DEVELOPMENT OF A NUMERICAL MODEL FOR UNSATURATED/ SATURATED HYDRAULICS IN ASH/ BRINE SYSTEMS

by

Mehari Tewolde Menghistu

Thesis

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DECLARATION

This thesis contains no material that has been submitted for the award of any other degree or diploma at this or any other University and contains no material previously published or written by any other person except where due reference has been made in the text. I furthermore cede copyright of the thesis in favour of the University of the Free State.

Mehari T. Menghistu

DEDICATION

This thesis is dedicated to my late uncle, Kesete Tsegay Mengistu, who has raised me to be the person I am today, for his unconditional love, guidance and support.

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LIST OF SYMBOLS

d = Thickness of an aquifer at **x** [L]

$f(x,t)$ = Strength of a source(+) or sink(-) $[T^{-1}]$

g = Acceleration of gravity $[L.T^{-2}]$

$h(x,t)$ = Peizometric water level, or pressure head [L]

n, m = Characteristic constants in the Van Genuchten's retention curve

n = Outward directed unit normal vector to a surface [L]

p = Fluid pressure [Pa]

p_w = Pressure of water [Pa]

p_c = Capillary pressure [Pa]

$q(x,t)$ = Magnitude of Darcy velocity $\boldsymbol{q}(x,t)$ $[L.T^{-1}]$

q_n = Normal Darcy flux over a boundary surface $[L.T^{-1}]$

$q(x,t)$ = Darcy velocity of fluid in a porous medium $[L.T^{-1}]$

r = Radius of a borehole [L]

w(x,t) = Pressure head along the inside of a borehole [L]

z = Elevation above a reference level [L]

C = Soil moisture capacity of a porous medium $[L^{-1}]$

D_t = Partial derivative with respect to t

E = Rate of evapotranspiration $[L.T^{-1}]$

$E(\tau)$ = Error associated with the Lagrange interpolation polynomial

K = Scalar hydraulic conductivity $[L.T^{-1}]$

$\boldsymbol{K}(x,t)$ = Hydraulic conductivity tensor of a porous medium $[L.T^{-1}]$

K_0 = Unsaturated Hydraulic conductivity [$L.T^{-1}$]

K_r = Residual Hydraulic conductivity [$L.T^{-1}$]

K_s = Saturated Hydraulic conductivity [$L.T^{-1}$]

L = Symbolic operator]

Q_a = The rate of discharge from the aquifer to the borehole [$L^3.T^{-1}$]

$Q(x,t)$ = Rate of water injection(+) or withdrawal(-) from a borehole [$L^3.T^{-1}$]

R = Rainfall intensity [$L.T^{-1}$]

$S_o(x,t)$ = Specific storativity of an aquifer [L^{-1}]

S_w = Water saturation [1]

T = Time [T]

V = Velocity of a unit mass [$L.T^{-1}$]

V = Volume of fluid [L^3]

V_0 = Proper volume element [L^3]

V_v = Volume of voids [L^3]

V_w = Volume of water [L^3]

X = Cartesian coordinates of a point in space (x,z) [L]

GREEK SYMBOLS

α = Parameter in Van Genuchten's moisture retention curve

α = The compressibility of porous medium [$L.T^2.M^{-1}$]

β = Coefficient of compressibility of water [$L.T^2.M^{-1}$]

δ = Dirac delta function [$L.T^2.M^{-1}$]

ε = Porosity of a porous medium [$L^3.L^{-3}$]

$\phi(x,t)$ = Piezometric head (also known as Hubert's potential) [L]

$\phi_0(x,t)$ = Initial piezometric head [L]

μ = Dynamic viscosity of water $[M.T^{-1}.L^{-1}]$

φ = Three-dimensional finite element basis function

θ = Volumetric moisture content $[L^3.L^{-3}]$

θ_r = Residual moisture content $[L^3.L^{-3}]$

θ_s = Saturated moisture content $[L^3.L^{-3}]$

ρ = Fluid density $[M.L^{-3}]$

ψ = Soil matric pressure head [L]

(ξ, η, ζ) = Coordinates of the local head domain Γ

Δ = Small increment [1]

Θ = Reduced water content [1]

∇ = Gradient operator in two dimensions $[L^{-1}]$

Ω = Global domain $[L^3]$

Ω_e = Boundary of the global domain Ω $[L^2]$

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CHAPTER 1

INTRODUCTION

1.1 GENERAL

Vast quantities of coal combustion residues (ash) and effluents are produced simultaneously in the coal processing facilities of Eskom and Sasol. These facilities are all located in the interior of South Africa in water sensitive catchment areas, where the re-use and recycling of water are mandatory. Although the re-use and recycling of the water reduces the volumes of effluent considerably, a large volume of salient effluents remains that has to be disposed of. The handling and disposal of saline effluents is a difficult and complex problem. The current practice used by both parastatals is to co-dispose of the effluents with the ash residue in waste disposal sites and ash dams. Although this practice provides a potentially elegant approach at least from the viewpoint of the generator of both the ash and effluent, the co-disposal of ash and brine in a landfill could have dire consequences on the environment (Mudd, 2002). This applies in particular to the release of environmentally deleterious and toxic constituents of the ash into the air, soil, surface and groundwater (Baba and Usmen, 2006), which can lead not only to environmental and land-use problems, but also jeopardizes the health of organisms living in the surrounding ecosystem. Pressure from social awareness groups has consequently caused many governments to try to stem damage from waste disposal sites through international agreements and laws on a worldwide scale. The question therefore arises as to how can Eskom and Sasol better manage their ash dams to not only satisfy all legal requirements and possible pressure from social awareness groups but also, more importantly, prevent, or at least limit, pollution of the natural environment.

An approach frequently applied in investigations of geohydrological pollution problems is to develop a so-called *model* (or models) that presumably captures the relevant features of the pollution mathematically (Huyakorn and Pinder, 1983; Princeton University Water Resources Program, 1984), and then simulates the migration of the contaminants through the environment with the view to taking corrective action if and when necessary. This is usually achieved by first developing a *conceptual model* of the site that is then cast into a set (or sets) of mathematical equations which can be implemented on a computer. This is achieved by using historical observations of the pollution at the site to first calibrate and verify the model(s), before using them to simulate the future evolution of the site. However, the migration of contaminants from waste sites into the surrounding ecosystems is a highly complex process that is not yet fully understood. It is consequently difficult (if possible at all) to ensure that the conceptual model does represent the migration of contaminants at a given site adequately and to prove that results derived from the approach are meaningful. In fact, (Bredehoeft, 2005) states that 25% of the conceptual models in the model analyses he investigated were incorrect and that the approach will always be accompanied by an uncertainty that is difficult to quantify. This observation supports the view of (Voss, 2005) in his editorial to Volume 13 of the Hydrogeology Journal, which is devoted to a discussion of the application of models under the title “The future of hydrogeology” that such investigations must be characterized as ‘faith-based’. “In other words, hydrogeologists … ‘believe’ that their approach is a meaningful and useful way to proceed, but cannot prove it objectively.” A similar view is expressed by (Orr and Meystel, 2005), who ascribe the limited successes achieved in the past using this approach to “… the ultimate reliance on first-principle models that lead to complex, distributed-parameter partial differential equations (PDE) on a given scale.” They therefore propose that there should be a paradigm shift towards a goal-oriented, flexible, adaptive, multi-resolutional decision support system. (It is perhaps worthwhile to mention that (Wolfram, 2002) raised a similar critique against Physics.) It is therefore of value to briefly review what the term model means; the difficulties associated with models and how to limit or account for these difficulties. The discussion below commences in section 1.2 with a brief definition of the term ‘model’, more precisely a ‘scientific model’ and its limitations in the study of geohydrological phenomena. This is followed by a discussion of the difficulties that may be experienced with the practical applications of models to environmental phenomena more specifically, geohydrological phenomena, in Section 1.3. The discussion is concluded with a description of the purpose and scope of this thesis in Sections 1.4 and 1.5 respectively.

1.2 SCIENTIFIC MODELS

1.2.1 Definitions and Properties

The word ‘model’ has so many meanings and is so over-used in science that it is sometimes difficult to know exactly what it refers to (Konikow and Bredehoeft, 1992).

(In fact, the encyclopaedia on the Internet, Wikipedia, listed 16 meanings of the word, when accessed on 2007-05-01.) One must therefore be very careful when using the word ’model ‘scientifically. However, Konikow and Bredehoeft’s definition of a model as: ‘a representation of a real system or process’ does not really help to clarify the confusion. For example, to what extent does their definition of the term ‘model’ correspond to the term ‘conceptual model’ used above?

Judging from the available literature, see, for example. (Morton, 1993; Narasimhan, 1999; Ritchey, 1991), the term ‘model’ (or to be more specific ‘scientific model’) may be viewed as the result of a process whereby ideas from an existing theory – sometimes merely heuristics – combined with observations of a specific phenomena to arrive at a mathematical description of that phenomenon. For example, the analysis of many physical, biological and social systems today are based on the theory of heat conduction, introduced by the French Egyptologist and mathematical physicist, Jean Baptiste Joseph Fourier, in his 1807 masterpiece: Théorie de la Propagation de la Chaleur dans les Solides and his classic monograph (Fourier, 1822). However, this raises the question as to what is meant by the term ‘theory’.

There is no doubt that the natural sciences known today have been developed through the quest of humankind to understand and control the natural environment. This has been achieved by using their inherent faculty for abstract philosophical reasoning to relate observations on natural phenomena to one another, themselves and nature. Judging from the vantage point of the twentieth century, the success reached thus far with this objective (particularly in the exact sciences, such as physics and chemistry) can be ascribed to three outstanding developments in the history of humankind (Botha, 1994).

(a) The development of numerals and the ability of humans to count and measure (in other words delineate ‘quantity’) by the ancient Mesopotamian and Egyptian civilizations.

(b) The recognition that physical phenomena, that is any thing, fact, or change perceived by any of the senses, the cause or explanation of which is in question, can be related to three basic measurable quantities: space, time and mass.

(c) The introduction of what is called ‘the principle of decomposition’, by the eminent British scientist, Sir Isaac Newton, in the seventeenth century. According to this principle, the behaviour of a complex physical phenomenon can be decomposed into hierarchical sets of simpler phenomena, called interactions or observables (if they can be observed by humans).

Since space, time and mass are measurable, and numbers form the basis of all mathematics, the question arises: is it not possible to combine the power of human reason with well-planned observations, and to describe natural phenomena in abstract mathematical terms? The result of this conceptualization of a natural phenomenon is commonly known as a theory in physics. A theory, therefore, could be regarded as a scheme or system of ideas established through observation or experiment and embodied in a set of mathematical equations with the functional form

$$\mathbf{Lu}(\mathbf{p},\mathbf{v}) = \mathbf{f} \tag{1.1}$$

that relates the set of unknown observables **u** to another set of known observables **v** through the relational operator **L**, relational parameters **p**, and forcing functionals **f**. These observations led (Botha, 1994) to distinguish between four types of models:

- Conceptual models – idealized verbal descriptions, and/or mental conceptions of a particular physical phenomenon that form a basis for further investigations of the phenomenon. (The term conceptual model above should be interpreted in this sense.)
- Mathematical models – the mathematical relation in an Equation (1.1).
- Analytical models – mathematical models where the relation in an Equation (1.1) can be expressed in terms of analytical functions, e.g. the Theis solution of the groundwater flow equation.
- Numerical models – mathematical models that can only be approximated numerically, e.g. finite element or finite difference approximations of the groundwater flow equation.

1.2.2 Difficulties Associated with Scientific Models

The possibility always exists that a model (even a theory) does not represent the observed behaviour of a natural phenomenon adequately. Experience in the exact sciences indicates that such situations are usually caused by an insufficient knowledge of small-scale interactions that play a vital role in the phenomenon. One solution in such situations is to investigate the phenomenon in detail with the view to identify, understand and quantify the unknown interactions in a cohesive, systematic manner. However, Nature behaves in its own subtle ways and not necessarily as envisioned by humans. As pointed out by Paul Roman, Alfred A. Brooks, and Lorenzo de la Torre in Physics Today (1998), the result of this is that while physical reality exists objectively, it is not fully or directly accessible to humans. Moreover, as already recognized by Einstein, such constructs cannot be extracted from experience but must be invented by humans (Neuman and Wierenga, 2003). It may therefore take a long time before a physical phenomenon reveals its nature to humans via sensory impressions and experiences (observations and experiments) that allow them to develop suitable mental constructs, a conceptual model of the phenomenon. No wonder it took centuries to develop some of the best-established theories in Physics. The luxury of time, unfortunately, is not available in situations involving the lives of living organisms, humans in particular. Various attempts have consequently been made through the years to develop suitable models for phenomena with an insufficient knowledge of the basic interactions.

The traditional application of a scientific model is to use its corresponding mathematical model in Equation (1.1) and compute values for the unknown observables (**u**) and estimates of the relational parameters (**p**). However, results derived from a scientific model for a phenomenon with an insufficient knowledge of its basic interactions, will obviously not be reliable. Nevertheless, a model is often the only alternative one has in practical situations. In such situations, it may be useful to have a measure of the uncertainties contained in results computed with a suitable but not necessarily perfect model. This is the reason why many of the models used in groundwater investigations are based on existing deterministic physical models and theories (Neuman and Wierenga, 2003). While this practice is often severely criticized, even to the extent that it should be dropped in groundwater investigations (Orr and Meystel, 2005), the fact remains that the existing deterministic models have served humans well, both qualitatively and quantitatively, in the development of the modern technological age. This suggests that the use of deterministic models can only be neglected in groundwater and similar geohydrological investigations at the cost of neglecting a perhaps limited, but often valuable and sometimes the only, independent source of information on unknown interactions.

An approach commonly used to circumvent insufficient knowledge of interactions for a given phenomenon is to postulate a deterministic conceptual model structure for the phenomenon and its associated mathematical model, Equation (1.1). The calculations are then subjected to a statistical analysis assuming that the relational parameters, although imperfectly known, can be quantified through a prior uncertainty model and Monte Carlo simulations (Bredehoeft, 2005; Neuman, 2005). There is sufficient reason to believe that the approach work in the short term, can be achieved if a sufficiently large enough database exists of relational parameter values that could be used to select a suitable prior uncertainty model (for the parameters) (Neuman and Wierenga, 2003). Nevertheless, the possibility always exits that such a model can neither reproduce nor explain new observations and experimental data no matter how large the supporting database may be – something that (Bredehoeft, 2005) refers to as "surprise". However, such "surprises" are understandable if it is kept in mind that geohydrological scientists must deal with phenomena whose characteristics are only unique over periods determined by the environmental and anthropogenic forcing experienced at a site. Moreover, these phenomena, like many other natural phenomena, are inherently non-linear (Scott, 2007). A slight change in the forcing function of the natural elements could therefore cause a rapid change in the behaviour of the phenomena (including bifurcation often observed in non-linear dynamical systems). For example, the hydraulic conductivity of an unsaturated fine sand varies over five orders of magnitudes from 10^{-7} m s^{-1} to 10^{-12} m s^{-1} when the matric potential varies from 10 m to 100 m (Yeh *et al.,* 2005). The behaviour of geohydrological phenomena is consequently complex and not fully amenable to controlled observations and experimentation. In fact, it is not unusual to find that observations of the phenomena may lead to the development of not just one, but multiple, conceptual models for the phenomenon (Beven, 2006; Botha and Verwey, 1992). (Beven, 1993) calls this the "equifinality thesis" or "equifinality problem". The description of such phenomena must therefore remain forever incomplete and imprecise and their conceptual mathematical models merely fallible scientific constructs, and not credible engineering tools (Neuman and Wierenga, 2003).

1.3 APPLICATION OF SCIENTIFIC MODELS IN GEOHYDROLOGY

A natural question that arises from the preceding discussion is: is there any useful purpose for a scientific model especially in Geohydrology? While there are many people who would answer in the negative, the reality is that models, how imperfect they may be, are often the only means one has to address complex geohydrological problems. The emergence of general principles and techniques to address uncertainties and equifinality in models is probably the best testimony to this. The real difficulty would seem to be a lack of well-accepted guidelines as to how to actually implement the principles and techniques in an integrated manner and to efficiently assimilate important information from the data into the models to produce improved hydrological predictions (Liu and Gupta, 2007).

One approach that seems to be particularly suitable for this purpose is data assimilation (DA), defined by (Liu and Gupta, 2007) as: procedures that aim to produce physically consistent representations or estimates of the dynamic behaviour of a system, by merging the information present in imperfect models and uncertain data in an optimal way to achieve uncertainty quantification and reduction. The advantage of this approach is that it describes the comprehensive problem of 'merging models with data' and therefore includes the three related problems of system identification, parameter estimation and state estimation, that are all critical to the reduction of uncertainty in model predictions. The question is how to implement the approach? It is important to remember that geohydrological modelling cannot take place in a vacuum as all field sites are unique and hence cannot be validly represented by a generic model, except for initial investigations. Instead, the models must be solidly grounded in a broad array of regional and data specific to the site under investigation (Neuman and Wierenga, 2003).

Among the three types of DA problems, system identification is the most important and, typically, the most difficult, as it may involve the development of qualitative, diagnostic measures and include the use of expert knowledge and subjectivity. This suggests that the investigations should be carried out systematically, and perhaps iteratively, in the order of system identification, parameter estimation, and state estimation.

1.4 PURPOSE OF THE STUDY

Present investigations arose from a request by Eskom and Sasol to provide them with a detailed proposal for a framework with the view to increasing the competency of both organizations in the management of the co-disposal of ash and brine and the dissemination of knowledge. Two sites were selected by the organizations for this purpose: the Tutuka Power Station and the Secunda Synthetic Fuel Plant.

It follows from the preceding discussion that the best approach would be to base the envisaged framework on a geohydrological model (conceptual and mathematical) for a given site. As both organizations have already invested in a number of speciation models, they requested that due notice should be taken of these models, before the development of new speciation and numerical models for the proposed framework. An initial survey of the existing models revealed that one area not covered by the models is unsaturated flow. It was consequently decided to adapt an unsaturated-saturated flow model originally developed by (Verwey and Botha, 1992) for this purpose. However, it became clear during the adaptation of the model that there is insufficient data to develop and implement a suitable framework at any one of the selected sites.

Gathering suitable data for the development of a geohydrological model is an expensive and time-consuming process (Fetter, 2001; Freeze and Cherry, 1979). Geohydrological modelling has benefitted significantly from developments over the past two decades, e.g. the dramatic growth in computational power; the ever-increasing availability of distributed hydrologic observations, and an improved understanding of the physics and dynamics of the hydrological system (Liu and Gupta, 2007), but these developments have paradoxically increased the observations required to drive the models. An attempt has consequently been made to introduce a few preliminary ideas on how to develop a structured methodology to reduce the cost and time involved in gathering the information needed to drive the models.

1.5 SCOPE OF THE STUDY

Geohydrological models for the management and control of waste disposal sites are conventionally based on historical data, or where that is not available, on generic data-sometimes even proxies (Botha *et al*., 2000). The discussion that follows in Chapter 2 therefore begins with a description of the data available for both the Tutuka and Secunda sites. To investigate the Tutuka and Secunda site would require the development of suitable flow and mass transport models. However, as discussed in chapter 2, there is not sufficient data to develop even proxy models for the sites. The present discussion is therefore limited to the development of conceptual models for both the Tutuka and Secunda sites in chapter 3 and the application of the unsaturated-saturated computer package of (Verwey and Botha, 1992) to the Tutuka site in chapter 5.

The application of geohydrological models to assess the behaviour of a waste disposal site has historically often been viewed as an attempt to predict the future behaviour of the site. However, this would require information on relational parameters and known interactions in Equation (1.1) whose behaviour cannot be determined with certainty far into the future (Van Blerk, 2000). A geohydrological model should therefore never be viewed as an attempt to predict the future of a given waste site, but rather as an aid to assess how effectively the site is managed and controlled. The best way to achieve this is to investigate the waste site systematically, preferably using well-established and accepted international methodology. Unfortunately, no documents exist, at least at this time that describe such a methodology, its implications and the steps necessary to implement it in practice in a way that can also be understood by interested members of the public.

Two techniques that could make valuable contributions to such an assessment are that of (Neuman and Wierenga, 2003) and (Liu and Gupta, 2007). Although both papers provide valuable insight into the philosophical and mathematical aspects of such an investigation, they lack guidelines as to how to obtain suitable site-specific data at minimum cost and time. Chapter 6 therefore describes an attempt to provide guidelines for the development of such a methodology, based on the ISAM Safety Assessment Methodologies for Near Surface Disposal Facilities (IAEA, 2002; Van Blerk, 2000). No attempt will be made though, to develop a fully-fledged methodology. This could only be achieved by using the information from various organizations, regulatory authorities and other interested parties.

CHAPTER 2

THE ASH DUMP SITES USED IN THIS INVESTIGATION

2.1 INTRODUCTION

2.1.1 General

Two ash dumpsites or dams, as they are also called, were selected for this investigation. The first is situated on the site of Eskom's Tutuka Power Station located 25 km, north-east of the town of Standerton, and the second, at Sasol the synthetic fuel production plant at Secunda. Both towns are situated in the Mpumalanga Province of the Republic of South Africa. The scale of operations on both stations is immense and therefore the potential to pollute the environment is, for this reason, real. Most of the ash generated at the two sites is dumped in landfills covering several hectares of valuable land near the plants.

At Tutuka, dry ash is dumped via conveyor belts on the ash dump, but is pumped as saline slurry to the dam at Secunda. Although dry ash disposal is, in principle, less dangerous to the environment than wet ash disposal, the dry ash at Tutuka is irrigated with highly salinated waste water from the water treatment plant to suppress excess dust (and as a co-disposal principle). Excess water that could drain to underlying aquifers is consequently present at both the dump and dam sites, thereby adversely affecting the groundwater quality at these sites (Carlson and Adriano, 1993).

As quoted by Dr. Hassett "Disposal is forever" and hence safe disposal of the ash without adversely affecting the environment is a major concern. So too, is the large storage area required for disposal. Globally, various attempts have been made in the past to use the ash in economically viable products such as building materials, soil improvement, the water holding capacity of soil, mine reclamation efforts and road construction (Adriano and Weber, 2001; Bin-Shafique, 2002; Cambell *et al.*, 1983). Even on a global level, however, despite positive uses, the rate of production of ash clearly far outweighs consumption. For the unused material, disposal practices involve holding ponds, lagoons, landfills and slag heaps; all of which can be regarded as unsightly, environmentally undesirable and a non-productive use of land resources as well as posing an on-going financial burden through their long-term maintenance. The efficient management of ash dumps/dams therefore presents a major challenge to both Eskom and Sasol.

While some preliminary work has been done to determine the possible pollution of the groundwater resources by the ash dump at Tutuka, no detailed geohydrological study has yet been undertaken at Secunda, except for the routine monitoring of the groundwater quality. However, no consistent methodology is currently in place to assess the long-term impacts of the ash management and disposal on the groundwater resources at both Tutuka and Secunda, nor is there enough data available. The following discussions in section 2.2 and 2.3 therefore concentrate more on summarising and evaluating the existing information at the sites with a view to developing suitable groundwater models for the sites. Knowledge of the physical and chemical properties of ash and engineering methods required are vital in ash disposal management. This is briefly discussed in section 2.4.

2.1.2 Ash Disposal System

Disposal of fly ash as a by-product of incineration of coal is becoming an increasing economic and environmental burden. Wherever coal is burned it is necessary to have an efficient ash handling system in place, especially in a coal-fired power station environment where large quantities of pulverized fuel ash (PFA) are created. Such ash can be a considerable environmental nuisance as well as being awkward to handle due to its abrasiveness and fine particle size.

Basically, there are two ash disposal placement methods: dry or wet ash disposal mechanisms. Dry ash placement involves any method that results in a solid material that does not drain water except during rainfall and irrigation. The ash is transported by truck or conveyor belt at the site and disposed of by constructing a dry embankment (dyke). Wet placement is any method that results in an excess of water that must be handled after the ash has been placed, that is, the fly ash is transported as slurry through pipes and disposed of in an impoundment called an ash pond. With the growing environmental awareness that hydraulic ash removal systems are costly with regard to water and land usage, emphasis has been placed on finding a better system. In South Africa, power station fly ash is disposed of in one of two ways; by dry dumping or by hydraulic deposition into dams. It has sometimes been observed that a marked hardening of the hydraulically deposited fly ash occurs, producing a very erosion-resistant surface Fourie *et al.*, (1997).

2.1.2.1 Wet ash disposal system

Similar to overseas experience, wet ash disposal systems have been the preferred methodology in South Africa power stations, but this method of ash management is being re-evaluated because of the cost of disposal and the potential for contamination of surface and ground waters by trace elements leached from the ash dams. Eskom power stations are in the process of transforming to dry ash disposal systems; yet wet ash disposal methodology is still in operation at the Sasol Synthetic Fuel facility and all old Eskom power stations. Wet ash disposal involves, ash being pumped from the power station to the ash dams in ash-to-water ratios of 1:10 to 1:5 by volume Hodgson and Krantz (1998). Excess water on top of the ash dams is decanted through a penstock arrangement, draining water into ash water return dams. From there, water is returned to the power station to pump more ash.

Wet disposal of FA (fly ash) is a simple operation and has minimal effect on the local air quality. On the other hand, the amount of water required forming the FA slurry is considerable and recirculation of water is a costly practice. During wet disposal, heavy metals (which are toxic in nature) leach from the matrix leading to pollution of the environment. A major disadvantage of wet disposal is that it demands large areas of land, which are practically irretrievable for future use Singh and Kolay (2002).

2.1.2.2 Dry ash disposal system

Although both dry and wet ash disposal methods have an impact on both surface and groundwater, dry ash disposal dumpsites (heaps), when properly constructed, are unlikely to produce leachate for many years. Factors that possibly play a role in reducing the leachate impact from dry ash are the pozzolanic property of dry ash and its inherent dry nature, and the saline (brine) content of water used to irrigate the heaps. Nowadays the wet ash disposal system has been abandoned in most Eskom plants due to the high cost factor and the potential environmental impact and has been replaced by dry ash disposal that is more cost effective and less dangerous to the environment.

In a dry ashing system, the ash is partially wetted at the power station by adding approximately 10-15% water before being transported by a conveyor belt to the disposal dumpsite. This moisture prevents the ash from blowing off the conveyor belt and a watering gun is also available in the area where the ash is being tipped to prevent it from drying out and creating a dust problem.

According to Hodgson (1999), this dry ash disposal system is similar to that used in all power stations in South Africa and the most common concentration of chemicals in the effluent are sodium and sulphate. The pozzolanic action of a wet ash system is very different from that of a dry ash system. In wet ash systems, water migrates from the inside of an ash dam to the outside, where evaporation occurs. The presence of carbon dioxide is essential for pozzolanic development but wet ash dams are usually saturated with water, so no carbon dioxide of any significance can permeate the dams. Although pozzolanic action is not possible within the wet ash dams, the presence of atmospheric carbon dioxide assists in the development of a skin of pozzolanic material. This layer covers the outer few millimetres of an ash dam and can easily be broken to expose the soft unaltered ash below.

At dry ash dumps, the upper layers go through alternate wetting and drying cycles, as they are exposed to rainfall and evaporation. This cyclic exposure allows sufficient water and air to exchange to establish a pozzolanic layer of up to a metre or more on the top and along the sides of these dumps. The controlling factor for pozzolanic action is not so much the amount of rainfall, but the irregularity of the event.

2.2 THE TUTUKA POWER STATION

2.2.1 General

The Tutuka Power Station, which commenced power generation around 1985, is one of the more recent power stations constructed by Eskom and a number of potential sources already exist, delineated in Figure 2-1, that could contribute not only to the pollution of the groundwater in the area, but also to the surface water (Hodgson, 1999). Some of the more significant of these sources, apart from the ash disposal site, include coal stockpiling, solid waste disposal, dirty water dams and the sewage works.

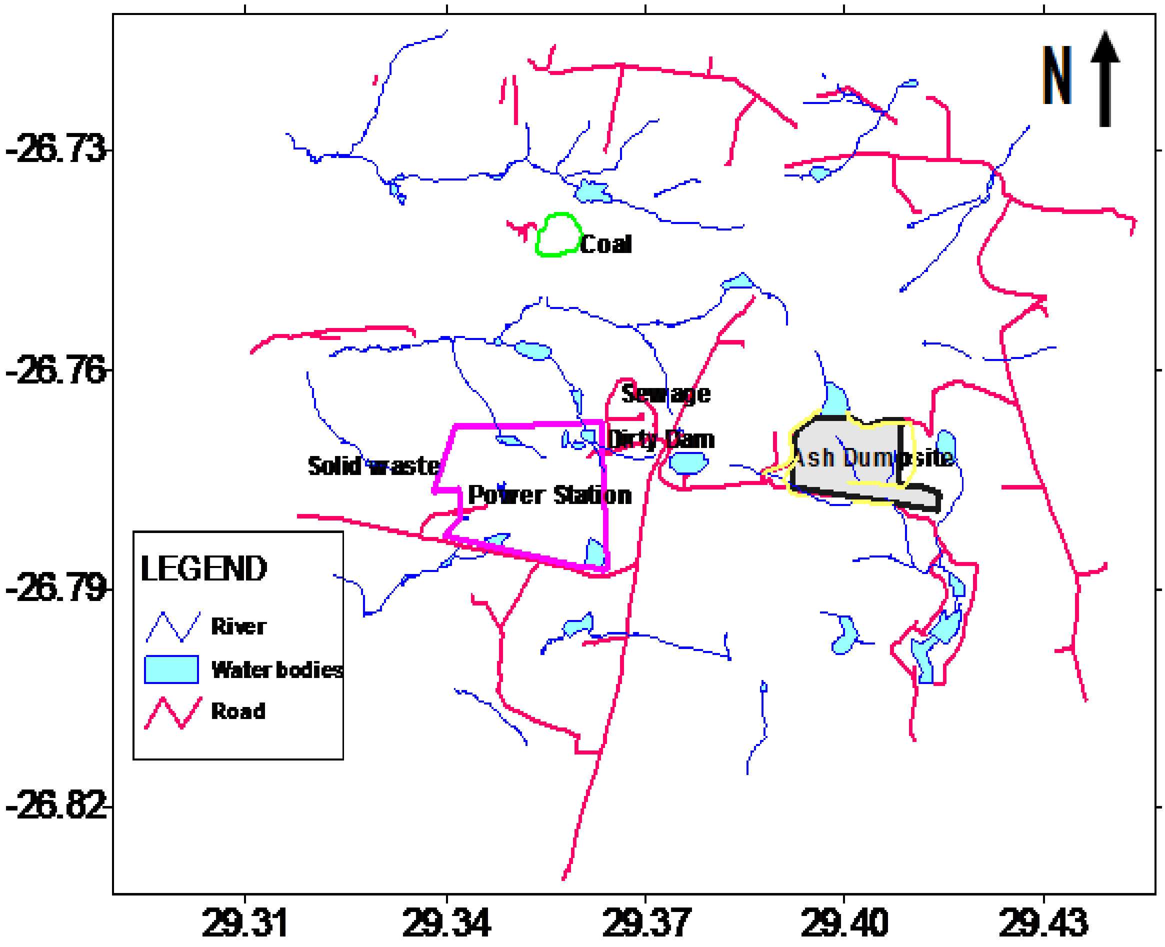

Figure 2-1: Topographical map of the area and facilities surrounding the Tutuka power station, (in relation to topography, ash dump, coal stockyard, dirty water dam, sewage plant and solid waste site.)

The ash dump in Figure 2-1, which currently covers approximately 190 ha, extends eastwards. The dump is approximately 40 m above ground level on the side where dumping takes place, and slopes gently towards the west. The coal stockyard lies approximately 5 km north-west of the ash dumpsite, and covers an area of approximately 28 ha. Solid waste is disposed of west of the power station. A dirty water dam is situated in the north-eastern corner of the power station security fence, with the sewage works approximately 400 m to the north and in the same drainage system. A small water body, in the form of a wetland or pond, lies approximately 400 m to the east of the ash dump.

