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4TH INTERNATIONAL CONFERENCE ON ACID ROCK DRAINAGE

SHORT COURSE
FOR

PREDICTION MODELS FOR ACID ROCK DRAINAGE

MAY 31, 1997
VANCOUVER, BC
13:30 - 16:30

Speakers:	Daryl Hockley	Steffen Robertson & Kirsten
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MODELLING PRINCIPLES (WASTE ROCK FOCUS) PART I

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1. TERMINOLOGY

Discussions of modelling are often confused by imprecise or inconsistent terminology. The following sections present and define modelling terminology as used in this report.

Conceptual Models

The term "conceptual model" refers to the set of ideas about the physical, chemical, biological and technological processes that govern the behaviour of the modelled system. The term is particularly useful to distinguish "the set of ideas .... " from the representation of those ideas, typically simplified, in physical or mathematical models.

Physical Models

The term "physical model" refers to laboratory tests, field tests, and any other physical simulation or analogue of the modelled system. By this definition, a humidity cell test is a physical model of some of the geochemical and hydrological processes involved in ARD. Many fields of engineering and science use the term “physical model,” for example where scale models are tested in wind tunnels. However, it is imprecise to use a single term to refer to the wide range of test methods applied to ARD studies.

Mathematical Models

The term "mathematical model" refers to the representation of the modelled system as a set of equations, inputs and parameters. Darcy's law is an example of a mathematical model describing the relationship between permeability, potential, and groundwater flow.

Several terms are used to further characterize mathematical models. They are presented in the following sections as pairs of opposites to make their definitions more clear. To aid the discussion, a generalized mathematical model, adapted from Box *et al.* (1978), is referenced. It takes the form:

$$\eta = f(\mathrm{x}, \beta)$$

where:

- η is the set of outputs from the model, for example the predicted pH and contaminant concentrations in seepage from a waste rock pile;
- x is the set of input variables, for example the precipitation rate and the sulphide content of the rock;
- β is the set of theoretical or empirical parameters, for example the rock permeability and the sulphide oxidation rate; and,
- f is the set of functions describing the assumed relationships among input variables, parameters, and outputs.

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Empirical vs. Mechanistic

The term "empirical" is used herein to refer to mathematical models wherein the functional relationships, f, among input variables, parameters, and outputs are either unknown or not explicitly considered. Since the functional relationships are not included, empirical models do not require input parameters β. A simple example of an empirical model is a graph showing historical contaminant loads vs. flowrates, used to predict future contaminant loads under similar flowrates.

The term "mechanistic" is used herein to refer to mathematical models where the functional relationship f is known or assumed known. The well-known program MODFLOW (McDonald and Harbough, 1988), is an example of a mechanistic model, based on the functional relationship expressed by Darcy's law.

It is rare to find a model which is either fully mechanistic or fully empirical. Most mechanistic models require at least some input parameters β that do not have a theoretical basis. The use of Darcy's law, for example, requires that hydraulic conductivities be measured or estimated. Similarly, most empirical models have some basis in mechanistic understanding, even if only in the choice of inputs x and outputs η for which correlations are sought. As a result, the terms "empirical" and "mechanistic" should be thought of as representing the end members in a continuum.

Deterministic vs. Stochastic

The term "deterministic" is used herein to refer to mathematical models where a single set of inputs x and a single set of parameters β are used to predict a single set of outputs η. An example is the use of a single reaction rate to predict sulphide oxidation in a small, uniform waste rock pile.

The term "stochastic" is used herein to refer to mathematical models where more than one set of inputs ($x_1, x_2, ... x_n$) and parameters ($\beta_1, \beta_2, ... \beta_n$) are used to predict multiple outputs ($\eta_1, \eta_2, ... \eta_n$). An example is the use of a range of reaction rates to predict sulphide oxidation in a large, variable waste rock pile.

Recent advances in computer technology have blurred the distinction between deterministic and stochastic models. In the past, stochastic models commonly described input variables and/or parameters as probability distributions. The functional relationships in the stochastic models were then required to operate on distributions. With today's computers, it is possible to take a deterministic model, even a very complex one, and run it many times with slightly different inputs, to produce the required range of outputs. The terms "deterministic" and "stochastic" can therefore also be seen as end members in a continuum, describing not a fundamental property of the model but rather the method in which the model is used.

Comprehensive vs. Process Specific

The term "comprehensive" is used herein to refer to models that attempt to deal with all of the processes f that govern all outputs η. Examples from other fields include MODFLOW, which is intended to be a comprehensive model of groundwater flow, and MINTEQA2 (Alison *et al.* 1989), which is intended to be a comprehensive model of equilibrium solution chemistry.

The opposite term used herein is "process specific", which denotes models that are concerned with only one of the governing processes, f, and a restricted set of inputs x, β, and outputs η. Examples are models that describe only the chemical oxidation of pyrite, or only the infiltration of water through the surface of a waste rock pile.

The degree to which a model is "comprehensive" depends on the scope of the modelled system. A truly comprehensive model of some ARD problems would need to include not only the underlying ARD processes but also the environmental, social and financial consequences of several possible courses of action. Similarly, whether a model is truly "process specific" will depend on how one classifies several inter-related mechanisms into individual processes. Nonetheless, the terms are useful to recognize the very different intent of groups of models that are currently available, and in discussing priorities for future development.

Engineering Models

The term "engineering model" is used herein to refer to models that are ultimately intended to support practical decisions, usually by predicting the field behaviour of real systems. Perkins *et al.* (1995) used the same term to refer to a group of ARD models that have been developed in the last five years, primarily for use in evaluating remediation alternatives. As is common in many fields of engineering, the models adopt simplifying assumptions about some or all of the processes f, and try to limit the required inputs x and parameters β to those that can be reliably measured or estimated given the current state of the art.

The report by Perkins *et al.* (1995) dealt only with geochemical processes, and defined engineering models to be distinct from empirical models. Chapter 4 below discusses engineering models that are currently in use, and concludes that they span the range from empirical to mechanistic. Hence what distinguishes an engineering model, as the term is used herein, is not empiricism, but the objective of providing support to practical decisions.

Earlier reports from this project used the term "applied model" and distinguished it from "research model". This terminology is avoided here, because most of the available ARD models remain the subject of ongoing research and development.

Engineering models can be deterministic or stochastic. They also need not be comprehensive. Often the best engineering approach is to recognize that only one process is important in a particular decision, and then adopt a process specific model.

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2. Process - Specific Models

This chapter introduces the processes that contribute to, influence, or are influenced by acidic drainage in waste rock. The processes are grouped into the following categories:

_ External processes and variables;
_ Construction of waste rock piles;
_ Infiltration and water flow within waste rock piles;
_ Oxygen and heat transport;
_ Local geochemical processes;
_ Contaminant transport within and discharge from waste rock piles;
_ Downstream impacts; and,
_ Remediation measures.

Many other groupings of the fundamental processes would be equally valid. The emphasis herein is on listing and briefly describing individual processes, and reviewing relevant process specific models.

Figure1 shows how the above listed groups of processes interact with each other and with external processes and variables. In discussing the modelling of inter-related process, the authors have found it helpful to first identify the types of coupling between processes. (See Tsang, 1987, for a full discussion of coupled processes.) The figure denotes strong one-way coupling as single headed arrows and strong two-way coupling as double headed arrows. Indirect coupling is indicated by dashed arrows. Each of the boxes and arrows is discussed in more detail in the following sections.

2.1 External Processes and Variables

- Site geology;
- Mine planning and operations;
- Site hydrogeology; and,
- Site meteorology.

The coupling between external processes and the other ARD processes is generally one-way. In other words, while external factors may influence the other ARD processes, the other ARD processes generally do not influence the external factors. The significance of the one-way coupling is that conceptual and mathematical models of the external factors can be developed independently from ARD models. In fact, for each of the four external processes and variables listed above, a well developed modelling methodology exists outside the ARD field.

2.2 Construction of Waste Rock Piles

The coupling between pile construction and other ARD processes is also exclusively one way. The process of pile construction determines the geometry, composition and to some extent, the physical properties of the pile, which in turn affect other processes. As a result, most mathematical models in the ARD literature treat pile construction as an external process, i.e. as input or a set of input parameters.

The construction process also has a direct effect on the distribution of material with different geochemical properties. Any of the ARD models that use a finite difference or finite element code are theoretically capable of simulating the location in a pile of material with different properties. Time dependent models, such as presented by Chapman *et al.* (1993) and SENES (1991), also have the capability to simulate the growth of a pile over time, by simple addition of new nodes. In general, the limitation of such models is not theoretical but practical. There is seldom sufficient information to justify a detailed model of the pile composition or pile development.

Exceptions to the above arise when remediation of only the most problematic material within a pile is planned. In such cases, greater efforts to model the spatial distribution of material may be justified. An example is provided by WISMUT GmbH, and SRK (unpublished work, 1995), who have recently attempted to estimate the distribution of acid generating material in several waste rock piles in the Ronneburg mining district of former East Germany. The overall reclamation strategy called for the most acid generating material to be relocated to the bottom of an open pit. In order to prioritize and schedule the relocations, it was necessary to create "block models" of the acid generating and neutralizing potential within each pile. The models divided each pile into a series of 50 x 50 x 10 m blocks, each of which were assigned a representative acid generating potential and a representative neutralizing potential. The block values were assigned by methods developed for the interpretation of ore bodies. Initially, a polygonal interpretation of each pile was attempted, based only on drillhole data. A subsequent review of the historical development of some of the piles allowed annual construction boundaries to be identified. New polygonal interpretations were then completed, with the construction boundaries treated as analogues of geologic structures.

One of the piles consisted of waste rock that had been mined in several areas of the pit and placed by conveyor. The only "structures" obvious from the historical information were the individual lifts. Three attempts were made to generate a block model of acid generating and neutralizing potential by geostatistical analysis of drillhole data. Two of the attempts used ordinary kriging, the third used indicator kriging. The conclusion was that all of the geostatistical interpretations were questionable. However, the results of the ordinary kriging were recommended because they allowed a quantitative estimate of the uncertainty associated with each block value, as shown in **Figure 2**

2.3 Infiltration and Water Flow within Waste Rock Piles

2.3.1 Infiltration

Hydrologists use the term "infiltration" to refer to the portion of precipitation that is not directly intercepted by surface vegetation, collected on the surface as ponded water, or transported directly to the stream as surface runoff. In the ARD literature, "infiltration" also refers to the process by which water penetrates the surface of a rock pile. As **Figure 3** shows, hydrologists also distinguish between “infiltration” and “net infiltration”, with the latter referring to only the portion of water that penetrates the ground surface and is not subsequently lost to evapotranspiration. In most ARD literature, this distinction is not accounted for and “infiltration” is used interchangeably with “net infiltration”. Exceptions are Gélinas *et al.* (1994), who distinguish between "shallow infiltration" and "deep infiltration", and C&E (1996) who use the term “hypodermic flow” for shallow infiltration that subsequently drains from the toe of the pile.

In most of the reviewed mathematical models of ARD, infiltration is assumed to be uniform across the pile, and is calculated by multiplying an average precipitation rate by an "infiltration coefficient". Differences arise in the method of estimating the infiltration coefficient. Gélinas *et al.* (1994), SRK (1993b, 1995b), and Brenk (1994) estimated infiltration coefficients from water balances. Cameco (personal communication, 1993) back-calculated the infiltration coefficient from the results of regional hydrogeological modelling. Regional estimates of evapotranspiration were used by SRK (1993b) and Gélinas *et al.* (1994) as a "reality check" on infiltration rates estimated in other ways. SENES *et al.* (1994) proposed to use regional evapotranspiration coefficients directly as a means to estimate infiltration rates.

More complex approaches have also been applied. Schafer *et al.* (1994) used the Soil Conservation Service (SCS) curve number approach, which accounts for surficial soil types and climatic conditions. SENES (1991), SRK (1993b) used the hydrological computer model HELP (Schroeder *et al.,* 1994a,b) which accounts for material variations and wetting/drying cycles. Both approaches were designed for fine-grained soils and not for coarse-grained rock. Their use in ARD models is typically restricted to covered rock piles and rock that weathers rapidly to fine-grained material.

Several researchers from the University of Saskatchewan have participated in the development of a mathematical model called SOILCOVER (O'Kane *et al.* 1993, Swanson 1995). As the name implies, the model predicts the performance of soil covers placed over waste rock piles. The model has been shown to predict infiltration measured by lysimeters placed under the till cover at the Equity Silver Mine (O'Kane *et al.*, 1995).

2.3.2 Water Flow within the Waste Rock Pile

As indicated by **Figure 3**, the flow of net infiltration through a waste rock pile can take place by at least three different processes:

- Uniform unsaturated flow;
- Preferential "channelling" above the water table; and
- Saturated flow below the water table.

In rock piles where sulphide oxidation reactions generate enough heat, evaporation and the movement of water as a vapour can also be important. As mentioned above, some models also distinguish shallow infiltration and/or hypodermic flows.

Uniform unsaturated flow

Uniform unsaturated flow refers to flow in response to the forces of matric suction and gravity. Matric suction results from the affinity of water for rock surfaces and capillary pores, and depends on the soil's grain size, degree of saturation, wetting/drying characteristics and wetting history.

Most models of unsaturated flow use Richard's equation, which expresses Darcy's law in terms of water content:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial}{\partial x}\left(K(\theta)\frac{\partial H(\theta)}{\partial x}\right)$$

where:

$K(\theta)$ is the unsaturated hydraulic conductivity(m/s)
$H(\theta)$ is the matrix potential or suction head (m)
θ is the volumetric water content (m^3/m^3)
x is the distance along vertical profile (m)
t is the time (s).

Written in the above form, it is clear that the unsaturated flow equation accounts for the fact that both the hydraulic conductivity and the matric suction vary with water content. Comprehensive discussions of unsaturated flow can be found in Freeze and Cherry (1979) and Hillel (1980).

The functions $H(\theta)$ and $K(\theta)$ have been a subject of active research by soil physicists for many decades. It is clear that both functions are dependent on the grain size distribution of the soil. However, the only currently available methods to measure the two functions have been developed for agricultural soils. Although they have been successfully applied to tailings, they may not be applicable to coarser waste rock.

Many models in the ARD literature consider unsaturated flow but do not attempt to solve Richard's equation. Scharer *et. al.* (1994), White *et. al.* (1994), and Bennett *et. al.* (1995) represent unsaturated flow as constant velocities in an advection-dispersion equation, or as constant residence times in a CSTR. Both approaches are equivalent to assuming steady state conditions, removing the need to solve Richard's equation. SRK (1993c) found that contaminant concentrations predicted by a mathematical model were affected by both the steady state flowrate and the assumed water content. In other words, faster porewater velocities through drier rock resulted in different contaminant concentrations than slower porewater velocities through wetter rock. The $K(\theta)$ relationship for the waste rock was used to predict the water content required to support steady state infiltration under a unit hydraulic gradient.

Channeling

Morin *et al.* (1991) discussed field evidence for "channelling" in waste rock piles, *i.e.* the flow of water through discrete channels. The most convincing experimental evidence was that provided by Elboushi (1975), who sprayed dilute white paint onto small scale rock piles and noted, after dismantling the piles, that the paint coated only 20% of the rock surfaces below 90 cm depth.

The factors that cause channelling are difficult to incorporate into deterministic models. They occur at finer scales than most models can conveniently incorporate, and they are to some extent random. Erikson and Destouni (1994) used stochastic methods to address the issue of channelling in waste rock piles. Flow along any path was represented by a residence time within the dump, and log-normal and bimodal distributions of residence times were used to show the effects of channeling.

Morin and Hutt (1994) compared sulphate production rates measured in the laboratory to sulphate concentrations measured at the Bell Mine, in Northern B.C. They attempted to account for the difference by claiming that only 5% of the rock in the field had been contacted by channelling water. Subsequently, Morin *et al.* (1995b) recognized that some of the sulphate produced in the field was also precipitated as gypsum, and that the method did not allow a reliable measure of flow channelling in such cases.

SRK (1995) modelled channelling by fitting a simple two-region flow model to a series of precipitation and runoff data. The data were collected from a catchment in southern B.C. that was dominated by a single waste rock pile. The two-region flow model divided net infiltration into two components. Approximately 20% of net infiltration was estimated to channel rapidly through the pile. The remainder passed through the pile more slowly. The two-region flow model was subsequently combined with a simple reaction model to demonstrate the effects of the flow pattern on contaminant loads.

Smith *et al.* (1995) applied a "kinematic wave approximation" to model water flow within waste rock piles. Their approach was similar in principle to the two-region model. However, the flow region was assumed to consist of a number of "channel groups", each with a different conductance. The model was able to match measured hydrographs.

SRK (1996) compared sulphate release and storage data from the Halde Beerwalde waste rock pile, and concluded that only approximately 60% of the pile was being flushed.

Saturated flow

Saturated flow refers to the process of water flow below the water table. In this zone, water is the only phase present within the pore spaces. Unlike channellized flow, the physics of saturated flow is well understood. The governing equation for saturated flow is given by Darcy's law. Comprehensive discussions can be found in many texts, for example, Freeze and Cherry (1979), and Domenico and Schwartz (1990).

2.4 Oxygen and Heat Transport

As **Figure 1** indicates the transport of oxygen through a waste pile plays a central role in controlling the local geochemical processes which influence ARD. At many sites oxygen transport has been shown to be the rate limiting step in generation of acidic drainage. The processes of oxygen and heat transport are tightly coupled such that one process cannot be discussed without discussing the other. As indicated in **Figure 1** oxygen and heat transport are also coupled with the local geochemical processes. Oxygen transport gives rise to sulphide oxidation reactions. The oxidation reactions give rise to heat transport. Heat transport gives rise to air movement and thus oxygen transport.

The main mechanisms by which oxygen is transmitted through a waste pile are:

- transport in infiltrating waters;
- advection of air by pressure difference;
- temperature convection of gases; and
- diffusion.

Figure 4 shows examples of field monitoring data from SRK (1997). The data indicate the complexity of oxygen transport processes in waste rock, and show how the dominant processes can change from one season to another. The following notes are a simplification.

2.4.1 Transport in Infiltrating Waters

Oxygen dissolved in infiltrating waters moves through the pile with the flow of water (advection) and diffuses out to the reactive surfaces. In flooded tailings pits, diffusion through water is the dominant oxygen transport process. Richie (1994a) calculated the sulphate flux through a "typical" dump which would be expected with water as the only oxygen source. He concluded that in terms of the sulphate fluxes measured in waste rock dumps, oxygen-saturated infiltrating waters are not a significant oxygen supply mechanism.

2.4.2 Advection

Advection is the process of air movement under a pressure gradient. In a waste rock pile, three mechanisms cause this: prevailing winds blowing over the pile surface; atmospheric pressure variations due to barometric patterns; and thermal convection through the pile. Thermal convection is a special case of advection and is discussed in the next section.

As with water flow, air convection is described by Darcy's law. The rate of advection through a pile is dependent on: the pressure gradient, the air permeability, and the water content. Higher pressure gradients result in higher rates of air flow through a pile. Higher permeabilities result in higher rates of air flow. The water content affects the amount of available pore space through which air can pass. Higher water contents decrease the air permeability of the material and thus decrease advection rates.

Wind blowing over a waste pile results in pressure differences across the surface of the pile much the same way as those over an aircraft wing (called the Bernoulli effect). Although this effect has been discussed (Ritchie, 1994a), the contribution of prevailing winds to oxygen transport has not been quantified in the field.

Barometric pressure effects are clearly evident in data collected from the Nordhalde waste rock pile in Germany (SRK, 1997).

2.4.3 Thermal Convection

Thermal convection is a special case of advection where pressure gradients are generated by temperature induced density gradients. In waste rock dumps, thermal convection is a significant process for two main reasons:

1) sulphide oxidation reactions are highly exothermic resulting in large temperature gradients; and
2) soil conducts heat poorly thus transferring it to the air phase.

Ritchie (1994a) showed that oxygen fluxes per unit area of waste material caused by thermal convection are much higher than fluxes resulting from diffusion, although occur over a much smaller area. Modeling and field(?) studies (references) have shown that convection is rapidly established in piles with air permeabilities of 10^{-9} m^2 or higher.

