	27000	28	14	
	35000	37	18	
	17000	18	9	
	59500	62	31	
	70000	73	37	
	71000	74	37	
	48000	50	25	
	45000	47	24	
	1000	1	0.5	