Of concern for this study is the water dam less than 30 m north of the ash dump, more clearly delineated together with the small water body in Figure 2-2. The dam is topographically up gradient from the disposal site and groundwater flow is towards the ash dump. According to Hodgson (1999), this dam sustains a shallow groundwater table beneath the ash dump, thereby causing salt to leach excessively from the ash dump into the surrounding areas. He therefore recommended that this dam should be emptied and kept dry.

Hodgson (1999) suggests that, on a regional scale, the run-off from the ash dump area is directed towards the Grootdraai Dam, which is situated approximately 9 km south of the power station. Locally, four catchments are involved. The ash disposal facility lies in its own catchment. The dirty water dam, sewage works and solid waste site are in one catchment. Run-off from the coal stockyard drains to the north, but groundwater seepage flows into dirty water dam catchment.

Figure 2-2: Tutuka locality site map ash dump, water dam to the north and small water body to the east. Scale 1;1000m

A significant effort is made by the operator of the power station to keep the site in a near perfect state through landscaping and rehabilitation Hodgson (1999). For example, a 300 mm thick soil layer has been placed at the top of the ash dump and planted with grass to minimize the problem of dust.

2.2.2 Dry Ash Disposal at Tutuka Power Station

Fly ash from a coal-burning power station is typically deposited by dry dumping and spread by a stacker and dozer. This is the system, used at Tutuka Power Station.

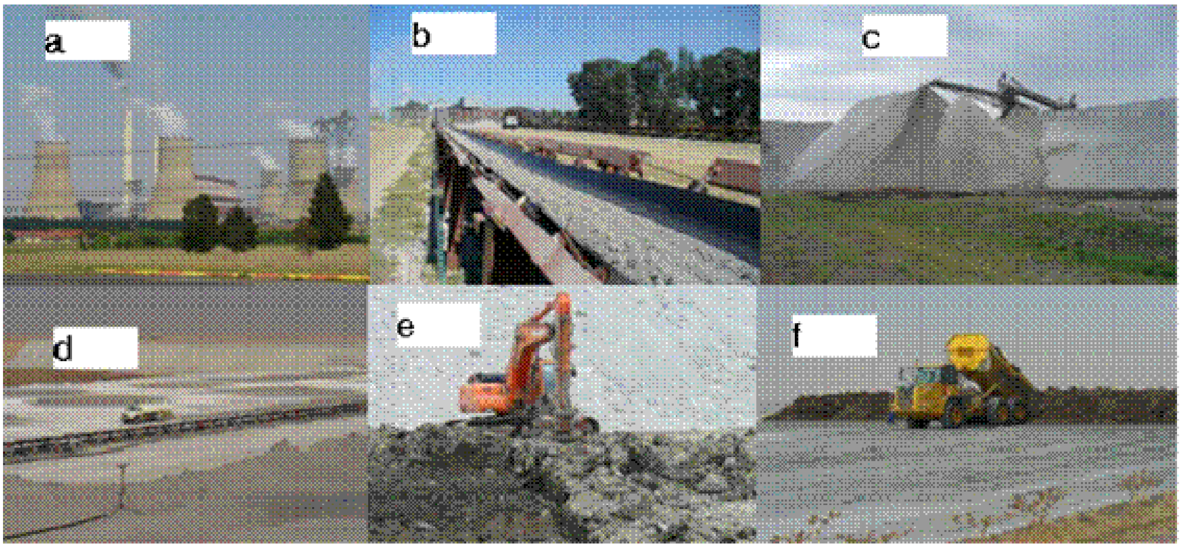

Figure 2-3: Photograph of dry ash disposal system at Tutuka ash dumpsite (UWC report to Sasol/Eskom January 2008).

The moist ash at Tutuka is transported by conveyor belt to the ash dump where it is dumped in a single or double stacking operation (Figure 2-3 b &c). No mechanical compaction of the ash, other than its own weight and the weight of machinery used on top of the ash dump is taking place (Figure 2-3 d, e & f). This is one of the convincing reasons why it is assumed that ash is a porous material.

In addition to the moisture added to the ash within the power station, the ash is again wetted by means of a pivot irrigation system as it is dumped off the conveyor belt to prevent the ash from drying out and creating a dust problem. Under severe windy conditions, dust does, however, still blow from the exposed ash.

In addition to its less negative environmental impacts and cost effectiveness, the rehabilitation of dry ash dumps is viable in the early stages of the process and Eskom has achieved significant success in this respect (Burgers, 2002). The main advantages of immediate rehabilitation are:

- dust and erosion are controlled/suppressed.

- rain water infiltration is minimized.
- rehabilitated dumps are more aesthetically pleasing than un-rehabilitated dumps.

The ash is levelled after placement and covered with soil as soon as possible. This cover is usually in the order of 100-300 mm thick. The soil cover prevents ash from blowing off the dump and serves as a growth medium for grass. While the top surfaces of most ash dumps are slightly graded, to allow rain to run off, ponding may occur in small areas especially after heavy rainfall events. Vegetation is quickly established under these conditions when irrigated with fresh or brine/saline water, especially on the side slopes where more moisture is available from lateral seepage and run-off from the top surface of the dump.

2.2.3 The Nature and Climate of Tutuka Site

The region surrounding the Tutuka site forms part of the Highveld plateau of South Africa with its characteristic flat topography and grasslands, well known for its maize and sunflower agricultural activities. As shown in Table 2-1 by the monthly temperature and rainfall data recorded at the official weather station at the nearby town of Bethal 40 km north-eastern of the Tutuka site, the area has a warm to cold temperate climate, characterized by two distinct seasonal weather patterns. The main wet season occurs in summer and extends from October to April, contributing to 89.9% of the total rainfall. Most of the heavy rain in the region is associated with thunderstorms. The average annual rainfall for the area is 682 mm per annum (SA Weather Service). The mean annual evaporation (MAE) of the region is 1563 mm, and the mean annual run-off (MAR) 55 mm (Midgley *et al.,* 1994).

The mean monthly temperature varies between 1 and 26℃ (Table 2-1).Summers in the study area are hot, and the winters cold.

The prevailing wind direction is north-west during the summer and east during winter. Winds are usually light to moderate.

Table 2-1: Monthly temperature and rainfall data for the 30 year period 1961 – 1990 observed at the official weather station of the South African weather service, Weather SA, at the nearby town of Bethal.

MONTH	TEMPERATURE (° C)				PRECIPITATION		
	Highest Recorded	Average Daily Maximum	Average Daily Minimum	Lowest Recorded	Average Monthly (mm)	Average Number of days with >= 1mm	Highest 24 Hour Rainfall (mm)
January	34	26	14	7	146	15	71
February	34	25	13	6	75	9	88
March	33	25	12	1	61	9	55
April	30	22	9	-1	48	7	64
May	27	20	4	-4	14	3	54
June	24	17	1	-9	7	2	19
July	25	17	1	-8	6	1	25
August	27	20	4	-8	13	2	29
September	32	23	8	-5	28	4	48
October	33	24	10	-1	78	10	61
November	33	24	12	3	129	14	58
December	33	25	13	3	106	13	87
Year	**34**	**22**	**8**	**-9**	**711**	**90**	**88**

Groundwater monitoring at Tutuka ash dam

A substantial number of groundwater monitoring wells have been installed in and around the ash dumps at Tutuka and Secunda in the course of various hydrogeological investigations conducted over the past 20-25 years. Unfortunately, only a few of them provide data that is useful for the present investigation. Preliminary water level monitoring data has been collected from the new core drilled holes for the period of 2006-2007.

The previous modelling studies conducted at the Tutuka ash dumpsite (Hodgson, 1999) have relied primarily on available water level data from monitoring boreholes for model calibration. Usually, when a groundwater flow model is calibrated using only water level data when hydraulic conductivities are not known (as applicable to this study) or are incorrect, a model may reproduce observed water levels very well but can still fail to accurately simulate flow rates.

Borehole monitoring for the ash dump at Tutuka was implemented to establish their water levels on a daily basis in order to establish rainfall and/or irrigation impacts on the levels in the short term.

Time series water level data from boreholes at the site, for example, AMB 79, shows that water levels fluctuate minimally due to external influences such as rainfall and irrigation. The highest maximum water level rise recorded in the borehole was 10.06 m, and the lowest, 10.47 m, a difference of 41 cm over a period of six months Figure 2-4.

Observed water level variations during the period November 2006 - November 2007 for a number of the coreholes are shown in Table 2-1, with well locations indicated in Figure 2-4. Water levels for all the boreholes measured (Table 2-2) show the same limited water level fluctuations.

Figure 2-4 below depicts the year-long water level record for AMB 79; the lowest water levels occurred during the winter months, while the highest levels occurred in the summer and are as expected based on climatological information. A possible explanation for the anomalous water level rise in August could be due to unexpected winter rainfall or ongoing brine irrigation where the infiltration possibly reached the water table.

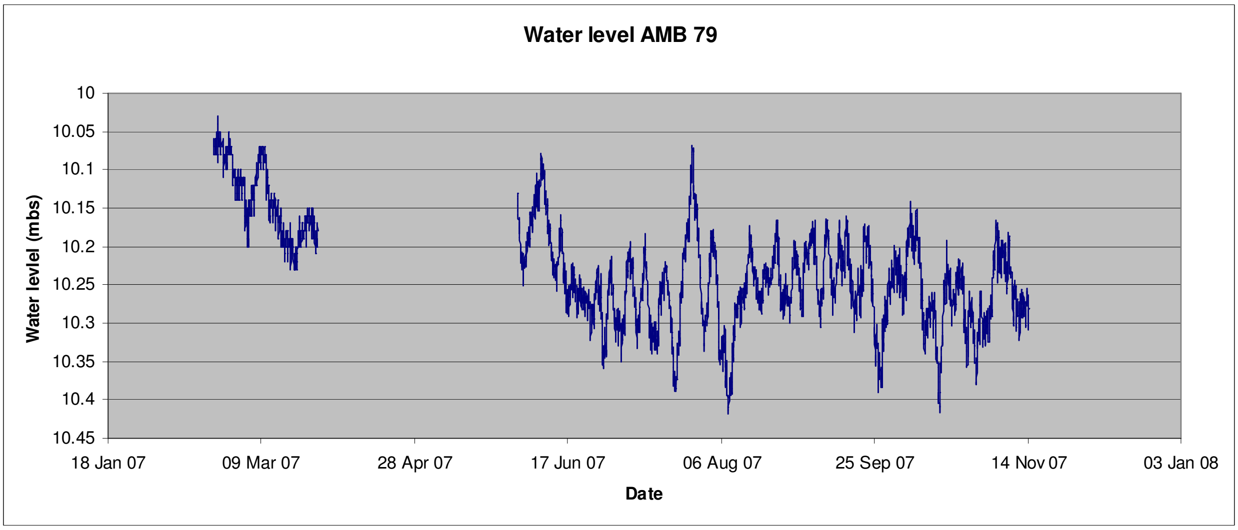

Figure 2-4: Water level fluctuations in Borehole AMB 79 observed by Nel (2007) at the Tutuka site.

Table 2-2: Water levels for boreholes AMB 79, 80, 82, 83, 85, and 86 of the Tutuka ash dumpsite.

Corehole name	**Depth to bedrock (m)**	**Borehole depth (m)**	**Date of measurement Water level (m)**				
			10 11. 2006	**21 Feb 2007**	**14 Jun 2007**	**06 Aug 2007**	**14 Nov 2007**
AMB79	12	12.04	9.93	10.07	10.31	10.32	10.28
AMB80	22	25.3	20.61	20.51	20.42	20.37	20.28
AMB82	25	23.87	23.07	23.06	23.09	23.06	23.06
AMB83	32	37.20	No water	29.13	29.12	29.11	29.10
AMB85	0.5	7	No water	2.07		1.71	1.16
AMB86	0.5	3.5	No water	2.14	2.13	2.14	1.29

With the exception of AMB 79 and AMB 83, the drilled coreholes did not penetrate the bedrock beneath the ash dumpsite. Corehole AMB 79 shows water levels within 10 m of the top ash heap during the entire monitoring period. Coreholes AMB 85 and

AMB 86 show consistently higher water levels, but these core holes were drilled on the virgin surface off the ash dump south of the dumpsite where leachate from the dam and drainage from the north water dam pass through. A number of factors probably contribute to the somewhat variable behaviour of the different corehole water levels. One consideration is the difference in position of the coreholes with respect to ash age, corehole depth and ash behaviour.

Surface run-off from the area is in the order of 8% of the annual rainfall. Groundwater recharge in undisturbed areas is in the order of 3% of the annual rainfall (Hodgson, 1999)

Generally, water level monitoring data shows that no drastic water level changes are taking place in the Tutuka rehabilitated areas.

2.2.4 Geology and Geohydrology of the Tutuka Ash Dump

There is no doubt that the geology of a dumping site will play a vital role in managing the impact of waste disposal on the environment of the site (Theis *et al.*, 1987 and Adriano *et al.*, 1983). It is therefore vital to have a good knowledge of the geology of such a site when starting to investigate the effects that a waste dump has on its environment. Ideally, natural soils at the base of the dumpsite with a high proportion of clay are associated with a low permeability barrier to force the salt to leach to the subsurface beneath the dam.

The Tutuka site is wholly underlain by sediments of the Permian Age Ecca Group of the Karoo Supergroup of formations, while quaternary deposits in the form of gravels containing cobbles and boulders occur along the rivers and streams in the area. The Ecca Group, which is often subdivided vertically into the Pietermaritzburg, Vryheid and Volkrust formations, overlies the Dwyka tillite conformably. By using this division, the area can be viewed as underlain by the Vryheid formation, which consists mainly of interbedded sand stones, siltstones, shales and coal. The sediments are mainly horizontally bedded, but slightly inclined in some areas, as witnessed by the gradual dip in elevation from 1 650 m in the north-west to 1 568 m in the south-east. The water dam north of the ash dump is consequently situated at a slightly higher elevation than the ash dump. Water could drain from the dam to the ash dump, thereby creating the shallow aquifer below the dump as theorized by Hodgson (1999).

The Karoo Supergroup has been intensely intruded by dolerite dykes and sills during the late Triassic and early Jurassic ages. As shown by the geological profile of a borehole at the Tutuka ash dump in Figure 2-5, the ash disposal site and surrounding area is largely underlain by highly-weathered and fractured dolerite at a depth of approximately 25 m. The ash dump could therefore easily pollute water contained by the pores and fractures in the sill and hence any aquifer present in fresh siltstones, sandstones, mudstones and shales that underlie the sill. This possibility has been investigated in the past through a set of monitoring and core boreholes drilled in and around the site. As these boreholes have all been capped and numbered and could yield valuable information for the present study, a census was undertaken to locate the boreholes. However, this was not an easy task as some of the older boreholes are situated in grasslands with tall grasses and in sunflower or maize fields. Figure 2-6 displays a map of the known boreholes.

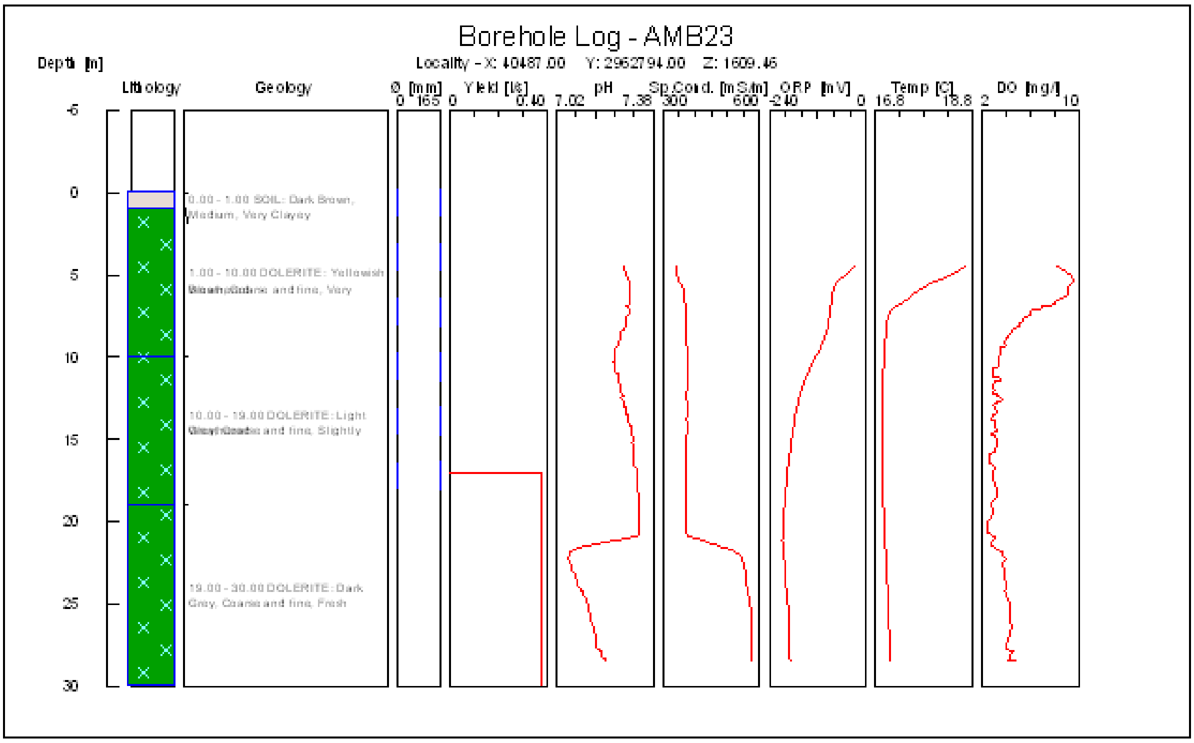

Figure 2-5: Geological profile of a borehole at the Tutuka ash dump. [After Hodgson (1999).]

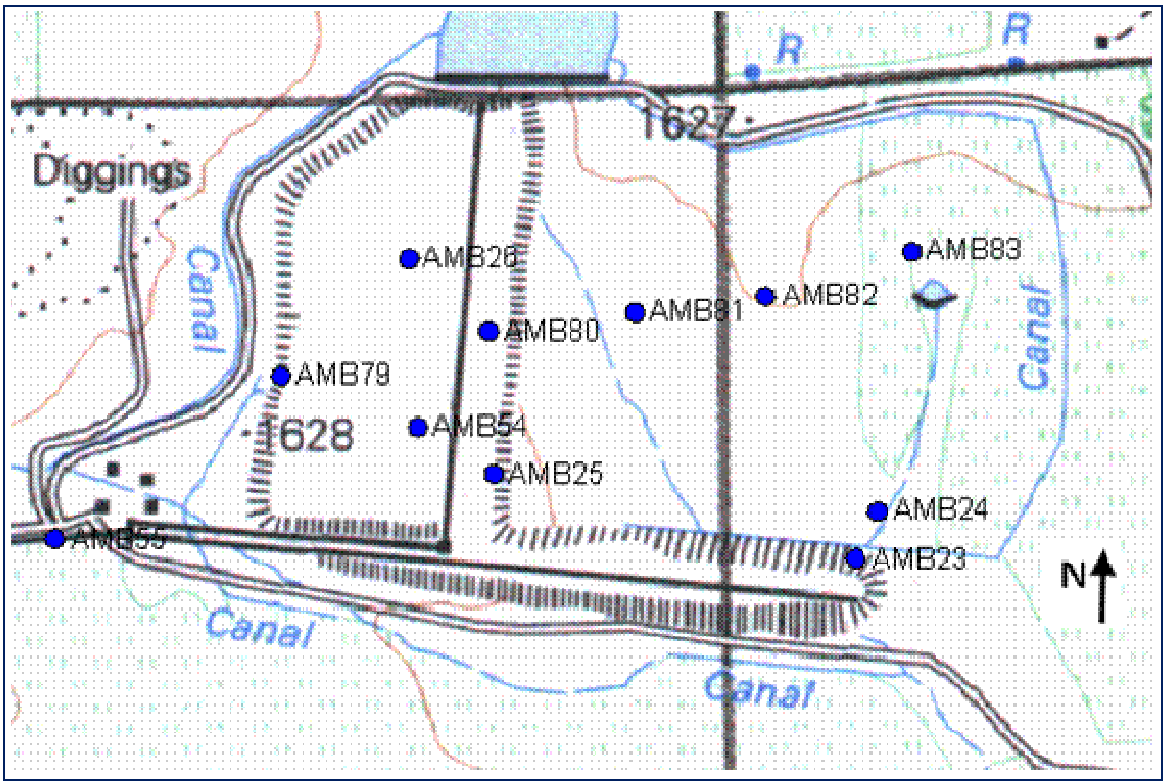

Figure 2-6: A map of the existing monitoring and core drilled boreholes in and around the Tutuka ash dump.

2.2.5 Geophysics Surveys

Resistivity Surveys

Electrical resistivity varies between different geological materials, dependent mainly on variations in water content and dissolved ions in the groundwater. Resistivity investigations are thus used to identify zones with different electrical properties which can then be referred to different geological strata. Resistivity is also called specific resistance, which is the inverse of conductivity or specific conductance. The most common minerals forming soils and rocks have very high resistivity in a dry condition, and the resistivity of soils and rocks is therefore normally a function of the amount and quality of water in pore spaces and fractures.

The internal nature of the ash at Tutuka was also investigated by profiling it with electrical resistivity surveys along the traverses indicated by the two red lines in Figure 2-7. The geophysics survey contributed to the choice of coreholes drilled sites based on the variable salt and moisture content in the ash as well as areas of different ash age at Tutuka (Figure 2-7).

In a further attempt to understand the geological and hydrogeological interaction between ash dam and ash disposal sites, cores holes were drilled at Tutuka ash dumpsite as a function of ash age and resistivity response in line with the geophysical traverse. A total of five drilling exercise were undertaken on sites typifying the decreasing age of the ash dumpsite at Tutuka.

The objectives of the geophysics survey program were to:

- Investigate the conductive nature of the subsurface
- Identify possible groundwater flow channels in the underlying bedrock.

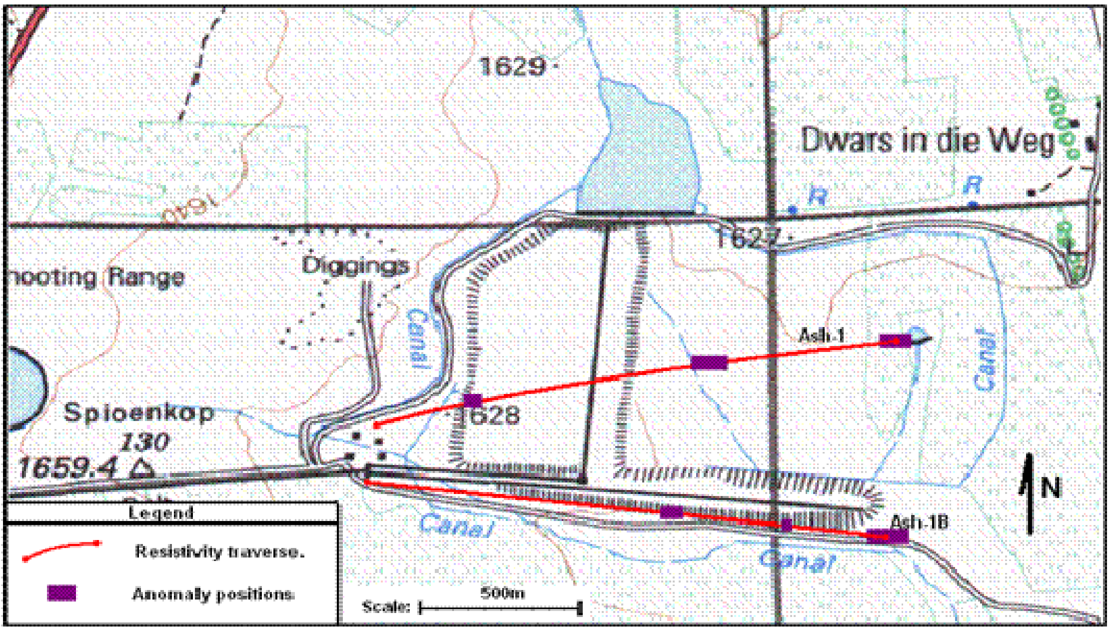

Figure 2-7: The Ash-1 and Ash-1B traverses used in the electrical resistivity surveys of the ash dump at Tutuka.

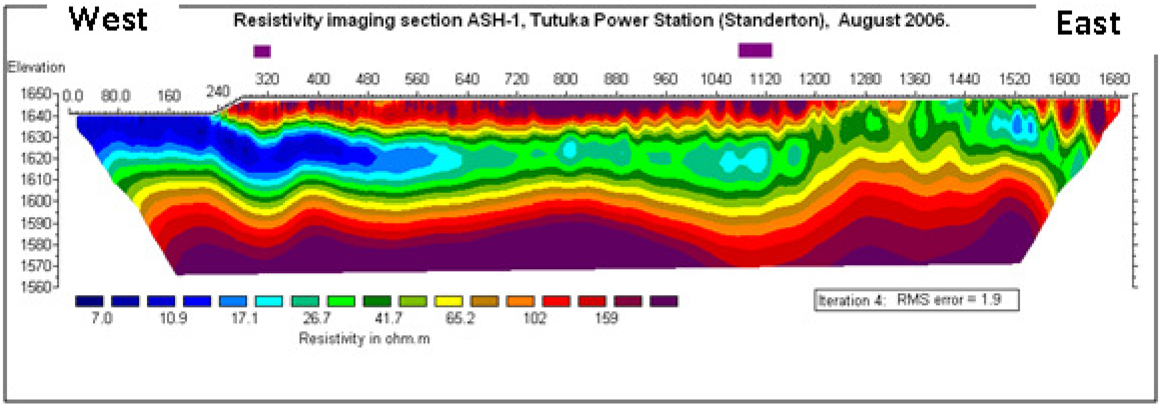

Figure 2-8: Resistivity profile along the ASH-1 traverse in Figure 2-7.

The shallow, approximately 18 m thick, highly-resistant layer (the red-purple contours in Figure 2-8) is associated with dry disposed ashes. This layer, which disappears at a distance of 1 280 m from the origin of the profile, reappears at approximately 1 550 m and attains its maximum thickness in the far eastern side of the profile. This behaviour of the layer can be ascribed to the ash having a different composition in that part of the profile. The more conductive nature (lower resistivity) of the ash in that area could result from surface irrigation (this is feasible as this is the fresh ash being deposited and conditioned with brine and has not yet reached equilibrium with the atmospheric CO_2 for mineral formation). The more conductive (less resistive) layer (blue-yellow contours) below the ash layer is associated with a weathered dolerite sill body of approximate 30 m thickness and an apparent resistivity of between 7 and 60 Ohm.m. This layer reaches minimum resistivity values on the western side of the profile where it is not covered by the ash layer and is consequently exposed to a higher rate of chemical weathering. Resistivity values below 10 Ohm m are normally associated with clayey formations. The resistive layer below this conductor can either be fresh or less weathered dolerite or a Karoo-sandstone layer. Of interest are the “valley” shaped anomalies in this layer at stations 320 and 1 100 metres. Positions are marked with purple squares on the model and locality map. These anomalies are probably associated with paleo valleys in the bedrock and are thus preferential groundwater flow paths. The valley feature at 1100 metres corresponds approximately with the old stream or drainage feature on the 1:50 000 map (Figure 2-7).

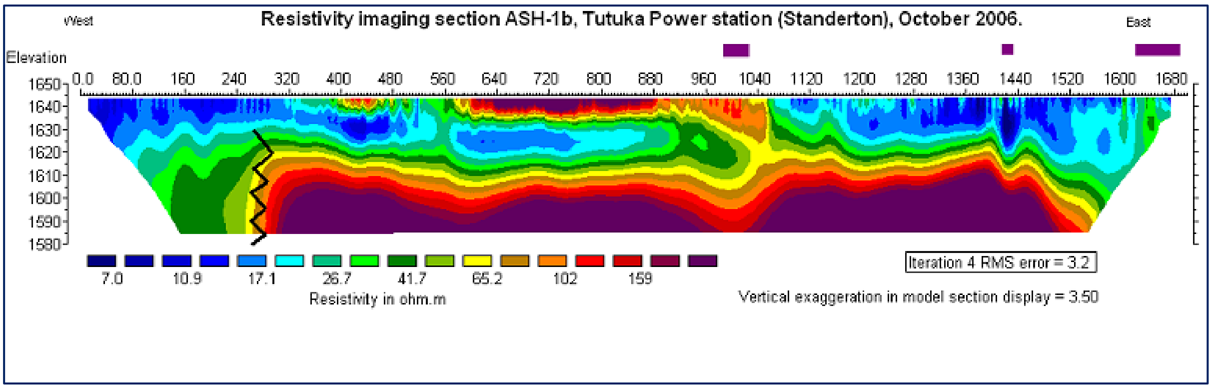

Figure 2-9: Resistivity profile along the ASH-1b traverse in Figure 2-7.

Profile Ash-1b: This model is contoured with the same resistivity contour scale as Ash-1 and the same interpretation criteria apply. Of interest is the lateral resistivity change between stations 240 and 320 metres. This lateral change is most probably caused by lithologies of different electrical resistivity (e.g. dolerite sill and Karoo layer) or vertical displacement due to a geological fault. This anomaly (lateral change) might be correlated with the downward curving contours on the far eastern side of profile Ash-1.

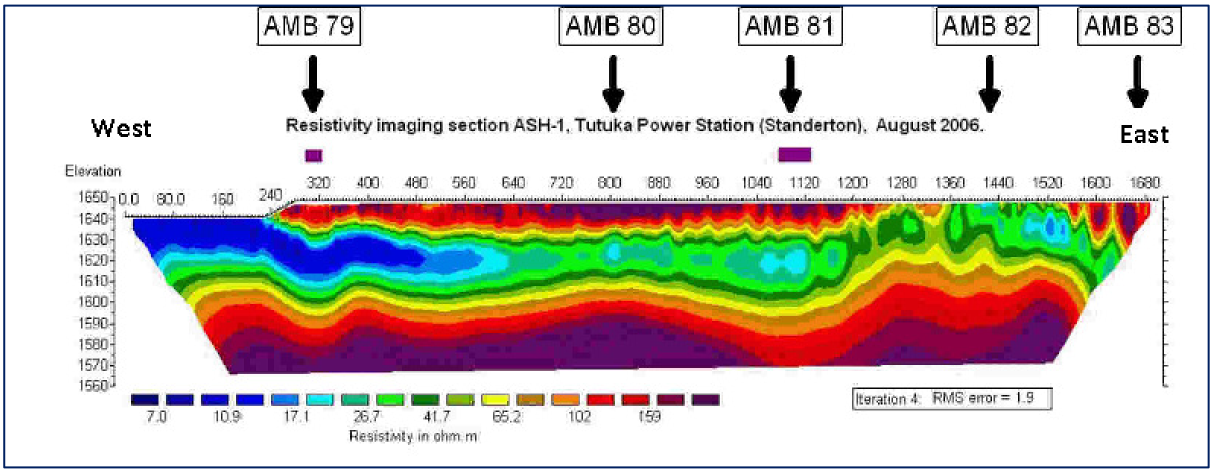

Figure 2-10: Approximate borehole positions in relation to the electrical resistance pseudosection profile results. The black line represents the inferred ash/bedrock contact (October *et al.* 2007).

Five core boreholes, numbered AMB79, AMB80, AMB81, AMB82, and AMB83 denoted in Figure 2-10 were drilled along profile Ash-1 to obtain more information (Table 2-3) on the ash age and subsurface properties of the ash dam.

The graphic log relating to core depth in the table below shows that at various ages and depths differences in the properties of ash were found. These varied from very hard coarse ash, to very hard fine ash that was fractured, soft fine powdery ash and clay, and mudstone or dolerite material where the bedrock was sampled.