Convection has been shown to be a significant process in uncovered piles. Steam rising from uncovered piles has been observed in Ronnenburg, Germany. On one pile where thermal convection occurred over half of a dump, that half remained covered in snow during the winter months while the other half remained bare. Convection generally ceases after emplacement of a cover. Covers limit the oxygen supply to the pile and therefore reduce oxidation.

2.4.4 Diffusion

Diffusion is the process of oxygen movement under a concentration gradient. The consumption of oxygen by sulphide oxidation results in a concentration gradient from the surface of the dump to the point of reaction. Although the diffusion process theoretically occurs in both water and air, for reasons discussed above the diffusion of oxygen through water is essentially negligible for the purpose of waste rock piles.

The primary controls on the rate of oxygen diffusion into a waste rock pile are: the pore space tortuosity, the water content; and the rate of oxygen consumption at the point of oxidation. Increased pore space tortuosity results in lower rates of diffusion. The water content also influences the tortuosity of the pore space; higher water contents result in more tortuous pathways. The oxidation rate influences the depth at which oxygen is totally consumed. Higher oxidation rates result in higher concentration gradients and thus faster rates of diffusion.

Diffusion is controlled to a lesser extent by the composition of the pore gas oxygen is diffusing into. In most cases nitrogen is the primary pore gas in a waste pile. However, if carbonate neutralization is significant, carbon dioxide may be the primary component.

Piles where diffusion dominates show a characteristic monotonic decrease in oxygen concentration with depth (Bennet et. al., 1995). Such piles are said to be oxygen limited. Piles where oxygen remains constant or increases with depth are most likely “advection dominated” and are said to be “oxygen abundant”. Ritchie (1994a) discusses a number of piles worldwide which have been shown to be diffusion dominated. Diffusion is generally considered to be the dominant process in covered piles.

2.5 Geochemical Processes

A recent review by Perkins *et al.* (1995) recognized four classes of geochemical processes that contribute to acidic drainage.

- Oxidation of sulphide minerals;
- Dissolution of carbonates, oxyhydroxides, and silicates;
- Precipitation of oxyhydroxides; and,
- Dissolution and precipitation of sulphate minerals.

The review also mentions co-precipitation, ion exchange and adsorption as having secondary effects.

All of the above processes are influenced by infiltration and water flow, and by the material properties resulting from pile construction. They are also influenced, although to a variable extent, by oxygen and heat transport. Some of the geochemical processes, in particular the sulphide oxidation reactions, consume oxygen and/or liberate heat. Hence **Figure 1** shows a two-way coupling between the relevant boxes. Contaminant transport within and discharge from waste rock is also strongly influenced by geochemical processes, and can in some situations have a feedback effect on them, leading to another two-way arrow in **Figure 1**.

Several recent publications offer good reviews of one or more of the above geochemical processes, notably Perkins *et al.* (1995), Otinowski (1995), Nicholson (1994), Gould *et al.* (1994), Alpers *et al.* (1994), and other papers in the collection edited by Jambor and Blowes (1994). The following sections provide only the minimum necessary to support further discussion of ARD models.

2.5.1 Oxidation of Sulphide Minerals

The oxidation of sulphide minerals releases acid, major and trace metals, and sulphate (Perkins *et al.* 1995).

The review by Morin *et al.* (1991) listed 28 examples of sulphide minerals. Iron sulphides are the most commonly mentioned in ARD literature, and include pyrite (FeS_2), pyrrhotite ($Fe_{0.8-1}S$), marcasite (FeS), as well as arsenopyrite (FeAsS). The significance of other sulphide minerals in ARD generation is strongly correlated with the mineralization. Chalcopyrite ($CuFeS_2$), chalcocite (Cu_2S), sphalerite (ZnS), and galena (PbS) are commonly noted in Canadian ARD literature, for obvious reasons.

Of the above list, pyrite is by far the best studied. The oxidation of pyrite, and other sulphides, has been shown to occur by several different mechanisms, including:

- Abiotic oxidation by O_2;
- Abiotic oxidation by Fe(III);
- Biologically catalyzed oxidation; and,
- Galvanic oxidation.

Figure 5 shows the influence of pH on the relative importance of pyrite oxidation mechanisms, as well as other reactions considered in this chapter.

Abiotic Oxidation by O_2

At pH values greater than 4, abiotic oxidation by oxygen dominates, and the resulting reactions can be summarized as follows:

$$FeS_2(s) + 7/2\ O_2 + H_2O = Fe^{+2} + 2SO_4^{2-} + 2H^+$$

$$Fe^{+2} + 1/4\ O_2 + H^+ = Fe^{3=} + 1/2\ H_2O$$

$$Fe^{3+} + 3\ H_2O = Fe(OH)_3(s) + 3H^+$$

Otwinowski (1994) reviewed experimental data on the above processes and concluded that the first reaction is kinetically controlled with a rate that depends upon the surface area of exposed pyrite, the oxygen concentration, and temperature. Equations to describe the effect of each parameter on the reaction rate were presented. Otwinowski (1994) also reviewed experimental data on the oxidation of ferrous iron. Equations were presented to describe the reaction rate as a function of the

Fe^{2+} concentration and pH. The participation of *Thiobacillus ferrooxidans* was found to have a much stronger effect than the other variables, as discussed below.

Nicholson *et al.* (1990a) concluded that the $Fe(OH)_3$, which is precipitated by the third reaction above, formed a coating around fine pyrite grains, and thereby slowed the reaction rate. Otwinowski (1994) accounted for this effect by considering the pyrite surface area to be a variable. Other authors have been more explicit, and used a shrinking core model to describe the reduction in oxidation rates caused by the $Fe(OH)_3$ coating. The shrinking core model is discussed further below.

Abiotic Oxidation by Fe(III)

At pH values less than 4, the ferric iron produced by the second reaction above remains in solution and can act as an oxidant in the further oxidation of pyrite:

$$FeS_2 + 14\ Fe^{3+} + 8H_2O = 15\ Fe^{2+} + 2SO_4^{2-} + 16\ H^+$$

Otwinowski (1994) reviewed experimental data on the oxidation of pyrite by ferric iron, and concluded that the reaction rate varies with ferric iron concentration and temperature, and inversely with the square root of pH.

The oxidation of pyrite by ferric iron, which can itself be a product of earlier pyrite oxidation, introduces a feedback loop into the above set of reactions. Similar "autocatalytic" reactions have been shown to produce unpredictable or "chaotic" results. Tuzynski *et al.* (1994) investigated whether mathematical models of the above processes would be inherently chaotic, and concluded, "no hallmarks of chaos, quasi-periodicity or intermittency have been found."

Another effect of the ferric iron may be to prolong oxidation in systems where oxygen has been excluded.

Biologically Catalyzed Oxidation

At pH values between 2 and 4, moderate or warmer temperatures, and in the presence of sufficient nutrients, the bacteria *Thiobacillus ferrooxidans* accelerate the oxidation of Fe^{2+} to Fe^{3+}, and can thereby increase the overall rate of pyrite oxidation.

Otwinowski (1994) cited over twenty studies of the influence of *T. ferrooxidans* on pyrite oxidation. Selected data from the studies were used to derive equations describing the dependence of the reaction rate on bacterial population, temperature, pH, oxygen, and Fe^{2+}. It was concluded that bacterial activity reaches its maximum at between 30° and 40° C and a pH of 2.3. Otwinowski (1994) also concluded that the rate of anaerobic pyrite oxidation, by ferric iron, was significantly greater in the presence of *T. ferrooxidans*. Only one set of quantitative data was found in Otwinowski's review, allowing a tentative mathematical model to be proposed.

White *et al.* (1994) included an equation describing *T. ferrooxidans* population growth rates as a function of H^+ and Fe^{2+}. The equation was intended only to provide reasonable limits on bacterial activity under varying conditions, and the authors state that the equation "is obviously not a comprehensive model ... more experimental work is needed".

Galvanic Oxidation

Galvanic oxidation can occur when two sulphide minerals with different electrical potentials come into electrical contact with each other. The mineral with the higher rest potential acts as a cathode and the mineral with the lower rest potential as an anode. The metal sulphide at the anode is oxidized to release metal ions and sulphur; the cathode is not affected. The overall reaction can be written as:

$$\mathrm{MeS} + 1/2\ \mathrm{O_2} + 2\mathrm{H}^+ = \mathrm{Me}^{2+} + \mathrm{S}^0 + \mathrm{H_2O}.$$

where Me is the metal in the anode.

Galvanic oxidation has been noted in studies of thin sections of waste rock, at both acid and neutral pH's (Kwong and Lawrence, 1994), and in other studies, such as those referenced in Perkins *et al.* (1995). It has recently been proposed as the mechanism behind the neutral pH release of zinc from sphalerite-pyrite assemblages in the Keno Hill mining district (Kwong, 1995). The same reference also suggested that galvanic oxidation of other minerals could delay pyrite oxidation, and thereby cause a delay in the development of acidic drainage.

Apart from the reaction stoichiometries and galvanic sequences that can be derived from conventional half-cell equations (*e.g.* Kwong, 1995), no other models of galvanic oxidation were found in the reviewed ARD literature. None of the reviewed engineering models accounted explicitly for galvanic reactions.

Lumped Parameter Models

Some authors have adopted a lumped parameter approach to modelling the abiotic oxidation of sulphides. This approach uses summary equations to describe the dependence of the overall oxidation rate, by any of the above reactions, on the most influential variables, such as oxygen concentration, pH, and temperature. An example is the pair of equations presented by Scharer *et al.* (1995):

$$k_c = A(0.33\mathrm{pH})^{0.7} e^{\frac{-E_a}{RT}} [O_2]$$

$$k_B = B\left[\frac{1}{1 + 10^{2.5-pH} + 10^{pH-4}}\right] e^{\frac{-E_a}{RT}}$$

The former defines the rate of abiotic oxidation of pyrite, the latter the rate of biological oxidation. Parameter definitions are provided under the discussion of the model "ACIDROCK" in Appendix C.

Lumped parameter approaches may be suitable for modelling a limited set of conditions. However, it is clear from the preceding discussion that very different mechanisms of sulphide oxidation can dominate under different conditions. Hence, one would expect different models to be necessary. For example, the equations presented by Scharer *et al.* (1995) cannot account for anaerobic or galvanic oxidation.

"Intrinsic Oxidation" Models

Discussions such as those presented by Otwinowski (1994) or Scharer *et al.* (1995) might lead to the erroneous conclusion that all of the functions and parameters necessary to simulate the processes of pyrite oxidation in waste rock are well understood. Similar compilations of experimental results are presented by Perkins *et al.* (1995) for pyrrhotite, asenopyrite, and marcasite. However, all of the reaction rate data has been obtained under carefully controlled laboratory conditions, most often using homogeneous samples of individual minerals and careful control of bacteria. Extrapolation to field conditions of heterogeneous, mixed mineral assemblages, variable bacterial populations, wet dry cycles and variable oxygen concentrations is not straightforward.

The use of "intrinsic" rates, measured in the field or derived from column tests, is an alternative adopted by some engineering models. The term "intrinsic oxidation rate" was used by Ritchie (1994a,b) to describe oxidation rates measured or estimated from field data. The intrinsic rate was adjusted to account for oxygen limitation and for the shrinking core effect. The term "production rate" was used by SRK (1993c) to refer to contaminant release rates measured in column tests. Monitoring of gas compositions in the field indicated that oxygen was not limited, so the "production rates" were extrapolated to field conditions by correcting for surface area and temperature. In SRK (1993a), the effect of oxygen limitations was also considered. SRK (1997) provides methods for relating the "production rates" of various metals to the pyrite oxidation rate.

Shrinking Core Models

Most of the above discussions deal with the effects of variables on the rate of oxidation at any point in time. However, in many engineering studies, the most important parameter is the rate of change in the oxidation rate as the available sulphide mineral is depleted. When natural depletion processes lead to a reduction in sulphide oxidation, the need for engineered solutions is less acute.

As mentioned above, shrinking core models have been used to simulate the long-term decrease in oxidation rate (*e.g.* Cathles 1979, Davis and Ritchie 1986). The shrinking core model was initially proposed by Wen (1968), and assumes that the reaction rate is controlled by the diffusion of reactants and/or reaction products through the gradually thickening surface layer. Nicholson (1994) used the shrinking core model in studies of sulphide oxidation.

Several of the engineering models in the literature use a form of a shrinking core model to describe the decrease in the rate of pyrite oxidation. The shrinking core model has been shown to allow simulation of some field data, for example the heap leach data analysed by Cathless and Murr (1980). However, the direct evidence for a shrinking core mechanism in waste rock is limited. SRK (1993c) attempted to fit various models of the depletion process to data from column tests, but were unable to find convincing evidence for any one mechanism.

2.5.2 Dissolution of Carbonates, Oxyhydroxides, and Silicates

The dissolution of carbonates, oxyhydroxides, and silicates consumes acid generated by sulphide oxidation (Perkins *et al.* 1995).

As indicated by **Figure 5**, the dissolution of carbonates is the dominant neutralizing reaction at near neutral pH. Morin *et al.* (1991) listed the carbonate minerals calcite and aragonite ($CaCO_3$), dolomite ($CaMg(CO_3)_2$), ankerite ($CaFe(CO_3)_2$), rhodocrosite ($MnCO_3$), and siderite ($FeCO_3$) as potential contributors to acid neutralization. Other authors (*e.g.* Otinowski 1994) have shown that siderite dissolution does not neutralize acid if the iron subsequently precipitates as a hydroxide. Siderite may, however, be important in controlling the soluble concentration of iron (*e.g.* Blowes and Ptacek 1994, and references therein).

Dissolution of oxide and hydroxide minerals can be the dominant neutralizing reaction at pH between 4 and 6. SRK *et al.* (1989) describe a simplified reaction path of typical ARD. The reactions are initially buffered at near neutral pH by carbonate dissolution. Iron released during the neutral pH oxidation of pyrite precipitates as a hydroxide. Once the carbonate buffering is exhausted, the system shifts to a lower pH, where the iron hydroxide becomes the principal neutralizing mineral. Blowes and Ptacek (1994) reported a similar reaction sequence in studies of acid generating tailings at the Heath Steele mine in New Brunswick.

Silicate minerals only participate strongly in acid neutralization at low pH (Blowes and Ptacek 1994, Perkins *et al.* 1995, and references therein). The dissolution may be total, or may involve rearrangement to a more stable phase. Phyllosilicate minerals such as clays and micas have been identified or indicated as neutralizing minerals in waste rock (e.g. Lefebvre *et al.* 1995). Perkins *et al.* (1995) concluded that clay minerals are the most reactive silicates.

Many conceptual models of ARD, such as the simplified reaction path presented by SRK *et al.* (1989), assume that the dissolution of neutralizing phases reaches local equilibrium. This assumption is supported by results such as those of Evangelou (1985), which indicated that the dissolution of calcite in hydrochloric acid reached equilibrium in about one hour. Blowes and Ptacek (1994) and Al *et al.* (1994) are recent examples of field studies of tailings which also indicated that neutralizing reactions reached equilibrium.

Several "all purpose" geochemical models have been developed to predict equilibrium concentrations. Perkins *et al.* (1995) presented a comprehensive review of equilibrium models that use an equilibrium constant formulation. Among those commonly cited in the ARD literature are MINTEQA2 (Alison *et al.* 1989), PHREEQ (Parkhurst *et al.* 1990), and EQ3/EQ6 (ref). For example, Al *et al.* (1994) used a transport-reaction code that employs a version of MINTEQA2 to simulate neutralization and other secondary reactions. The model "ACIDROCK" (Senes 1991, Brenk Systemplanung 1994) is an example of an ARD model that uses the equilibrium constant approach to describe neutralizing reactions.

The Pitzer ion interaction approach (Pitzer 1973, 1979) to model high ionic strength solutions has also been applied in the ARD literature (*e.g.* Alpers and Nordstrom 1991). Pitzer modifications of some of the above models exists, but their application is limited by the availability of input parameters.

Perkins *et al.* (1995) and other reviews (e.g. Mangold and Tsang 1991) neglected a third type of equilibrium model that actually predates the equilibrium constant approach. The initial computer models of chemical equilibria, developed by the Rand Corporation (1965) calculated equilibrium concentrations by direct minimization of the total Gibb's free energy of the system. For the purposes of ARD modelling, the Gibb's free energy approach has the advantage that all phases can be considered at the same time. In contrast, the equilibrium constant method requires that all aqueous equilibria be evaluated first, followed by solubility constraints. The result is an iterative process which often proves to be unstable, especially when mineral dissolution and re-precipitation reactions are numerous. Unfortunately, with the exception of the model described by Clasen *et al.* (1985), the Gibb's free energy approach is largely neglected in current practice. No mention of it was found in the reviewed ARD literature.

As pointed out by Morin *et al.* (1991), the rapid movement of water in some waste rock may prevent equilibrium from being reached. Other factors that may interfere with neutralization reactions are the low surface area of some carbonate and silicate bearing rocks, and the uneven distribution of acid generating and neutralizing minerals. For example, SRK (1994a) measured pH values in the field and laboratory that were below the level expected for buffering by carbonate, even though the rock clearly contained carbonate minerals. Neutralization was therefore modelled as kinetically controlled.

2.5.3 Precipitation of Oxyhydroxides

The precipitation of oxyhydroxides releases acid and consumes major and trace metals (Perkins *et al.* 1995).

The precipitation of iron hydroxide, and its influence on pyrite oxidation, was mentioned above. The reaction not only releases acid, it also removes ferric iron from solution, and thereby interferes with the oxidation of sulphide minerals by the Fe(III). Freshly precipitated iron and aluminum oxyhydroxides can also provide sorption sites for trace metals, as discussed further in Section 3.5.5. As indicated by **Figure 5**, the precipitation of oxyhydroxides is prevalent at pH above 5. As a rough "rule of thumb" iron hydroxide phases generally precipitate at one pH unit lower than aluminum hydroxides.

The precipitation of oxyhydroxides is rapid, and is most commonly modelled as an equilibrium reaction. The "all purpose" geochemical equilibrium models reviewed by Perkins *et al.* (1995) are examples. One weakness of current geochemical models is their inability to predict which of the many stable and metastable oxyhydroxide minerals will form in a natural systems (Alpers *et al.* 1994). For example, Bigham (1994) reviewed the complex relationships among the iron oxyhydroxide minerals ferrihydite, lepidocrite, goethite, and the sulphates schwertmannite and jarosite, and noted that the mineralogy of oxydroxides has been "oversimplified" in many studies of ARD.

2.5.4 Dissolution and Precipitation of Sulphate Minerals

The dissolution and precipitation of sulphate minerals mediate dissolved metal and sulphate concentrations (Perkins *et al.* 1995).

For sulphide oxidation at or near neutral pH, where the acid is neutralized by calcium carbonates, precipitation of gypsum results. Gypsum ($CaSO_4*2H_2O$) is a relatively insoluble sulphate, and equilibrium with gypsum maintains total dissolved solids (TDS) concentrations in the range of 2000-3000 mg/L. SRK (1993b) discussed water quality monitoring data from some of the waste rock piles in the Ronneburg mining district in the former East Germany. For piles where the buffering is instead dominated by magnesium carbonates, TDS concentrations as high as 20,000 mg/L were measured. Although acidity was effectively neutralized, the resulting sulphate and hardness concentrations exceeded receiving water criteria.

Alpers *et al.* (1994) reviewed reports of secondary sulphate minerals associated with ARD. It was concluded that melanterite ($Fe^{II}SO_4*7H_2O$) is "probably the most common" of the iron sulphate minerals. Of the hydroxy-sulphate minerals, aluminum hydroxy-sulphate ($Al_4SO_4(OH)_{10}*H_2O$) and schwertmannite ($Fe_8^{III}O_8SO_4(OH)_6$) were noted.