Table 2-3: Depth vs borehole characteristics of Tutuka core drilled boreholes

Corehole	**Ash age (Years)**	**Location**	**Corehole**	**Ash age (Years)**	**Location**
AMB79	20	S26.77259; E29.39340	AMB80	15	S26.77179; E29.39865
Depth (m)	**Description**	**Sample collected**	**Depth (m)**	**Description**	**Sample collected**
0-0.75	clay top soil	no	0-0.55	clay top soil	no
0.75	ash	yes	0.55	ash	yes
6.25	solid ash	yes	}	no description	yes
7	fractured porous	yes			yes
7	fracture very hard	yes	8	ash porous	yes
8	hard ash	yes	11	ash very porous & brittle	yes
9	coarse ash, moist	yes	13		yes
10	coarse ash	yes	}	ash very porous & brittle	
11	ash wet (1st water observed)	yes			yes
12	dolerite (light brown/orange clay)	yes	21	ash	yes
13	dolerite	yes	22	moist clay soil	yes
14	dolerite	yes	23	moist clay soil	yes
15	dolerite	yes	24	dry mudstone	yes
			25	dry mudstone	yes
NB: water level encountered at a depth of 9.93 m;3350 µS/cm			NB: water level encountered at a depth of 20.61m; EC 5113µS/cm		

In cases where the dump had been irrigated there were deeper layers and zones that were still unconsolidated, friable and loose, indicating that no or few pozzolanic reactions had taken place over time and hard and soft layers were found directly adjacent to each other. Unconsolidated ash was prevalent in more recently placed areas of the dump. The water level differed in each part of the dump sampled, ranging from between 9 to 23 metres from the surface and in two cores no water was observed. Some portions of cores were moist and others dry. Dry zones were found in cores where the water level was non-existent or deeper lying. EC of core water sampled varied from 315 to 571 mS/m, indicating differences in conductivity/resistance. This is in all likelihood due to the differences in the brine irrigation regime practised on different areas of the dump. Not much homogeneity was observed within each core, nor between different cores, and there were many fractured zones; once again highlighting the heterogeneous nature of the ash and the difficulty of predicting its chemical or geophysical characteristics. Thus it is not reasonable to expect predictable hydrogeological behaviour and uniform stability of ash in contact with brine flows.

The position of the drilled coreholes relative to the geophysical survey is given in Figure 2-11. The complete corehole logs are given in Table 2-3.

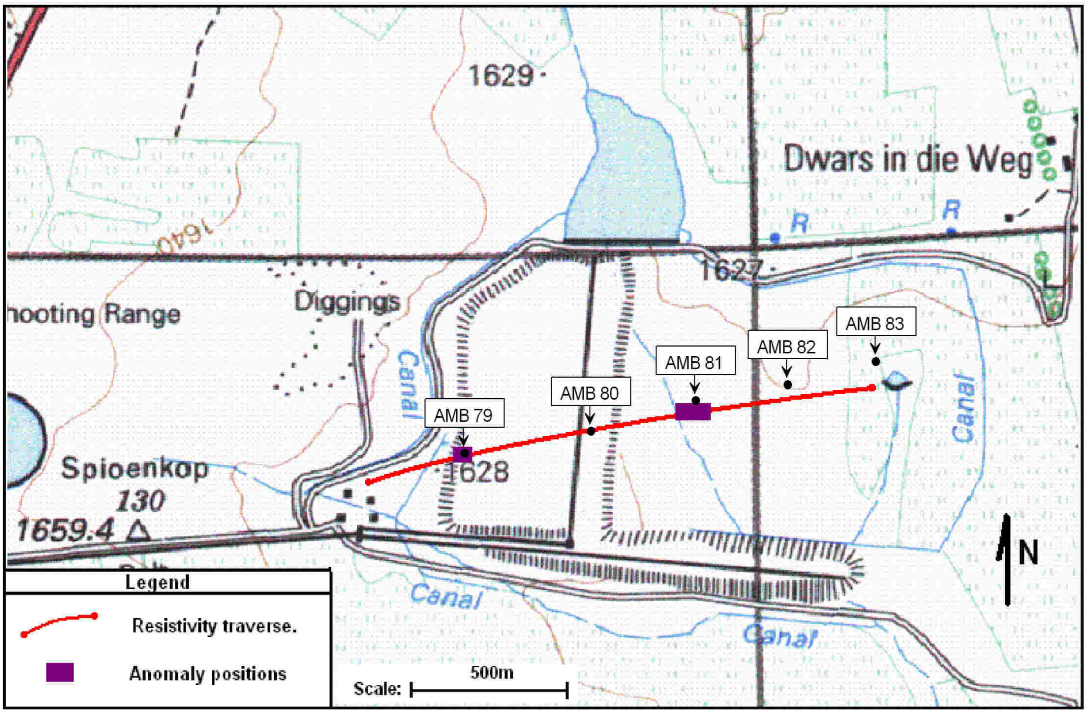

Figure 2-11: Borehole positions in relation to the geophysical line Ash-1 and ash dump age at Tutuka Power station

Although it is not possible to determine the geohydrological parameters (such as porosity, transmissivities) of a formation with measured geophysical parameters, lower electrical resistivities in a homogenous formation are normally associated with higher porosity and transmissivities. Low resistivities on the other hand, are normally associated with clayey formations and consequently low transmissivity values, or a formation filled with groundwater with a high EC (electric conductivity). Geophysical pseudosections do, however, assist in conceptualizing the ash and underlain aquifer

2.3 DESCRIPTION OF SECUNDA SYNTHETIC FUEL PLANT

2.3.1 General

The Sasol complex at Secunda commenced producing synthetic fuel, diesel, and petrochemicals from coal gasification between 1975 and 1982. This enormous complex is located in the upper Vaal River catchment on the Eastern Highveld of South Africa, which drains into Vaal Dam – the prime source of freshwater for the Gauteng area. The landscape is characterised by low-gradient streams winding over small alluvial plains.

The complex at Secunda utilises a low-grade bituminous coal in gasification and combustion processes to produce synthetic gas (also referred to as syngas) and steam respectively. Approximately 28 million tonnes of coal (70 % of the coarse coal feedstock) is consumed annually by the gasification process, which results in the production of about 7 million tonnes of gasification ash (Matjie *et al.,* 2004). The remaining 30 % of the coal utilized, a finer coal fraction, is combusted to produce steam and electric power. Coal ashes, gasification ash and fly ash are the by-products of these processes.

The Secunda site is much more complicated than the Tutuka site, as illustrated by the locality map of the site in Figure 2-12. Several different salty water, dirty water and evaporating ponds and dams exist around fine ash Dam4. About 50 m towards the north of the dam are evaporation ponds; to the east, there are evaporation ponds and coarse ash stacking. To the west, is another fine ash dam and on the southern side, are dirty water dams of different sizes. The water dams are deemed to be hazardous. As mentioned in Section 2.1, except for routine groundwater monitoring, no previous investigation has taken place over the entire site. A geological survey has been conducted for geological profile investigation and brine/salt content detection, and positions have been sited for core drilling, yet to date drilling has not taken place.

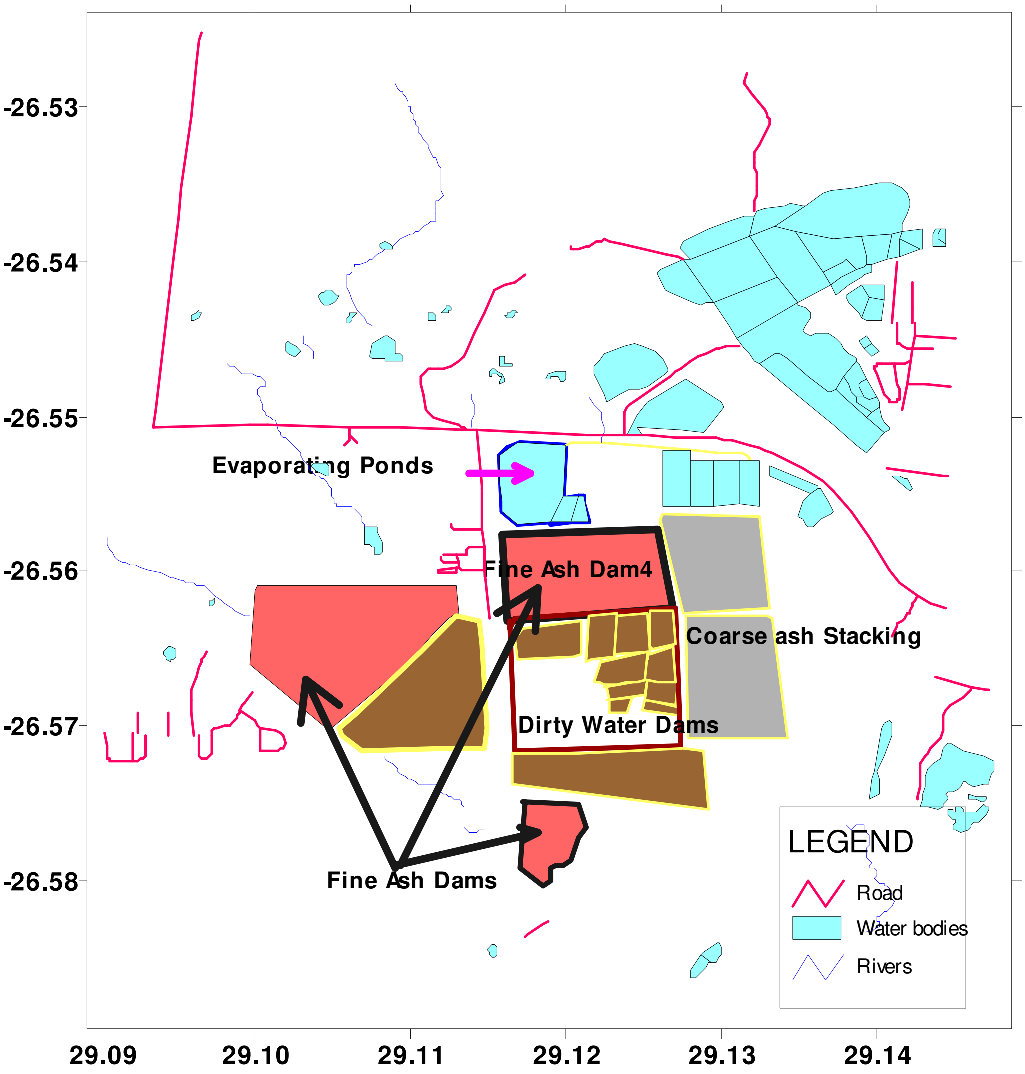

Figure 2-12: Topographical map of the area and facilities surrounding the Secunda Synfuel Plant, in relation to the topography, ash dump, evaporating ponds, dirty water dam, sewage plant and solid waste site. Scale from left to right is 1 430 m.

Figure 2-12 above depicts the general surroundings of the fine ash Dam4 at the Secunda synthetic fuel plant. The complexity of the study area is clear as several different waste dumps exist in a close proximity to each other. The ash dam itself is not dry, so a water pond on top of it bears testimony to the fact that it is fully saturated. It should be assumed to be a fully saturated porous medium.

2.3.2 Ash Disposal System at Secunda

Unlike the Tutuka ash disposal systems both wet and dry ash disposal systems are practised at the Secunda facility. Coarse ash is placed on dumps by a conveyor belt and fine ash is disposed of as slurry.

2.3.2.1 Wet ash disposal at Secunda ash dam

The coarse ash and the other material rejected from the mills are crushed and fed into sumps, and pumped to the ash dam. The fly ash sluiced from the precipitator hoppers is pumped separately to the ash dam, where it is used to build up ash dam walls. Water from the dam is decanted and reused in the ash system in a closed loop to pump the ash from the processing plant.

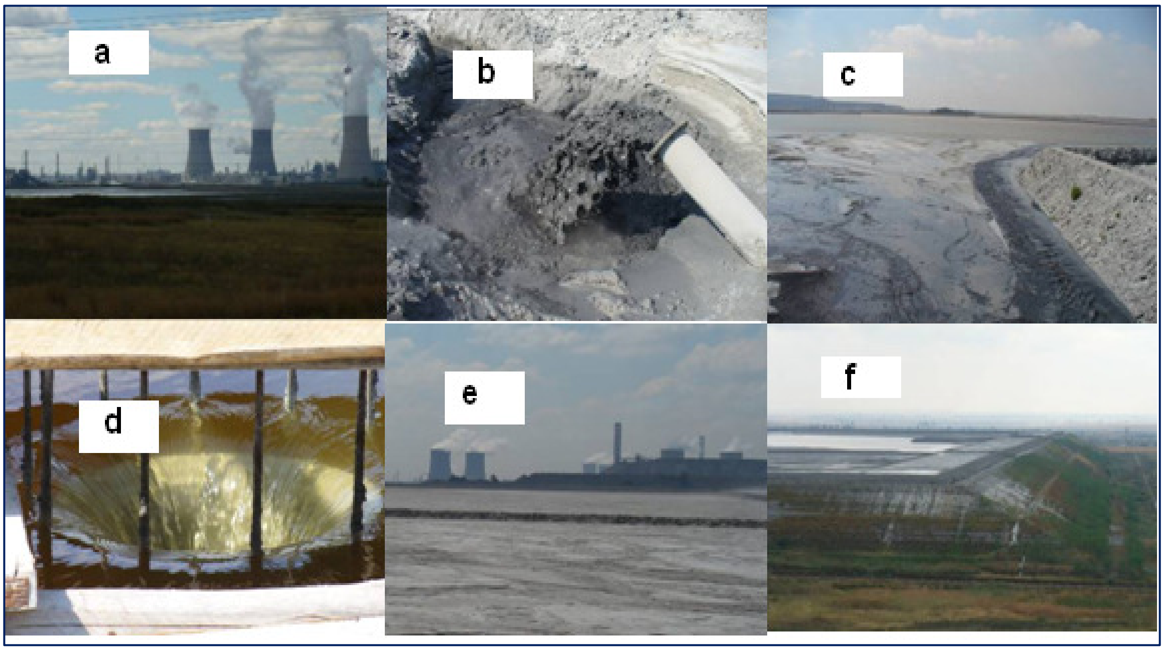

Figure 2-13: Photographs of the wet ash disposal system at the Secunda synthetic fuel plant.

Figure 2-13a shows an aerial view of the Secunda complex. The fly ash (FA) is mixed with water and then pumped through pipelines into ash ponds, (Figure 2-13b and c.) The FA ponds are then subdivided into smaller lagoons (Figure 2-13f), by creating a partition. The lagoon formation helps in compartmentalization of the ponds and the FA is disposed of alternatively in each lagoon, to pre-determined levels before switching to another lagoon.

2.3.3 The Nature and Climate of the Secunda Site

On a regional scale, both the Tutuka and Secunda sites are located on the same topographical elevation. The region surrounding the Secunda site forms part of the Highveld plateau of South Africa with its characteristic flat topography and grasslands, at an average height of 1 620 m above sea level, and is well known for its maize and sunflower farming activities. As shown by the monthly temperature and rainfall data recorded at the official weather station at Secunda and shown in Figure 2-14, the area enjoys a subtropical climate with hot summers and mild to dry cold winters. The average maximum daily temperature in January (summer) is 26℃, while in June (winter) the average minimum daily temperature is 1℃. The average annual rainfall is 682 mm, with approximately 10 times more rain falling in summer than in winter (Weather SA).

Rainfall is seasonal with most rain occurring in the summer period (October to April) and peaking in December and January. Rainfall occurs generally as convective thunderstorms and is sometimes accompanied by hail. Frost occurs in winter and there is occasional light snow on high lying areas. The prevailing wind direction is north-west during the summer and east during winter. Winds are usually light to moderate.

Rainfall and temperature records from the Secunda Weather Station are presented in Figure 2-15 and Figure 2-16. Figure 2-16 depicts the average monthly climatic parameters from the Secunda weather station. The maximum rainfall distribution is recorded during the months of January-February.

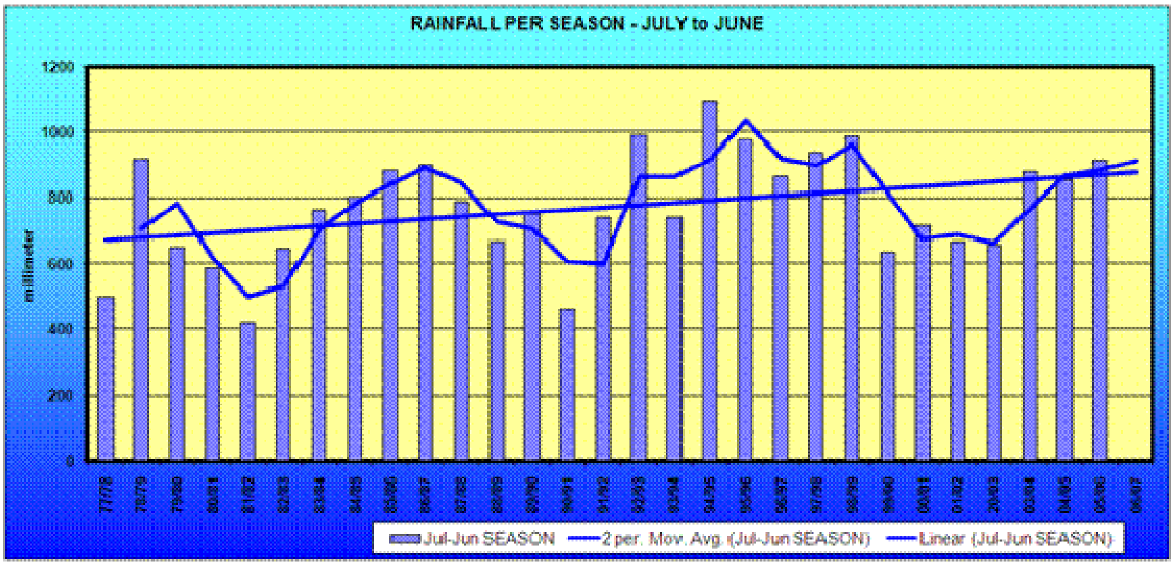

Figure 2-14: Monthly rainfall bars as measured by the Secunda Weather Station for June-July season (Sasol Data base)

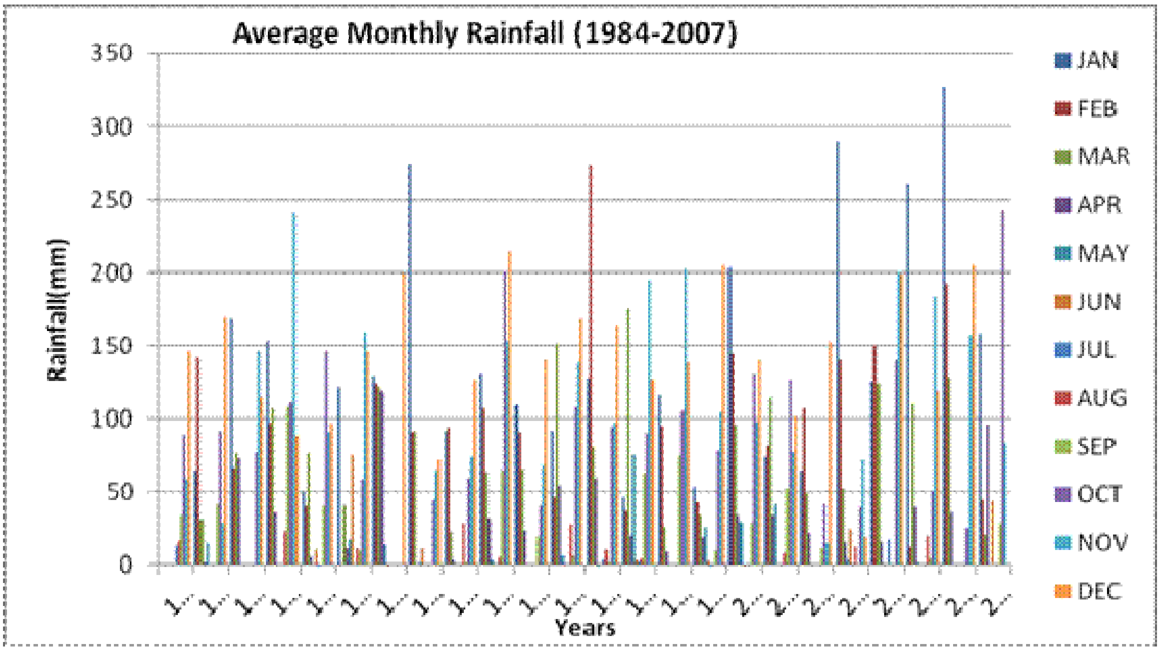

Figure 2-15: Monthly rainfall bars distribution of Secunda

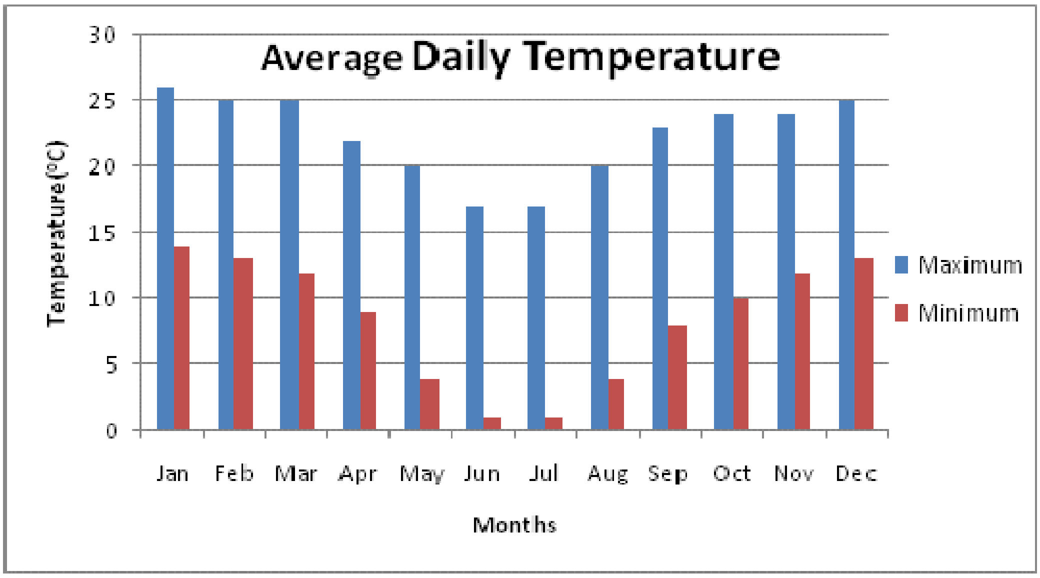

Figure 2-16: Average Daily Temperature at area close to Secunda (Bethal, 37 km north eastern of Secunda)

2.3.4 Geology and Geohydrology of the Secunda Ash Dump

2.3.4.1 Geology

As mentioned in the introduction to this chapter, the Secunda fine ash Dam4 and Tutuka dry ash dump are situated approximately 36 km apart from each other so the regional geology is therefore the same for both sites.

The Secunda site is entirely underlain by sediments of the Permian age Ecca Group of the Karoo Supergroup of formations. The Ecca Group, which is often subdivided vertically into the Pietermaritzburg, Vryheid and Volkrust formations, overlies the Dwyka tillite conformably. According to these divisions, the study area is underlain by the Vryheid formation, which consists mainly of interbedded sandstones, siltstones, shales and coal. The sediments are mainly horizontally bedded, but slightly inclined in some areas as evidenced by the gradual dip in elevation from 1 640 m in the east to 1 520 m above mean sea level in the south-west. The coarse ash stockyard and salty ponds east and north-east of the ash dam (Figure 2-12) are consequently situated at a slightly higher elevation than the ash dam itself. Water could therefore drain from these dirty water dams to the ash dump.

Quaternary deposits in the form of gravels containing cobbles and boulders occur along the rivers and streams in the area.

2.3.4.2 Geohydrology

The Karoo Supergroup was intensely intruded by dolerite dykes and sills during the late Triassic and early Jurassic ages and consists mainly of fractured-rock aquifers characterised by sediments with low permeability (Botha *et al.*, 1998). This implies that groundwater movement occurs mostly along secondary structures such as fractures, cracks and joints in the sediments. The Karoo aquifers are the most extensive type of aquifers found in South Africa.

As shown by the geological profile of a borehole at ash dam4 (Figure 2-17) at Secunda, the ash disposal site and surrounding area are largely underlain by a highly-weathered and fractured dolerite sill at a depth of approximately 25 m. The ash dump could therefore easily pollute water contained in the pores and fractures in the sill as well as any aquifers present in fresh siltstones, sandstones, mudstones and shales that underlie the sill.

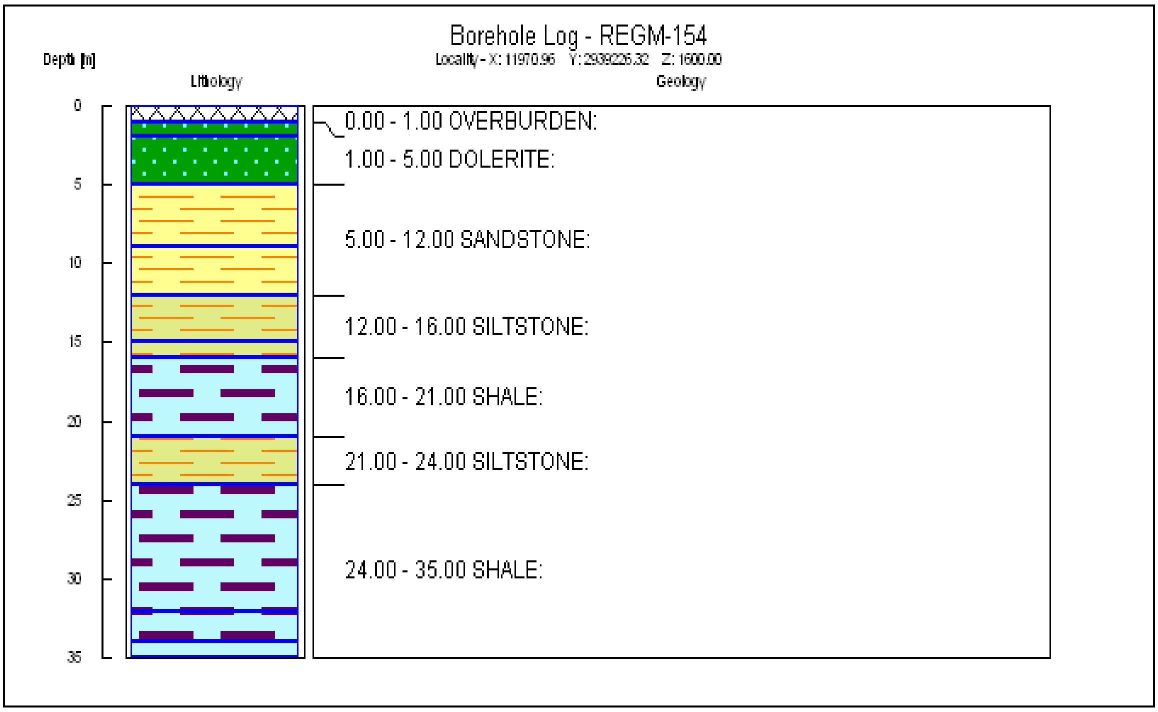

Figure 2-17: Geological profile of a borehole at the Secunda Fine ash dam4

Almost all South African power and synthetic fuel stations are situated in area with underlying shallow weathered rocks, ranging in thickness from 5-15 m. Water easily penetrates these weathered rocks. Deeper down, alternating layers of sandstone and shale exist and as the latter is impermeable to the movement of water it acts as a no-flow boundary at the bottom of the model (Hodgson and Krantz, 1998).

2.3.5 Geophysics at Secunda

Existing data is coupled with a geophysical survey to gain a thorough understanding of the topic under discussion. Resistivity imaging survey reveals the difference in the ash disposal methods in use for Secunda and Tutuka sites.

Tutuka ash dump profile is mainly characterised by high resistivity (102-159 Ohm m) due to the presence of the dry ash, while the Secunda profile is characterised by low resistivity (3- 10 Ohm m) due to wet ash disposal. The low resistivity indicates retention of the saline effluents as an interstitial solution in the Secunda ash dumps.

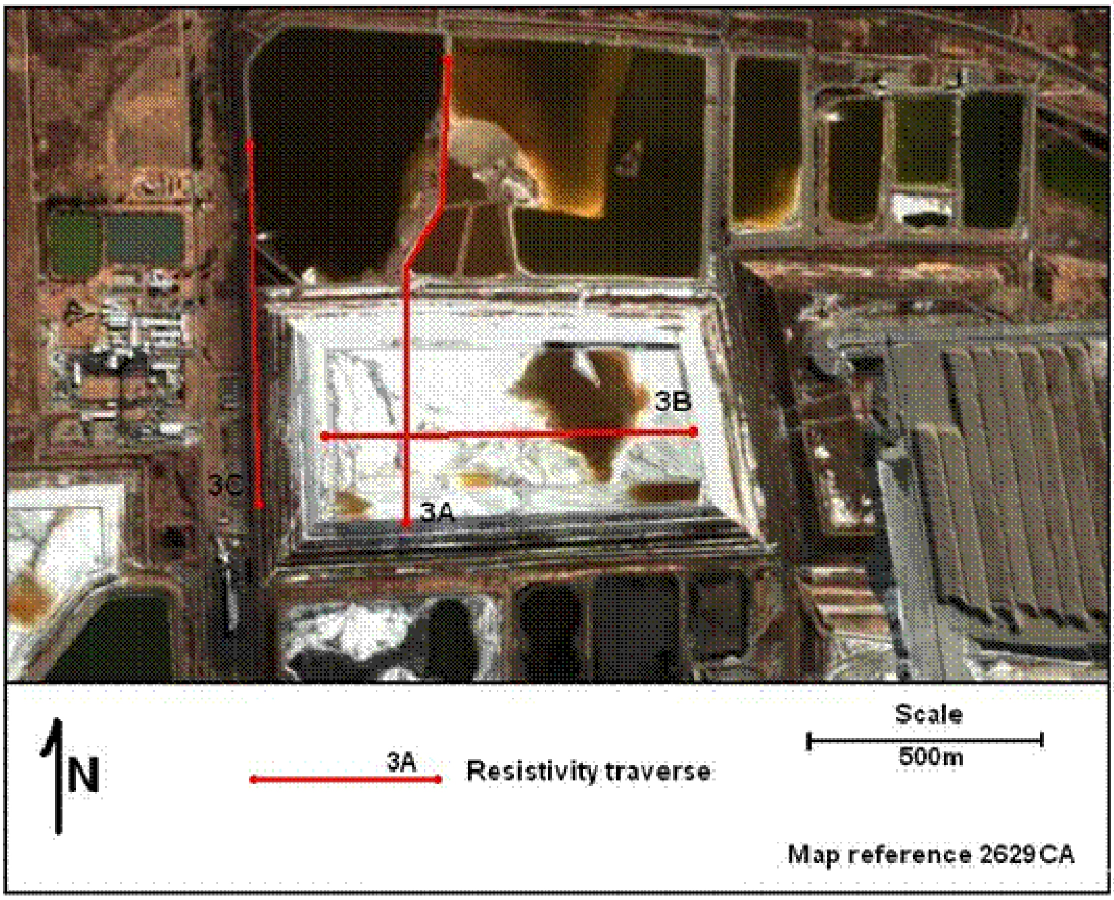

Figure 2-18: Resistivity Profile lines for Secunda synfuels fine ash Dam4

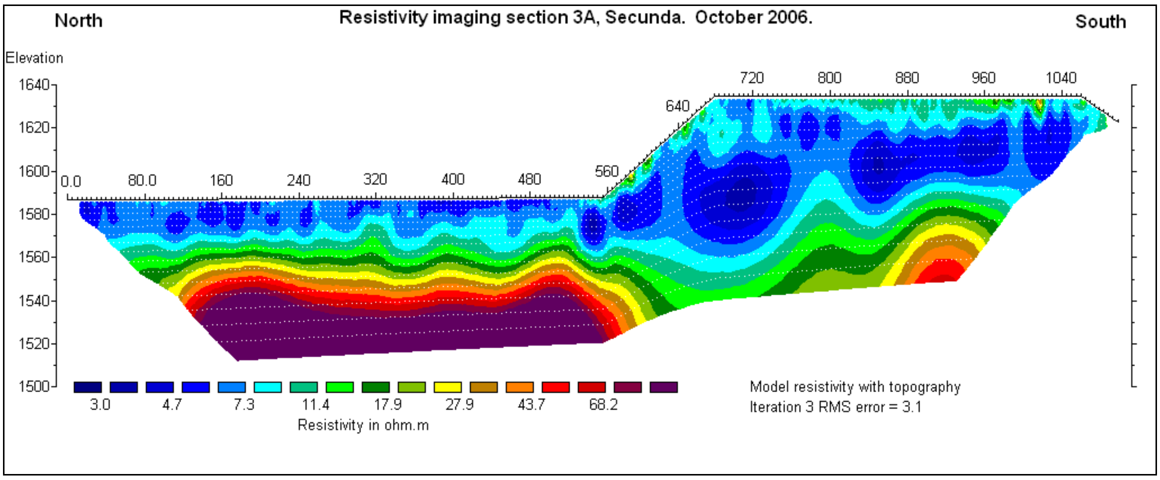

Figure 2-19: Profile 3A (profile length 1100m)

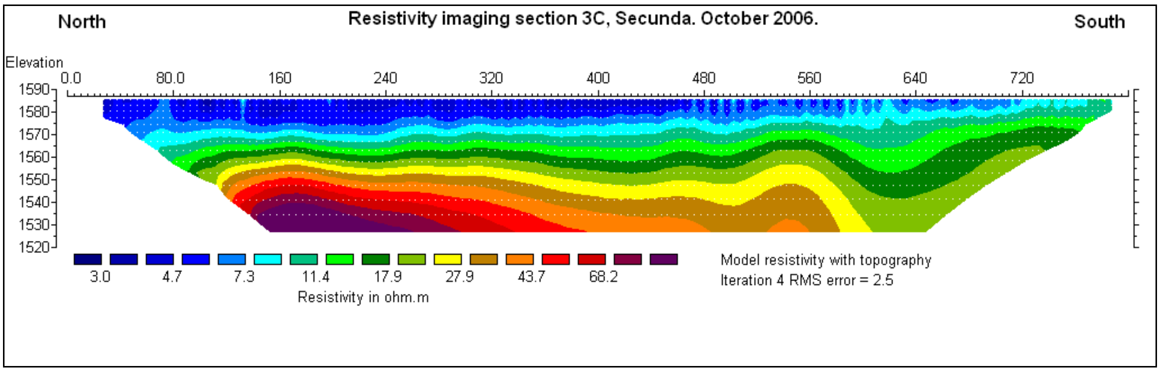

Figure 2-20: Profile 3C (profile length 800 m)

As shown in Figure 2-18 three different profiles were taken. Profile 3C and 3A are parallel and were drawn from south to north, while profile 3B is drawn from east to west.