Examples of ARD models that incorporate sulphate precipitation were found in the reviewed literature. SRK (1993d) used MINTEQA2 to successfully predict calcium, barium and sulphate concentrations in tailings porewater at the Key Lake mine in Northern Saskatchewan. Brenk Systemplannung (1994) discussed the effects of jarosites on the sulphate levels anticipated after flooding of waste rock in the Lichtenberg open pit, but it was not clear whether any mathematical model was applied.

2.5.5 Co-precipitation, Ion Exchange and Adsorption

Perkins *et al.* (1995) describe sorption processes as having a secondary effect on trace metal concentrations in acidic drainage.

Sorption reactions occur between aqueous species and reactive surfaces. In ARD, the most reactive surfaces are those formed by the precipitation of iron and aluminum hydroxides. For example, Alpers *et al.* (1994) presented electron micrographs showing the arsenic enrichment of iron oxyhydroxide coatings on pyrrhotite grains retrieved from the Delnite tailings impoundment in Ontario.

Leckie *et al.* (1980) described laboratory studies and mathematical models of the reactions between iron oxyhydroxide and trace metals. Subsequent studies (*e.g.* Davis *et al.* 1986, Honeyman 1984, Westall and Hohl 1980) have improved upon the mathematical models. The current understanding is that the strength of the sorption reactions depend on the trace metal, the mineralogy, crystallinity, and surface area of the adsorbent, and the ionic strength and pH of the solution. Application of the laboratory models to complex natural systems like mine wastes is therefore difficult. Some attempt has been made to quantitatively model the adsorption/coprecipitation of arsenic by ferric hydroxide in mine tailings (personal communication with W.J. Snodgrass, Beak Consultants, 1991).

More commonly, sorption reactions are either neglected by ARD models or accounted for by a simple "distribution coefficient". The distribution coefficient is assumed to represent the (constant) relationship between the aqueous and sorbed concentrations of a trace metal. For example, SRK (1993c) modelled the adsorption of nickel, arsenic and radium-226 onto sandstone waste rock from the Key Lake mine using literature values of distribution coefficients. A similar approach was adopted by Brenk Systemplannung (1994) to model the adsorption of radionuclides to organic carbon in waste rock at the Ronneburg mining district.

2.6 Contaminant Transport within and Discharge from Rock Piles

Figure 1 shows the processes of contaminant transport within and discharge from rock piles as being the result of the geochemical and water flow processes. The two-way coupling with geochemical processes arises because the transport can provide new inputs to local reactions.

2.6.1 Transport Mechanisms

Mechanisms of contaminant transport mentioned in the ARD literature include:

- Advection in water;
- Molecular diffusion in water;
- Hydrodynamic dispersion in water;

Transport of airborne contaminants, such as radium-226, is also discussed in the literature.

The importance of advection in comparison to diffusion or dispersion can be assessed by calculating the dimensionless Peclet number, $Pe = VL/D$, where V is the (advective) velocity, D is the diffusion or dispersion coefficient, and L is the length scale of interest. Peclet numbers greater than 10 indicate that advection is the dominant transport process.

For a waste rock pile with a depth of 10 m, and assuming a molecular diffusion coefficient of $1\text{x}10^{-5}$ cm/s (**ref.**), advection would be dominant whenever the average velocity exceeds 0.1 mm/day, or 4 cm/ year. Clearly, molecular diffusion is unlikely to be an important contaminant transport process in acidic drainage.

Hydrodynamic dispersion is caused by the variability of flow rates. Models such as the ones presented by Erikson and Destouni (1994) and Smith *et al.* (1995), both of which are discussed in

Section 3.3.2, account for the variability in flowrates by considering more than one flow channel. However, it is also possible to account for hydrodynamic dispersion using Fick's law, with the diffusion coefficient replaced by a "dispersion coefficient". The results is a so-called "advection-dispersion equation", where the water is assumed to be advected at a mean velocity, and dispersed both ahead and behind the mean velocity. SRK (1993a) is an example of an ARD model that incorporates an advection-dispersion equation.

It is clear from the above examples that a number of models are capable of simulating the dominant contaminant transport processes in waste rock piles. However, as indicated by Figure 1, all require inputs describing the flow of water within waste rock piles. Hence weaknesses in the fundamental understanding of flow patterns, in particular channelling, limit the value of such models.

2.6.2 Coupled Transport and Reaction

In some situations, say where a waste rock pile contains layers of material with different geochemical properties, it is necessary to consider the coupling of contaminant transport and geochemical process. In other cases, mathematical models treat the reaction of contaminants after their release from primary phases as part of the transport process, normally for computational convenience.

The coupling of transport with reaction leads to unexpected phenomena and to equally unexpected computational difficulties, to the extent that it is now customary to speak of "transport-reaction modelling" as a specialty in itself. Rubin (1983) presented a discussion of transport-reaction modelling which remains a good survey of the field. Rubin classified current modelling efforts distinguish between two broad classes of chemical processes:

- Processes or reactions sufficiently fast and reversible so that equilibrium may be considered to exist; and,
- Reactions that are relatively slow and irreversible where assumption of local equilibrium conditions are inappropriate.

Rubin (1983) has two additional levels of classification of chemical reactions within each of the classes above as follows:

- Reactions are distinguished by the number of phases involved, as either homogeneous (single phase) or heterogeneous (more than one phase); and,
- Within the heterogeneous class of reactions are the surface reactions (i.e. adsorption and ion exchange), and chemical reactions in the classical sense of the word (precipitation, dissolution, oxidation/reduction and complex formation, although the latter two items are not necessarily heterogeneous).

This classification leads to six classes of reactions with their typical mathematical formulations. For example, local equilibrium may be described by chemical relation equations which are algebraic, kinetic models on the other hand involve partial differential equations. Rubin presented simplifications of each type of problem. These simplifications still represent the state of the practice today.

The most commonly used simplification is the "retardation factor", which represents the sorption of a contaminant (see Section 2.5.5) as a decrease in transport rates. The approach leads to a very simple transport reaction model, but is only strictly correct when the adsorption can be described by a liner, reversible, equilibrium isotherm. SRK (1993c) and Brenk Systemplanung (1994) are examples of ARD models where a retardation factor was used to account for the sorption of contaminants during their transport through the waste rock.

Mangold and Tsang (1991) and Yeh and Tripathi (1989) have reviewed generalized approaches to transport-reaction modelling (i.e. approaches which do not use Rubin's simplifications). Mangold and Tsang (1991) emphasized the capabilities of publicly available software. Yeh and Tripathi (1989) concentrated on the advantages and disadvantages of the underlying formulations. Their conclusion was that a sequential iteration between transport and reaction algorithms offered the most flexible and stable approach. The sequential solution of transport and reaction algorithms is common in finite difference models of acidic drainage, *(e.g.* SRK 1993a, Brenk Systemplanung 1994). However, none of the reviewed literature explicitly mentioned the use of iterations to assure convergence.

3. ENGINEERING MODELS

As discussed in Section 1, the term "engineering models" refers to models that are intended to support practical decisions about real systems. Examples of the decisions supported by the engineering models reviewed herein are the amount of a bond required to cover the long term costs of ARD collection and treatment, the effectiveness of material segregation in reducing contaminant loads, and the effectiveness of covers for the same objective.

The engineering models reviewed for this study are summarized in Table 1. The models are described in terms of the processes outlined in Section 2. The descriptions of some of the models were found to be incomplete in the reviewed literature, and some models were developed for applications other than waste rock (usually tailings or analysis of results from a particular laboratory test). Examples are the models TRABAD and MINTOX.

Looking quickly through the table, two conclusions become apparent. The first is that there is a wide disparity in the number of processes explicitly accounted for by the various models. The table is organized so that more empirical models are in the first columns, and more mechanistic models in the latter columns. The second conclusion is that the most significant differences among the more mechanistic models are in their method of handling oxygen and heat transport, geochemical processes, and contaminant transport within the rock pile.

Engineering models will be discussed in more detail during the short course, using examples from the instructors' experiences.

These notes were excerpted (with minor revisions) from:

Steffen Robertson & Kirsten (Canada) Inc., "Modelling Acidic Drainage from Waste Rock Piles",
Draft Report S1202P9 for Ministry of Energy Mines & Petroleum Resources and Environment Canada,
October 1995.

Welcome Screen Search Report List

MODEL	Technical Committee	AMD TIME	Morin and Hutt Empirical
Parent Codes	n/a	n/a	n/a
Reference	xxxx (xxxx)	Ziemkiewicz (1995)	Morin and Hutt (1994)
developed for	estimating long term lime addition for ARD	predicing effluent chemistry from waste rock piles	predicing effluent chemistry from waste rock piles
dimensions	n/a	n/a	n/a
Solution Method	empirical	empirical	empirical
Construction of Waste Rock Piles	n/a	n/a	n/a
Infiltration and Water Flow within Rock Pile	not accounted for	- infiltration coefficient - requires estimation of % rock flushed	- infiltration coefficient - % rock flushed back/calculated from field data
Oxygen and Heat Transport within Rock Pile	n/a	n/a	n/a
Geochemical Processes leading to Contaminant Release	n/a	estimated from ABA data	estimated from laboratory kinetic tests and field observations
Contaminant Transport within and Discharge from Rock Pile	n/a	?	fails to account for secondary mineralization of species

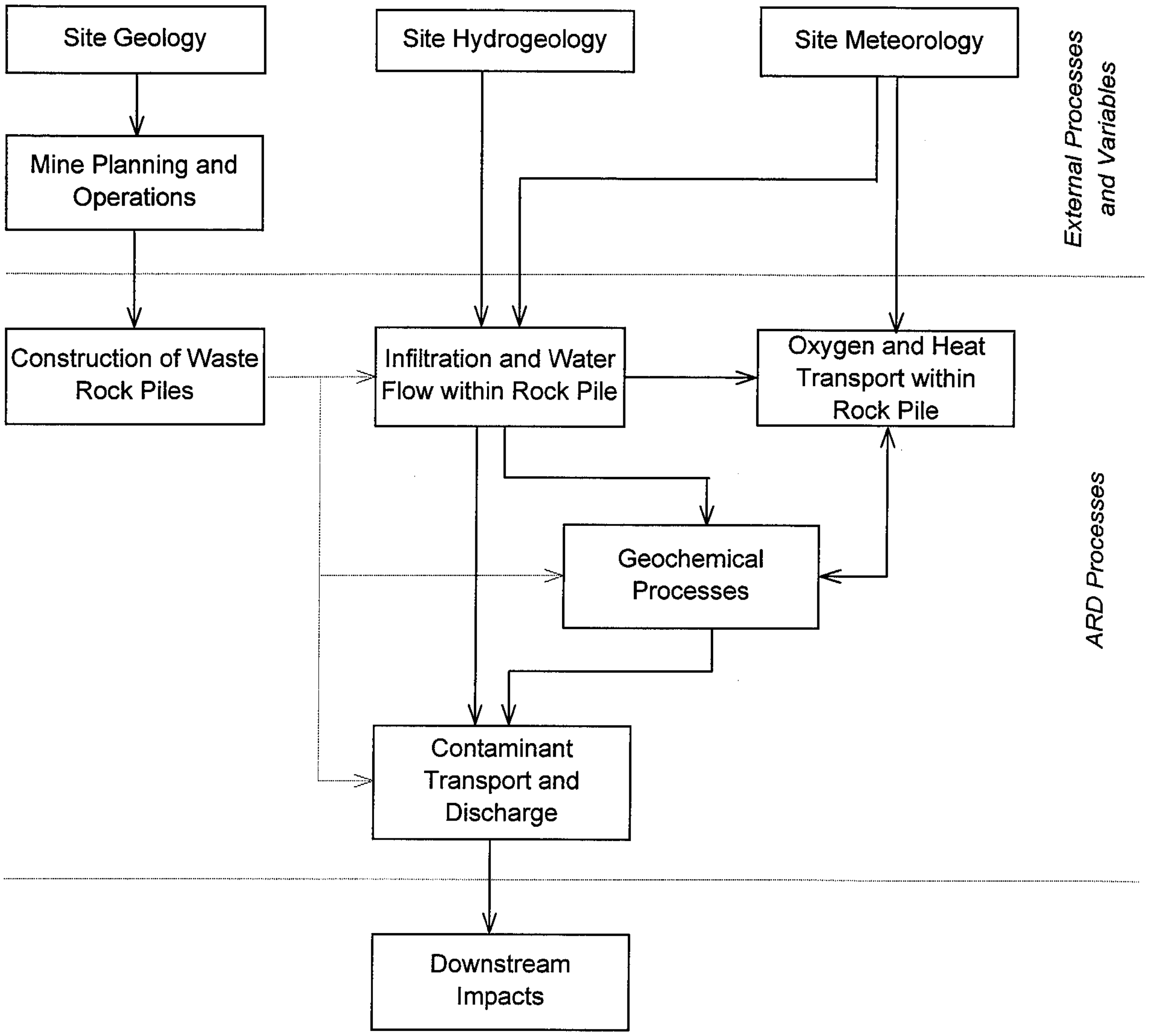
Welcome Screen Search Report List

MODEL	Q-ROCK	ACIDROCK	FIDHELM
Parent Codes	KINDYN	RATAP	-
Reference	SRK (1993a,b) Chapman et. al. (1993)	Brenk (xxx) SENES (1991) Scharer et. al.(1994)	Ritchie (1994) Bennett et. al. (1995)
developed for	estimating ARD for waste rock piles	estimating ARD from waste rock piles	studying oxygen transport mechanisms in waste rock piles
dimensions	1	1	2
Solution Method	finite difference	finite difference	finite difference
Construction of Waste Rock Piles	blocks added during simulation to simulate pile growth with time	fixed throughout simulation	fixed throughout simulation
Infiltration and Water Flow within Rock Pile	- infiltration coefficient - assumes steady state flow through pile	- xxx (199x) used HELP model to estimate infiltration - assumes steady state flow through pile	- infiltration coefficient - water flow described by continuity equation for multiphase flow
Oxygen and Heat Transport within Rock Pile	- oxygen diffusion - no heat transport	continuity equations for oxygen and heat transport	continuity equations for oxygen and heat transport
Geochemical Processes leading to Contaminant Release	oxygen dependant oxidation model	- shrinking particle oxidation model for fine fraction - shrinking core model for coarse fraction	temperature dependant oxidation model
Contaminant Transport within and Discharge from Rock Pile	- mass transport by advection and dispersion - considers decay, ppt. and sorption of radionuclides - equilibrium reaction, ppt. and dissolution of aqeous species	- mass transport by advection - considers decay, ppt. and sorption of radionuclides - equilibrium reaction, ppt. and dissolution of aqeous species	- mass transport by advection - no geochemical component

Welcome Screen Search Report List

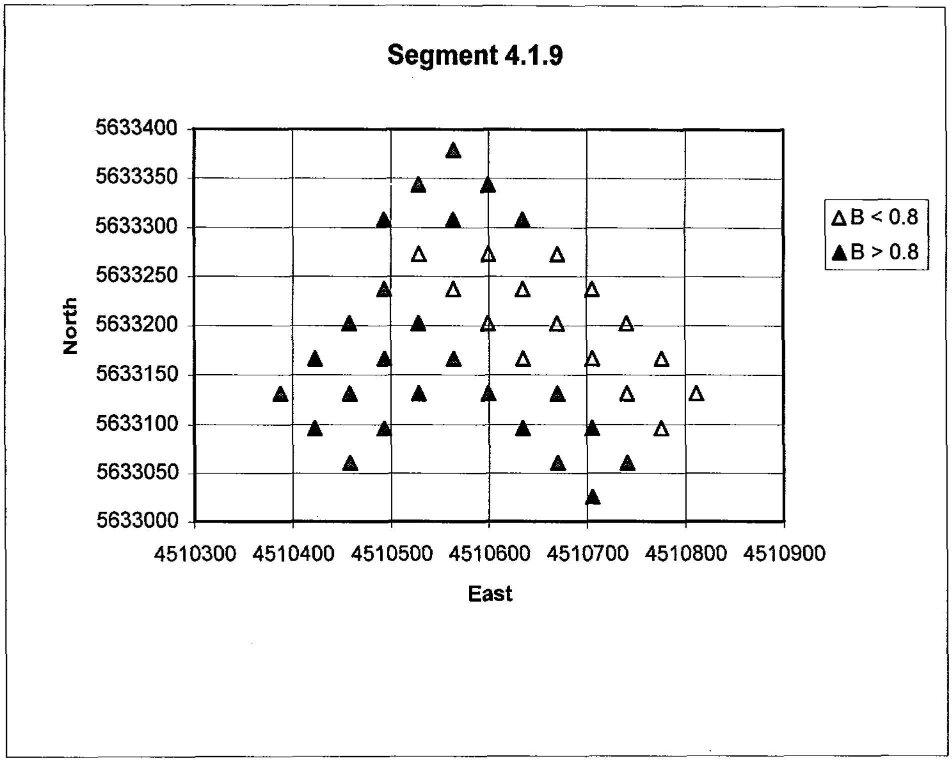
MODEL	TOUGH AMD	TRABAD	MINTOX
Parent Codes	TOUGH2	TRACR3D	PLUME2D MINTEQA2 PYROX
Reference	Gelinas et. al. (1994) Lefebvre and Gelinas (1995)	Bridwell and Travis (1995)	Wunderly et. al. (1995)
developed for	studying oxygen transport mechanisms and water flow in waste rock piles	prediction of ARD from mine wastes	simulation of oxygen diffusion, pyrite oxidation and reactive transport through a tailings impoundment
dimensions	2	3	2
Solution Method	integral finite difference	integrated finite difference	finite element
Construction of Waste Rock Piles	fixed throughout simulation	fixed throughout simulation	fixed throughout simulation
Infiltration and Water Flow within Rock Pile	- infiltration coefficient - water flow described by continuity equation for multiphase flow	- infiltration coefficient - water flow described by continuity equation for multiphase flow	- infiltration coefficient - assumes steady state flow through pile
Oxygen and Heat Transport within Rock Pile	continuity equations for oxygen and heat transport	- continuity equation for oxygen transport - no heat transport	- oxygen diffusion - no heat transport
Geochemical Processes leading to Contaminant Release	reactive core oxidation model	empirically determined fixed oxidation coefficient	shrinking core model
Contaminant Transport within and Discharge from Rock Pile	- mass transport by advection - no geochemical component	- mass transport by advection - equilibrium reaction, ppt., dissolution of aqeous species	- mass transport by advection and dispersion - equilibrium reaction, ppt., dissolution of aqeous species

Welcome Screen Search Report List



Presented at the Fourth International Conference on Acid Rock Drainage

Figure 1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5633000
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East
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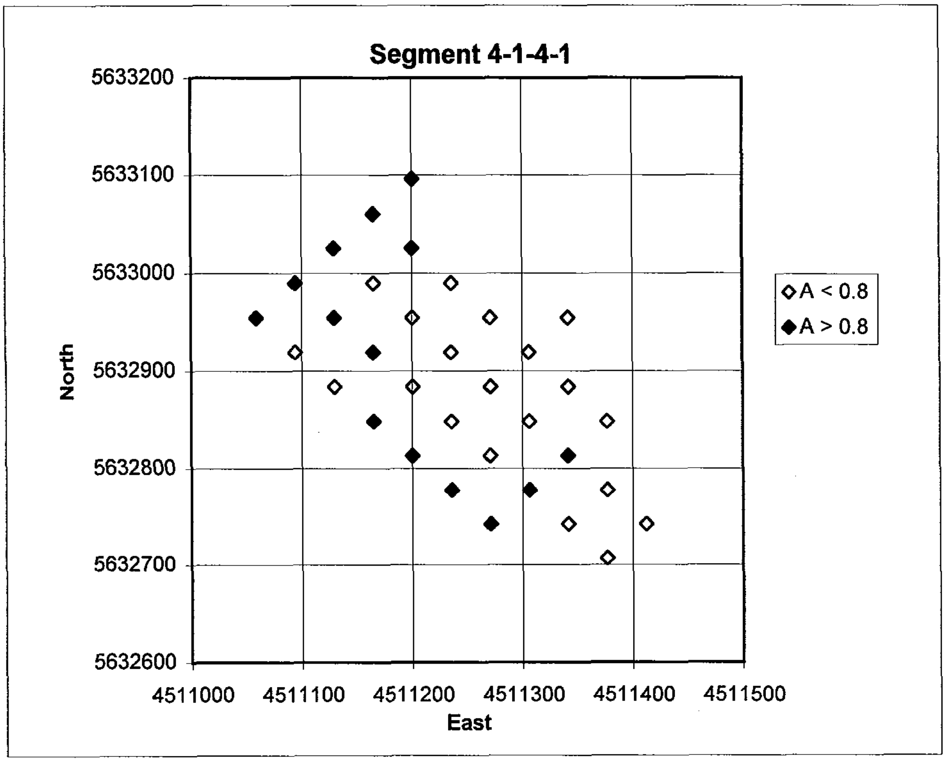
▲ B > 0.8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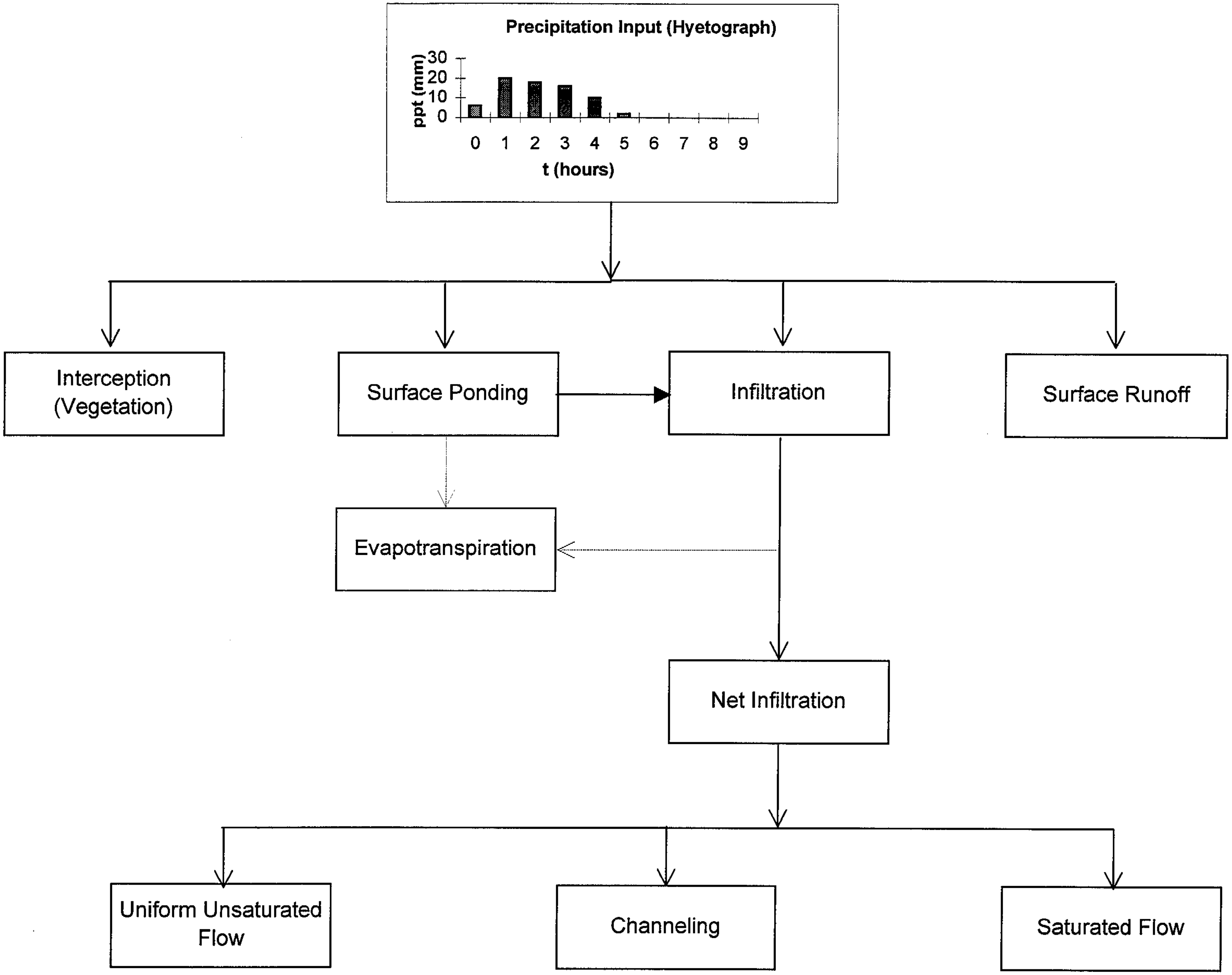
East
◇ A < 0.8
◆ A > 0.8

Figure 2



Interception (Vegetation)

Surface Ponding

Infiltration

Surface Runoff

Evapotranspiration

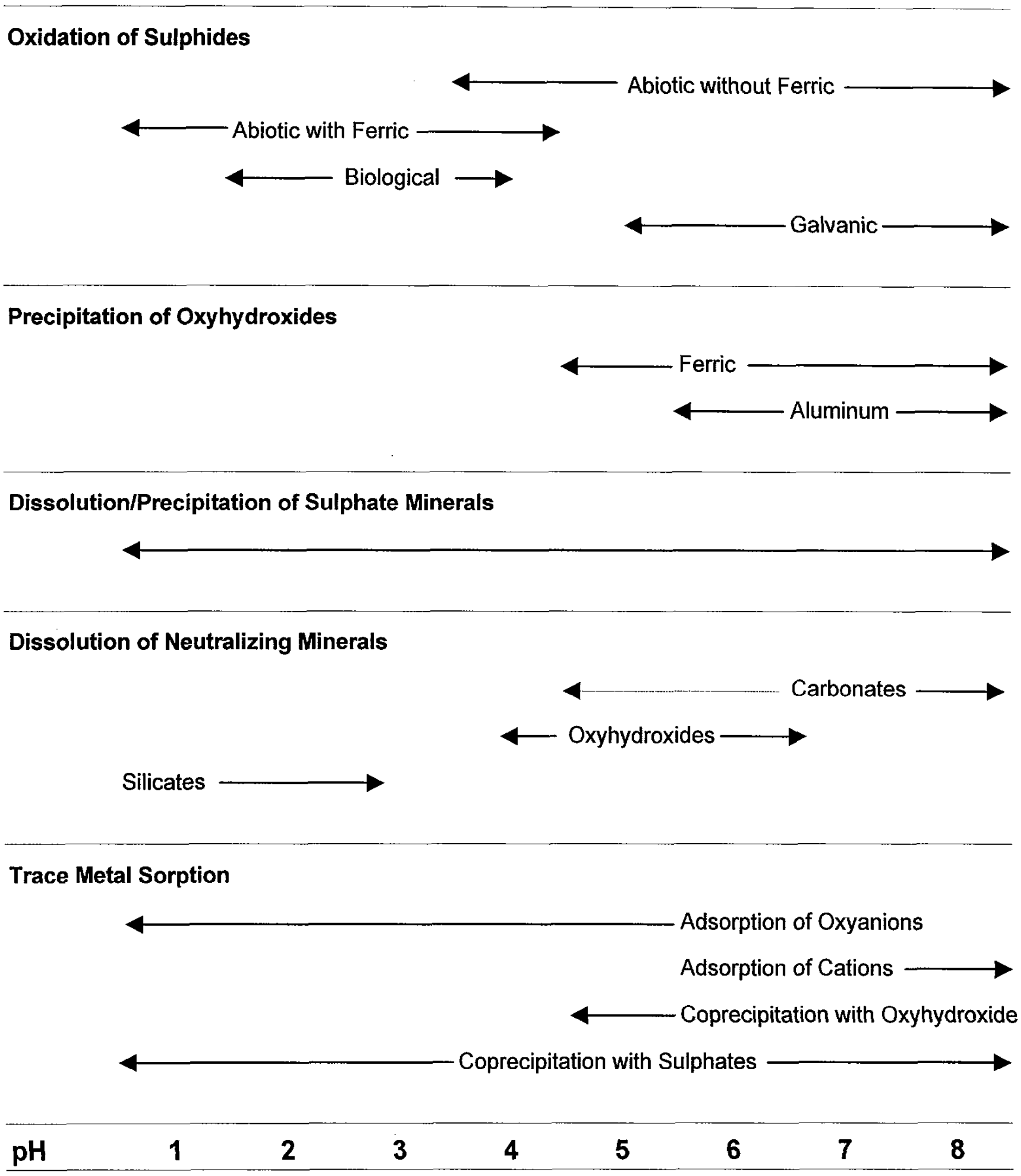
Net Infiltration

Uniform Unsaturated Flow

Channeling

Saturated Flow

Figure 3



Presented at the Fourth International Conference on Acid Rock Drainage

Figure 5

4TH INTERNATIONAL CONFERENCE ON ACID ROCK DRAINAGE

MODELLING PRINCIPLES
(TAILINGS FOCUS)
PART II

MAY 31, 1997
VANCOUVER, BC
13:30-16:30

MODELLING CONCEPTS AND OBJECTIVES WITH A FOCUS ON TAILINGS

by:

R.V. Nicholson

Beak International Incorporated

> *"When the only tool in your toolbox is a hammer, all of your problems begin to look like nails"* Anon

Focus on:

1) Selecting the correct concepts for key processes in tailings
2) Defining objectives - "What do we need to know and for what purpose?"
3) Selecting the correct tools to answer the critical questions

COMPARISON OF TAILINGS AND WASTE ROCK CHARACTERISTICS

Tailings	Waste Rock
• "Relatively" Homogeneous	• Heterogeneous
• Fine Grained (<0.5 mm)	• Variable Particle Size
• Minerals Exposed (Sulphides/Carbonates/etc.)	• Mineral Exposure Highly Variable
• Relatively Simple Hydrology and Chemical Transport	• Complex Chemical Transport

IMPLICATIONS FOR BEHAVIOUR OF TAILINGS

- "Homogeneous" chemical reactions (buffering/sorption etc.)
- Retain more water/greater resistance to oxygen migration above water table
- Water Table in Waste isolates portion from rapid oxidation
- Mineral exposure - greater availability for reactions
- Longer contact times between water and solids results in more complete neutralization or secondary reactions

TOOLS FOR ASSESSMENT (Prediction)

- Measurements
- Modelling

BRIEF REVIEW OF MEASUREMENTS

Lab

- Mineralogy (Identification)
  - Sulphide Content (Pyrite/Pyrrhotite/others)
  - Carbonate Content (Calcite/Dolomite)
- Acid-base-accounting (ABA) Testing with "Critical" Interpretation
- Sulphide, sulphate
- Carbonate
- Grain Size Distribution (for water content and hydrogeologic behaviour)

Field

- Conventional
  - Shallow wells in tailings
  - Porewater above water table (core squeezing)
  - Depth to Water Table
  - Moisture Content above Water Table gravimetric, neutron probe, time domain relfectometry (TDR)
  - Oxygen in gas above Water Table (O_2 profiles - oxygen gradients)
- New
  - Oxygen Consumption Rates at Surface (gives oxidation rates across tailings surface) that gives:
    - mapping
    - input for model calibration

See Figure 1

See Figure 2

MODELLING OF TAILINGS

"Back-of-the-Envelope"

- AP/NP calculations
- Inventories of Sulphide above water table (Oxidation Zone)
- Inventories of Neutralizing Solids along flow paths (Neutralization Zone)

"Research Models"

- more detailed
  - chemistry
  - hydrology
- Focus on "Potential" Controls on Concentrations of Metals (Equilibrium Processes)
- Fundamental process studies
- Testing hypotheses

"Engineering Models" (e.g., WATAIL)

- Assess Loadings of Major Oxidation Products
- Compare Management Options (e.g., Covers)
- Important Trends in Loadings with Time (How long is treatment required?)

CONCEPTUAL FRAMEWORK FOR TAILINGS ASSESSMENT

Above Water Table

- Inventory of Sulphide Mineral(s) (Acid Generation/ Metals Release)
- Rates of Oxidation (converts to loadings)
- Other Chemical Reactions (some neutralization/leaching of metals)

Below Water Table

- Buffering reactions (Ca, Mg - Carbonates)
- Precipitation/Sorption of Metals and Others

CONTROLS ON OXIDATION

- With Free Access to Oxygen (i.e., "The Lab")
  - Surface Reaction Controlled - Key Variable
  - Bacterially Enhanced
- In a Tailings Impoundment
  - Oxygen Availability controlled (diffusion through tailings)
  - Resistance of Tailings and Water to Oxygen Movement
  - Oxidation from Surface Downward (oxygen transport controls rates).

LABORATORY RATES ON PURE SULPHIDES (No Oxygen Restriction - Similar to "IDEAL" Humidity Cell Tests)

	Oxidation Rates*		Typical Tailings**
	(Mol $m^{-2}s^{-1}$)	(mg-SO_4 $m^{-2}wk^{-1}$)	(mg-SO_4 $kg^{-1}wk^{-1}$)
Pyrite	5 x 10^{-10}	60	1,500
Pyrrhotite	5 x 10^{-8}	3,000	75,000

* Rates given per area exposed sulphide and per kg of typical tailings

** Typical tailings may have 5% S with a surface area of 0.5 m^2g^{-1} of sulphide or 25 m^2kg^{-1} of tailings

EXAMPLES OF CALCULATED FIELD RATES (Ignoring Oxygen Restriction):

Percent Sulphur (Pyrrhotite)	1	15	30
Pyrrhotite Content (kg m^{-3})	50	750	1,500
*Calculated Oxidation Rate (kg-$SO_4$$m^{-3}a^{-1}$)	450	6,800	13,608
Measured Oxidation Rate (kg-SO_4 $m^{-2}a^{-1}$) (Oxygen Consumption measurement on fresh tails in impoundment	1	10	240
**Calculated/Measured	450	680	60

*Based on laboratory rates (e.g., Humidity Cells)

**Lower Measured rates are due to restriction by Oxygen Diffusion

SUGGESTED APPROACH TO ASSESSMENT OF PLANNED SULPHIDE TAILINGS

1) Quantify - Sulphides
   - Carbonates
2) Mineralogic Identification
3) "Back of the Envelope" for Magnitude of Problem
   - Above the Water Table
     - Acid Potential
     - Neutralization Potential
   - Identify Flow and Transport Pathways and Estimate Rates of Flow
   - Below Water Table
     - Neutralization Potential

4) Identify other Water Quality Issues (some non-acid waters can have elevated metals)
  - Ferrous Iron (Fe^{2+})
  - Zinc
  - Nickel
  - Arsenic
  - TDS

  (Others NOT Attenuated at Neutral pH?)

5) Laboratory Testing (e.g., Humidity Cells) to Verify Potential Water Quality Problems ***Not to Assess Anticipated Rates in an impoundment***

6) Modelling/Assessment (Experience Required)
  - Chemical Kinetics
  - Aqueous - Solids Reactions
  - Physics of Diffusion
  - Surface and Subsurface Hydrology, etc.

MODELLING OBJECTIVES

- Many possible objectives
  - assess magnitude of potential problem
  - test hypotheses for uncertain processes
  - compare rehabilitation options
  - **Develop Management Strategies**
    - Focus on Calculated Loadings over time
    - Identify critical variables
    - Compare scenarios
    - Provide basis for decision making

KEY PROCESSES AND CHARACTERISTICS THAT CONTROL OXIDATION REACTIONS, ACID GENERATION AND LOADINGS TO THE ENVIRONMENT

Processes

1) Chemical Kinetics
   - some basic information available
   - may require some characterization
2) Oxygen Diffusion
   - controlled by moisture content
   - highly variable
   - may require "uncertainty analysis"
3) Neutralization Reactions
   - requires knowledge of neutralizing minerals present
   - most are well-defined reactions

Characteristics

1) Sulphide Content
   - represents inventory of potential acid production
   - affects rates of acid and metal loadings
2) Carbonate Content
   - represents inventory of potential acid consumption (or NP)
   - can also affect rate of oxidation
3) Depth of Water Table
   - rapid oxidation rates occur above
   - low to insignificant rates below
   - neutralization possible above and below
4) Moisture Content above Water Table
   - controls rate of oxygen diffusion and net loadings transit time
5) Infiltration Rate
   - affects transit time in subsurface

The WATAIL Model

- Control Volume Reactors (Nodes)
- Coupled Oxygen Diffusion/Oxidation Kinetics in vertical profile above water table
- Secondary solids reactions
- Water flow/solute transport
- Provides loadings (and concentrations) to downstream location

See Figure 3

MODELLING OBJECTIVES

- Develop some simple scenarios to compare effects of management options
- compare incremental benefits of management options
- define critical tailings and environmental variables that influence effluent quality
  - investigate time trends
  - highlight major uncertainties
  - highlight Measurements/Monitoring required to verify expected behaviour

See Figure 4

CONCLUSIONS

- Assessment and Modelling of tailings can be conducted at different levels of detail and for different purposes.
- Critical to develop appropriate conceptual models for the questions to be addressed.
- Some simple issues may be addressed by simple acid-base-accounting and "back-of-the-envelope" calculations.
- Major issues involve rates and flows and need more sophisticated approach (the simplest and most transparent models are usually best)

- Loadings are more reliable (certain) than concentrations because hydrology can be much more variable over time than oxidation.
- Uncertainty analysis should be used to better understand effect of variables on loadings.
- Appropriate field and laboratory measurements are the key to assessment and verification of model predictions and future tailings performance.