The annotated section indicates the associated geology with the different modelled subsurface resistivities. It is assumed that the site is underlain by a Karoo dolerite sill and that no ash has been dumped north of the existing dump in the past. Modelled resistivities between 3 and 10 Ohm.m (approximately), can be associated with highly weathered dolerite (clay) as well as ash. This is clearly visible on profile 3A where the boundary of the ash dump is visible. The red–brown contours are associated with less weathered to fresh dolerite.

Profile C is parallel to profile A and is thus inserted directly after Profile A in the text for easy comparison. Two models for profile A (iteration 3 and 4) are shown. Iteration 4 (top model) show a more prominent lateral change in ground resistivity below stations 640 and 840 metres in the form of trough or valley shaped anomalies. This lateral change was initially interpreted as a vertical conductor (geological fault) on each flank of the conductive area. These features, however, are less prominent on iteration 3. A lateral change in ground resistivities clearly exists. It is, however, questionable whether these changes are associated with geological faults or whether the lower resistivity zone is merely caused by a preferential weathered zone in the dolerite.

Profile 3C was done to determine the extent and direction of the low resistivity zone (640-840 m) seen on profile 3A. The lateral change in resistivities below station 600 metres on profile 3C, probably form the northern side of this low resistive zone. Of interest is the thickness of the conductive (dark blue) layer in the southern part of profile 3C when compared with the same layer on profile 3A. A hypothetical surface (ground level) below the dump should be visualised. If this is indeed the scenario, this layer may thicken to the east of profile 3A.

Profile 3B only indicates the conductive ash layer above the more resistive uniform bedrock.

The above interpretations and assumptions are made purely based on the resistivity model. Drilling information is crucial for geophysical calibration purposes. Drilling information and any other available information need to be incorporated into the model for a final or more accurate geological/geohydrological interpretation.

2.4 PHYSICAL, CHEMICAL AND HYDRAULIC PROPERTIES OF ASH

Safe disposal of ash without adversely affecting the large storage area and environment are a major concern of coal-based thermal power plants. In this regard utilizing the ash rather than dumping it is the most desirable option. Coal ash can be utilized in bulk only in geotechnical engineering applications such as construction of embankments or as a remediation backfill material for sites, etc. For these uses, an in-depth understanding of the physical and chemical properties, and the engineering and leaching behaviour of the ash are required. Even when the ash is dumped as a bulk into a disposal site, as applicable to both Tutuka and Secunda, knowledge of these properties would assist in where to dump it and what monitoring mechanisms should be implemented. The physical properties of ash are therefore, extremely important from both a geohydrological and engineering standpoint. The way in which the ash is put together, or its architecture, is related to its structure, which in turn is a reflection of texture, aggregation and porosity. The movement of air, water and solutes through the ash dump is dependent on the spaces and their configuration among the soil/ash particles. Information available from field studies indicates that the actual effects/impacts of ash disposal on groundwater quality largely depend on the physical and chemical characteristics of the ash and the hydrogeologic characteristics and climate of the disposal site (Theis *et al.*, 1978; Kopsick and Angino, 1981).

The physical and chemical properties of ash are dependent on the composition of the parent coal, conditions during coal combustion, efficiency of emission control devices, and practises used during storage and handling (Adriano *et al.*, 1980). Physical properties assist in classifying the coal ashes for engineering purposes. The properties discussed are specific gravity, grain size distribution, index properties, free swell index and specific surface as well as classification.

Much of the work published on fly ash hydraulics pertains to its strength when used in highway construction and cement industries. Little is known about ash dump hydraulics and its connectivity to the large subsurface beneath it.

Hydraulic conductivity and moisture retention characteristics of the fly ash also depend, among other things, on the degree of change that the ash has undergone in the ash dam, through pozzolanic crystallization. Laboratory results have shown that hydraulic conductivity of an ash dam after the engineering process is less than that of the same ash taken at the rear end of the slurry (van den Berg *et al.*, 2001). As the ash goes through different stages during dumping processes, mineral precipitation and pozzolanic crystallization of the ash particles could be the reason for the reduced hydraulic conductivity at the ash dam according to van den Berg *et al.* (2001). Further, fly ash in the ash dam is a heterogeneous medium because of the grain size variation and crystallization.

2.4.1 Physical Properties of Ash

Physically, fly ash is a very fine, powdery material, composed mostly of silica, and nearly all particles are spherical in shape as a result of cooling and solidifying from molten droplets of inorganic coal residues. Some of the basic physical properties that play a role in understanding the ash dump hydraulics are described in the following paragraphs.]

Note that hydraulic conductivities of coal combustion residues (ashes) may vary significantly based on the degree of compaction methods.

For simulation purposes two typical layers are assumed; a top ash layer and a clay layer beneath the ash. Soil hydraulic properties are available for clay soil from literature, but are not plausible for ash curve fitting parameters. As has been shown by Case *et al*., (1983) in their encyclopaedic work on moisture retention curves, the approximation can be applied successfully, provided that the interest is centred only on the domain for which the experimental data is available. The moisture content vs pressure head relationship for ash was therefore, determined from uranium mill tailings data. For this particular work uranium mill tailing with a particle size ranging from 92% passing 1 000 μm to 3.4% passing 9 μm was used for a case scenario simulation.

2.4.2 Hydraulic Properties of Ash in Ash Dump

While much has been written on the composition, trace metal content, leachability, physical and chemical properties of fine-grained or coarse ashes (i.e. fly or bottom ash), there is a dearth of information on the hydraulic parameter properties (porosity, moister content, hydraulic conductivity, etc.) of ash particles. The hydraulic conductivity and moisture retention properties of fly ash is a major impacting factor if it is to be applied in an open cast situation. Apart from limiting the through flow of water, it will also determine the amount of air ingress into the ash (Hodgson and Krantz, 1998). And since ash hydraulic conductivity is a function of effective porosity, it decreases as porosity decreases (van den Berg *et al.,* 2001).

The hydraulic properties (hydraulic conductivity, storativity and porosity and/or curve fitting parameters in case of an unsaturated zone) of an ash dump must be known/estimated to properly evaluate the environmental impact of ash on the porous dump site. The hydraulic conductivity and moisture retention characteristics of the fly/coarse ash will depend, among other things, on the degree of change that the ash has undergone in the ash dump, through pozzolanic crystallization (Hodgson and Krantz, 1998), the way the ash is placed and the engineering of the ash dump. Also, as mentioned above, fly ash in an ash dump is not a homogeneous medium because of grain size variations and crystallization. The heterogeneity of the size of the particles contributes to the difference in hydraulic conductivity.

For the purpose of this work it has been assumed that the hydraulic conductivity of the ash is higher than that of the underlying aquifer (typically clay). An assumption that is reasonable according to Hodgson and Krantz (1998) as the average hydraulic conductivity of fly ash is in the order of 10^{-1}m/d, whereas that of the underlying clays is usually less than 10^{-4}m/d. Van den Berg *et al.*, (2001) also estimated hydraulic conductivity: K-values of ash on ash dams range between 0.02 – 0.1 m/d on a laboratory scale while Mudd, (2002) estimated a value of 0.3024 m/d for both vertical and horizontal isotropic saturated fly ash. Although these estimates are empirical, they demonstrate the high permeability of the ash with high volumetric water content. Mudd (2002) also estimated that the unsaturated K values range from 0.167-0.886 m/d, compared to the estimated saturated K value of approximately 0.3 m/d. The variation can be attributed to the different inflow rates and the respective change in the outflow rate. This suggests a small change in volumetric water content in response to different inflows, with a small subsequent change in K. After the inflow ceases, however, the fine-grained nature of the ash is effective in limiting further drainage of pore waters, indicating a rapid decrease in the hydraulic conductivity function as the volumetric water content falls.

From the hydraulic conductivity literature review one can argue that leachate/ drainage of waste from an ash dump to the underlying aquifer (clay specifically) is not a serious concern for groundwater quality, specifically if the ash forms a pozzolanic crystallization as it then acts as a barrier. Seepage to the surface could be a point of concern for surface water especially if it joins some streams.

Permeability is another important parameter in the design of liners or dykes to contain leachate migrations.

The coefficient of permeability of ash depends on the grain size, degree of compaction and pozzolanic activity.

2.4.3 Chemical Properties

The chemical properties of coal ash also greatly influence the environmental impacts that may arise out of their use/disposal as well as their engineering properties. Adverse impacts include contamination of surface and subsurface water with toxic heavy metals present in the coal ashes, loss of soil fertility around the plant sites, etc. This therefore, calls for a detailed study of the chemical composition, morphological studies, pH, total soluble solids, etc of the ash.

The disposal of FA in dams or heaps presents a huge problem due to its alkalinity (pH >12) and chemical characteristics (Hodgson, 1999).

Many fly ashes are also characterized by high alkalinity and high concentrations of soluble salts (Carlson and Adriano 1993). The compaction and crystallization processes are due to the chemical interaction of coal residue constituents. (Pandian, 2004) argued that a chemical composition with a relatively high percentage of carbon dioxide can decrease pozzolonic activity.

The density of coal ashes is an important parameter as it determines strength, compressibility and permeability. Densification of ash improves the engineering properties. The compacted unit weight of the material depends on the amount and method of energy application, grain size distribution, plasticity characteristics and moisture content at compaction.

To appreciate the real order of degree of compaction and corresponding water contents of different ashes with reference to soils, the compaction curves were plotted on a volume basis using void ratio and volume water content. Pandian, (2004) found that most fly ash compactions curves plot the same as ordinary soils.

Generally speaking, geotechnical modelling would be advisable to integrate with the groundwater flow model thus incorporating all the flow and reaction processes. Pozzolanic crystallization also takes place as a result of the carbon dioxide calcium reaction, where precipitation causes the formation of cementation and compaction.

2.4.4 Impact of Ash Disposal on Saturated Flow Zone

In the saturated zone, given similar pressure conditions, groundwater flow will be greatest in high-hydraulic conductivity materials. The impacts on groundwater flow will depend on the hydraulic conductivity of the surrounding geologic materials as well as the extent of compaction during emplacement. If the surrounding materials are relatively intact strata with a lower hydraulic conductivity than the ash dumpsite, groundwater will flow through the dumpsite. Alternatively, if the hydraulic conductivity of the surrounding geologic materials is higher than that of the dumpsite, water will tend to flow around the dumpsite (Al and Blowes, 1996a). The contrasts in hydraulic conductivity will further alter the groundwater flow. Under these conditions, the impacts on groundwater flow will depend on the orientation of the groundwater flow direction relative to the orientation of the layers of ash dumpsites and spoil. If the groundwater flow direction is parallel to the ash dumpsite layers, water will flow preferentially through the coarse spoil layers, with only minor flow through the ash residues. This scenario is seen from the geophysical pseudo section where the ash is underlain by an impermeable dolerite sill; the flow is then parallel to the ash dam layer beneath it. If the groundwater flow direction is perpendicular to the ash dumpsite layers, the fine-grained ash residues will impede the flow and reduce groundwater velocities through the emplacement zone.

2.4.5 Impact of Ash Disposal on an Unsaturated Flow Zone

As will be discussed in section 3.4, predictions of unsaturated flow are complex, even without the addition of ash residues, and research on unsaturated flow through coal combustion residues (ash dumpsites) is extremely limited. Nevertheless, some observations on the potential impacts of coal residue (ash waste) on unsaturated flow at mine sites are provided here based on relevant studies of unsaturated flow through layered fine- and coarse-grained materials and through waste rock piles at coal and metal mine sites.

The impacts of ash dumps on unsaturated flow will depend on a number of factors, including the degree of contrast in hydraulic properties between the ash dumpsite and the surrounding spoil or geologic strata, the moisture content, and the geometry of dumpsite emplacement (Hillel, 1998). As discussed previously, research on unsaturated flow suggests that at times of low infiltration, water in the unsaturated zone may flow preferentially through fine-grained ash dump layers rather than through the coarser-grained ash materials.

Thus, large uncertainties remain regarding flow in the unsaturated zone in complex mine settings, especially those with great contrasts in hydraulic conductivity.

When ash dumps (coal residues) are placed close to the water table, a thick capillary fringe could form within the materials. Studies of groundwater flow through mine tailings with similar particle size distributions and hydraulic conductivities as fly ash, noted a thick capillary fringe, ranging from tens of centimetres up to six metres in thickness (Blowes and Gillham, 1988; Al and Blowes, 1996a). Under such conditions, the addition of only a small amount of water, such as a minor precipitation event, can lead to a pronounced rise in the water table and increased potential for contaminant transport to surface water bodies.

2.5 DISCUSSION

The physical engineering and chemical properties of ash dam/dump play a major role in shaping the hydraulic composition of an ash dam. To properly evaluate the potential impact of the disposal of coal combustion by-products on groundwater quality, the physical and chemical properties of these by-products, transport processes in groundwater, and the solution techniques of mathematical models must be understood.

The ash nature, disposal system and activities on and around the dumpsites suggest that ash dams/dumps are complicated entities. Based on the physical, chemical, geological and dumping mechanism of ash at the dam sites, it can be concluded that ash dam/dumpsites are heterogeneous porous mediums.

If scientifically valid conclusions are to be made concerning the potential for the environmental impact of disposal materials, then valid tests must be performed. The site should be conceptualized thoroughly so that all the physical features are incorporated in the conceptual model.

CHAPTER 3

DEVELOPMENT OF CONCEPTUAL AND MATHEMATICAL MODELS FOR THE TUTUKA AND SECUNDA ASH DUMPSITES

3.1 INTRODUCTION

Understanding the movement of water and chemicals into and through the subsurface of the earth is of vital importance in managing, using and protecting our natural resources. As these processes are very dynamic, and the subsurface environment is not easily observable or accessible (Botha *et al.*, 1990), such investigations are often based on so-called models of the earth's surface and subsurface that underlies the site of interest. The normal way to achieve this objective is to gather as much information as possible about the geology, geohydrology, hydrochemistry and topography of the site and to study the features, events and processes and their interactions that may have an impact on the movement of the water and chemicals at the site. The advantage of this approach is that one can then combine a study of the evolving interactions between the features, events and processes and the basic laws of physics and chemistry to develop first a conceptual model and then a mathematical model for a given site (Botha, 1996).

As pointed out by (Botha *et al.*, 1990; Robinson *et al.*, 2006) and (Van Waveren *et al.*, 1999) the success of this procedure depends entirely on a sound knowledge and understanding of all the interactions controlling the flow of water and mass transport at a given site. It is not surprising therefore, to learn that it may take years – even centuries, or perhaps, never – to determine the features, events and processes and their interactions at a specific location. It is therefore rarely, if ever, possible to develop a full-scale conceptual and mathematical model for the site. Nevertheless, the approach has achieved such successes in the exact sciences that it is difficult to think of a science where modelling is not applied in one form or another. These successes, unfortunately, have also lead to a misplaced trust in mathematical models as it is expected that such models are able to describe and predict the future evolution of a site precisely, although nothing could be further from the truth (Bredehoeft, 2003, 2005; Oreskes *et al.*, 1994). However, the procedure has so many advantages (Botha, 1996) that it is nearly always worthwhile to try to develop suitable conceptual and mathematical models when investigating sites.

It is not always easy to develop site-specific conceptual and mathematical models for a given site, at least not during the initial phase of an investigation. What is often more important, is to remember that a true mathematical model for any site must account for the laws of physics and chemistry governing the behaviour of the features, events and processes characteristic to the site. As these laws are universally valid, one can often use existing models and develop a so-called generic model for a given specific site.

There are essentially two advantages in the use of a generic model:—a model based on existing information gathered from several sites including the one under investigation, or to be investigated. The first advantage is that the model can provide considerable physical insight into the features events and processes that should be included in more site-specific conceptual and mathematical models; the second advantage of a generic model is that it can assist in determining the field investigations needed to develop such site-specific models. For example, flow through a porous medium will never be equivalent to flow through a fractured rock aquifer. Nevertheless, a porous flow model based on variable porosities, might yield not too unrealistic description of flow through a fractured rock aquifer, and at the same time, delineate aspects that need to be investigated further (Botha *et al.*, 1998).

Generic models are especially useful where there is simply not enough information available to develop site-specific conceptual and mathematical models.

Groundwater is, by its very nature, a three-dimensional phenomenon; in other words, it depends on all three dimensions of space, $x = \{x, y, z\}$, and the time t. Thus, it would seem that a conceptual model based on only two spatial dimensions would not be much worth in the study of groundwater phenomena. However, a three-dimensional model is also worthless without the support of sufficient observational (experimental) evidence. This poses a major difficulty in the use of conceptual models for groundwater studies. Fortunately, it is theoretically possible to obtain useful information on the behaviour of a three-dimensional physical phenomenon by reducing its dimensions, either physically or mathematically (Bear, 1977; Botha, 1996), a conclusion supported by the historical successes achieved with two-dimensional versions of conceptual models for groundwater phenomena. The discussion below in Section 3.2 therefore begins with a preliminary attempt to derive a conceptual model for the Tutuka site followed by a brief discussion of the differences between the Tutuka and Secunda sites that need to be taken into account in the development of a suitable conceptual model for the Secunda site outlined in Section 3.3.

As a perusal of the existing literature will show, a large number of mathematical models for the study of groundwater resources exist (Bear, 1972, 1979; Bear and Verruijt, 1987; Domenico and Schwartz, 1990; Huyakorn and Pinder, 1983; Pinder and Gray, 1977). As many of these models have been developed for specific purposes, they may not be suitable for all sites. For example, the models in the references above have been developed for flow in saturated porous media and may therefore not apply to the variable-saturated flow present in the ash and the unsaturated and saturated members of the fractured Karoo Super Group of geological formations that underlie both the Tutuka and Secunda sites. However, a porous flow model based on variable porosities, may be able to yield not too unrealistic results for flow through fractured rock aquifers, especially aquifers in the Karoo Supergroup, and at the same time highlight aspects that need to be investigated further (Botha *et al.*, 1998). Section 3.4 therefore describes the three-dimensional mathematical model for the flow of water through variable-saturated porous media. As not enough data exists, only a vertical two-dimensional version of the model is implemented in Chapter 4 and used in Chapter 5 to investigate the flow of water through the ash dam at Tutuka and its underlying geological formations.

There is no doubt that the main topic of concern at both the Tutuka and Secunda sites is the potential pollution of the surrounding environment by water that infiltrates the ash dams to ultimately seep into nearby streams and rivers and aquifers that may underlie the ash dams. The main objective should therefore be to develop site-specific mass transport models of both the Tutuka and Secunda sites. Unfortunately, there is simply no data available at this time to warrant the development of even rudimentary generic mass transport models for the sites. No attention will therefore be devoted to the development of even rudimentary conceptual and mathematical models for both sites.

The discussion ends in section 3.6 with a brief summary of the importance of a reliable conceptual model.

3.2 A CONCEPTUAL MODEL FOR THE TUTUKA ASH DUMP SITE

There is no doubt that one would need a three-dimensional model to fully describe the interactions between the ash, the water used to irrigate the ash, any aquifers that may underlie the ash dump and the natural environment. However, the development of such a model would require far more data and resources than that available for this project, and would not necessarily contribute to a better understanding of the interactions at the site. The present discussion therefore will be limited to two vertical cross-sections with locations shown in Figure 3-1.

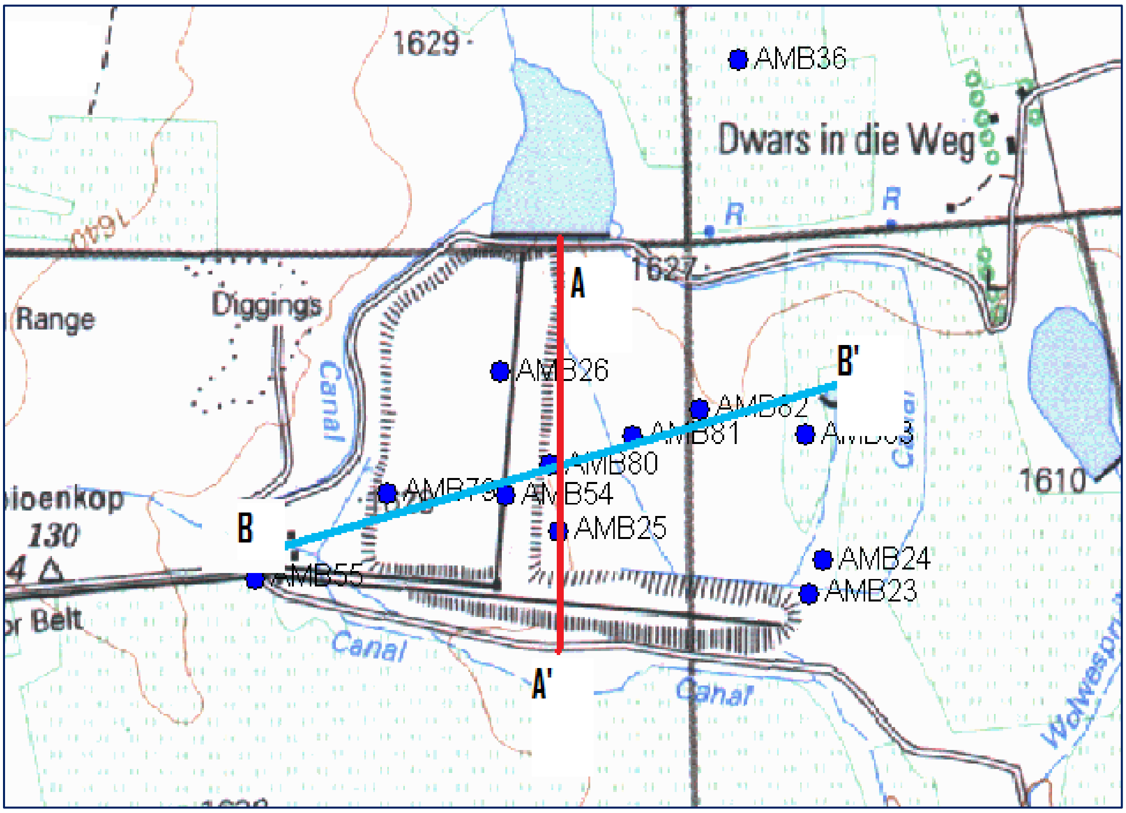

Figure 3-1: Locations of the cross-sections considered in the development of a vertical flow model for the Tutuka ash dump.

The first cross-section (B-B') in Figure 3-1 is the same as the ash-1 cross-section in Figure 2-7 used in the geophysical survey of the ash dump. The reason for this choice is that the resistivities provide a suitable proxy for the water content in and below the ash dump, as will be discussed in Chapter 4 and 5. The ash-1B cross-scetion in Figure 2-7 is less useful as it runs along the edge of the ash dump and is therefore not fully representative of the ash itself. It will consequently not be considered further here.

The second cross-section, (A-A’), which is oriented from north to south across the ash dump is a sub-section of the profile (Hodgson, 1999) uses in his preliminary model of the site. The main advantage of this cross-section is that it can be used to study the remark by Hodgson (1999) that the water body at point A in Figure 3-1 sustains a shallow groundwater table beneath the ash dump that might facilitate the leaching of water from the dump. Unfortunately, there is no information available on the water content across the profile, nor is there a suitable proxy. This cross-section will therefore not be considered here. Nevertheless, it may be advantageous if more attention could be paid to the cross-section in future investigations, particularly because such investigations could verify or negate the remark of (Hodgson, 1999).

The simplest way to construct a conceptual model for a given site is to visually represent the major features, events and processes at the site. The geological logs of existing boreholes and the core boreholes discussed in Section 2.2.4 were consequently used to interpolate a geological profile of cross-section B–B' in Figure 3-1. This profile, illustrated schematically in Figure 3-2, shows that the ash above the virgin soil surface is from 30 to 40 m thick. The ash is underlain first by a thin layer of saturated clay (1000 mm thick), followed by a layer of undulating weathered dolerite and an unweathered dolerite sill

As mentioned in Chapter 1, the main purpose of the present investigation was to investigate the extent to which saline effluents and ash can be co-disposed. As illustrated in figures 3-2 and 3-11, part of the water applied on the surface of the ash, be it in the form of rain or the saline effluents, will either evaporate from the ash heap or seep from the ash dam to ultimately flow as runoff towards the surface streams in the area, as indeed observed at the interface between the ash and the clay on the southern side of the dump. The remaining water will infiltrate into the subsurface of the earth below the ash. There are thus two pathways and their associated features, events and processes that need to be included in a conceptual model of any ash dam: one along the surface of the area around the ash dam, and the second through the subsurface of the earth below the ash dam. The present investigation of the Tutuka ash dam, however, will be restricted to the subsurface pathway illustrated in

Figure 3-2.

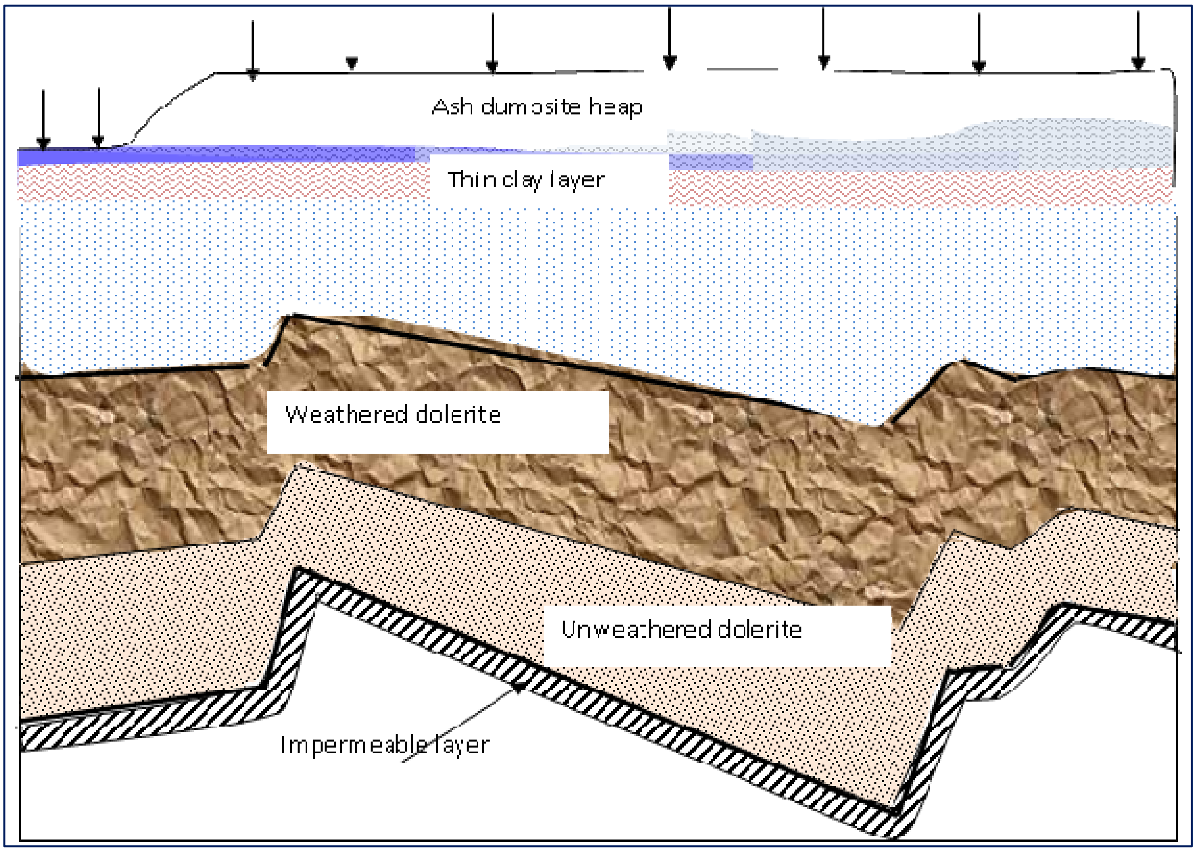

Figure 3-2: Schematic geological profile of cross-section (B-B') as inferred from the geology of the site discussed in Section 2.2.4.

3.3 A CONCEPTUAL MODEL FOR THE SECUNDA ASH DAM

The arguments above obviously also apply to the Secunda site. However, there are a number of features that may need special consideration when developing a conceptual model for the Secunda site, of which the following three are the more important.

a) The ash is disposed of as fully saturated slurry.

b) A number of hydraulically connected waste disposal sites and wastewater bodies border the main ash dump (see Figure 2-12).

c) It is claimed that the water released by the slurry at the ash dump is pumped back to the power station and re-introduced into the general water distribution system at the site. Unfortunately, there is no indication as to how efficiently the water is reclaimed.

These features, and the almost complete lack of any suitable information (compare the discussions of the information available for the two sites in Sections 2.2 and 2.3), make it difficult to develop even a crude vertical cross-sectional model for the site at present. No attempt will therefore be made to develop a conceptual model for the Secunda site. This situation should, however, not be viewed negatively, but rather as an opportunity to use the model for the Tutuka site and other guidelines discussed in this thesis and develop a more realistic conceptual and ultimately site-specific model for the Secunda site.

3.4 MATHEMATICAL MODEL FOR SATURATED-UNSATURATED FLOW IN A POROUS MEDIUM

3.4.1 General

A fluid will only flow through a porous medium if the force driving the flow is larger than the frictional forces that exist between the molecules of the fluid themselves and their interactions with the grains of the porous medium. A fluid will, consequently, only flow through a porous medium if it has sufficient energy to overcome the frictional forces. The mathematical description of a fluid is therefore invariably based on the energy of the fluid.