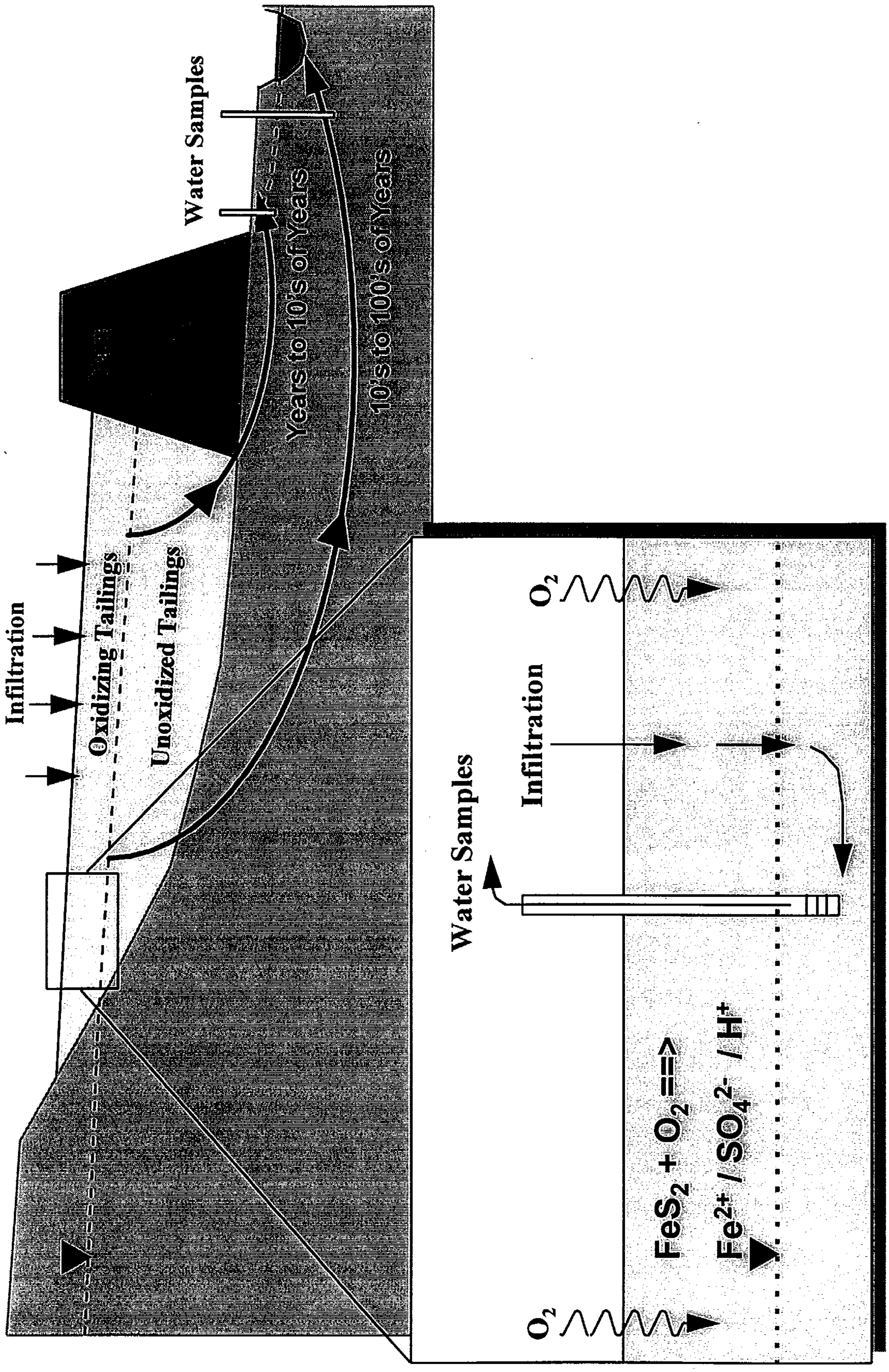

Infiltration
Oxidizing Tailings
Unoxidized Tailings
Water Samples
Years to 10's of Years
10's to 100's of Years
O_2
Infiltration
Water Samples
$FeS_2 + O_2 ==>$
$Fe^{2+} / SO_4^{2-} / H^+$
O_2

Figure 1

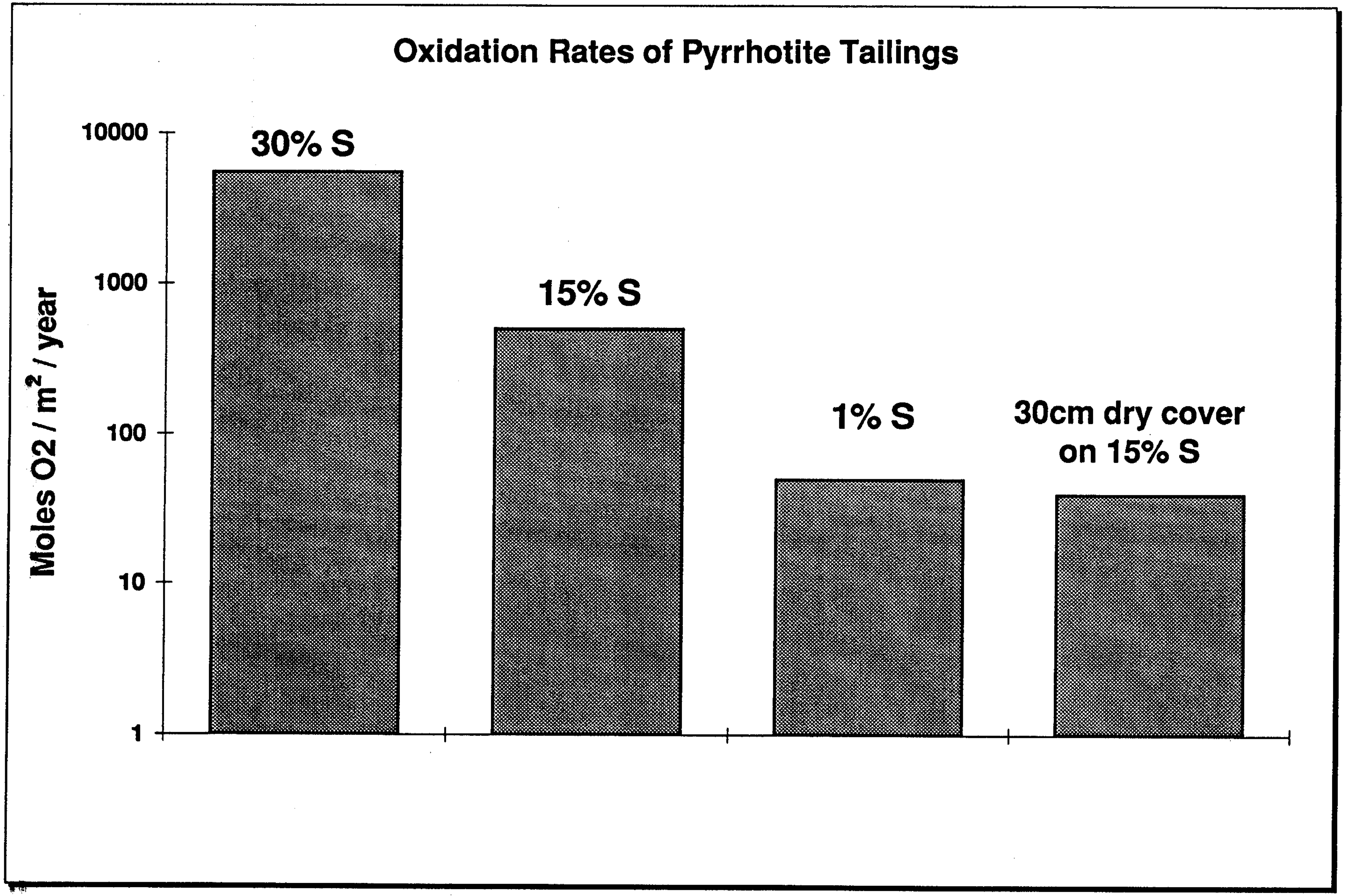

Oxidation Rates of Pyrrhotite Tailings
Moles O2 / m² / year
10000
1000
100
10
1
30% S
15% S
1% S
30cm dry cover on 15% S

Figure 2

Schematic Section of Model Node

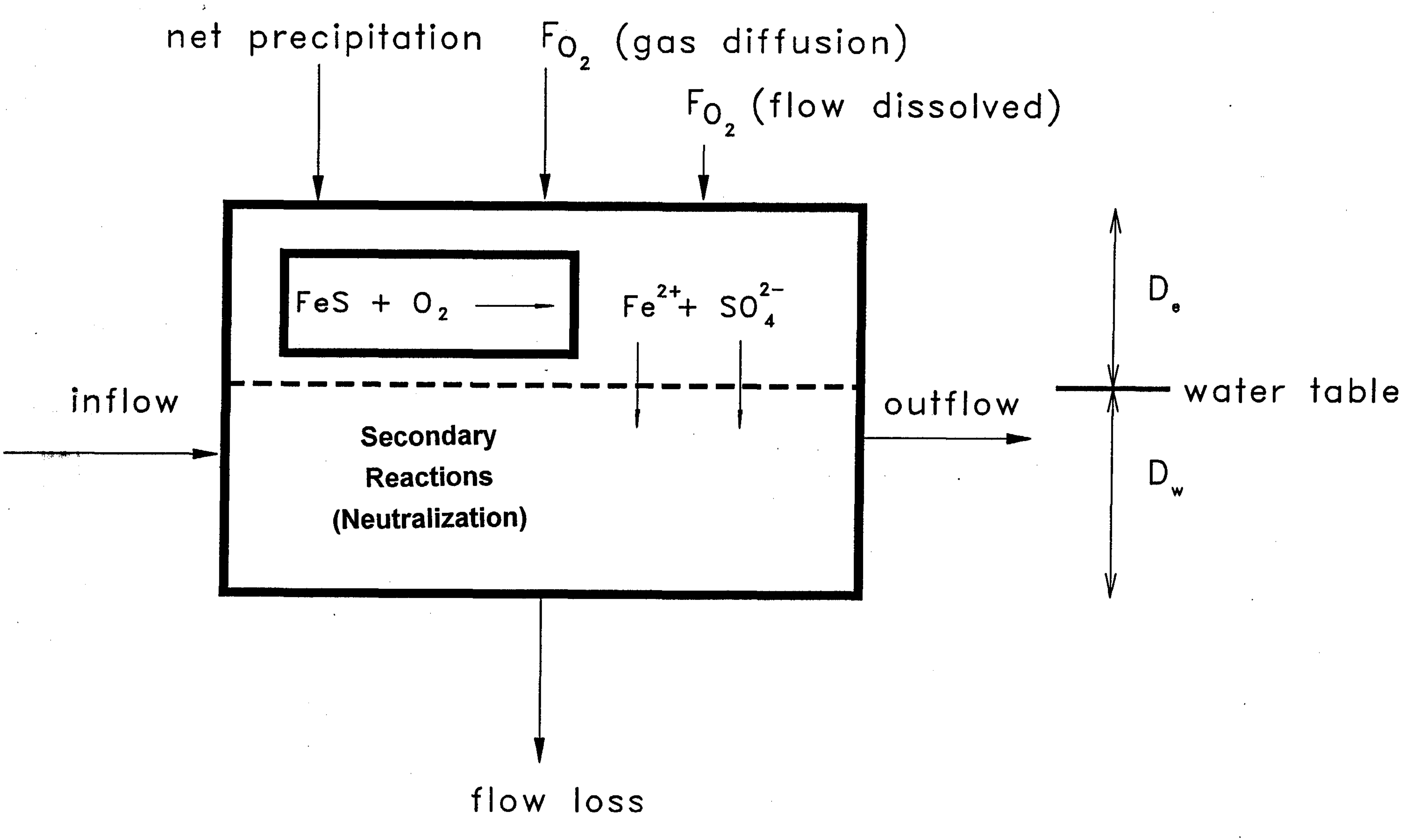
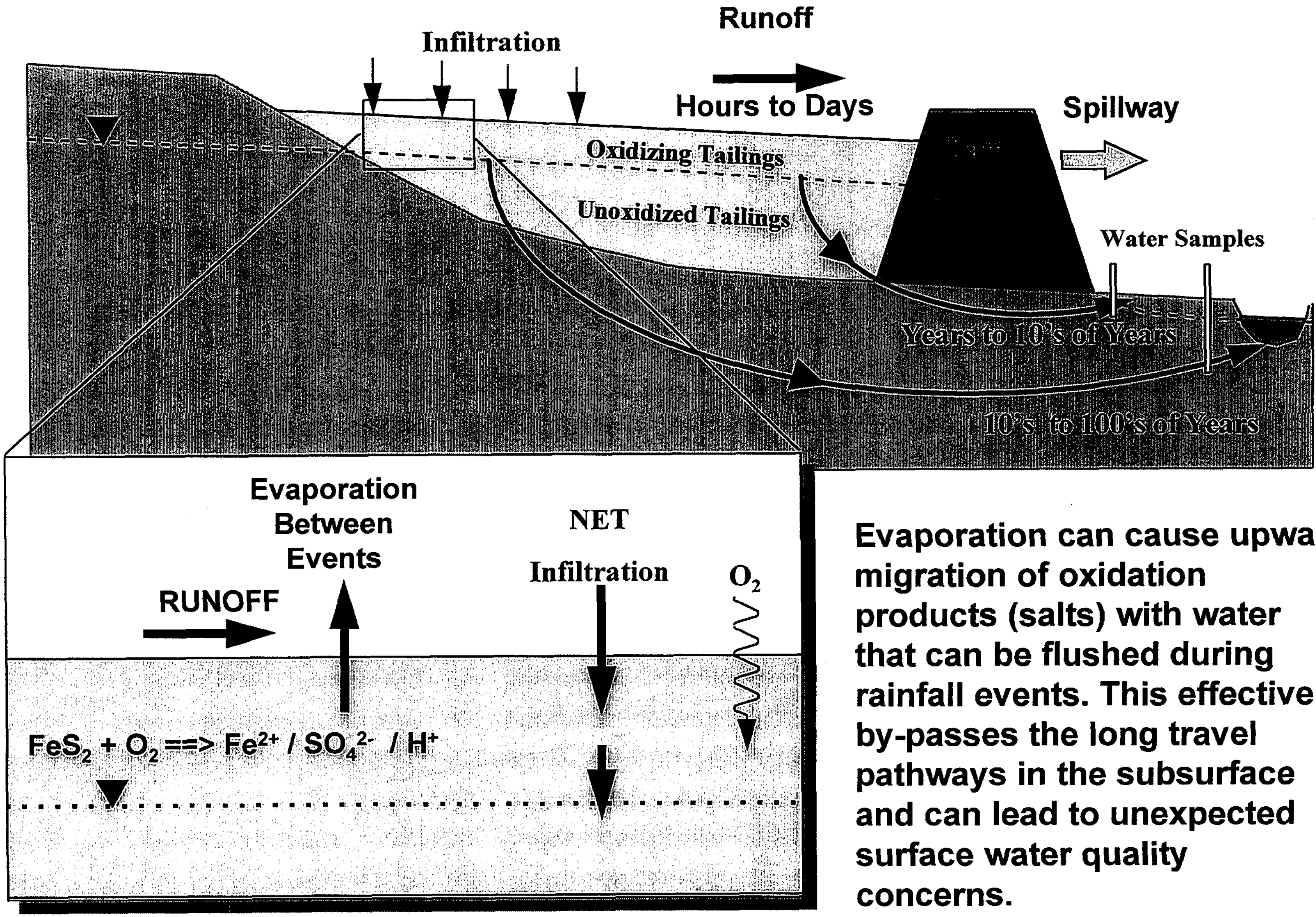


Figure 3



Evaporation can cause upward migration of oxidation products (salts) with water that can be flushed during rainfall events. This effectively by-passes the long travel pathways in the subsurface and can lead to unexpected surface water quality concerns.

Figure 4

Plan View of Tailings Impoundment

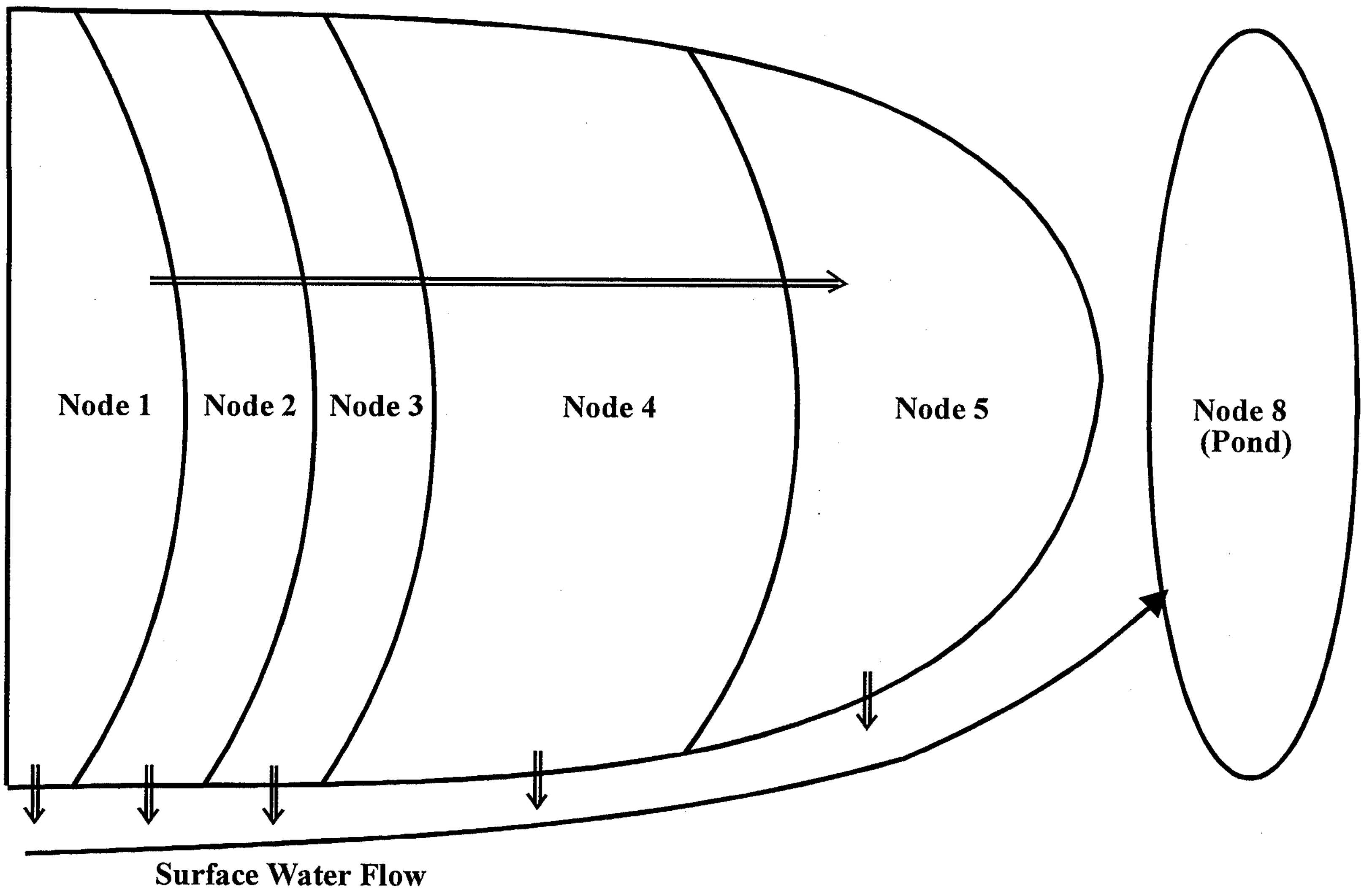


Figure 5

Cross-Section in Direction of Flow

E = Evaporation (salt migration to surface and pond)
EPF = Evaporation + pore water flushing (to pond)
Seepage = Steady-state seepage from subsurface (to pond)

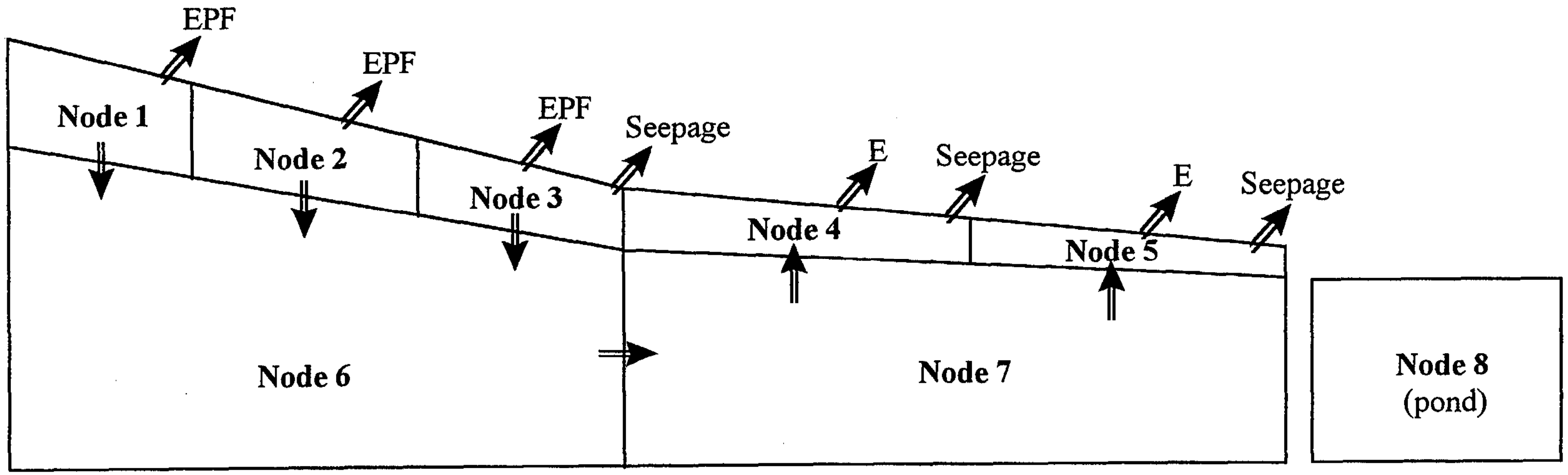
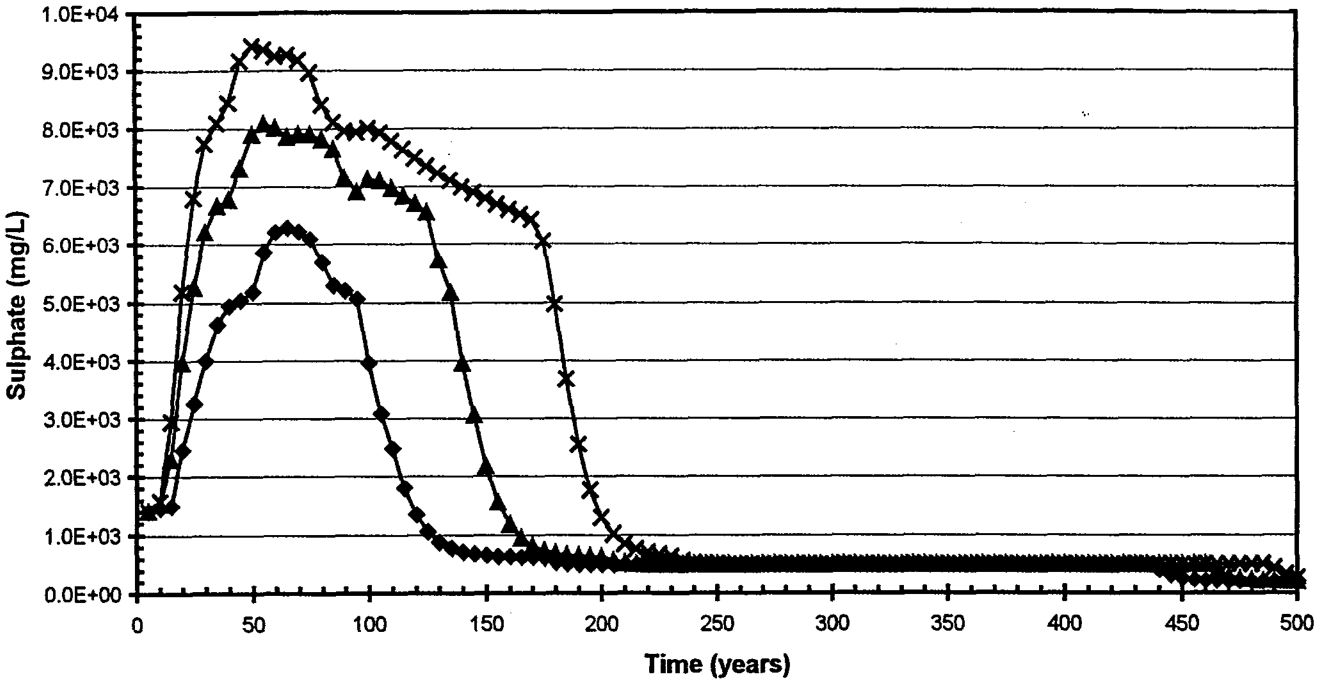


Figure 6

Sulphate Concentrations in the Pond for Various Sulphide Mineral Content



Zinc Concentrations in the Pond for Various Sulphide Mineral Content

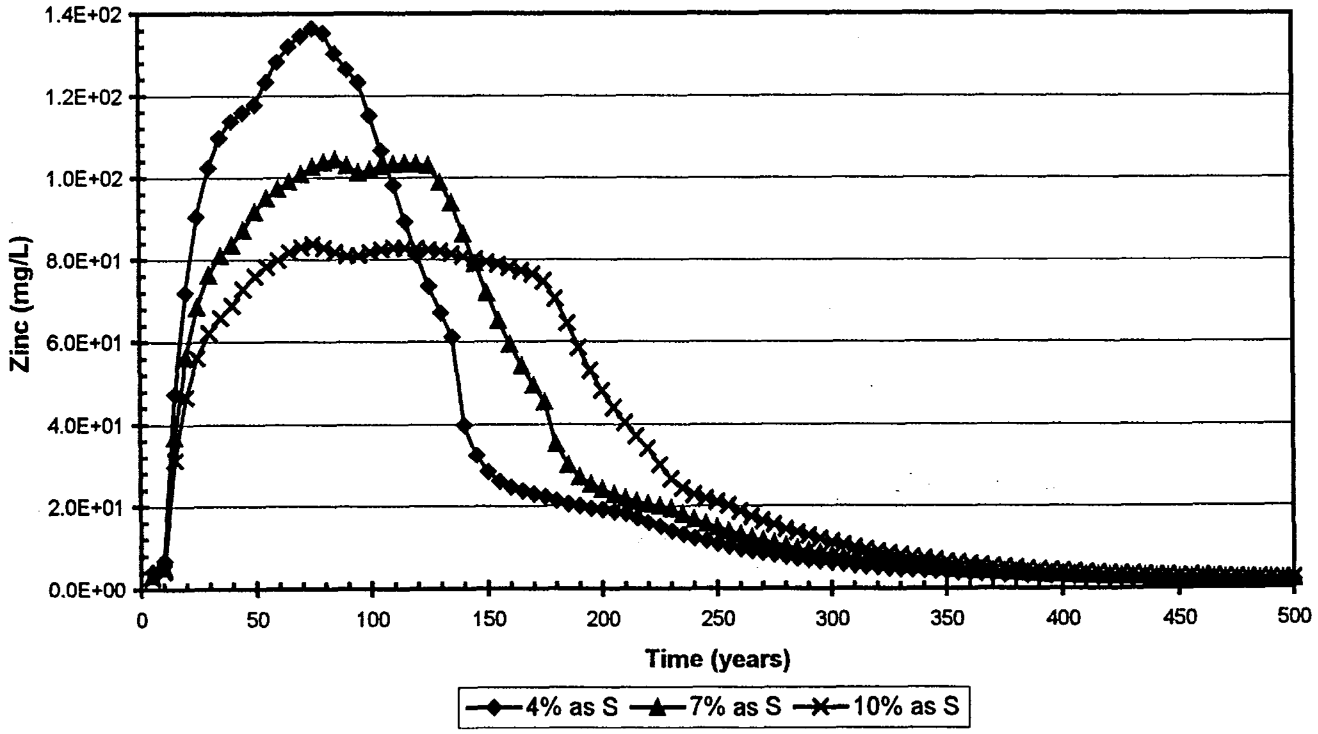
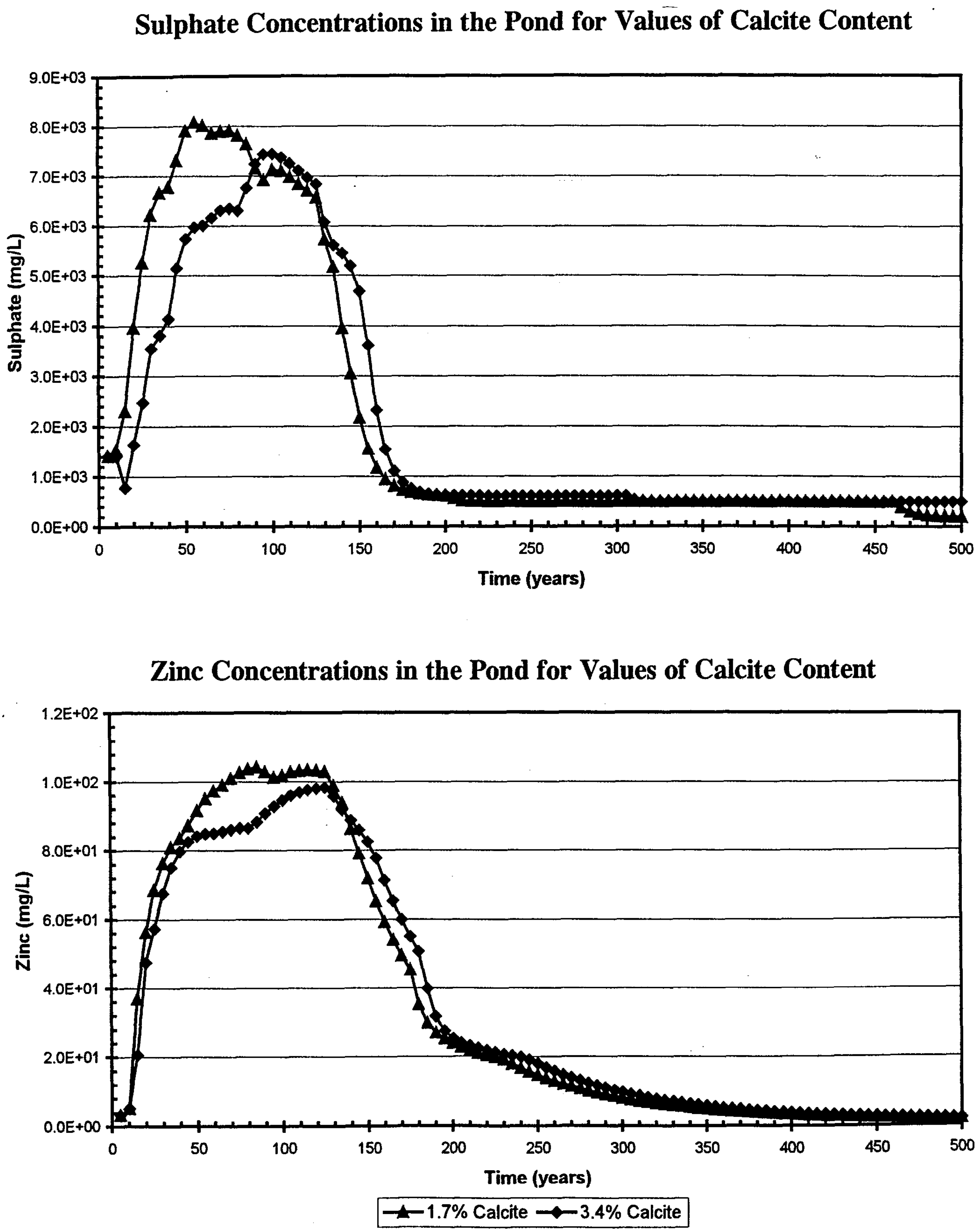


Figure 7



Sulphate Concentrations in the Pond for Values of Calcite Content

Zinc Concentrations in the Pond for Values of Calcite Content

Figure 8

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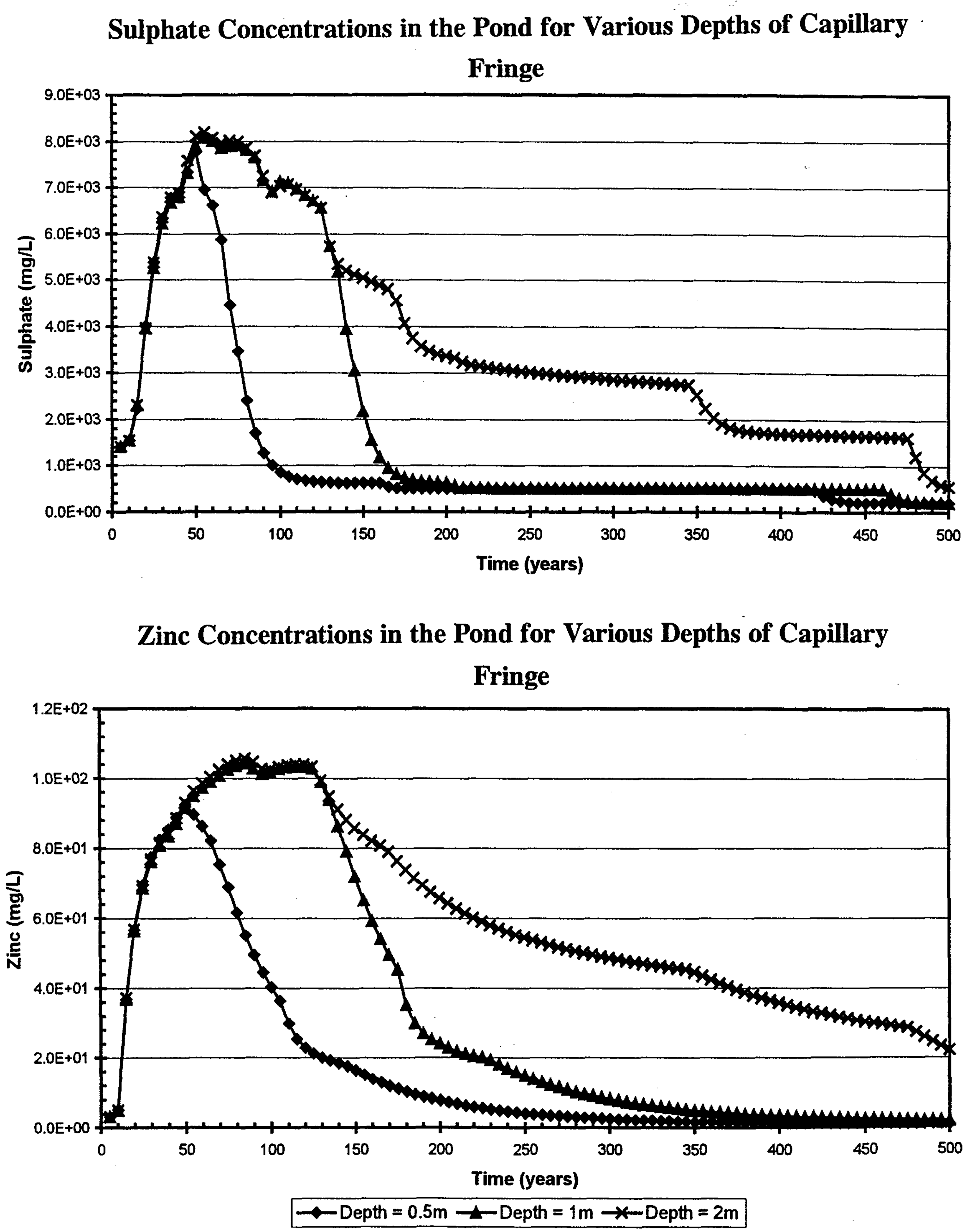
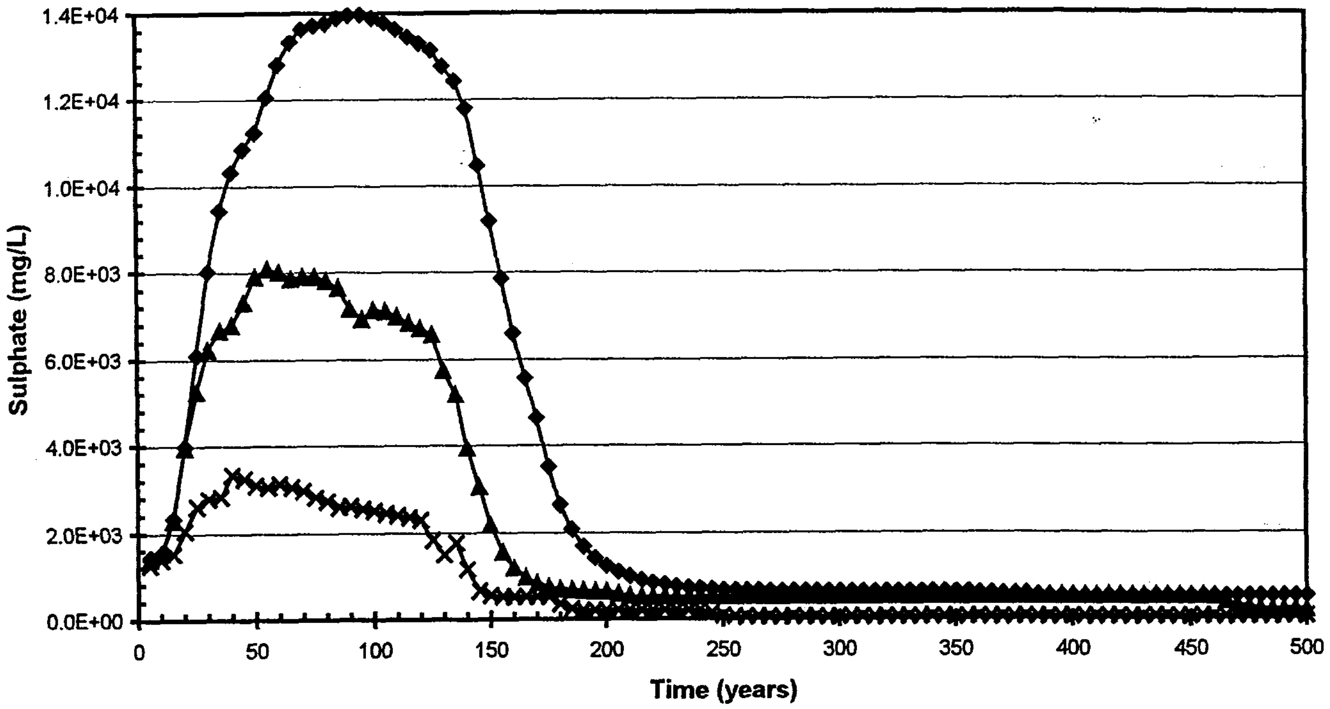