Although there are other sources of energy, the flow of a fluid in a porous medium is conventionally based on the gravitational potential energy of the fluid, the energy of fluid pressure and the kinetic energy of the fluid. This allows the introduction of the so-called fluid potential, the mechanical energy per unit mass of the fluid given by (Bear, 1979; Freeze and Cherry, 1979) as

$$E = gz + \frac{v^2}{2} + \int_{p_0}^{p} \frac{dp}{\rho}$$

where g is the acceleration of gravity, z a suitable reference elevation, v the velocity of a unit mass of the fluid, p the fluid pressure at the elevation z and ρ, the density of the fluid. As the fluid velocity is normally small in a porous-medium, the velocity term is usually neglected in the studies of fluid flow through a porous medium, thereby giving rise to the so-called Hubert's potential (Bear, 1979; Freeze and Cherry, 1979; Hubbert, 1940) as

$$\Phi = gz + \int_{p_0}^{p} \frac{dp}{\rho}$$

which reduces, in the case of an incompressible fluid, a fluid with a constant density, to

$$\Phi = gz + \frac{(p - p_0)}{\rho}$$

It is customary in groundwater literature to equate p0 to atmospheric pressure taken as zero. This allows one to introduce the so-called piezometric head φ, and the pressure head h defined by

$$\varphi = z + \frac{p}{\rho g} = z + h \tag{3.1}$$

The pressure head is thus nothing other than the pressure exerted by a column of water with height h at a point P in the porous medium. The piezometric head can thus be interpreted as the sum of the elevation of the point P above a suitable reference elevation, often taken as the mean sea level, and the pressure head h, as illustrated in Figure 3-3.

3.4.2 Porosity, Volumetric Moisture Content and Water Saturation

Water can only occur in voids or pores of a porous medium. The volume and sizes of the pores are thus of the utmost importance in studies of the motion of fluids through a porous medium. It is therefore important to have a measure that can be used in the comparison of different porous media. However, to define such a measure uniquely, is not easy, especially when the porous medium relates to the subsurface of the earth, which consists of at least three components: water, air and the solid matrix. It is therefore customary to introduce a number of parameters to measure the pores and the distribution of water in the subsurface of the earth. The first such measure is the porosity of the medium, defined as the ratio (Botha, 1996)

$$\lim_{V \to V_0} \frac{V_v}{V} \tag{3.2}$$

where V_0 is the so-called proper sample volume and V_v the volume of voids in V_0.

A measure closely related to the porosity of a porous medium, is the volume of fluid that the medium contains within a proper sample volume. This measure is conventionally expressed by either one of two variables: the moisture content, defined in terms of the volume of water, V_w in V_0 as

$$\theta = \lim_{V \to V_0} V_w / V \tag{3.2}$$

and the water saturation defined by

$$S_w = \frac{\theta}{\varepsilon} = \lim_{V \to V_0} {}^{V_w}\!/_{V_v} \tag{3.3}$$

The moisture content of a fully-saturated porous medium must clearly be equal to the porosity of the medium. In unsaturated flow, this value of θ, also known as the saturated moisture content, is conventionally denoted by the symbol θ_s. The moisture content and water saturation of a porous medium must thus satisfy the inequalities

$0 \le \theta \le \varepsilon (= \theta_s)$ and $0 \le S_w \le 1$

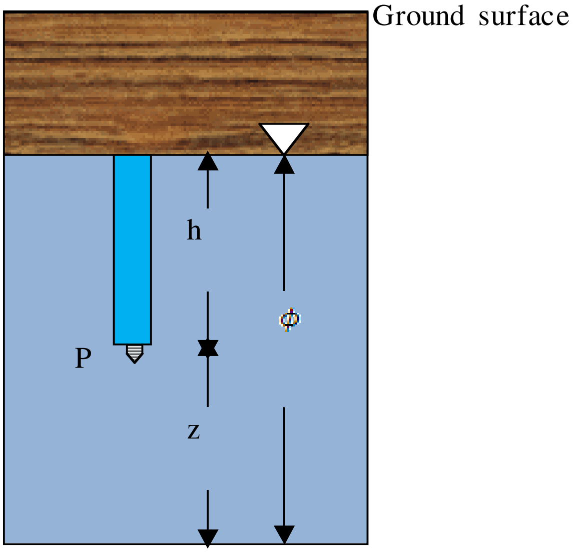

Figure 3-3 Diagram illustrating the definition of the piezometric and hydraulic heads.

3.4.3 Moisture Retention Curve

The pressure, p_w, experienced by water in an unsaturated porous medium is generally less than atmospheric pressure. In other words, the pressure is negative if atmospheric pressure is equated with zero. This means that the water pressure (p) and pressure head (h) are positive below the water level in a partially-saturated porous medium and negative above it. The idea of a negative pressure was not intuitively very attractive to the early soil scientists so they therefore introduced the positive quantity capillary pressure, defined by the equation

$$p_c = -p_w$$

to describe the distribution of water in an unsaturated soil. However, as discussed by (Botha, 1996), this pressure is the result of the interaction between the capillary water, soil grains and adsorbed water. The modern term ‘matric pressure’ is thus more descriptive.

The idea of a negative pressure has nonetheless an important advantage from the theoretical point of view. The reason for this is that the vertical distribution of water in the subsurface of the earth usually ranges from unsaturated to saturated conditions. The use of a negative pressure thus allows one to describe the entire water profile in the subsurface with a single, continuous pressure function, such as the one in Figure 3-4. Nevertheless, there are situations where the term ‘matric pressure’ has significant advantages.

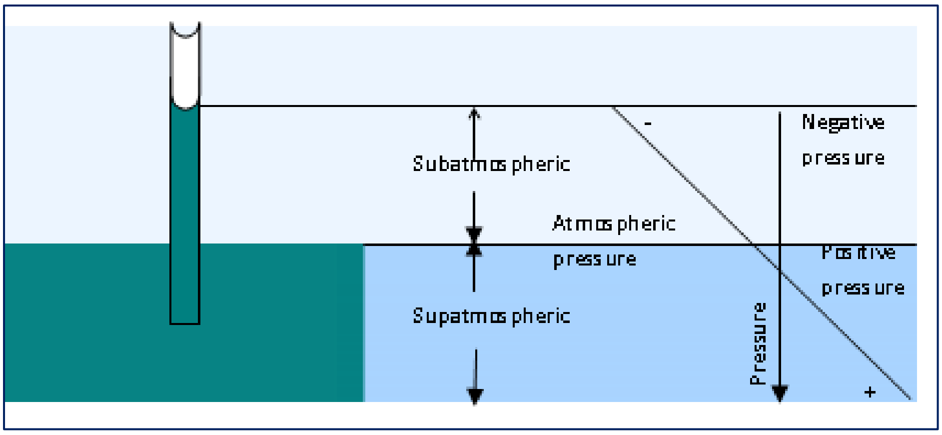

Figure 3-4: Distribution of pressure below and above the water level in a partially saturated porous medium.

Experiments have shown that if water is removed from an unsaturated porous medium, the curvature of the menisci, the remaining capillary water formed with the soil grains, decreases. However, Laplace’s law (Botha, 1996) requires that a decrease in radius of the menisci must be accompanied by an increase in the matric pressure. The volume of water present at any point in an unsaturated porous medium is thus closely related to the matric pressure (or pressure head) at that point. This relation, known as the water or moisture retention curve, is conventionally expressed mathematically in terms of the pressure head h in Equation (3.1) as

$$\psi = -\mathrm{h} = \psi(\theta) \tag{3.4}$$

The schematic graph of a moisture retention curve in Figure 3-5 indicates that Equation (3.5)is not a simple, but a highly non-linear relation of the moisture content. In more physical terms, θ(ψ) is said to a show a hysteresis effect. This means that the curve is at least double legged, with one leg valid during the drying cycle (desorption) and the other during the wetting cycle (sorption). Moreover, as the surface of the earth is intermittently subjected to both drying and wetting cycles, the curve can change abruptly from the sorption to the desorption leg, and conversely. For example, a very dry soil may be soaked by rain that stops when its moisture content reaches the point A in Figure 3-5. After that, desorption will set in, which, if allowed to continue unchecked, will follow the path indicated by the line segment AB in Figure 3-5, and ultimately the normal desorption leg. These secondary curves are commonly referred to as scanning curves. Care must therefore be exercised when using the retention curve in practical applications.

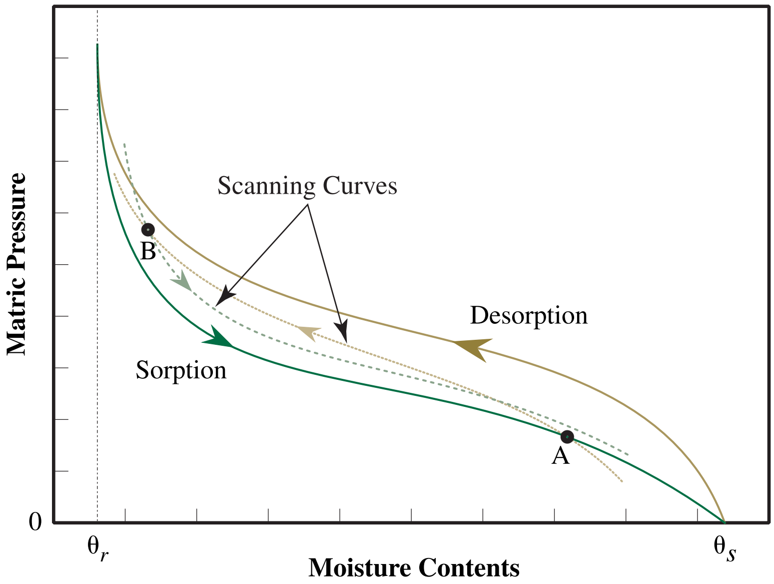

Figure 3-5: Schematic water retention curves for clayey and sandy soils.

The major reason for this behaviour is the dependence of the capillary pressure on the contact or wetting angle between the water and the soil, which is larger during sorption,(when water moves upwards in the pore), than during desorption, when the water moves downwards. The capillary pressure in a pore is thus always larger during desorption, than sorption (Baker, 1998).

It is interesting to note that the moisture retention curve does not generally approach the matric pressure axis as the moisture content decreases, but rather follows an asymptote that runs parallel with the matric pressure axis through a small positive value of θ, called the residual moisture content and denoted by θ_r in Figure 3-5. The moisture retention curve is consequently commonly expressed not in terms of the moisture content, but the reduced moisture content, defined by the equation,

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{3.5}$$

It would be most useful if an explicit expression for the retention curve could be derived from basic physical principles. Although attempts have been made to achieve this, see, for example. (Ferrand and Celia, 1990), the necessary computations are rather complex. The experimental determination of the curve is thus still the preferred alternative. While this is a relatively simple (but laborious) experimental exercise that has been conducted for years by soil scientists, the interpretation and application of moisture retention curves are not straightforward. For example, can one really apply the concept of a moisture retention curve to the many important dense geohydrological formations, such as fresh dolomites and dolerites, or to alluvial deposits with large boulders? Although some progress has been made in this direction (Bouwer and Rice, 1984; Guarracino, 2006), the question cannot yet be considered as fully answered. Nevertheless, it will be assumed in the discussion to follow that a moisture retention curve can be determined for the geological formations and ashes at Tutuka and Secunda.

The absence of an analytical expression for the moisture retention curve makes it difficult to use the curve in practical calculations, not only at off-experimental points, but also in general. All practical applications of the curve therefore usually rely on approximations of the curve. There are essentially two approximation methods that can be used for this purpose. The first, and most obvious, method is interpolation. It must be kept in mind though, that the moisture retention curve is highly non-linear. Interpolation, particularly linear interpolation, can thus only be applied successfully in cases where the experimental points are closely spaced and distributed over the full range of θ–values ($\theta_r \leq \theta \leq \theta_s$). Unfortunately, it is impractical to determine the curve at a large number of points experimentally, with the result that its true behaviour is seldom, if ever, known precisely, especially near θ_r and θ_s. Many scientists thus opt for the second alternative: approximation of the experimental values by an empirical or semi-empirical analytical expression. Although any suitable analytical expression would do, much can be gained if the expression is chosen judiciously. For example, the expression selected should be able to represent the experimental results accurately and not require an exorbitant computational effort to evaluate. This is exemplified by the form of the curve in Figure 3–5 that very much resembles the sigmoidal shape of a cubic polynomial. As a polynomial is able to match the experimental points exactly and is easy to evaluate, this would seem to be an ideal choice. Unfortunately, a polynomial approximation often introduces more difficulties than it is supposed to solve. Two errors, often committed by inexperienced users when using interpolations, are: (a) extrapolate the variable beyond the range for which experimental data points are available, and (b) approximates the data with a polynomial of too high a degree. Nevertheless, as shown by (Case et al., 1983) in their encyclopaedic work on moisture retention curves, a cubic polynomial approximation can be applied successfully, provided that interest is centred only on the domain for which experimental data is available. Unfortunately, one is not only interested in the retention curve itself when modelling variable saturated flow in practical applications, but (more importantly) also in its derivative:

$$C = -\mathrm{D}\theta(\psi)$$

This derivative, commonly referred to as the moisture capacity of an unsaturated soil (an analogy to the heat capacity of a body defined as the change in its heat content per unit change in temperature) can cause severe difficulties in practical computations if not continuous at the transition from unsaturated to saturated flow and inversely. This requirement has lead to the development of a large number of semi-empirical expressions (Botha, 1996; El-Kadi, 1985; Seki, 2007) of which the best-known is that of (Van Genuchten, 1980)

$$\Theta = [1 + (\alpha\psi)^n]^{-m} \tag{3.6}$$

where α, n, and m are empirical curve fitting parameters with m = 1 – 1/ n in the original formulation, from which follows

$$\mathrm{D}\Theta(\psi) = -\frac{\alpha m n(\alpha\psi)^{n-1}}{[1+(\alpha\psi)^{n}]^{m+1}} \Rightarrow \mathrm{D}\Theta(0) = 0 \quad \text{iff}\, n > 1$$

The Van Genuchten approximation is thus able to represent the moisture capacity continuously, not only at the transition from unsaturated to saturated flow, but also in unsaturated flow if $n \geq 1$. Although there are indications that the Van Genuchten approximation may not be applicable to all soil types (Ippisch *et al.*, 2006; Seki, 2007; Vogel *et al.*, 2008), it is still the preferred approximation used in mathematical models of unsaturated flow (Jhorar *et al.*, 2002), including this investigation

3.4.4 Variable-saturated Groundwater Flow

The flux of groundwater through a saturated unit area in the earth's subsurface is conventionally described with Darcy's law (Bear, 1972, 1979; Botha, 1996)

$$\mathrm{q} = -\mathrm{K}\nabla\varphi = -\frac{\mathrm{k}\rho g}{\mu}\nabla\varphi \tag{3.7}$$

where q is known as the Darcy velocity, φ is the pizometric head defined in Equation (3.1), ρ the density and μ the dynamic viscosity of water, g the acceleration of gravity and K and k the hydraulic conductivity and permeability tensors of the subsurface respectively, with

$$\nabla = \mathrm{iD_x} + \mathrm{jD_y} + \mathrm{kD_z}$$

the well known nabla operator, expressed in terms of the Cartesian unit vectors {i, j, k} and the Cartesian derivatives $D\zeta$ (ζ = x, y, z).

It follows from the preceding discussion that there is no difference between the piezometric head distribution in saturated and unsaturated flow from the mathematical point of view, provided that one is willing to accept that the pressure is negative in unsaturated flow. One would therefore expect that Darcy's law is also applicable to unsaturated flow. However, it must be kept in mind that unsaturated flow only occurs in pores that remain filled at the given matric head and the fluid films that surround partially-drained pores (Botha, 1996). The Darcy velocity for unsaturated flow therefore should be less than that of saturated flow and steadily decrease as the moisture content of the porous medium decreases. The hydraulic conductivity should thus be smaller in unsaturated flow than in saturated flow; in other words, the unsaturated hydraulic conductivity of a porous medium is a function of the moisture content, or the matric head in unsaturated porous flow. Following (Richards, 1931), Darcy's law for unsaturated flow is thus conventionally expressed in the form

$$q = -K(\psi)\nabla\varphi \tag{3.8}$$

This dependence of K on ψ (hence on θ) implies that values of K, like the moisture retention curve, can only be obtained from measurements in the field, or in the laboratory. However, this is one of the most difficult and time-consuming procedures in soil physics to achieve. As ψ is a highly non-linear relation of the moisture contents, it is not always easy to distinguish between the tensorial and non-linear properties of K. However, because the force of gravity dominates the flow in the unsaturated zone of the earth's surface, the dominant direction is vertically downwards. The hydraulic conductivity is therefore usually taken as the scalar, $K(\psi)$, although there are situations where one might need to use its tensorial form, albeit only as a diagonal tensor (Yeh *et al.,* 2005).

The equation of K with the scalar K has the advantage that one may approximate $K(\psi)$ with analytical expressions, of which the best known are the (Brooks and Corey, 1966) and (Van Genuchten, 1980) approximations. Following (Van Genuchten, 1980), see also (Botha, 1996), this relation can be expressed as

$$K(\Theta) = K_s \Theta^{1/2}\left[1 - \left(1 - \Theta^{1/m}\right)^m\right]^2 \tag{3.9}$$

where K_s is the saturated hydraulic conductivity of the soil. This approximation will be used in the numerical model for the Tutuka site in Chapter 4

3.4.5 The Groundwater Flow Equation

The easiest way to derive an expression for the transient flow of water in unsaturated-saturated porous media is to combine the law of mass conservation with Darcy's law. This yields what may be termed as the generalized Richards equation, which assumes for an isotropic porous medium and density-dependent flow the form (Bear, 1979; Botha *et al.*, 1990; Huyakorn and Pinder, 1983; Reeves and Duguid, 1975)

$$D_t\left[\rho\theta(\mathbf{x},t)\right] = \nabla\cdot\left[\rho K\nabla\varphi(\mathbf{x},t)\right] + \rho f(\mathbf{x},t) \tag{3.10}$$

or if the fluid is incompressible (ρ = constant)

$$D_t\left[\theta(\mathbf{x},t)\right] = \nabla\cdot\left[K\nabla\varphi(\mathbf{x},t)\right] + f(\mathbf{x},t) \tag{3.11}$$

where

$$\mathrm{f}(\mathrm{x},\mathrm{t}) = \frac{\text{Volume of fluid entering a volume of porous material per unit time}}{\text{Volume of porous material}} \tag{3.12}$$

is known as the strength of any sources or sinks that may be present in the medium.

Equations (3.11) and (3.12) differ somewhat from the equations normally used to describe variable-saturated flow (McDonald and Harbaugh, 1988; Voss, 1984; Yeh and Ward, 1980), in that they contain two dependent variables (θ and φ). However, they do have an advantage in that they present one with uniform descriptions of density dependent and density-independent variable-saturated flow in the earth's subsurface (Verwey and Botha, 1992). Moreover, it is not difficult to show that they can always be reduced to equations containing only the dependent variable φ(x, t). Take, for example, the left hand side of Equation (3.11), which can always be expressed in terms of the water saturation S_w as (Botha, 1996)

$$\begin{aligned} D_t\left[\rho\varepsilon S_w(\mathbf{x},t)\right] &= \left[S_w(\mathbf{x},t)D_p(\rho\varepsilon) + \rho\varepsilon D_p S_w(\mathbf{x},t)\right]D_t p(\mathbf{x},t) \\ &= \left[\varepsilon S_w(\mathbf{x},t)D_p(\rho) + \rho S_w(\mathbf{x},t)D_p(\varepsilon) + \rho\varepsilon D_p S_w(\mathbf{x},t)\right]D_t p(\mathbf{x},t) \end{aligned}$$

This equation can be simplified somewhat by the introduction of the compressibility coefficients for water and the porous matrix, given respectively by

$$\alpha = \left(\frac{1}{1-\varepsilon}\right)\mathrm{D_p}\varepsilon, \quad \beta = \left(\frac{1}{\rho}\right)\mathrm{D_p}\rho(\mathrm{p},\mathrm{c},\mathrm{T})$$

and observing that the time derivative can be expressed as

$$D_t\,p(x,t) = D_\varphi p(x,t) D_t \varphi(x,t) = \rho g D_t \varphi(x,t)$$

This yields the equation for the density-dependent flow of water in a variable-saturated porous medium

$$\rho\left[C(\varphi) + S_w S_0\right] D_t \varphi(x,t) = \nabla g \left[\rho K \nabla \varphi(x,t)\right] + \rho\, f(x,t) \tag{3.13}$$

or if the fluid is incompressible (ρ = constant)

$$[C(\varphi) + S_w S_0] D_t \varphi(x,t) = \nabla g \left[K \nabla \varphi(x,t)\right] + f(x,t) \tag{3.14}$$

where

$$C(\varphi) = \varepsilon D_\varphi S_w(x,t) \quad \text{and} \quad S_0 = \rho g[\alpha(1-\varepsilon) + \beta]$$

are known as the moisture capacity and specific storativity of a porous medium respectively.

The saline effluents used in the disposal of the ash implies that the mathematical model for the ash dam at Tutuka should be based on the density-dependent Equations (3.11) or (3.14). However, as suitable data does not exist and as this investigation does not include the establishment of a full model of the site, the model discussed in Chapter 4 will be restricted to the density-independent Equation (3.12).

3.4.6 Initial and Boundary Conditions

The solution of any partial differential equation, such as Equation (3.12), always contains a number of integration constants that have to be determined in one way or another. The method, universally used for this purpose, is to prescribe suitable initial and boundary conditions on the domain Ω, over which the differential equation is defined, and its boundary δΩ (Bear, 1979; Botha and Pinder, 1983). Such boundary and initial conditions must obviously relate to the physical nature of the flow and should therefore represent the initial and boundary conditions in the field as accurately as possible.

It is usually not difficult to choose a suitable initial condition for a given differential equation. All that is required is the selection of a set of observations on the dependent variable, θ and φ in Equation (3.12), at a suitable time ($t = t_0$, say) and to use that as the initial condition. As $\theta = \theta(\psi)$ and φ is related to ψ through Equations (3.1) and (3.5), an initial condition for Equation (3.12) can assume either one of two forms

$$\varphi(x, t_0) = \varphi_0(x) = z + \psi_0(x), \qquad \theta(x, t_0) = \theta_0(x) \tag{3.15}$$

The choice of suitable boundary conditions is, unfortunately, not that simple as the theory of partial differential equations allows only three types of boundary conditions: Dirichlet, Neuman and Cauchy conditions (Morse and Feshbach, 1953; Verwey and Botha, 1992). If u(x, t) denotes the solution of the generic partial differential equation

$$\mathbf{L}\mathbf{u}(\mathbf{x}, t) = \mathbf{f}(x, t) \tag{3.16}$$

and $\alpha(x, t)$, $\beta(x, t)$ and $\gamma(x, t)$ are known functions of x and t on the boundary $\delta\Omega$ of Equation (3.17), these conditions assume the forms

a) Dirichlet conditions (or boundary conditions of the first type)

$$\alpha(x, t)u(x, t) = \gamma(x, t)$$

b) Neuman conditions (or boundary conditions of the second type)

$$\beta(x, t)u(x, t) = \gamma(x, t)$$

c) Cauchy conditions (or boundary conditions of the third type, also known as Robin's boundary conditions).

$$\alpha(x, t)u(x, t) + \beta(x, t)u(x, t) = \gamma(x, t)$$

If $\gamma(x, t) = 0$, the conditions are said to be homogeneous, otherwise they are known as non-homogeneous boundary conditions.

Dirichlet boundary conditions are usually associated in groundwater flow with a body (or bodies) of surface water (rivers, lakes or oceans) that intersect an aquifer. If $\varphi1(x, t)$ is the known piezometric head in the body of surface water, a suitable Dirichlet boundary condition for Equation (3.12) will thus be of the form

$$\varphi(x,t) = \varphi_1(x,t), \qquad (x \epsilon \delta\Omega_1, t > 0) \tag{3.17}$$

Neumann boundary conditions, also referred to as flux boundary conditions, are probably the most frequently used (and misused) type of boundary conditions in groundwater flow phenomena. This type of boundary condition is usually associated with a flux of material across and normal to the boundary of the differential equation. A suitable Neumann condition for Equation (3.12) will thus be of the form

$$q(x,t).n = -[K\nabla\varphi(x,t)].n \quad (x\varepsilon\delta\Omega_2, t>0) \tag{3.18}$$

where n is the outwardly directed unit vector, normal to the boundary $\delta\Omega_2$. Cauchy boundary conditions are usually associated with semi-permeable boundaries in groundwater flow phenomena and will not be discussed further here.

It is important to note that the types of boundary conditions can be mixed freely when applied to a given differential equation. The only constraint is that the conditions should fully cover the boundary

$$\delta\Omega = \delta\Omega_1 + \delta\Omega_2 + \delta\Omega_3$$

Moreover, the theory does not prohibit a change in boundary condition from one type to another as time progresses. Two types of boundary conditions of this nature that occur quite frequently in groundwater flow phenomena are precipitation-evaporation and seepage boundary conditions, which will now be discussed in more detail.

3.4.7 Precipitation-Evaporation Boundary Conditions

Precipitation-evaporation boundaries are usually associated with the surface of the earth. They differ mathematically only in the sense that the fluxes associated with them have opposite directions. However, as the physical processes involved are quite different, the boundaries are usually treated as separate boundaries.

To derive suitable expressions for precipitation events, consider the situation of an unsaturated soil with a hydraulic conductivity K(x, t), subject to a precipitation intensity R(x, t). Everyday experience indicates that on reaching the soil surface, the precipitation immediately begins to infiltrate into the soil. If n denotes the outwardly directed unit vector normal to the soil surface in Figure 3-6 and the soil is able to absorb all the rain, the two fluxes must satisfy the Neuman boundary condition

$$\mathrm{n \cdot R(x,t) = n \cdot K(x,t) = \varphi(x,t) = n \cdot q = q_n} \qquad (3.19)$$

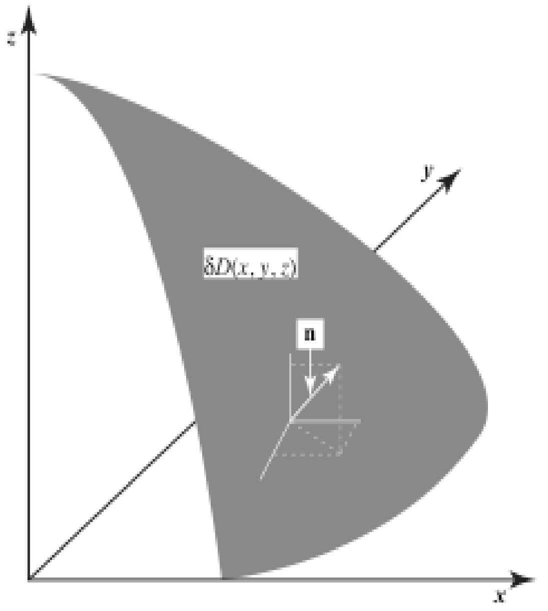

Figure 3-6: Geometric representation of the unit vector n normal to the soil surface δΩ(x, t).

However, it is common knowledge that the soil is not always able to absorb all the water. In such situations the rain tends to pond on the surface and to run off towards shallower areas if the rain continues long enough. This phenomenon, known as ponding, can be explained by observing that the law of mass conservation requires that the flux of water normal to the top of the soil must equal the flux normal to the bottom of the surface. Ponding therefore will occur whenever $R \geq q_n$. It should not be interpreted though, that ponding will only occur when the soil surface is fully saturated. On the contrary, it is known that ponding often also occurs over unsaturated soil surfaces, especially after long periods of drought. In such situations the Neuman boundary condition in Equation (3.20) must be replaced by the Dirichlet boundary condition

$$\varphi(\mathrm{x},t) = \mathrm{h_p(x},t) \quad (\mathrm{x} \in \delta \mathrm{D_1},\ \mathrm{t} > 0)$$

where $h_p(x, t)$ is the depth of the water during ponding.

It is important to note that the pressure across a saturated soil surface during ponding is constant. This means that the gradient of the pressure head (or pressure for that matter) must vanish across the soil surface.

$$=h_p(x,t) = 0$$

Thus, there exists a limit to the rate at which a soil can absorb precipitation during ponding, given by

$$q = -K= \varphi(x,t) = -K= [h_p(x,t) + z] = K$$

This limit reaches an absolute maximum when the soil surface is fully saturated, i.e., when K assumes its saturated value K_S.

A rainfall boundary condition is clearly a highly non-linear function of the surface matric head y(x, t) that can only be applied iteratively. This is usually achieved by using an assumed value of y(x, t) to compute the Darcy velocity at the soil surface from Equation (3.9) by using either the full tensor

$$K = \begin{pmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{xy} & K_{yy} & K_{yz} \\ K_{xz} & K_{yz} & K_{zz} \end{pmatrix} \quad (3.20)$$

or its equivalent scalar expression in Equation (3.10). If the magnitude of q = q ≥ R at the soil surface, Equation (3.12) is solved using the boundary condition in Equation(3.20). This procedure is repeated as long as the solution yields a q with magnitude q ≥ R. Otherwise, a value for $h_p(x, t)$; must be computed or estimated, taking R the piezometric head at the soil surface, and possible run-off from the area into account, and then solve the equation with the Dirichlet boundary condition in Equation (3.18).

The earth's surface loses water through either one of two phenomena: evaporation and transpiration. Although there are situations where one of the processes completely dominates the other (bare soil surfaces and dense forests, for example), they usually occur simultaneously, hence the designation evapotranspiration. This is a highly-complex phenomenon controlled by a process commonly referred to as the atmospheric evaporation demand (AED)—and consists of the atmospheric and soil conditions prevalent at the surface of the earth and at the roots of plants. However, just as the infiltration rate of rain is controlled by the hydraulic properties of the soil, so is the rate of evapotranspiration. For, no matter how large the AED may be, the earth's surface simply cannot supply more water than that be transmitted through the upper soil layers and the roots of plants and thus, it is not easy to compute the evapotranspiration rate for a vegetated site. The unsaturated flow models used in geohydrological investigations are consequently often restricted to evaporation from bare soils, E(x, t). If the magnitude of E(x, t) satisfies the inequality

$$\mathrm{n}\cdot\mathrm{K}(\mathrm{x},t)\nabla\varphi(\mathrm{x},t) \geq \mathrm{n}\cdot\mathrm{E}(\mathrm{x},t)$$

then the non-homogeneous Neumann boundary condition

$$\mathrm{n}\cdot\mathrm{K}(\mathrm{x},t)\nabla\varphi(\mathrm{x},t) = \mathrm{n}\cdot\mathrm{E}(\mathrm{x},t) \tag{3.21}$$

Can be used to describe evaporation from the soil surface when solving Equation (3.12). However, just as the rate at which a soil may absorb water during infiltration is limited by its saturated hydraulic conductivity, so is its ability to release water limited by its residual water contents θ_r, see Figure 3-5, or the equivalent residual matric head, h_r. This situation can be accounted for by replacing the Neumann boundary condition in Equation (3.22) with the Dirichlet condition

$$\varphi(\mathrm{x},t) = \varphi_{\mathrm{r}}(\mathrm{x},t) = \mathrm{h}_{\mathrm{r}}(\mathrm{x},t) + \mathrm{z} \tag{3.22}$$

A modeller of unsaturated groundwater flow must therefore have a good knowledge of both the prevailing climatic and soil conditions at the site to be modelled.

Experimental evidence suggests that precipitation is always accompanied by evapotranspiration from the earth's surface. However, the magnitude of the evapotranspiration is usually much smaller than the rainfall and is therefore often neglected. One noteworthy exception to this rule is a hot barren surface, where the rain may evaporate on contact with the soil surface, at least until the surface has cooled sufficiently.