Sulphate Concentrations in the Pond for Various Depths of Capillary Fringe

Zinc Concentrations in the Pond for Various Depths of Capillary Fringe

Figure 9

Sulphate Concentrations in the Pond for Various Infiltration Rates



Zinc Concentrations in the Pond for Various Infiltration Rates

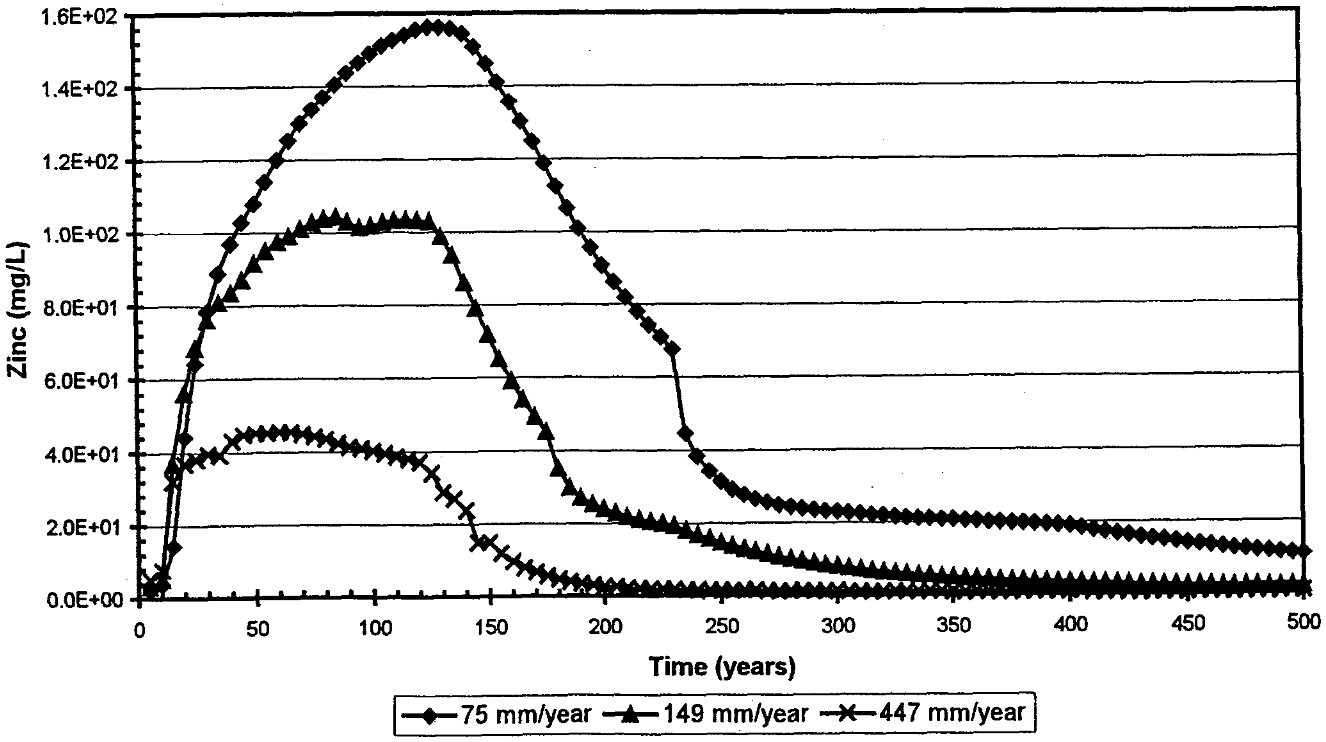


Figure 10

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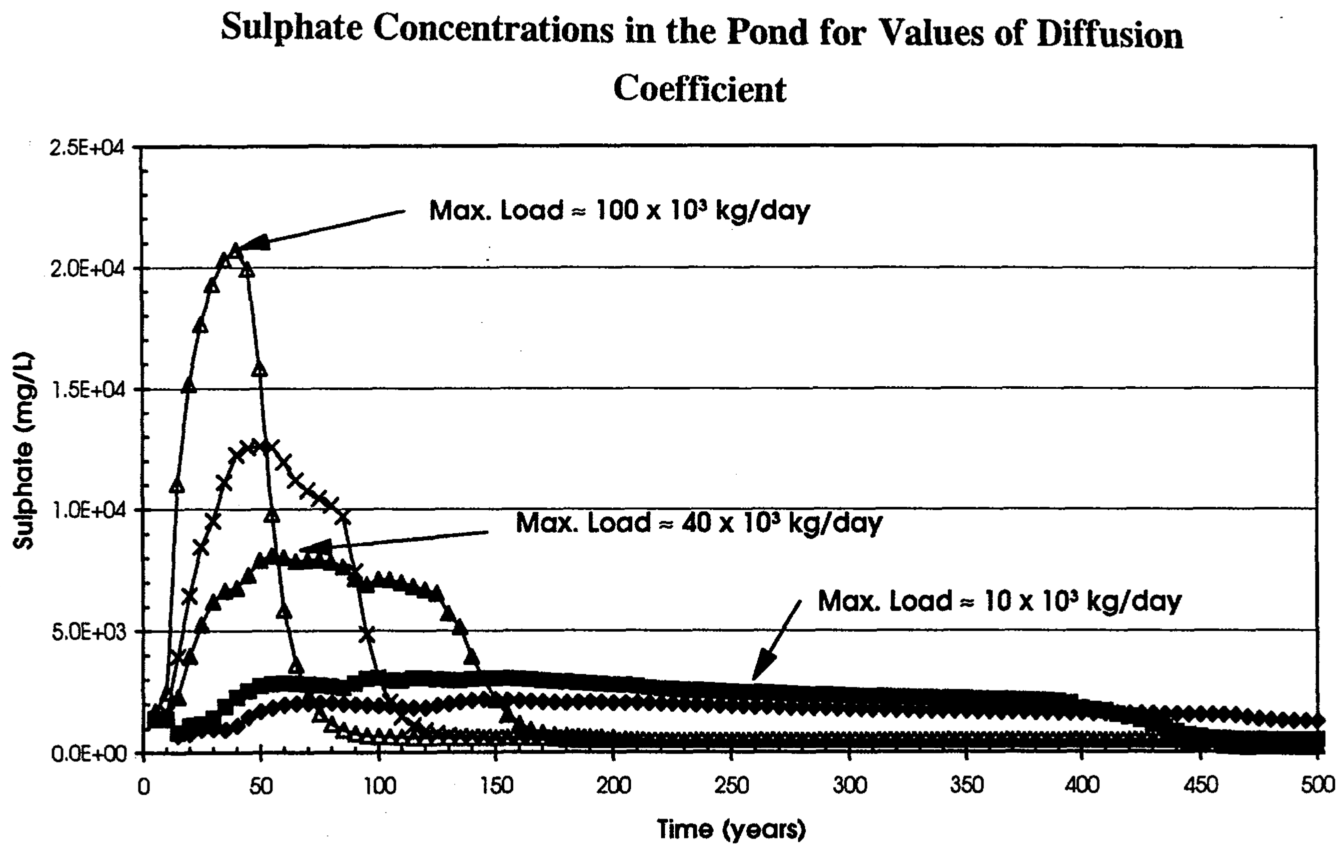

Sulphate Concentrations in the Pond for Values of Diffusion Coefficient

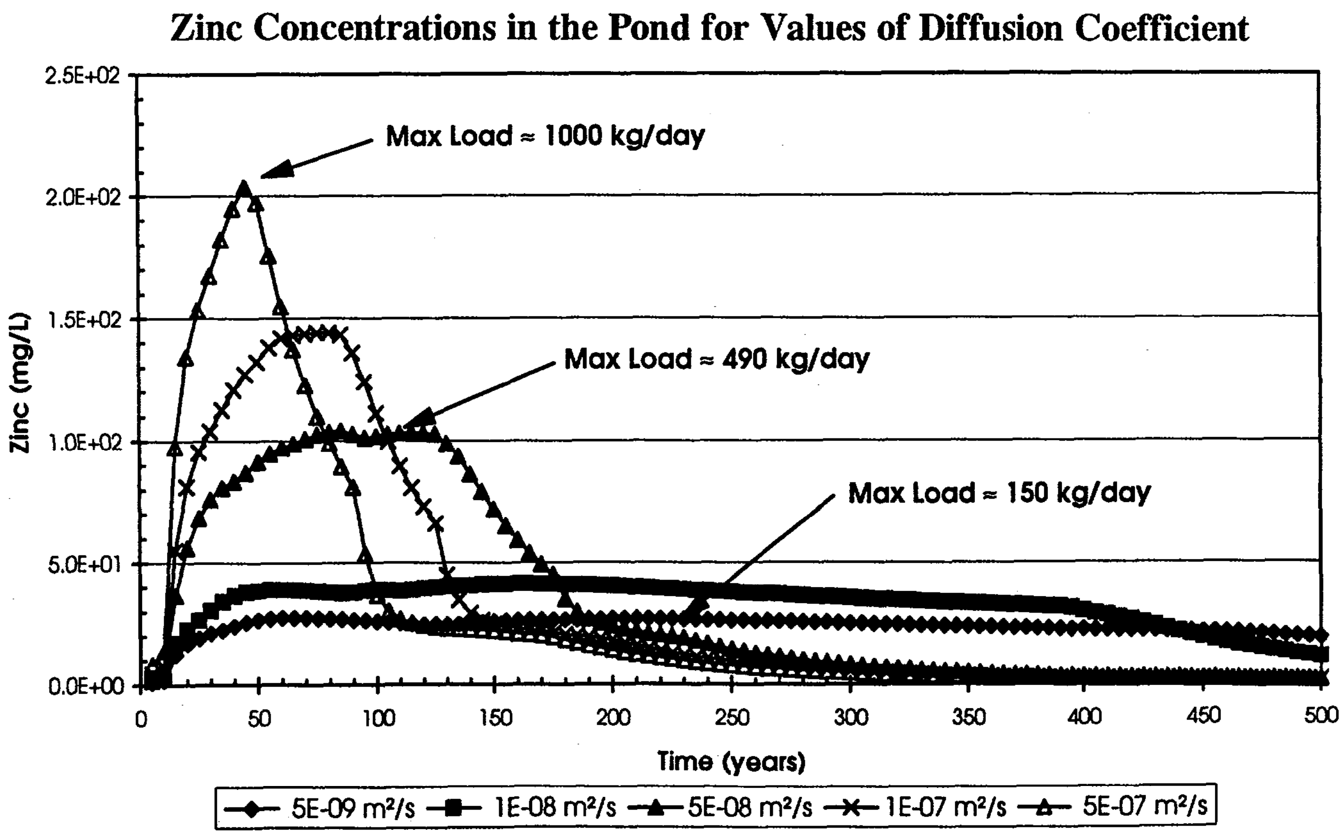
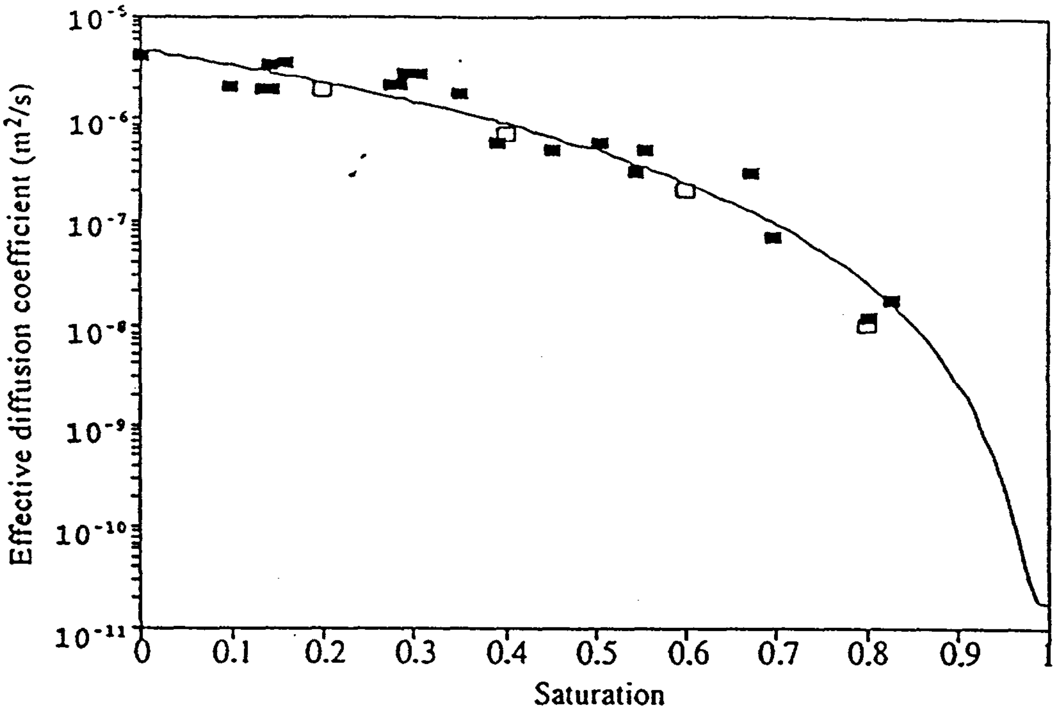

Zinc Concentrations in the Pond for Values of Diffusion Coefficient

Figure 11



Oxygen diffusion coefficient versus water saturation of tailings (Elberling et al., 1994)

Figure 12

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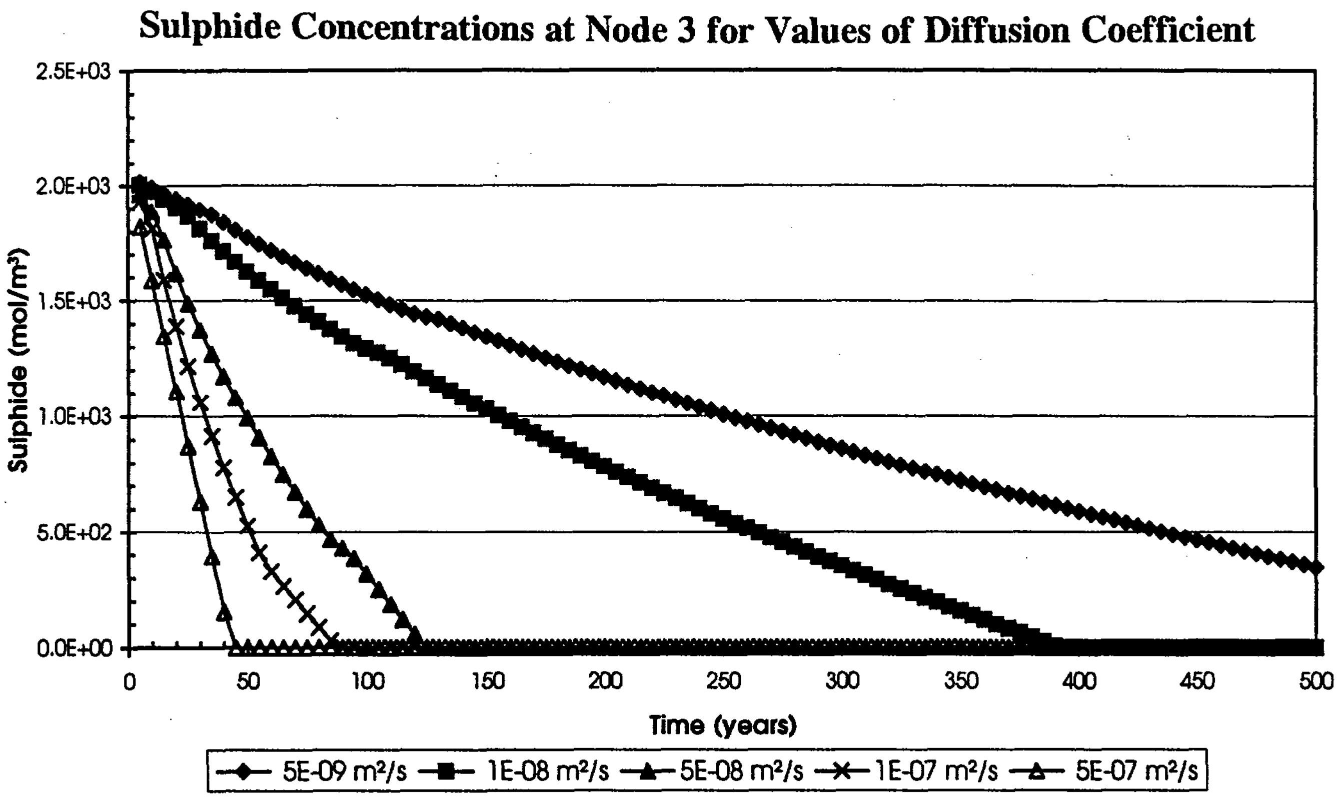
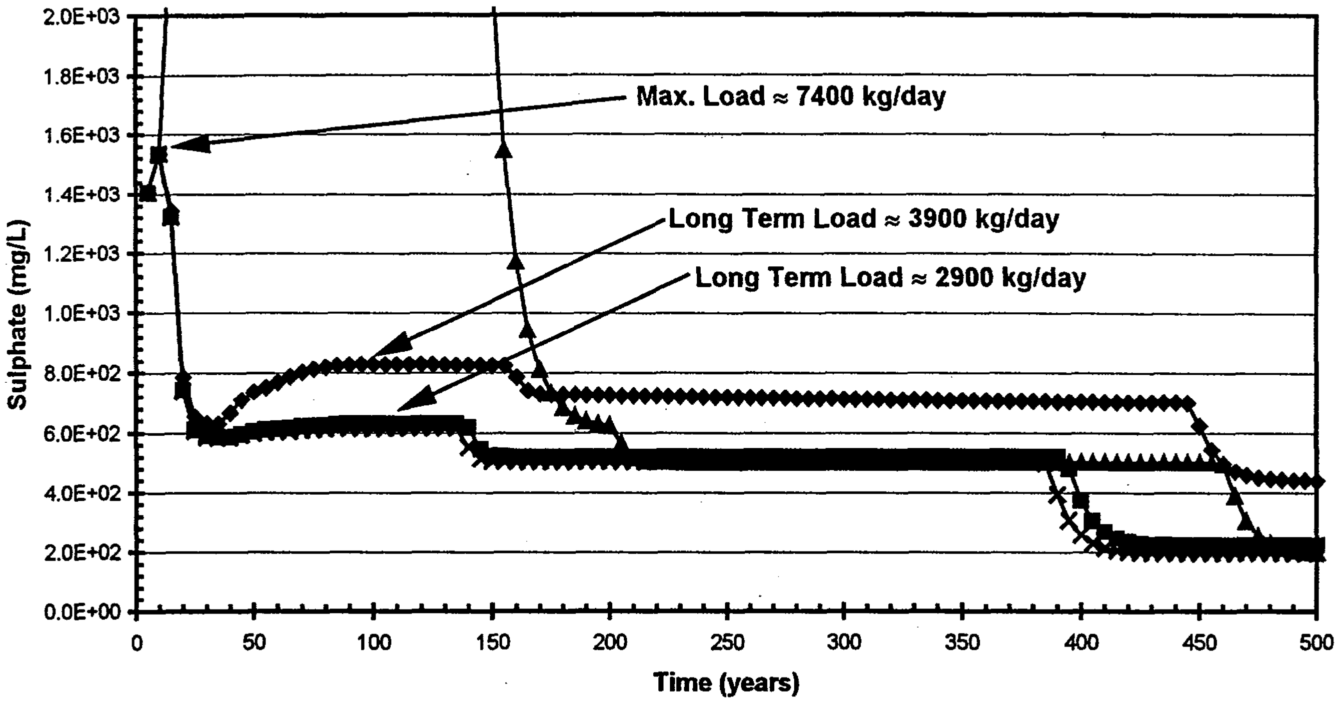


Figure 13

Sulphate Concentrations in the Pond for Various Cover Scenarios



Zinc Concentrations in the Pond for Various Cover Scenarios

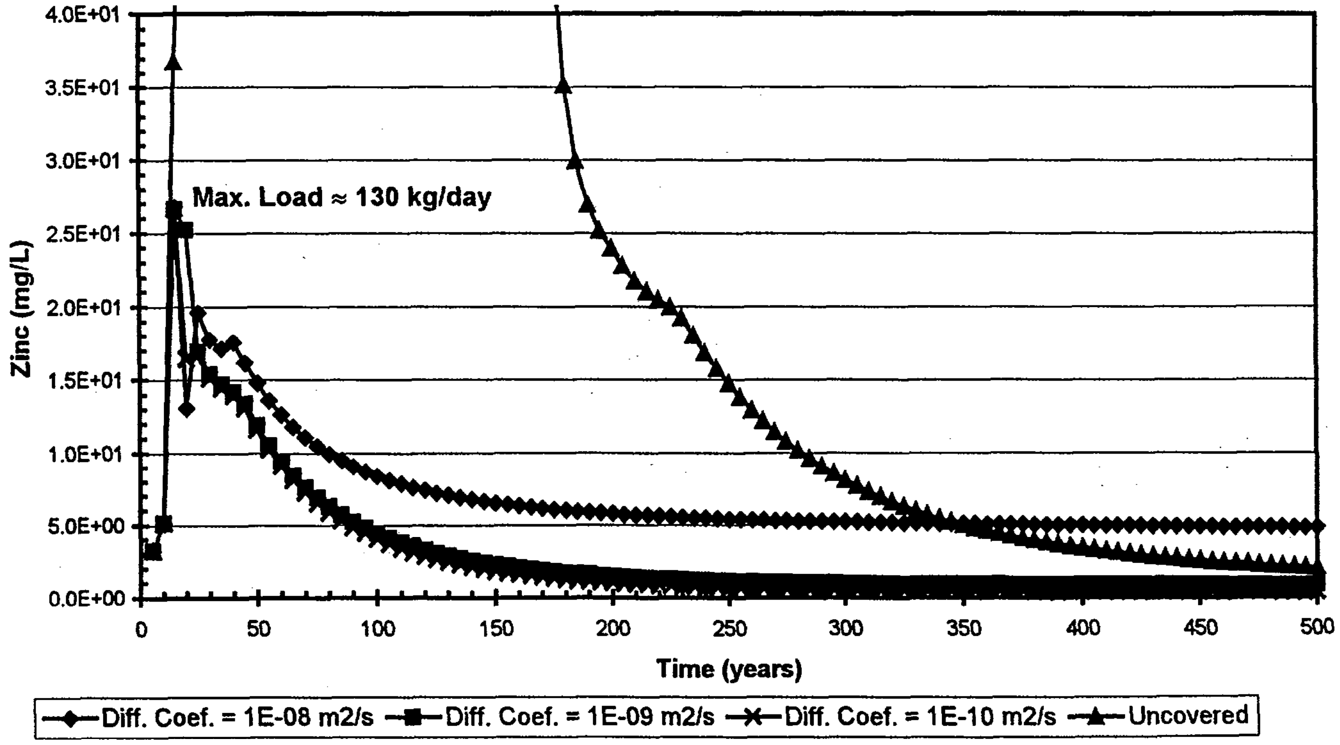


Figure 14

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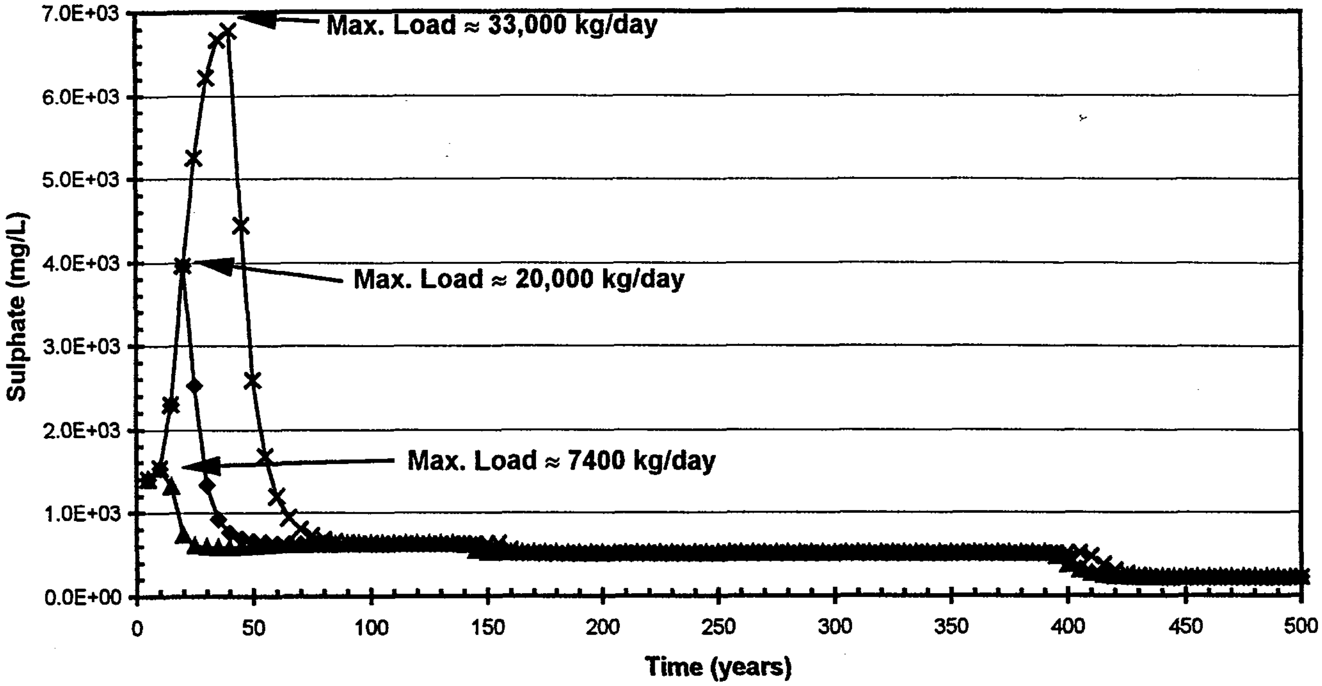
Sulphate Concentrations in the Pond for Various Years of Cover Construction