3.4.8 Seepage Boundary Conditions

The domain of an aquifer can be divided conveniently into three zones: a permanently unsaturated zone, a drainable zone and a permanently saturated zone, see Figure 3-8. As used here, the term drainable zone refers to an unsaturated part of the aquifer that could become saturated during recharge events, and then recharge the saturated and unsaturated zones. The drainable zone is thus not static.

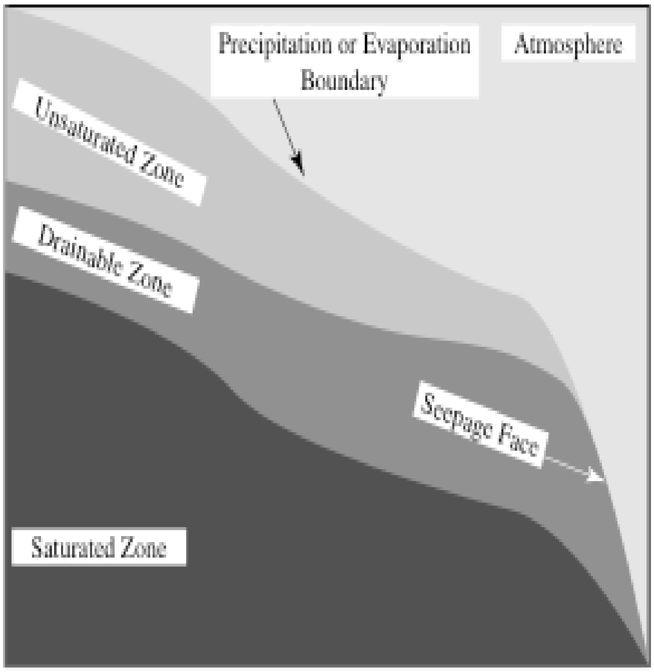

Figure 3-8 Schematic representation of the different zones in an aquifer.

The drainable zone of an aquifer is often exposed to the atmosphere along valleys, the shores of oceans, lakes and riverbanks. Thus, water may drain from the drainable zone towards the atmosphere if the domain is saturated; thereby creating a seepage face, see Figure 3-8. As long as $h(x, t) \geq 0$ on the interior and the seepage face of the drainable zone, the seepage face can be described mathematically through a Dirichlet boundary condition of the form.

$$\varphi(x,t) = \varphi_s(x,t) = z \qquad (3.23)$$

This condition will obviously no longer apply if rain sets in or if $h(x, t) < 0$. In such situations the boundary condition has to be replaced with the rainfall boundary condition, given by Equations (3.19) and (3.20), and the evaporation boundary condition of Equations (3.22) and (3.23) respectively. Which one of these conditions applies at a given time can be determined only from the model. Seepage boundary conditions, such as precipitation and evaporation boundary conditions can thus only be applied iteratively.

3.5 SOURCES AND SINKS

There are, in general, two types of sources and sinks associated with groundwater resources (Botha, 1996):—areal and discrete. Areal sources and sinks include, for example, rain and evapotranspiration, while boreholes are classical examples of discrete sources and sinks. It follows from the preceding discussion that areal sources can be incorporated into groundwater flow models as boundary conditions; this leaves the discrete sources. Although it is unlikely that water will ever be withdrawn through boreholes from an ash dam, it may be necessary to include boreholes in future models of ash dams to study the evolution of the dams and their immediate environments. Thus, it is considered worthwhile to include a brief discussion of how boreholes may be included in groundwater flow models.

It is common practice to associate discrete sources and sinks with Discrete the Dirac delta function, defined by the equation

$$\int_{\Omega} g(x)\delta(x - x_0)dx = g(x_0)$$

where x0 is the position of the discrete source or sink. When applied to boreholes this can be achieved by viewing them as line sources and express the source term, f(x, t) in Equation (3.12) in the form

$$f(x,t) = Q(t)\delta(x - x_0)$$

where Q(t) is the discharge or recharge rate of the borehole and $x_0 = \{x_0, y_0\}$ the position of the borehole in the plane of the earth's surface. Unfortunately, this approach cannot be applied when Equations (3.11) to (3.15) are used to simulate saturated-unsaturated flow in the vertical plane of the earth's subsurface, or in three dimensions, because the transmissivity properties of the geological layers in the earth's subsurface vary from layer to layer and with depth.

The first alternative that comes to mind to avoid this difficulty is to determine f(x, t) directly from its definition in Equation (3.13). However, this implies that the volume of the aquifer from which the water is withdrawn at the time *t* is known – a constraint that can never be satisfied. (Voss, 1984) tried to circumvent the problem by equating the volume of porous material with the total volume of the aquifer. This may be an acceptable approximation for a uniform aquifer, but not for a heterogeneous, anisotropic, layered aquifer.

An interpretation that avoids any prior knowledge of the strength of a borehole is to view the borehole as forming a boundary within the aquifer. One difficulty with this interpretation though, is what type of boundary condition must one use to account for the discharge from the borehole? An idea, originally introduced by (Theis, 1935) in deriving his analytical solution for the flow of groundwater in a confined aquifer, is to represent the borehole as a Neumann boundary. The idea is very useful when working with a uniform, confined aquifer with vertical thickness d and a fully penetrating borehole, as illustrated in Figure 3-9. If n is the unit vector normal to the inside of the borehole wall, r the radius of the borehole and Q(x, t) the rate at which water is pumped from the borehole, the borehole can be described with a Neumann boundary condition given by the component of the Darcy velocity normal to the borehole wall (Huyakorn and Pinder, 1983)

$$q_n(x,t) = n \cdot K \nabla \varphi(x,t) = \frac{\text{total discharge}}{\text{total area of borehole}} = \frac{Q(x,t)}{2\pi r\, d} \tag{3.24}$$

However, this boundary condition is again only valid for a homogeneous confined aquifer continuously in contact with the borehole and does not apply to a phreatic or multi-layered aquifer (Huyakorn and Pinder, 1983).

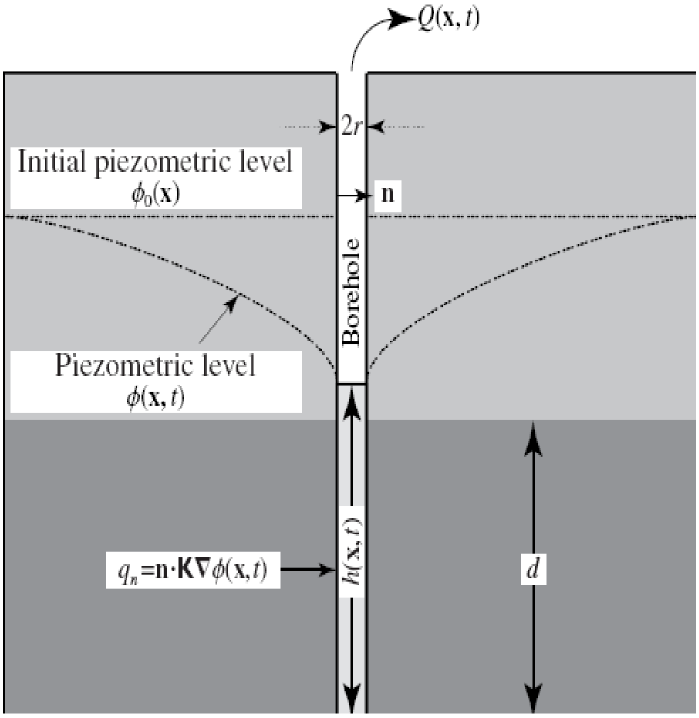

Figure 3-9: Distribution of the piezometric head near a borehole, before and after pumping was initiated.

One remaining possibility to represent a borehole as a boundary in the aquifer is to consider it as a Dirichlet boundary, subject to the boundary condition

$$\varphi(\mathrm{x},\mathrm{t}) = \varphi_{\mathrm{b}}(\mathrm{x},\mathrm{t}) = \mathrm{w}(\mathrm{z},\mathrm{t}) \quad [\,\mathrm{p}(\mathrm{x},\mathrm{t}) \geq 0] \tag{3.25}$$

where w(z, t) is the piezometric pressure along the wall of the borehole, as illustrated for a phreatic aquifer in Figure 3–9. Initially it would seem to be impossible to specify a discharge rate for the borehole using this approach. However, let Q(x, t) be the rate at which water is discharged from the borehole, and Q_a(x, t) the rate at which the aquifer discharges water to the borehole, subject to the boundary condition in Equation (3.26). The water level in the borehole will clearly rise, if Q(x, t) < Q_a(x, t), with a corresponding increase in w(z, t), and conversely. The effect that Q(x, t) has on the borehole, and thus the aquifer, is therefore implicitly contained in w(z, t). The real difficulty is how to determine w(z, t). One approach would be to view unsaturated and drainable parts of the borehole wall as evaporation or seepage boundaries and apply Equations (3.25) and (3.26) iteratively. However, Huang (1973) has shown that this is not necessary when solving Equations (3.14) or (3.15) numerically. It is merely necessary to solve the equation twice; first by prescribing an arbitrary Dirichlet boundary condition along the full length of the borehole, and then a homogeneous Dirichlet boundary condition. The true values of the piezometric heads along the borehole wall are then given by a linear combination of these two solutions. This concept has been applied with excellent results in modelling the multi-layered aquifer on the Campus Test Site (Botha *et al.*, 1998) and has recently been extended to any number of boreholes by Cloot and Botha (2004). The method can also be applied to Equations (3.11) and (3.12).

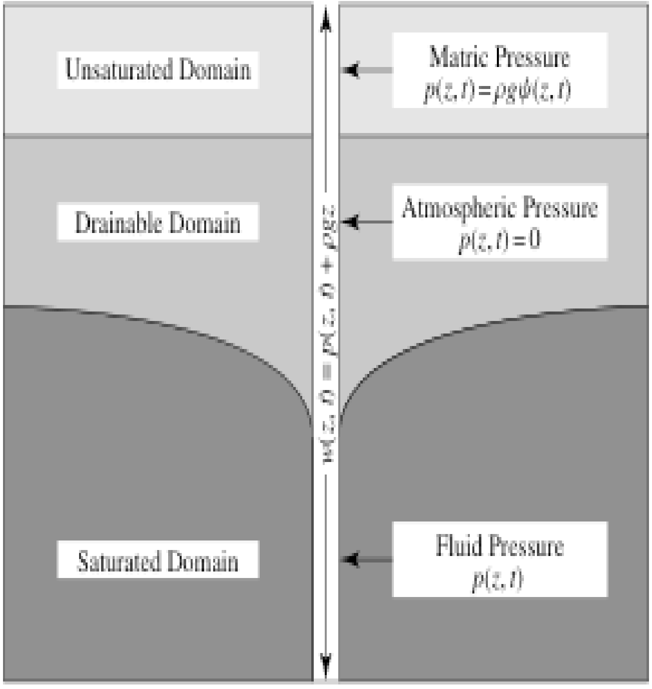

Figure 3-10: Graphical illustration of the application of Dirichlet boundary conditions to simulate the behaviour of a borehole in a numerical model of an aquifer.

3.6 SUMMARY

It is not unreasonable to summarise the preceding discussion by stating that the mathematical model for flow in a variable-saturated porous medium can only be applied successfully in practice if supported by a suitable conceptual model for a site under investigation or a site to be investigated. There are essentially two reasons for this conclusion. The first is that it would be difficult to implement the mathematical model for such a site in practice without some knowledge of the underlying geology and its effect on the various parameters present in the mathematical model. The second is that the conceptual model can be used to evaluate the quality and quantity of existing data, to identify missing data and even to evaluate the suitability of the assumed mathematical model.

Development of the conceptual model is the most important part of the modelling process. The conceptual model is the foundation of the quantitative, mathematical representation of the field site (i.e., the mathematical model), which in turn is the basis for the computer code used for simulation.

No single mathematical equation can estimate or predict the direction and rate of fluid flow with any accuracy. However, Darcy's law remains the first hand tool to apply for porous media fluid flow for a saturated/unsaturated zone. This forms the basis of the discussion of chapter four.

With the assumption that the ash dump is a porous medium, the hydraulic conductivity in the vadose zone is a function of volumetric moisture content, and is dependent on the porosity of the system. That is K increases if the porosity increases, and porosity is a time-dependent variable of the ash dump.

Based on the discussion above, it is evident that the unsaturated zone is of a challenging nature because of the interdependence of its hydraulic parameters. This gives rise to the nonlinearity of the governing mathematical equations in the vadose zone and makes it difficult to find analytical solutions except with some reserved assumptions.

Groundwater flow in the unsaturated zone is further complicated by the fact that both

K and ψ may change as water content θ varies and, by its very nature, unsaturated flow involves many changes in volumetric moisture content as waves of infiltrated water pass through. The nonlinearity of the flow equations compounds the difficulty of applying analytical solution methods.

The changes in the porosity, moisture content and unsaturated hydraulics applied to an unsaturated zone occur in the unsaturated as well the saturated parts of an ash dump. It is thus of the utmost importance that laboratory and field experiments are conducted in such a way that the time dependence of these parameters can be studied correctly. The ensuing model would also be more robust and efficient in simulating the flow of fluids into and through the unsaturated and saturated ash dumpsite as well as the underlying aquifer.

It is important to note the following physical properties of an ash dam:

- specific characteristics of the ash dam are probably time dependant,
- porosity: due to compaction and through pozzolanic crystallisation, the ash

porosity will decrease with time (e.g. experiments conducted at IGS have shown properties of virgin fly ash to be in the order of 60%). If the porosity changes, the kinematic porosity (flow porosity) will also change. Ash is not a homogeneous medium because of grain size variations and recrystallisation.

- hydraulic conductivity: K-values estimated by van den Berg et al., (2001) on ash dams range between 0.02 – 0.1 m/d. If porosity decreases, the K-value also decreases.
- the exchange/adsorption/absorption of the ash will change with time
- unsaturated zone hydraulics (i.e. soil water retention curves and the unsaturated K-values which are a function of the water content).

The construction of the correct conceptual flow model is of vital importance, i.e. the amount of flow is not only a function of the vertical K-value of the ash, but also a function of the underlying geological formation, e.g. weathering of dolomite and dolerite will give rise to a layer below the ash that has totally different K-values! The vertical flow will thus also differ for the two scenarios. Where dolerite underlies the ash, the water from the ash dam will probably drain downwards until it reaches the water level. If the dolerite occurs [if the K-value of the weathered clay is less than that of the ash], the flow will be horizontal and seepage would occur at the surface.

It is believed that the model will be of practical interest in understanding the unsaturated and saturated ash dam/dump and underlying systems undergoing simultaneous desaturation and deformation.

Based on the discussion in Section 2.2, the various processes associated with these interactions can be conceptualized as illustrated in Figure 3-11

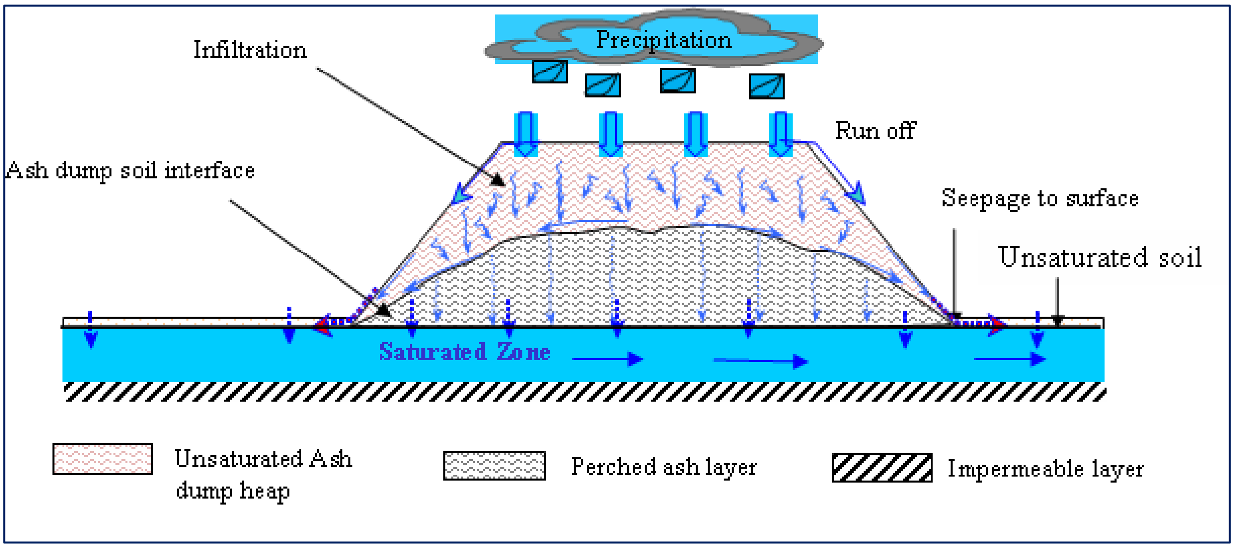

Figure 3-11: Schematic conceptualization of the Tutuka ash dumpsite

CHAPTER 4

NUMERICAL APPROXIMATION OF THE TWO DIMENSIONAL SATURATED-UNSATURATED GROUNDWATER FLOW EQUATIONS

4.1 INTRODUCTION

Methods used to solve the differential equations governing the flow of fluids and mass transport in groundwater can generally be divided into analytical methods, semi-analytical methods and numerical methods (Miroslav and Nielsen, 1994). However, the applicability of analytical and semi-analytical methods is limited to homogeneous domains with relatively simple geometries. Partial differential equations defined over complex domains, as is usually the case in groundwater studies, can consequently only be solved numerically.

Two numerical approximations are commonly used in groundwater investigations: the finite element method and the finite difference method. The finite difference method has the advantage in that it is easy to implement using a computer. However, the method lacks some useful features of the finite element method, such as the direct implementation of mixed or flux boundary conditions, curved boundaries and mass conservation in multiphase flow (Allen, 1985; Bear, 1979; Botha and Pinder, 1983; Verwey and Botha, 1992 and Istok, 1989). The present investigation is for these reasons based on the two-dimensional finite element approximation of the saturated-unsaturated groundwater flow equation, SUFF, originally developed by (Botha, 1985) and later enhanced and extended to three dimensions by (Verwey and Botha, 1992) and is described in Section 4.2.

One difficulty experienced with computerised implementation of both the finite difference and finite element methods, and especially the finite element method, is the generation of a suitable spatial grid or mesh (Botha and Pinder, 1983 and Istok 1989). A finite element mesh generator, discussed in section 4.3, and based on the MATLAB Toolkit of (Zaiceno, 2004) and the cardinal finite element mesh generator CFEM of (Botha *et al.*, 1993), was consequently developed for the present investigation.

4.2 METHOD OF SOLUTION

4.2.1 The Galerkin Finite Element Method

The use of finite element approximation for the solution of a differential equation is so well-known and described in literature, (Botha and Pinder, 1983; Pinder and Gray, 1977; Verwey and Botha, 1992 and Istok, 1989), that only the basic principle as it applies to the present investigation will be discussed here.

The highly non-linear nature of Richard's equation (3.11) in the unsaturated zone due to the dependence of the hydraulic conductivity on the moisture content and pressure head, in combination with the non-trivial forcing conditions that are often encountered in engineering practice, makes Richards equation practically impossible to solve using analytical approaches except in a few special cases (Kulabako, 2006); when it is assumed that the soil medium is homogeneous.

In a numerical method, the flow domain is often divided into many cells. The differential equation, as well as the boundary and initial conditions, are approximated by discrete equations. Solving these discrete equations (on a computer) yields the head in discrete locations (nodes) and time. The numerical solution of Richard's equation requires a decision about the form of the equation to be solved, the constitutive relations used to close the equation, the spatial approximation, the temporal approximations, the non-linear equation and the non-linear equation solution methods.

Generally, numerical methods to solve the pressure head/matric head-based form are most common because they have the advantage of being applicable to both saturated and unsaturated conditions and of accommodating heterogeneous soils (Verwey and Botha, 1992 and Kulabako, 2006). However, numerical approximations based on this formulation generally exhibit very poor conservation of mass, unacceptable time-step limitations (Milly, 1985) and relatively low convergence which seriously undermine its physical basis (Kulabako, 2006). The mixed form of Richard's equation is generally considered superior to the *pressure head*-based form because of robustness with respect to mass balance (Kulabako, 2006). However, conservation of mass alone does not guarantee acceptable numerical solutions as demonstrated by (Celia *et al.*, 1990). The choice of an appropriate interface nodes approximation for unsaturated hydraulic conductivity, as well as proper treatment of the time derivative, have been pointed out as critical in the numerical solution of unsaturated flow (Kulabako, 2006).

The solutions of the general saturated/unsaturated flow equation in this approximation are pressure head based and also density independent. The discretization of the general flow equation is given below.

4.2.2 Discretization of the General Flow Equation

The fundamental concept in the finite element approximation of differential equations is the discretization of the global domain, $\Omega(x,z)$, into smaller (usually irregular) subdomains, or elements $\Omega_e(x,z)$. However, it is not easy to perform all the necessary calculation, if Ω_e is not rectangular.

The established variable order, variable step-size backward difference method for time integration with an evolving spatial discretization approach is applied based upon the local Galerkin method.

The governing equation of flow in (3.11) contains two dependent variables. As shown in Section 3.4.4, the relation between the moisture content and pressure head is highly non-linear. Due to the highly nonlinear nature of relations between relative permeability, water saturation, and pressure head, the governing flow equation given by (3.11) is also highly non-linear, at least in the unsaturated part of the domain (Huyakorn and Pinder,1983).

The general flow equation in (3.11) contains two different dependent variables on its left- and right-hand sides. Such a formulation is not very useful when a differential equation has to be solved analytically. Equation (3.11) is consequently usually transformed into an equation with one dependent variable. This can be achieved by using the water retention curve, defined in Equation (3.5), to replace θ with $\phi(x,t)$. This yields the equation (Botha *et al.*, 1990).

Practically, it is not only difficult but also impossible to solve two dependent variables with a single differential equation such as Equation (3.11), with two dependent variables, θ and $\phi(x,t)$. One possibility mentioned here to prevent this double-dependent variable formulation, is to replace $\theta(x,t)$ with $\phi(x,t)$. This can be done quite easily by using the moisture retention curve in Equation (3.5), which leads to

Equation (4.1). Unfortunately, an efficient numerical approximation for this ϕ-based equation that conserves mass does not exist (Milly, 1985).

However, (Allen, 1985), Verwey and Botha, (1992) and (Celia *et a*l., 1990) have shown that this difficulty can be avoided, if equation (3.11), is used directly.

Allen's method is based on the observation (Botha and Pinder, 1983) that any function, such as $\rho\,\theta(x,t)$, can always be expanded over an interval $[t_n, t_{n+1}]$ in terms of the linear Lagrange interpolation polynomial as

$$\rho\ \theta(x,t) = l_n(t)\,\rho\,\theta(x,t_n) + l_{n+1}(t)\,\rho\,\theta(x,t_{n+1}) + E(\tau)$$

Substitution of this expression for $\theta(x,t)$, excluding the error term $E(\tau)$, into equation (3.11) and collecting the resulting equation at $t_n = t_{n+1}$, yields the non-linear, backward finite difference approximation for time, that is

$$\rho\ \theta^{n+1}(x) - \rho\ \theta^{n}(x) = \Delta t \nabla \bullet \left[\rho\, K(x,t_{n+1}) \nabla \phi(x,t_{n+1})\right] + \Delta t \rho\, f(x,t_{n+1}) \tag{4.1}$$

where the subscripts, n and $n+1$, refer to an approximation of $\rho\theta(x,t)$ at times t_n and t_{n+1}, respectively.

Although there are a number of methods that can be used to solve the non-linear equation (4.1) iteratively (Botha and Pinder ,1983), a very effective Newton-Raphson type iteration method exists. To derive this method, let $h_m^{n+1}(x)$ be the solution of Equation (4.1) after m iterations at the time step t_{n+1}. The solution after $(m+1)$ iterations can then be expressed in the form

$$h_{m+1}^{n+1}(x) = h_m^{n+1}(x) + \delta h_{m+1}^{n+1}(x) \tag{4.2}$$

where $\delta h_{m+1}^{n+1}(x)$ represents a presumably small correction to $h_m^{n+1}(x)$. As $\theta^{n+1}(x)$ and $K(x)$ are both functions of $h(x,t)$, Equations (3.11) and (3.5), Taylor's theorem, can be invoked to write:

$$\rho\theta_{m+1}^{n+1}(x) = \rho\theta_m^{n+1}(x) + \delta h_{m+1}^{n+1}(x) D_h \rho\theta_m^{n+1} \tag{4.3}$$

$$\rho K_{m+1}^{n+1}(x) = \rho K_{m}^{n+1}(x) + \delta K_{m+1}^{n+1}(x) D_h \rho K_{m}^{n+1} \tag{4.4}$$

Substitution of Equations (4.2) to (4.4) into Equation (4-1), yields the following

$$\begin{aligned}\left[\rho\theta_m^{n+1} + \delta h_{m+1}^{n+1} D_h \rho\theta_m^{n+1} - \rho\theta^n\right] = \Delta t \nabla \bullet \left[\{\rho K_m^{n+1} + \delta h_{m+1}^{n+1} D_h \rho K_m^{n+1}\}\nabla\{h_m^{n+1} + \delta h_{m+1}^{n+1} + z\}\right] \\ + \Delta t \rho f(x, t_{n+1})\end{aligned}$$

Rearranging the terms on the right-hand side and assuming that the terms

$$\Delta t \nabla \bullet \left[\delta h_{m+1}^{n+1} D_h \rho K_m^{n+1} \nabla\{h_m^{n+1} + \delta h_{m+1}^{n+1} + z\}\right]$$

are of second order in magnitude,

$$\begin{aligned}\left[D_h \rho\theta_m^{n+1} - \Delta t \nabla \bullet \{\rho K_m^{n+1}\nabla\}\right]\delta h_{m+1}^{n+1} = -\left[\rho\theta_m^{n+1} - \rho\theta^n\right] + \Delta t \nabla \bullet \left[\rho K_m^{n+1} \nabla \phi_m^{n+1}\right] \\ + \Delta t\, \rho\, f(x, t_{n+1})\end{aligned} \tag{4.5}$$

The major advantage of Equation (4.5) over the former similar approximations for the variably saturated flow equations according to (Milly,1985) is that it conserves mass-yielding significantly better balance of mass for a fixed amount of computing efforts.

Consider the integral on the right hand side of equations (4.5) over the domain Ω

$$\begin{aligned}\int_\Omega R_m^{n+1} d\Omega &= -\int_\Omega \left[\rho\,\theta_m^{n+1} - \rho\,\theta^n\right] d\Omega + \Delta t \int_\Omega \nabla \bullet \left[\rho\, K_m^{n+1}\, \nabla \phi_m^{n+1}\right] d\Omega + \Delta t \int_\Omega \rho\, f(x, t_{n+1}) d\Omega \\ &= -\int_\Omega \left[\rho\,\theta_m^{n+1} - \rho\,\theta^n\right] d\Omega + \Delta t \int_{\partial\Omega} \left[\rho\, K_m^{n+1}\, \nabla \phi_m^{n+1}\right] \bullet n ds + \Delta t \int_\Omega \rho\, f(x, t_{n+1}) d\Omega\end{aligned}$$

where **n** is a unit normal vector to the boundary $\delta\Omega$ of Ω, and use was made of the divergence, or Gauss' theorem (Verwey and Botha,1992). The three terms on the right hand side of this equation represent, respectively, a change in water content of Ω, the flux of water through the boundary of Ω and the yield of source/sink during the period Δt. The right hand side therefore represents in effect the mass balance for variably saturated flow. That is if equation (4.5) is iterated until R_m^{n+1} satisfies a prescribed tolerance. The solution of Equation (4.5), $\phi^{n+1}(x,t)$ will also satisfy the law of mass conservation within this tolerance.

To avoid the difficulty of collapsing Equation (4.5) into a saturated situation only, the term $D_t[\rho\theta(x,t)]$ can also be expressed as

$$D_t(\rho\theta) = D_h(\rho\theta) D_t h$$

through the chain rule of differentiation. The first term on the right hand side of this equation can be further written in a more convenient form by replacing θ with the water saturation, S_w as defined in section 3.4.2.

This yields

$$D_h(\rho\theta) = D_h(\rho\varepsilon S_w) = S_w D_h(\rho\varepsilon) + \rho\varepsilon D_h(S_w)$$

$$= S_w[\varepsilon D_p\rho + \rho D_p(\varepsilon)] D_h p + \rho\varepsilon D_h(S_w)$$

$$= S_w[\varepsilon\rho\beta + \rho(1-\varepsilon)\alpha]\rho g + \rho\varepsilon D_h(S_w)$$

$$= \rho S_w[\rho g\{\varepsilon\beta + (1-\varepsilon)\alpha\}] + \rho\varepsilon D_h(S_w)$$

$$= \rho S_w S_o + \rho C(h)$$

where S_o is the specific storativity of the medium, $C(h)$ is the fluid moisture capacity and $h(x,t) = \int_{p_o}^{p} \frac{dp}{\rho g}$ was used to express h in terms of p. The other two parameters incorporated in the above simplification are

$$\alpha = (1-\varepsilon)^{-1} D_p\varepsilon$$

the compressibility coefficients of the medium and

$$\beta = \rho^{-1} D_p\rho$$

is water compressibility, respectively. Substitution of this expression into Equation (3.11), and using the same assumption as the derivation of Equation (4.5), allows one to express Equation (4.5) in the form

$$\left[\rho S_0 - \Delta t\nabla \bullet \{\rho K_m^{n+1}\nabla\}\right]\delta h_{m+1}^{n+1} = -\left[\rho S_0(h_m^{n+1} - h^n)\right] + \Delta t\nabla \bullet \left[\rho K_m^{n+1}\nabla \phi_m^{n+1}\right] + \Delta t\, \rho\, f(x, t_{n+1}) \tag{4.6}$$

This is the approximation to use in the saturated domain of the variably saturated flow.

It is important to note that Equations (4.5) and (4.6) have been derived from the density-dependent flow.

However, the programs discussed in the section below, are consequently based on the density-independent versions of Equations (4.5) and (4.6) and the program developed in this thesis is based on the density independent flow equation.

Equations (4.5) and (4.6) are fundamentally just two elliptic partial differential equations. The finite element method is thus the most efficient method with which to solve them numerically (Botha and Pinder, 1983). After applying the Galerkin method of weighted residual to the governing differential equation and backward difference for time stepping, the resulting set of matrix equations for a transient analysis are given as follows:

$$(A - B)\delta h_{m+1}^{n+1} = -C + \Delta(B\Phi_m^{n+1} + D + F) \tag{4.7}$$

where the symbols A and B are matrices with elements

$$a_{ij} = \iint_\Omega [C(h_m^{n+1}) + S_0 S_w(h_m^{n+1})]\varphi_i(x)\varphi_i(x)d\Omega$$

$$b_{ij} = \iint_\Omega K(h_m^{n+1})\nabla \varphi_i(x)\varphi_i(x)d\Omega]$$

and C, D, F, and Φ_m^{n+1} vectors with element components

$$c_j = \iint_\Omega (\zeta^n - \zeta_m^{n+1})\varphi_i(x)d\Omega$$

$$d_i = \iint_\Omega n \bullet [K(h_m^{n+1})]\phi_m^{n+1}]\varphi_i(x)ds \quad = \quad \iint_\Omega q_n \nabla \varphi_i(x)ds$$

$$f_i = \iint_\Omega f(x, t^{n+1})\varphi_i(x)d\Omega$$

$$\phi_{m,i}^{n+1} = \phi_m^{n+1}(x_i, t_{n+1})$$

The variable ξ is used here to denote either θ or $S_0 h$, while $\varphi_i(x)$ denotes the i-th two dimensional, finite element basis function. Care should be taken not to confuse $\varphi_i(x)$ and the piezometric head $\phi(x)$. These algorithms have been implemented in the program SUFF (discussed in chapter five), that can be used to simulate saturated-variably saturated flow.

The above is the solution to the general equation of saturated/unsaturated groundwater flow equation.

To find the solution for a particular dimension, two-dimension in this case, the two-dimension horizontal or vertical equations were considered.

The primary basis for the iteration schemes in Equations (4.5) and (4.6), is the assumption that the correction term δh_m^{n+1} will vanish if m is sufficiently large. The left hand sides of both equations must thus also vanish when this is true. Since z is independent of time, Equation (4.7) can be rewritten as

$$S_o(\varphi_m^{n+1} - \varphi^n) = \Delta t \nabla \bullet [\rho K_m^{n+1} \nabla \varphi_m^{n+1}] + \Delta t \rho f(x, t_{n+1}) \tag{4.8}$$

in this case. However, this is exactly the well-known backward finite difference approximation for the fully saturated flow equation, Equation (3.11). This shows that Equation (4.8) is indeed the correct approximation to use with saturated flow in the model for variably saturated flow.

It is important to note that Equation (4.8) reduces to a linear elliptic equation for fully saturated flow, as K does not then depend on the piezometric head.

4.3 GRID GENERATION AND FINITE ELEMENT MESH

The accuracy attainable with the finite element method in solving partial differential equations depends ultimately on the sizes of the elements in the grid used for this purpose. The grid must therefore often be refined a number of times before an acceptable solution is obtained.

The generation of a finite element grid is, at best, a very time consuming exercise, the more so the higher the dimensions of the problem. A grid generator is thus almost a necessity when solving two- or three-dimensional partial differential equations with the finite element method.

The main objectives of a grid generator are threefold: (a) to divide the domain of interest into a number of elements, (b) to compute the coordinates of the nodes of each element and (c) to number the nodes and elements uniquely and hence solve the problem iteratively.

The form of a finite element grid and the sizes of its elements depend very much on the problem for which it is required (Botha and Pinder, 1983). An automatic grid generator should therefore always be able to display the grid visually, so that the user can verify and change the grid interactively.

It is standard practice in finite element work to number the nodes anti-clockwise around an element, and in such a way that the bandwidth of the coefficient matrix is minimized (Botha and Pinder, 1983, and Istok, 1989)

A special two-dimensional mesh generator was therefore adapted as part of the investigation in combination with CFEM (Botha *et al.*, 1993) to generate the element, nodal and boundary incidence. This finite element mesh was generated using MATLAB Toolkit by (Zaicenco, 2004).

The CFEM program code was used to divide the domain of interest into blocks and a number of elements and compute the x, z coordinate of the node of each element, element incidence and nodal boundary incidence globally. The node-coordinates and element-nodal incidence are then used as an input to the toolkit to generate the FE mesh using the MATLAB program.

The groundwater flow is modelled in a two-dimensional vertical (x-z plane) cross-section. The preliminary conceptual model domain is depicted in Figure 4-1. This figure also shows the spatial coordinate convention used in the modelling. The x-coordinate origin is taken to be directly underneath the centre of the experimental plot. The modelled region extends 379.8 m to the right. The vertical z- coordinate is taken to be positive upwards. The top ash surface is thus located at an elevation of 81.4 m above the datum level.

The finite element discretization of the model domain is shown in Figure 4-1. Using the x, z coordinates from the preliminary FE data, it was not possible to visualize all the numbers of elements and nodes. A total of 231 rectangular elements were used, along with the element size. The chosen discretization provided sufficient resolution in the flow simulations without requiring excessive computational effort.

The finite element mesh of 81.4 m by 379.8 m domain consisted of x rows and z columns of rectangular finite elements with variable sizes to prevent numerical oscillations, requiring columns as thin as 0.001 m along the interface and top surface as illustrated in Figure 4-3.

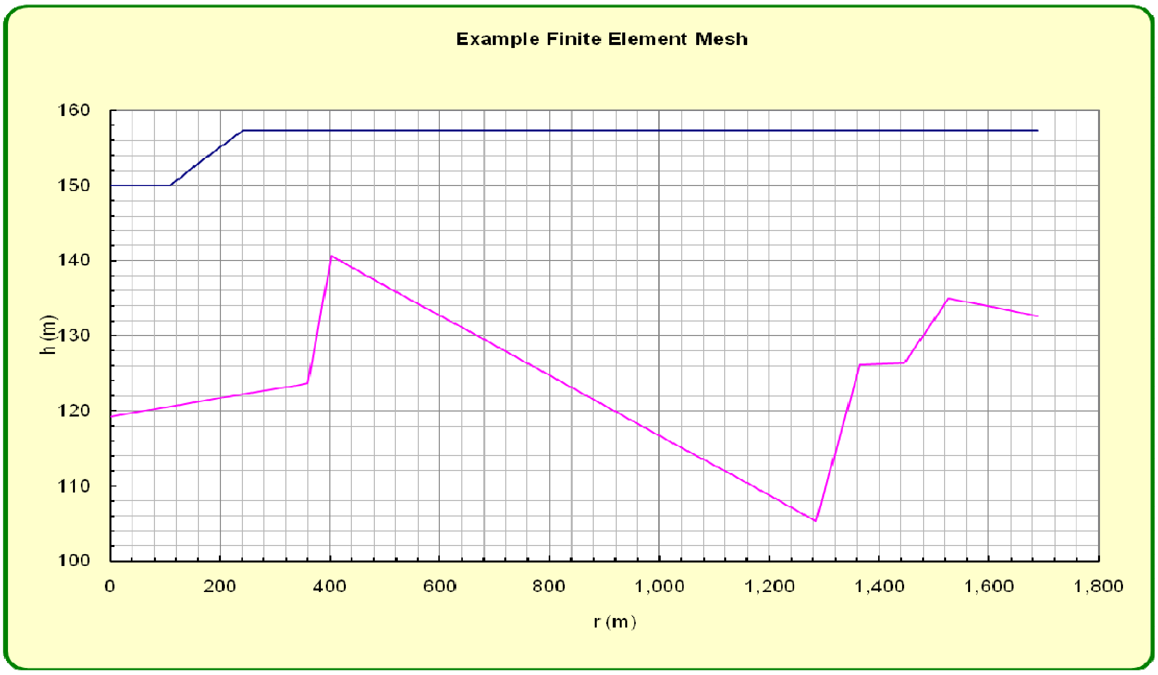

Figure 4-1: Finite element mesh (FE) for BB' cross-section at Tutuka ash dumpsite

For the purpose of convergence, a more refined finite element mesh was also generated where emphasis was given to regions where according to (Istok, 1989 and Botha *et al*., 1990), areas are exposed to boundary changes such as the top ash dump and the two boundary sides. Figure 4-2 below illustrates the initial FE mesh generated for cross-section BB' at Tutuka ash dumpsite. A refined FE mesh with more refinement at the top and the two sides of the conceptual model is illustrated in Figure 4-3.

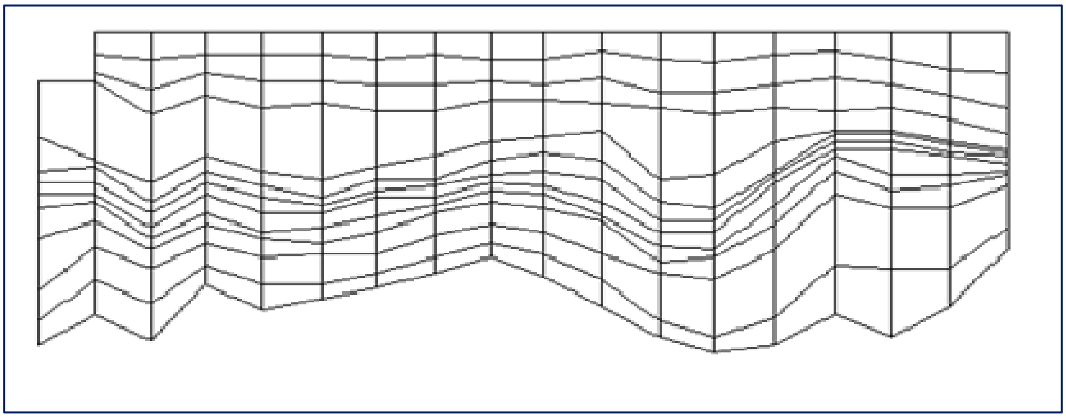

Figure 4-2: Finite element mesh for cross-section BB' at Tutuka ash dumpsite.

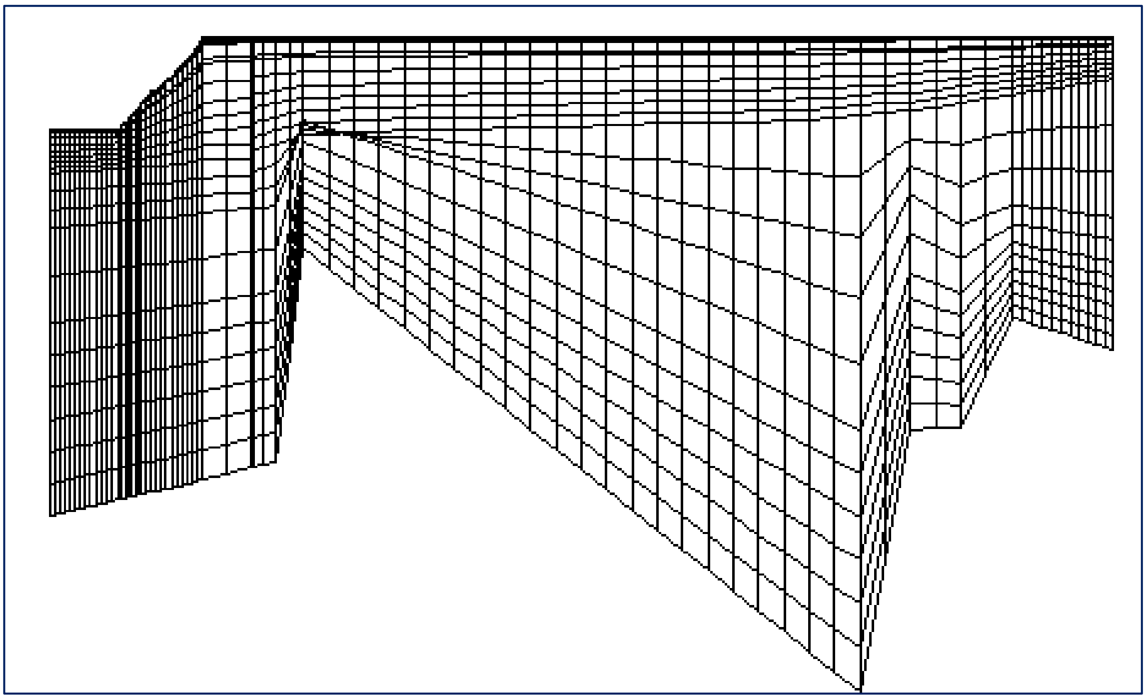

Figure 4-3: A more refined finite element mesh for cross-section BB' at Tutuka ash dumpsite.

4.4 DISCUSSION

While solving such problems, some information with regard to the problem and its structure is lost during the discretization that replaces the partial differential equation by a system of algebraic equations. Numerical method approximations are by far the most powerful methods of solution in addressing such complex equations.

Temporal discretization and spatial discretization is done over the entire study area to minimize the error of approximation.

The purpose of a mesh is merely to provide the computer package with the necessary geometrical information of the site and not the physical information.

CHAPTER 5

APPLICATION OF THE NUMERICAL MODEL

5.1 INTRODUCTION

The first step taken to evaluate the numerical algorithms derived in Chapter 4 was to develop a computer program in FORTRAN and apply it to a hypothetical aquifer/ash dump located in the ash dam at Tutuka which is theoretically underlain by layered clay, weathered and unweathered dolerite. The aquifer, together with the dump, is 81.4 m thick. The water table is at the interface of the ash dump and subsurface aquifer. The basic techniques of implementation, the assignment of initial and boundary conditions and size of the domain are discussed in section 5.2.

Two possible flow case scenarios for the Tutuka ash dumpsite across the geophysical cross-section are discussed to investigate the convergence and robustness of the model as well as the model's sensitivity to change in parameters to different ash types of different age and aquifer parameters. The scenarios were simulated using different boundary and parameter assumptions and a number of modelling scenarios were analysed that differed in the processes taken into account for the transient flow simulation. The emphasis in this study is on saturated-unsaturated flow modelling with the understanding that an accurate description of water movement is the first and most essential step in addressing the assessment of the migration of dissolved chemicals which in many instances will be of ultimate environmental concern. These results are generic and are presented in section 5.3.

5.2 COMPUTER IMPLEMENTATION

SUFF (**S**aturated **U**nsaturated **F**luid **F**low) is a two-dimensional, saturated-unsaturated flow code. The flow solution is based on the pressure head form of the general Darcy's equation and/or Richard's equation. One objective of this study was to test the applicability and numerical accuracy of the code for the difficult Tutuka dry ash dumpsite simulation problem.

Models should be supplemented by carefully conceived fieldwork that not only provides data for estimating model inputs, but also provides an independent confirmation of conditions in the subsurface environment. A FORTRAN program, originally developed by Verwey and Botha (1992), for three dimensional saturated-unsaturated groundwater flow and mass transport modelling was modified to suit the Tutuka study area as a two-dimensional model where the vertical dimension is assumed to be z-axis and the horizontal one x-axis.

5.3 MODEL PARAMETERS

The SUFF code uses the Galerkin finite element technique (Botha and Pinder, 1983) to solve (3.11) in combination with (4.1). The implementation of the program depends on the solution of the governing partial differential equation as discussed under Method of Solutions in chapter 4.

5.3.1 Description of Input Data

The parameters required for simulation of the model are saturated hydraulic conductivity, porosity, moisture retention curves (pressure head versus moisture content, and curve fitting parameters) for unsaturated porous media from laboratory or field samples.

The necessary input data for a simulation include:

- specification parameters: two-dimensional; steady state or transient; all saturated, all unsaturated, or saturated-unsaturated material, region shape and size, and mesh design
- values of ρ, β, and g
- values of the over-relaxation factor and other parameters that control numerical solutions
- initial conditions
- configuration of soil types and geologic formations and hydrologic properties for each soil type; functional relations $\theta(\psi)$ and $K(\psi)$) with the saturated-soil values n and K_o, and the compressibility α.

The input data for SUFF is given in a single file. This file comprises one or more identified groups and data must be mathematically arranged, otherwise an error message of invalid characters will be displayed when trying to execute (run) the program.

5.3.2 Initial and Boundary Conditions

Initial head specification:

The reaction of a groundwater system can only be judged from its observed water level pattern. When modelling an ash dumpsite such as the one at Tutuka, particular attention should be given to obtaining a reliable set of initial hydraulic head (phi) as possible in order to obtain accurate and realistic answers. After a careful examination of the geophysical and borehole log information data, it was decided to use the water level pattern that corresponds with the interpolated resistivity profile for the case scenarios.

At any boundary node, boundary conditions can be imposed that specify the flux, the head, or no-flow conditions. One can write the boundary conditions in terms of either the total hydraulic head ϕ or the pressure head ψ.

Prescribed head (Equation. 3.18) and prescribed flux (Equation. 3.19) boundary conditions are quite straightforward and do not require further elaboration. The seepage face boundary condition applies at boundaries where instantaneous drainage takes place and is physically described as a condition where the pressure head is fixed at *b* = 0, when the soil is saturated and no-flow conditions occur or when a groundwater divide exists and the soil is unsaturated.

For example, along an x-z boundary, we can impose any of the following conditions:

$$\phi = \phi_c \quad \text{or} \quad \psi = \phi_c - z;$$

$$\frac{\partial \phi}{\partial z} = 0 \quad \text{or} \quad 1 + \frac{\partial \psi}{\partial z} = 0;$$

5.3.3 Description of Data Output Files

The file ***suff.itr*** contains a complete description of the finite element mesh, the boundary code of each node, and the hydraulic and transport properties of each soil material. The output data condition depends on the manner in which the logical variable KOW (Kind of Output Wanted) is set.

The file ***suff.prn*** contains output from the program and includes the Darcy velocity in both x and z directions, moisture content and a list of the boundary changes that could take place during simulation. The list of output data depends on how many parameters the KOW conditions have been set for; if the KOW is two, then only the output flow and mass transport values are obtained,, and if the KOW is set to three, the output is flow mass transport plus Darcy's velocity.

5.4 APPLICATION AND DISCUSSION OF RESULTS

5.4.1 General

Output from the program is in the form of plots of pressure-head (ψ), hydraulic head (ϕ), and moisture content (θ) fields for any desired cross-section at any time step. From the pressure-head diagram one can locate the position of the water table; from the hydraulic-head diagram, the flow velocity can be determined at any point as well as the times of travel along various flow paths, the rate of infiltration at the waste source and the rate of discharge to the surface at the exit point.

A reasonable starting point in the siting of a waste disposal project is a steady state analysis of the natural regional flow system. Such an approach provides a prediction of the long-term-average flow conditions without considering the transient influences of the time-dependent climatic conditions and occasional artificial perturbations at the surface.

5.4.2 The Flow Equation

Groundwater flow is modelled in a two-dimensional vertical (x-z plane) cross-section. The modelled domain and assigned boundary condition are depicted in Figure 5-1. This figure also shows the special coordinate convention used in the modelling. The x-coordinate origin is taken to be directly underneath the centre of the experimental plot. The modelled region extends 379.8 m to the right. The vertical (z-) coordinate is taken to be positively upwards. The soil surface is thus located at an elevation of 81.4 m. The dimensions of the modelled region were defined to be large enough so that boundary effects on flow and transport would be negligible. As shown in Figure 5-1, the left and right side boundaries are assigned Dirichlet boundary conditions for flow. The upper boundary that corresponds to the soil surface is also assigned a no-flux condition, except for the zone that corresponds to the irrigation area.

Figure 5-1 outlines a more refined two-dimensional vertical cross section through a hypothetical basin. The mathematical model for this section consists of a 96 x 38 nodal grid with uniform nodal spacing of 30 m in the horizontal direction and 3 m in the vertical direction.

The finite element mesh used for the 379.8 m by 81.4 m domain consists of x rows and z columns of rectangular finite elements with variable sizes to prevent numerical oscillations, and requires cells as thin as 0.001 m along the interface and top surface as illustrated in Figure 4-3. The initial head distribution used for simulation is illustrated in Figure 5-1.

Figure
5-1

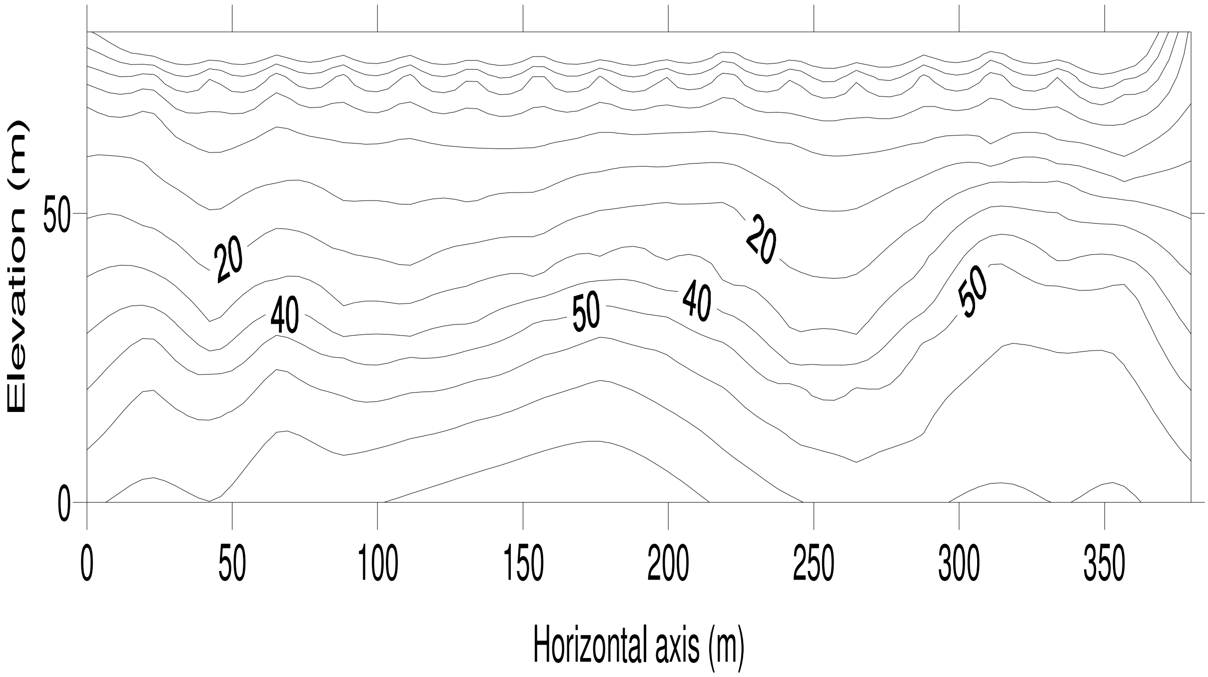

Figure 5-1: Initial piezometric head distribution for cross-section BB' at Tutuka ash dumpsite.

Figure 5-1 above shows the position of initial head distribution for the Tutuka ash dumpsite. The water table is approximately 20 m below surface.

For the purpose of convergence of data, a more refined finite element mesh was also generated with emphasis placed on regions exposed to boundary changes such as the top ash dump and the two boundary sides (Istok, 1989).

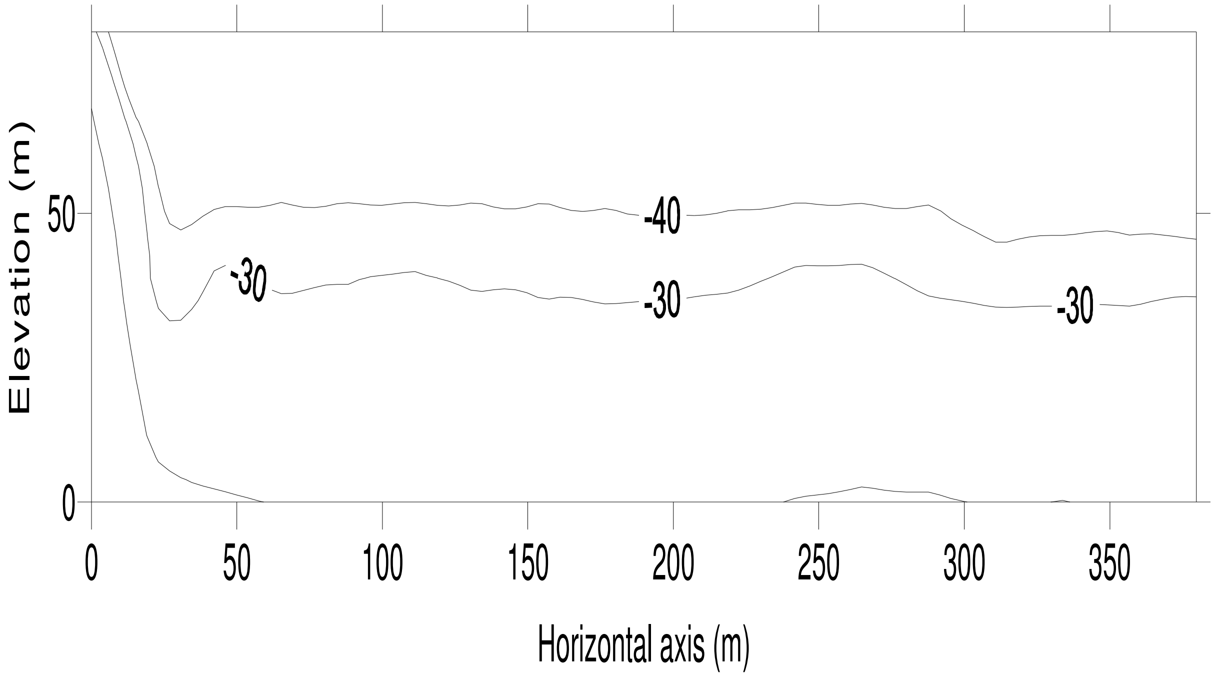

Figure 5-2: Piezometric head distribution for cross-section BB' at Tutuka ash dumpsite after 5 time steps.

Scenario 1: Homogeneous and isotropic ash dump across BB' cross-section.

A 81.4 m profile was set up consisting of two layers: an upper layer, which has a thickness of 6 m composed of ash particles, and a lower layer which has a thickness of 45.151 m and is composed of clay with an undulating weathered and unweathered dolerite layer. The depth of the groundwater table is 7.5 m below the top of the dump. The simulation was run for one day.

In response to the brine water irrigation on top of the ash dam, the water level will rise from 20m to approximately15 m below surface.

The parameters of the profile materials are given in the table below:

Table 5-1: Curve fitting Input values for SUFF

Soil type	**Hydraulic conductivity(m/d)**	**Porosity**	θ_r	θ_s	α**(1/m)**	**n**
Uranium mill tailings	8.64×10^{-4}	0.44	0.09	0.35	1.7	3
Clay	8.64×10^{-4}	0.43	0.068	0.38	0.80	1.09
Weathered dolerite	4.8×10^{-2}	0.43	0.068	0.38	0.80	1.09

The curve fitting input values in Table 5.1 above were used for two scenarios: a two layer model and three layer models. As discussed in the previous section, the two layers represent ash underlined by clay. Uranium mill tailing characteristic values were used to represent the ash. A three layer scenario was also simulated for comparison of results with the two layer model. In the three layer model layers represent ash, clay underlined by weathered dolerite.

Figure 5-2 above shows that the piezometric head and saturation stabilized at a new position after 5 time steps from the moment when the ash was placed on the dump. The excess of water has infiltrated down to the aquifer. The nature of the aquifer underlying the ash dam therefore plays a significant role in potential contamination.

A second scenario was simulated with different hydraulic conductivity values. The higher the conductivity, the faster the flow rates (according to the higher Darcy's velocities). Other factors that play a significant role on the model are position and suitable boundary conditions. The level of the water table may also be altered by changes in the permeability of the underlying foundation material.

The top of the model was assumed to be a rainfall flow boundary with the possibility of changing to a seepage boundary during irrigation or after rainfall; the two sides a flux boundary (Neumann type) and the bottom a no-flow boundary.

5.5 DISCUSSION

The analysis drawn from this chapter is that the model has been simulated for different grid sizes at different time steps.

It is often wise to check the accuracy of a numerical solution by re-running it again with smaller time and space steps. However, the results using smaller time steps and grid size confirm a large convergence error. Conventionally, the more refined the grid size, the more accurate or close the result obtained. Regardless of the laborious data input process, especially so when using the FE method model, approximations are useful to provide guidance as to what management or control mechanisms can be implemented.

The results discussed in this work are all based on conclusions derived from a generic model for the Tutuka ash dump. While such a model can provide a valuable insight into the physical behaviour of such study areas it can never replace field observations. Field observations and models must complement each other.

Models should be supplemented by carefully conceived fieldwork which not only provides data for estimating model input but also provides an independent confirmation of conditions in the subsurface environment.

A tacit assumption, in both the flow and transport simulations, is that the ash dump and underlying Karoo aquifer can be adequately represented by a porous medium flow and transport model. The use of the porous medium such as the SUFF code for the simulation was motivated by the fact that it incorporates many other features that were required in modelling the site, including the ability to accommodate transient infiltration and seepage face boundaries. Another consideration is that there is insufficient quantitative information available on fracture characteristics such as fracture aperture and connectivity. However, these are aspects that can be addressed in future investigations as fracture flow.

Evaporation and infiltration into initially dry soil profiles typically create local mobile regions with large gradients of water head. The highly non-linear relationship between hydraulic conductivity and pressure heads contribute to very steep saturation fronts during infiltration into initially dry soil. Insufficient local resolution for such instances of water flow can result in numerical oscillation and numerical smearing (Milly, 1985). Solutions to these problems have resulted in the advent of temporal and spatial adaptive approaches. General categories of numerical approaches reported in literature to ensure accurate solutions of PDEs for water flow and solute transport in porous media are: i) a better mathematical approximation of the governing PDEs, (Voss, 1984), ii) an incorporation of adaptive grid refinement algorithms and iii) combinations of both of these].

As sufficient field data was not available for this investigation, generic data was used for simulation scenarios with two and three layer options. For the two layer scenario, the top layer comprises ash with a clay layer immediately below the ash. In the conceptual model scheme, the largest portion of material after the ash layer is probably the weathered dolerite. To account for this portion a three layer model was also simulated and results were compared with the two layer model. The conclusion is that if the ash dam is underlain by a low permeability clay layer, seepage from the dam is most probably to the side of the dam regardless of whether a three layer or a two layer scenario exists.

The use of a near surface disposal option requires design and operational measures to provide for the protection of human health and the environment, both during operation of the disposal facility and following its closure, as inappropriate management of landfill waste could result in severe health problems and permanent damage to the surrounding environment.

CHAPTER 6

PROPOSED METHODOLOGY FOR THE DISPOSAL OF FLY ASH AND BRINE

6.1 INTRODUCTION

All living organisms produce by-products, most of which are of little economic value and must therefore be disposed of, preferably using a method that is cost effective and acceptable to the public. Few people are aware of serious consequences that could ensue, if the disposal method being used is ultimately found to be inadequate. Few other methods are as inexpensive as internment/burial and humans have used this method from time immemorial as the preferred and presumably natural one for the disposal of wastes.

Before the advent of the industrial, and particularly the present technological age, the volumes of waste produced were insignificant and consisted mainly of natural substances. The earth's surface could thus easily absorb the waste without any apparent detrimental consequences to humans. What people did not realise though, is that the earth's surface has only a finite capacity to absorb waste. With the ever-increasing population of the world and the large volumes of waste produced by industry, the situation has arisen in many parts of the world where the earth can no longer absorb all the waste produced. Moreover, many of the wastes produced nowadays are of an artificial origin and foreign to the natural environment. Contact with the geological formations in the earth's subsurface, therefore, tends to 'harden' instead of decomposing the waste (Piet and Zoeteman, 1980). Large quantities of waste, previously thought to be safely disposed of, can thus re-emerge on or near the earth's surface, with detrimental consequences for all living organisms (Botha, 1996; Botha *et al.*, 1990).

One of the primary pathways for the migration of waste is the water cycle. Although it has been known for a long time that surface water is very susceptible to contamination, it took disasters such as the Love Canal to show that contamination of groundwater may present an even greater danger (Princeton University Water Resources Program, 1984). The main reasons for this state of affairs can be briefly summarized as follows (Botha, 1996).

(a) All groundwater, with the possible exception of connate water, originates from precipitation that infiltrates the earth's surface. Any water that percolates through a waste disposal site will obviously dissolve and transport some of the waste to an underlying aquifer.

(b) As most contaminants cannot be seen in water and groundwater is, with the exception of springs, not visible, it is difficult to detect the contamination of an aquifer without a suitable monitoring system.

(c) While most people would agree that surface water can transport dissolved solids over large distances, few seem to realise that groundwater is always subjected to the natural groundwater gradient and is thus in a constant state of motion. Groundwater can also transport dissolved solids to areas far from the waste disposal site.

(d) Groundwater generally moves very slowly. Contamination of the source may therefore not be detected until many years after land disposal of the waste (In the case of Love Canal, it took almost fifty years for the detrimental effect of the waste to be noticed.)

(e) Groundwater flows naturally towards any nearby surface stream, river, lake or ocean so surface sources of water can be polluted by groundwater without being noticed, even if the sources are effectively screened from other sources of pollution.

It is of the utmost importance that all possible steps should be taken to prevent a waste disposal site from polluting its natural environment and any groundwater resources underlying the disposal site. The combination of the waste disposal site, its natural environment and underlying groundwater resources will henceforth be referred to as the waste disposal system.

The first step in managing a waste disposal system would be to study the disposal site and its immediate surroundings and use this information to guide the management and control of the waste site. However, as this statement does not provide any guidelines the question may be asked how? And in what detail? These would be easy questions to answer if suitable global (or even local) guidelines were available. Unfortunately, this is not the case, except for radioactive waste, which will be discussed in more detail below. Two reasons can be advanced for this situation.

The first is that the majority of non-nuclear waste sites in the world have, in the past, often been used for a relatively short time. The second is that operators of such sites have not been held accountable for the future evolution of the site and its environment once the operations that generated the waste have been discontinued and the site abandoned. No (or very little) attention was consequently paid to any adverse effects the waste may have on the natural environment and living organisms of waste disposal sites. Indeed, the sites were often managed by what might be called the Least Cost Approach (LCA). In other words, forget about the site and its environment; just keep the cost to the operator as low as possible. This was, for example, the case with Love Canal and the mining of asbestos in South Africa. However, as shown by both examples such a view can cause extreme problems, not only for future inhabitants of areas surrounding historic waste sites, but also the generators of the waste. It is therefore of the utmost importance for both future generations and the generators of waste to manage waste sites with what may be called Least Damage to the Environment (or LDE) methodology rather than the LCA. In other words, minimize damage to the environment of the waste site rather than the cost to the operator.

One consequence of the Love Canal disaster was that many generators of waste began to use geohydrological models to keep track of the pollution of the groundwater by the waste on their sites (Princeton University Water Resources Program, 1984). Implicit in this approach, albeit not often expressed explicitly, is the belief that the geohydrological model could be used to predict the evolution of the site accurately and far into the future. This view and the fact that field investigations are prohibitively expensive, ultimately led to the conclusion that waste sites can be managed with models based on only a few haphazard field observations and generic data; this not only leaves much to be desired but, in fact, often contributed significantly to the cost of managing a waste site. The most desirable scenario is a management system that minimizes field observations and, at the same time, maximizes the managerial information to minimize damage to the environment for any type of waste disposal site. Although difficult, it is possible to develop such a management system from scratch. However, as will be shown below in Section 6.2, much can be gained by borrowing ideas from the ISAM methodology developed by the IAEA for the post-closure assessment of radioactive waste repositories. The following discussion therefore begins with a brief description of the nature of a management strategy for an ordinary chemical waste disposal system. This is followed in Section 6.3 by a discussion on the basic principles of the ISAM methodology, and a summary in Section 6.4 of the five phases into which the methodology is conveniently divided in Section 6.4.

6.2 THE NATURE OF MODELLING A WASTE DISPOSAL SYSTEM

The management of any waste disposal system, including the post-closure safety assessment of a radioactive waste disposal system, is concerned with the long-term future performance of the disposal system. The procedures are consequently often viewed as scientific exercises, carried out by scientists sitting in front of computers trying to predict the actual behaviour of every physical aspect of the disposal system (post-closure assessment of a radioactive waste disposal site) and to how provide solutions far into the future for, thousands or even millions of years. However, what is really required is a defensible estimate of the impact on individuals, directly or indirectly affected by the waste, and their environment as a function of time. This implies that it must be determined how the waste may escape from the waste repository, along which paths it may migrate and what effect it will ultimately have on human beings. The main essence behind a management system for a waste disposal system is thus to investigate, quantify and explain the effects that a waste disposal system will have on its surroundings. Although considerable attention has been given to this problem since the Love Canal disaster, there does not seem to be a universal view of what should be done in this regard, how it should be done and for what reason.

One observation that could aid in developing a more comprehensible view of the management of waste disposal sites is that any such site will be active for two periods.

(a) The *pre-closure period* – the time from inception of the site until its closure, also referred to as the operational period.

(b) The *post-closure period* – This period theoretically begins from the moment the site is closed and extends to the time when the waste does not pose any further threat to living organisms and the environment.

The safety assessment of a radioactive waste disposal system is consequently divided into two phases: namely pre-closure safety and post-closure safety assessments. As it is expected that people will operate the disposal site during the pre-closure period, but not necessarily during the post-closure period, the assessments may differ considerably. For example, the operators of the site will certainly be able to monitor and investigate the site and take corrective actions where necessary during the pre-closure period. Risks to humans pre-closure will also differ from those in the post-closure period. For example, the risk to workers being exposed directly to the waste after the site is closed is zero. A pre-closure assessment of the site could therefore be based on sound scientific principles and procedures, but this does not apply to a post-closure assessment when assumptions and guesses are resorted to.

There is ample evidence that many stable chemical compounds can affect humans and the environment adversely long after the closure of a waste disposal site, indeed in many cases indefinitely, (Botha *et al.*, 1990). This means that both pre- and post-closure management systems are required to fully manage a waste disposal site. However, this is far beyond the capabilities of one person. The following discussion therefore will concentrate only on the establishment of suitable guidelines needed to develop a pre-closure management system for waste disposal sites, based on principles the IAEA developed for the post-closure assessment of radioactive waste disposal sites.

A pre-closure management system for a waste disposal site may briefly be described as a performance assessment of the waste disposal system, which following (Van Blerk, 2000) may be formally defined as: ‘The (iterative) process involving site-specific prospective valuations of the pre-closure phase of a waste disposal system with three primary objectives:

a) identify the data; design and other needs to give defensible assurance that the system will not affect the environment and living creatures adversely during the pre-closure phase.

b) derive the necessary criteria to give reasonable assurance that the system complies with any regulatory requirements.

c) identify any factors that may limit the type of waste that can be disposed at a given site’.

The term iterative in the definition above means that it may be necessary to repeat the process two or more consecutive times. The advantage of such an approach is that it allows one to use information from the previous cycle to refine the management system and the collection of additional data. It also reduces the tendency that the management system may have to focus on one component of the system at the expense of others.

The term 'site-specific prospective evaluations' emphasizes the fact that the management system should use data from the actual disposal system. Not so much with the intent to predict its actual future behaviour, but to better understand the system and its behaviour and to reflect on the importance that specific components may have on the management model. The management of a waste disposal system will never be an exact procedure hence the 'term reasonable assurance' in the definition of a performance assessment above. The management of waste disposal is therefore more a decision tool to determine the conditions for which reasonable assurance of compliance with objectives can be provided, than as a method to predict the actual behaviour of a disposal system into the future.

6.3 BASIC PRINCIPLES OF THE ISAM METHODOLOGY

The original purpose of the IAEA with the development of the ISAM methodology was to assess the post-closure evolution of land-based facilities for the disposal of low and intermediate level nuclear waste (IAEA, 2002, 2004a, 2004b; Van Blerk, 2000). It may seem strange to recommend a methodology developed specifically to assess the behaviour of radioactive waste far into the future for the more mundane day-to-day management of a waste disposal site. Nevertheless, as the following discussion will show, there is little doubt that the management of many waste sites can gain considerably by applying the basic principles of the ISAM methodology. It is not the purpose though, of the following discussion to describe the ISAM methodology in detail which the interested reader can find in the references cited above, but to emphasize those aspects the author deems to be particularly significant for chemical waste disposal sites.

The IAEA introduced the ISAM methodology as a tool to assure stakeholders (government, regulatory authorities, the public at large and interested technical and scientific groups) that the disposal facility has been or will be sited, designed, constructed, operated and closed in a manner that will protect humans and the environment now and in the future (IAEA, 2004a). This applies in particular to so-called critical groups, which following the ICRP (International Commission on Radiological Protection),may be described as: individuals or groups thought to be representative of individuals or populations that may be at the highest risk of being affected adversely by the presence and operation of the waste disposal site (ICRP, 1998).

When viewed from the perspective of a chemical waste site, the purpose of the ISAM methodology can perhaps be best summarized as follows:

a) to provide pertinent information on the future evolution of a disposal system and its environment subject to the current management practices.

b) to use the information gathered in (a) to minimize the risks the disposal system may pose for present and future inhabitants of the waste site and its surroundings—particularly the critical group.

There are at least two differences between the ISAM methodology and the current methodology used in the managing of waste disposals. The first is that a waste disposal site should be viewed holistically as a system consisting of the following components:

- the near field – the waste, the disposal area, the disposal facility and waste, and any engineered barriers including the disturbed zone of natural barriers that surround the disposal facility.
- the geosphere – the rocks and other material situated between the near field and the biosphere (described below). The geosphere normally consists of an unsaturated zone or a saturated zone, or both. (See the discussion in Chapter 3.)
- the biosphere – the physical media (atmosphere, soil, sediments and surface waters) surrounding both the near field and geosphere and how they interact with living organisms (including humans).

The second is the insistence that all actions taken should be practical and executed in a logical, well structured, well documented, transparent, and auditable manner. This constraint can be applied to any management and assessment methodology, but its application is particularly enhanced if the management of a disposal system is divided into five often overlapping but distinct phases. These are: specification of the assessment context; description of the waste disposal system; development and justification of scenarios; formulation and implementation of models; analysis of results and building of confidence among the stakeholders.

6.4 THE FIVE PHASES OF THE ISAM METHODOLOGY

6.4.1 Specification of the Assessment (Management) Context

Central to the ISAM methodology is the idea of assessment context, or more appropriately for the present discussion, management context, the main aim of which is to answer two basic questions: what is it that one wants to assess or manage? And why does one want to manage it? In other words, what is the purpose of the development of a management system for a given waste site, and for whom is it intended? The answer from someone who has employed the historical modelling methodology discussed above would probably be to predict the future concentration of the waste at points of interest to the operator of the site or a regulatory authority. However, this answer does not provide a very precise description of what has to be considered in the management of a given site (the ash, brine or both), nor why it is necessary to manage the waste at all. The geohydrological models used in historical management models often lacked consistency individually and when compared with different models, historical management models usually ended with graphical illustrations of how the concentration of the waste would be dispersed across the site at various times in the future and not much more.

Although the historical modelling methodology is still in use today, the operators of waste sites are experiencing increased pressure from the critical group of stakeholders to ensure their health both now and in the future. It is therefore anticipated that future management methodologies for waste disposal sites will have to demonstrate that the waste will never affect human health and the environment adversely and also ensure that the disposal system satisfies any regulatory framework. A good management methodology will also allow management to test new disposal concepts covering aspects such as assessment philosophy, disposal system characteristics and timeframes.

6.4.2 Description of the Waste Disposal System

The division of the disposal site into the three components, described above: the near field, geosphere and biosphere, especially the geosphere and biosphere, is somewhat arbitrary for a disposal facility located at, or within a few metres, of the ground surface. However, the divisions can significantly be used to ensure that the chosen management system is well documented, transparent, and auditable. It is therefore important to provide a clear definition of these components and their interfaces (e.g. the geosphere biosphere interface) in the description of the management model. Such a description should therefore include some, or all, information of the following nature.

- the near field – the origin, nature, quantities and properties of the waste, engineered barriers (if any), disposal units, the extent and properties of the disturbed surface area (the area underlying the disposed waste) and whether the waste is capped or not.
- the geosphere – of particular importance here are: the geology, geohydrology, geochemistry of the rocks that underlie the site and the historic tectonic and seismic activities at the site.
- the biosphere – this includes the climatic and atmospheric conditions of the site, the presence and positions of surface water bodies, the near surface lithostratigraphy, topography and geographical extent and location of the site, the biota and human activities that may affect the disposal activities.

Note though, that the description of the disposal system must maintain a level of detail consistent with the management context (in particular the purpose, philosophy and timescales). It should also be kept in mind that the development of a system description will always be accompanied by two significant sources of uncertainty. The first is the uncertainty associated with characterising the present nature of the disposal system, and the second, the uncertainty associated with the future evolution of the disposal system.

6.4.3 Development and Justification of Scenarios

It follows from the discussion in the preceding section that the management of a disposal system must include both its present and future conditions. Nevertheless, it may sometimes be necessary to include other anticipated events even less probable events as well. This means that the contributions of many different factors must be consistently, considered and evaluated, often in the absence of quantitative data. The method used in the ISAM methodology to circumvent this problem is to collate and screen all historical and currently available information on the characteristics of the disposal system (e.g. the conceptual model, management practices, climate change, geohydrological conditions, the behaviour of people and any other natural or human induced condition). Personal judgment is then used to develop scientifically sound but hypothetical descriptions, commonly referred to as scenarios, of the disposal system. However, the word scenario (like model) has so many meanings and is so overused that it is not always possible to determine its precise meaning according to the Oxford English Dictionary. The word will consequently only be used in this thesis in the following sense, see also (Van Blerk, 2000).

‘A scenario is one member in sets of hypothetical and real features, events and processes (FEPs) that may affect the rational behaviour of a disposal system.’

The advantage of scenarios is that they allow one to use a mixture of quantitative analysis and qualitative judgments in the management of a waste disposal system. The only difficulty is that the behaviour of a disposal system could potentially be affected by so many FEPs that an unwieldy number of scenarios may result. The approach commonly used to prevent this is to construct a list of FEPs that potentially, or actually, could influence a given disposal system directly or indirectly. This list and the description of the particular disposal system are then used to select and document an appropriate base set of FEPs representing the scenario judged to represent the behaviour of the disposal system as best as possible. This procedure is often supplemented by the selection of alternative and disruptive scenarios that are most likely to have the greatest impact on system performance. Nevertheless, care should be exercised that the selected scenarios are consistent with the assessment context and system description and provide an appropriately comprehensive and credible picture of the system, its possible evolutionary pathways and critical events.

Several methods can be used to generate scenarios; none of them claiming to be the only or right one (IAEA, 2004a). They include methodologies such as expert judgment, fault tree and event tree analysis. However, it is advantageous to use transparent and systematic techniques, as they allow for the development of a justified and documented audit trail for the scenario, thereby enhancing the transparency and defensibility of the exercise, and this can be an advantage in building confidence for the management methodology in the stakeholders.

As mentioned above and illustrated conceptually for the ash brine co-disposal system in Figure 6-1, a waste disposal system can, in general, be divided into two segments, an internal segment and an external segment. It is therefore customary to refer to FEPs associated with the internal segment, such as the waste, the way in which the waste is placed and any engineered or natural barriers, as internal FEPs, and those associated with the external segment as external FEPs, often abbreviated as EFEPs. Nevertheless, there are FEPs, human behaviour in particular, that may affect the behaviour of the disposal system both internally and externally.

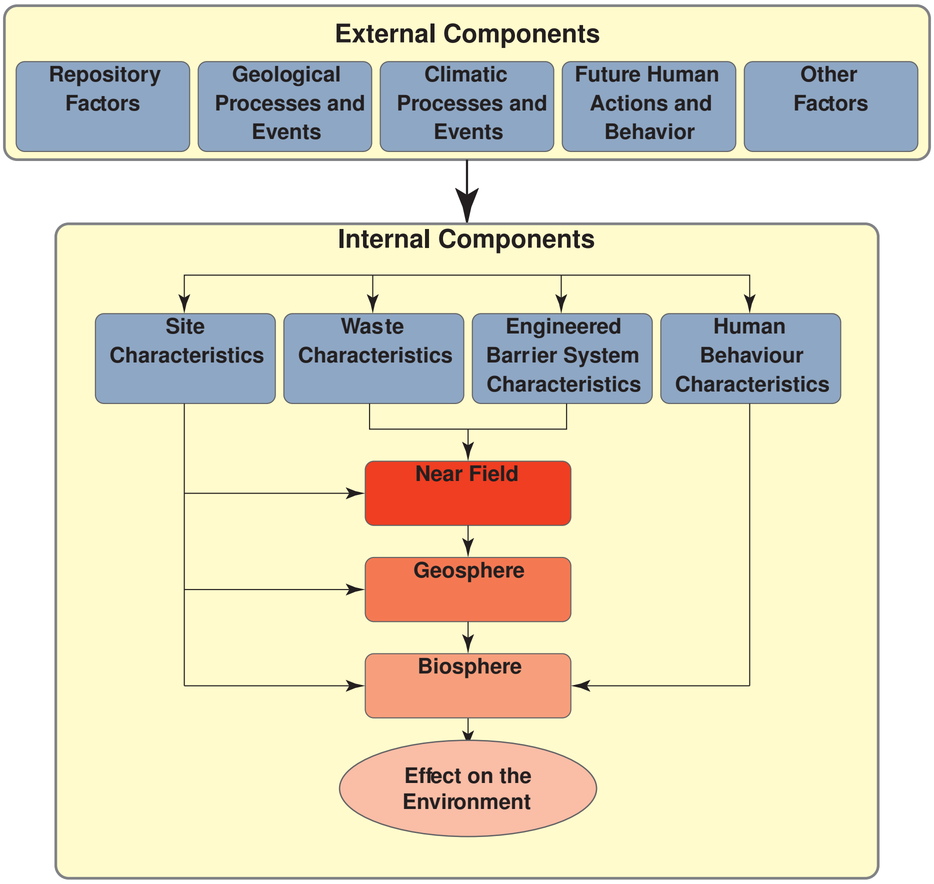

Figure 6-1: Conceptual illustration of the external and internal factors associated with a waste disposal system and the flow of information through them.

The way in which the waste migrates within the disposal system is largely controlled by the external FEPs. Any changes in them will consequently change the migration of the waste and would therefore require the development of new scenarios. External FEPs are, for this reason, often referred to as scenario-generating FEPs. Changes in the internal FEPs, on the other hand, will change the way in which the waste is released to the environment. They therefore may require different conceptual models, rather than different scenarios.

6.4.4 Formulation and Implementation of Models

Once the scenarios have been developed, their consequences must be analysed in terms of the assessment context. The most direct approach to achieve this is to develop a mathematical model for the selected scenarios. As discussed in Chapter 1, this can be achieved by either using ideas from an existing theory or even just simple heuristics, depending upon the level of information available for the disposal system at the time.

The scenarios associated with the near-surface disposal of waste will usually be closely related to subjects such as groundwater flow, heat flow and the dispersion of solids in both water and air, for which a large number of mathematical models exist. Thus, it will seldom be necessary to develop and implement new mathematical models for the scenarios encountered in waste disposal systems. Only if interactions are identified that are not included in established models, or if significant discrepancies between observations and the chosen model, may it be necessary to develop new mathematical models.

As explained in Chapter 1, the mathematical model associated with a conceptual model can be expressed either in the form of an analytical model, or a numerical model. Numerical models and in some cases, analytical models are today often implemented in commercial computer software packages. Unfortunately, the literature accompanying these packages does not describe the mathematical model underlying the package in enough detail and it is often difficult to establish whether a package represents a scenario or conceptual model accurately. The possibility therefore exists that the operator of a management system may use a computer package that is not suitable for the purpose. It is essential that the operator ensures that the mathematical model implemented in the software package to be used is consistent with the selected scenario. In many cases it will not be desirable, nor feasible, to model a disposal system using a single software package.

As illustrated by the discussion in Chapter 2, the observational data available at waste disposal sites, especially older sites, is often limited. The discussions in Chapters 3 to 6 show that it will be difficult to develop comprehensive scenarios and their associated mathematical models for such sites. In such cases, it may be advisable to begin the management model with the simplest possible scenario consistent with the available information and use this to guide the gathering of additional field data before proceeding to more complex scenarios and their associated conceptual models. According to the discussion in Chapter 1, data mining could be of considerable value in developing these more complex scenarios and their associated mathematical models.

6.4.5 Analysis of Results and Building of Confidence

The major objective of using models in the management of a disposal system is to determine how a scenario selected to represent the disposal system will evolve in time and how long it can be regarded as representative of the disposal system. The selected scenario and its associated mathematical model therefore form the core of a management strategy for the disposal system and it is important to know how to handle the uncertainties that are always present in models of waste disposal systems. For example, will a deterministic model (perhaps adjusted for statistically relational parameters and boundary conditions) be sufficient? Or would one need a full probabilistic model? Unfortunately, there are no easy answers to these questions, except to note that they will be dependent on the type and quantity of the available data (Carrera *et al.*, 2005; De Marsily *et al.*, 2005; Neuman, 2005). All that can be said is that the model must be consistent with the management context and provide insight into the behaviour of the system and the role played by specific components of the disposal system in the dispersion of the waste. The results derived from such mathematical models and field observations also often provide the only means by which to build confidence among the various stakeholders. Judging from the available literature, data mining once again would seem to provide the best approach to satisfy both the previous requirements.

6.5 CONCLUSION

The methodology advanced in this chapter for the management of waste disposal sites and their associated disposal systems may seem alien and elaborate. However, judging from local and international developments it may be difficult to develop and maintain waste disposal sites in the not too far future without a management methodology based on these or similar principles.

CHAPTER 7

GENERAL DISCUSSION AND CONCLUSION

Industrial waste management is a worldwide problem for industry, authorities and scientific institutions. The impacts and implications of waste management strategies have not yet been fully identified or quantified.

As indicated in Chapter one, the objective of this thesis arose from a request by parastatals, Eskom and Sasol to provide a detailed proposal for a framework with a view to increasing the competency of both organizations in the management of the co-disposal of ash and brine and the dissemination of knowledge with regard to the impacts of current disposal practice. The main objective of this study should therefore be to develop site-specific mass transport models for both the Tutuka and Secunda sites. Unfortunately, there is simply not enough relevant and critical data available at this time to warrant the development of even rudimentary generic mass transport models for the sites.

Because of the dearth of data, only a vertical two-dimensional version of the model could be implemented to investigate the flow of water through the ash dam at Tutuka power station and its underlying geological formations.

From existing literature and available geohydrological information it can be concluded that ash dumps are heterogeneous porous media, with changes within the assumed ash layer from medium-fine to coarse or the reverse, or with decreasing permeability from fresh to mature ash and from top to bottom of the layer. This is due to compaction, cementation, pozzolanic processing and also the aging of the ash from the time it was dumped on the site.

As discussed above, the hydraulic measurements available to date are relatively limited and therefore specific conclusions cannot be reached regarding the hydrology of ash systems. The only conclusion that can be reached with any certainty is that if the underlying aquifer is clay with less permeability than the ash dump, seepage will occur to the side of the ash dump but will have no adverse impact on the groundwater. If the underlying aquifer is presented in the weathered sediments of

Karoo aquifer, as is applicable to Tutuka, however, waste can drain to this layer and would have an impact on the quality of water.

Modelling continues to pose many challenges, the greatest of which is the data deficiency relative to the needs of a good predictive porous-flow model. We still know little about the control of the compressive subsurface flow system, and there is an accompanying data need for sound management models of the disposal systems. A geohydrological model should therefore never be viewed as an attempt to predict the future of a given waste site, but rather as an aid to assess how effectively the site is managed and controlled. The best way to achieve this is to investigate the waste site systematically, preferably utilizing well-established and accepted international methodology. Unfortunately, no documents exist, at least not at this point in time, that describe such a methodology, its implications and the steps necessary to implement it in practice in a way that can also be understood by interested members of the public.

As shown by the discussion in Chapters 3 to 6, it will be difficult to develop comprehensive scenarios and their associated mathematical models for such sites. It may be advisable therefore to begin the management model with the simplest possible scenario consistent with the available information and use this to guide the gathering of additional field data before proceeding to more complex scenarios and their associated conceptual models. According to the discussion in Chapter 1, data mining could be of considerable value in developing these more complex scenarios and their associated mathematical models.

A two-dimensional transient model for flow through saturated/unsaturated porous ash dump media has been developed. This model numerically solves the governing partial differential equations, which are highly non-linear. The model code uses quadrilateral finite elements for the geometrical assembly: the bilinear Galerkin interpolation for the spatial integration, and the Gaussian elimination for the solution of the resulting matrix equations. In addition to the usual constant-flux and constant-head boundary conditions, the code is capable of applying pressure-dependent boundary conditions at the ground surface. Thus, infiltration into, or seepage from, this surface may be simulated. Each element may be assigned different material properties that allow the investigation of layered geologic formations.

The results discussed in this work are all based on conclusions derived from a ***generic model*** for the Tutuka ash dumpsites. While such a model can provide valuable insight into the physical behaviour of such a study area, it can never replace field observations. Field observations and models must complement each other.

An attempt was also made in this study to provide guidelines for the development of data collection methodology, based on the ISAM Safety Assessment Methodologies for Near Surface Disposal Facilities. No attempt was made though, to develop a fully-fledged methodology as this can only be achieved by using the information from various organizations, regulatory authorities and other interested parties. Once this has been investigated and established building of a structured methodology for this kind of scientific problem – which can become a reference in the specific research field of waste disposal, is vital.

The main conclusion of the present investigation is that a waste disposal site is a complex system that can only be understood through a multi-scale methodology comprising appropriate experimental and modelling tools in association with an effective data acquisition system.

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SUMMARY

Vast quantities of coal combustion residues (ash) and effluents are produced simultaneously in the coal processing facilities of South African parastatals, Eskom and Sasol. The handling and disposal of saline effluents is a difficult and complex problem. The current practice used by these parastatals is to co-dispose the effluents with the ash in landfills; so-called ash dams. Although this practice provides a potentially elegant approach, at least from the viewpoint of the generator of both the ash and effluent, the co-disposal of ash and brine in a landfill could have dire consequences on the environment of the landfill site. This applies in particular to the release of environmentally deleterious and toxic constituents of the ash into the air, soil, surface and groundwater which can lead not only to environmental and land-use problems, but also jeopardize the health of organisms living in the surrounding ecosystem. The question therefore arises as to how Eskom and Sasol better manage their ash dams, to not only satisfy all legal requirements and possible pressure from social awareness groups, but also more importantly, prevent, or at least limit, pollution of the natural environment.

The present investigation arose from a request by Eskom and Sasol to provide them with a detailed proposal for a framework with a view to increasing the competency of both organizations in the management of the co-disposal of ash and brine and the dissemination of knowledge with regard to the impacts of the sites. Two sites were selected by the organizations for this purpose: the Tutuka Power Station and the Secunda Synthetic Fuel Plant.

The application of geohydrological models to assess the behaviour of a waste disposal site has historically often been viewed as an attempt to predict the future behaviour of the site. However, this would require information on relational parameters and known interactions whose behaviour far into the future cannot be determined with certainty. A geohydrological model should therefore never be viewed as an attempt to predict the future of a given waste site, but rather as an aid to assess how effectively the site is managed and controlled. The best way to achieve this is to investigate the waste site systematically, preferably utilizing well-established and accepted international methodology. Unfortunately, at this time, no

documents exist that describe such a methodology, its implications and the steps necessary to implement it in practice in a way that can also be understood by interested members of the public.

A two-dimensional transient model for flow through saturated/unsaturated porous ash dump media has been developed. This model numerically solves the governing partial differential equations, which are highly non-linear. The model code uses quadrilateral finite elements for the geometrical assembly: the bilinear Galerkin interpolation for the spatial integration, and the Gaussian elimination for the solution of the resulting matrix equations. In addition to the usual constant-flux and constant-head boundary conditions, the code is capable of applying pressure-dependent boundary conditions at the ground surface. Thus, infiltration into, or seepage from, this surface may be simulated. Each element may be assigned different material properties that allow the investigation of layered geologic formations.

The results discussed in this work are all based on conclusions derived from a ***generic model*** for the Tutuka ash dumpsites. While such a model can provide valuable insight into the physical behaviour of such a study area, it can never replace field observations. Field observations and models must complement each other.

An attempt was also made to provide guidelines for the development of site-specific data investigation methodology, based on the ISAM Safety Assessment Methodologies for Near Surface Disposal Facilities.

Key words: ash dam/dumpsite saturated unsaturated flow zones, moisture content, ash moisture content, numerical model, flow Equations Finite Element method, FEP methodology.

OPSOMMING

Groot hoeveelhede koolstof verbrandingsreste (as) en vloeibare aflope word gelyktydig in die steenkool prosesserings-fasiliteite van die Suid-Afrikaanse semi-staatsinstellings, Eskom en Sasol, gevorm. Die hantering en wegdoening van hoë southoudende aflope is ŉ moeilike en komplekse probleem. Die praktyke wat tans aangewend word deur hierdie instellings, behels die gelyktydige vrylating van die afvalstowwe en as in die stortingsterreine, wat as die “as-damme” bekend staan. Alhoewel hierdie praktyk na ŉ potensieel aanloklike benadering lyk, ten minste uit die oogpunt van die vervaardigers van die as-afvalstof en die afvloei, kan dit sekere nagevolge vir die omgewing in en om die stortingsterrein inhou. Hierdie is veral van toepassing op die toksiese en beskadigende elemente teenwoordig in die as wat in die atmosfeer, grond, oppervlakte- en grondwater vrygelaat word. Die nagevolge is nie slegs beperk tot die omgewingsgebruike en grondgebruik probleme nie, maar hou ook nadelige gevolge vir die gesondheid van organismes binne die omliggende ekosisteem in. Die vraag ontstaan dus hoe Eskom en Sasol hul as-damme beter kan beheer, om nie net die wetlike verpligtinge en enige moontlike druk van sosiaal-bewuste groepe te hanteer nie, maar belangriker nog, die besoedeling van die natuurlike omgewing te verhoed of, ten minste te beperk.

Die ondersoek wat tans onderneem word, het ontstaan op versoek van Eskom en Sasol. Die versoek behels ŉ indiepte voorstel met die doel om ‘n raamwerk daar te stel om die vermoëns van dié twee organisasies te verhoog ten einde die bestuur van die wegdoening van die as en soutwater, asook die verspreiding van kennis met betrekking tot die impakte van die afvalstowwe op die stortingsterreine, te bevorder. Twee terreine is deur die organisasie vir hierdie doeleindes gekies, naamlik die Tutuka Kragstasieterrein en die Secunda Sintetiese Brandstof Aanlegterrein.

Die aanwending van geo-hidrografiese modelle om die gedrag van ŉ stortingsterrein te bepaal, is op ŉ historiese grondslag gesien as ŉ poging om die toekomstige gedrag van die betrokke terrein te voorspel. Alhoewel hierdie benadering inligting sou benodig aangaande verwante parameters en bekende interaksies, sou gedragspatrone ver in die toekoms strek wat natuurlik nie met sekerheid bepaal kan word nie. ŉ Geo-hidrografiese model moet dus nooit gesien word as ŉ poging om die toekomstige gedrag te voorspel van ŉ gegewe stortingsterrein nie, maar verkieslik as ŉ hulpmiddel vir die bepaling van die effektiwiteit van die beheer en kontrole van die terrein wat toegepas word. Die beste manier om dit te verkry is om die stortingsterrein sistematies te ondersoek, verkieslik deur die aanwending van reeds gevestigde en aanvaarde internasionale metodologieë. Tans bestaan daar geen dokument wat so ŉ metodologie beskryf, of die implikasies en stappe aantoon om dit aan te wend in die praktyk op so ŉ manier dat die beginsels ook verstaan kan word deur belangstellende lede van die publiek nie.

ŉ Twee-dimensionele oorgangsmodel vir die vloei deur ŉ versadigde/onversadigde poreuse stortingsterrein media is al reeds voorheen ontwikkel. Hierdie model los die hoogs nielineêre oorheersend parsiële differensiale vergelykings numeries op. Die model kode gebruik kwadrilaterale eindige elemente vir die geometriese samestelling: die biliniêre Galerkin interpolasie vir die ruimtelike integrasie en die Gaussiese eliminasie vir die oplossing van die gevolglike matriks-vergelykings. Bykomend tot die gewone konstante vloei en konstante drukhoogte grenstoestande, is die kode in staat daartoe om druk-afhanklike grenstoestande toe te pas op die heersende toestand van die grondoppervlakte. Sodoende word infiltrasie na of die sypeling vanaf hierdie oppervlakte gesimuleer. Verskillende materiaal-eienskappe kan aan elke element toegeken word wat die ondersoek van gelaagde geologiese formasies sal toelaat.

Die resultate wat bespreek word in hierdie verhandeling is almal baseer op gevolgtrekkings wat afgelei is uit ŉ ***generiese model*** vir die Tutuka as-stortingsterreine. Terwyl só ŉ model waardevolle insig kan bied in die fisiese gedrag van die studieterrein, kan dit nooit veld waarnemings vervang nie. Veld waarnemings en modellering moet mekaar komplimenteer.

ŉ Poging is ook aangewend om riglyne te voorsien vir die ontwikkeling van ŉ terrein-spesifieke data ondersoek-metodologie wat gebaseer is op die "*ISAM Safety Assessment Methodologies for Near Surface Disposal Facilities*."

Sleutelwoorde: as-dam/-stortingsterrein, versadigde/-onversadigde vloei- sones, voginhoud, as-voginhoud, numeriese model, Vloei Vergelykings Eindige Element Metode, FEP Metodologie.