Zinc Concentrations in the Pond for Various Years for Cover Construction

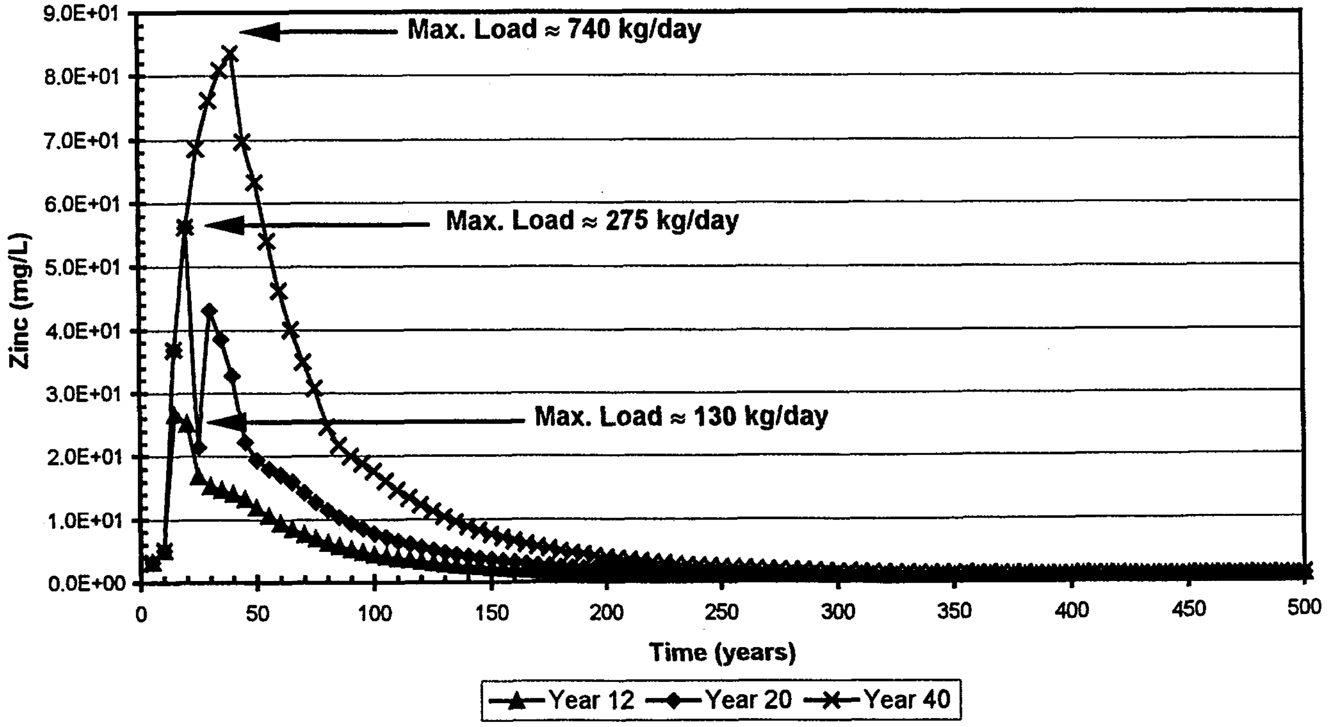


Figure 15

Prediction Models for Acid Mine Drainage

Luc St-Arnaud

Predictive Models for Acid Rock Drainage Short Course
Fourth International Conference
on Acid Rock Drainage
May 31, 1997

Possible Prediction Objectives

- identification of soluble and mobile metals
- maximum metal concentrations
- maximum metal loadings
- comparison of decommissioning options
- duration of dissolved metal production
- concentration and loading vs time

Outline

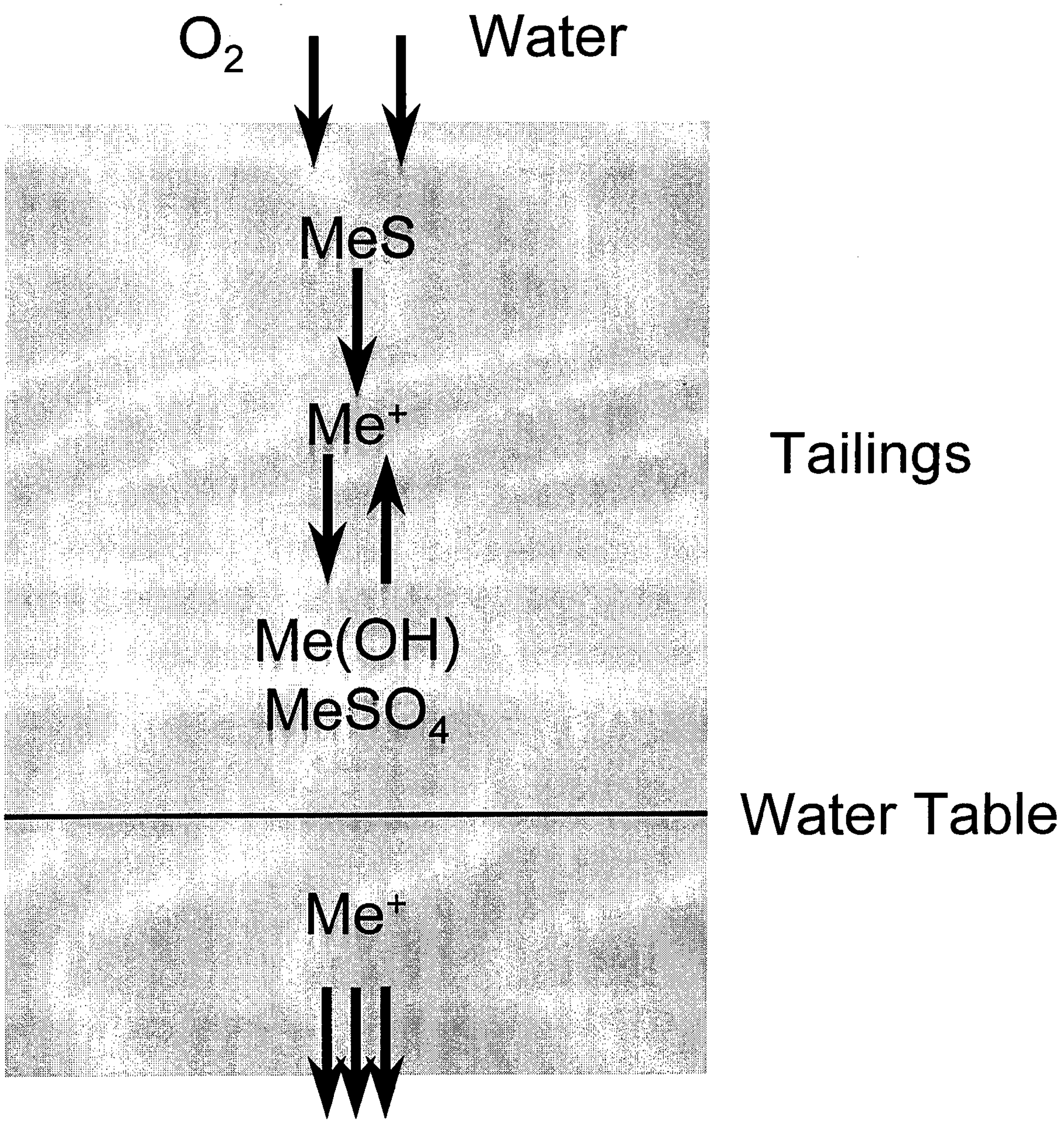
- Review of Physical and Chemical Systems
- Computer Models for AMD Prediction
  - Definitions
  - Classification
  - Applicability

Review of Physical and Chemical Systems

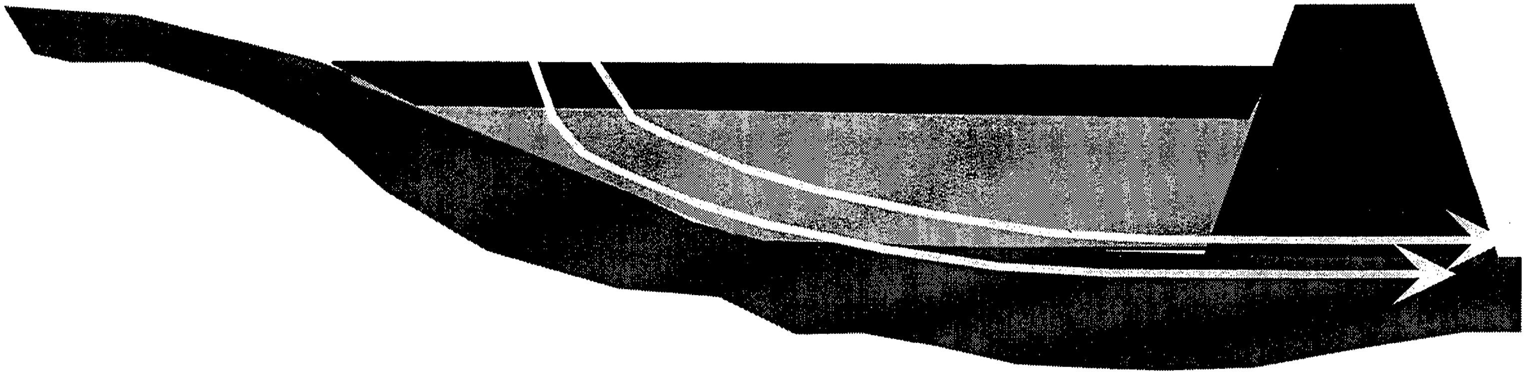
Acid-Base Balance

- Acid Potential (AP) %S
- Neutralization Potential (NP)

Acidity Dissolved Minerals	+	Carbonate Minerals Al-Si Minerals	→	Metal Carbonates Metal sulphates Metal hydroxides Dissolved ions

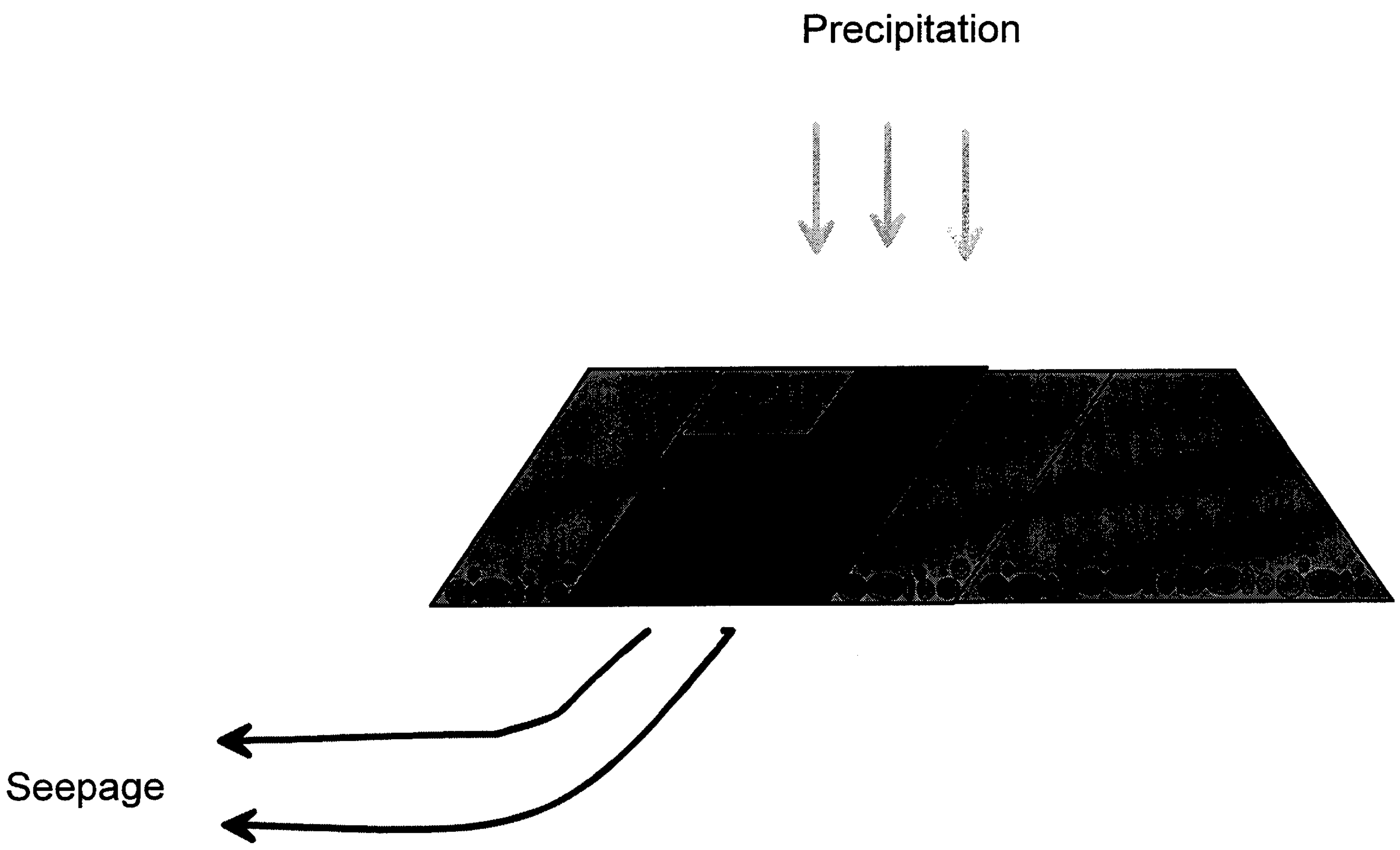

O_2
Water
MeS
Me^+
Tailings
$Me(OH)$
$MeSO_4$
Water Table
Me^+

Flow System

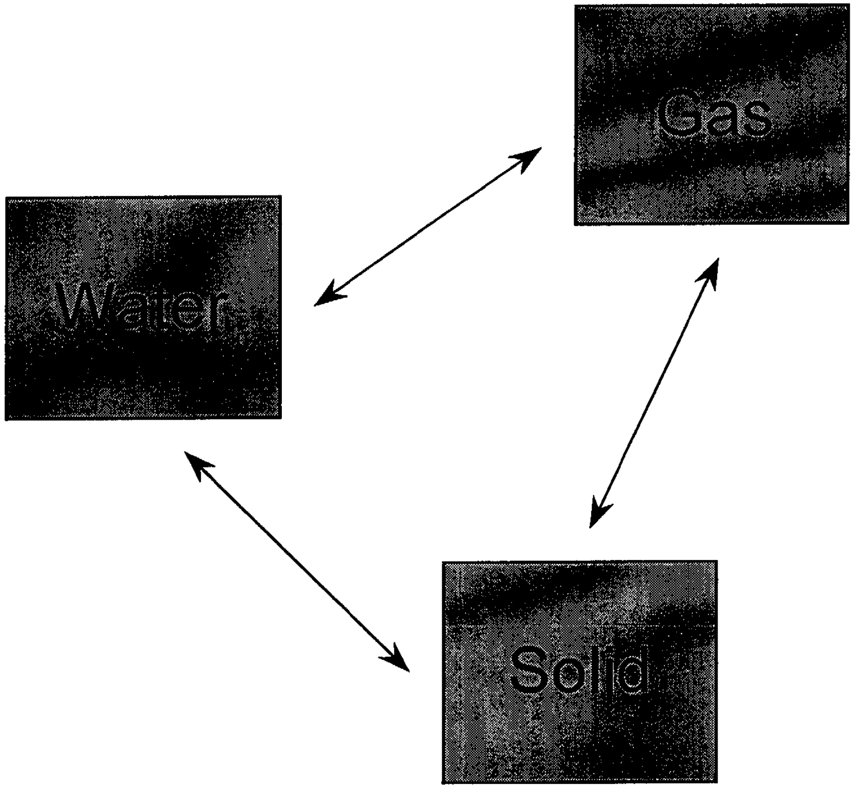


- define boundary conditions
- solve for hydraulic potentials
- calibrate to field data
- calculate velocities and discharges

Waste Rock Pile



Mass Transfer



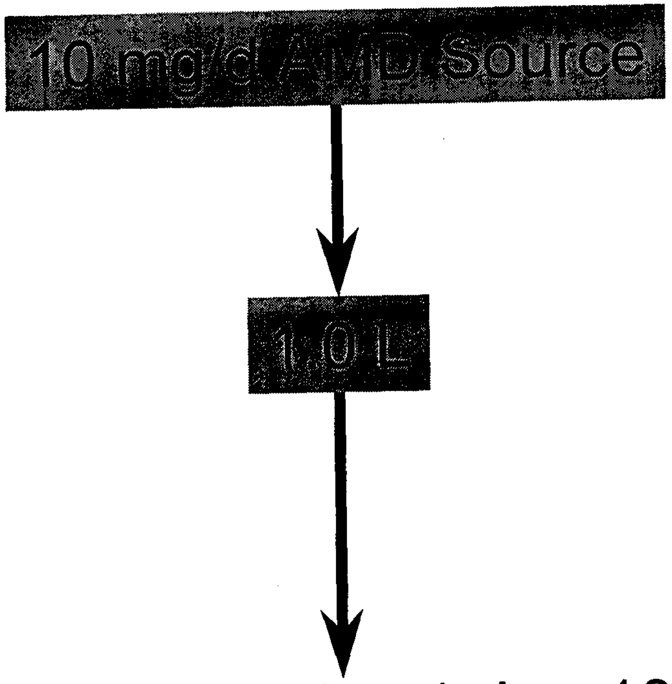
Geochemical Reactions in Mine Waste

PROCESS	*MASS TRANSFER EFFECT*
Oxidation of sulphides	H^+ and Me release
Precipitation of hydroxides	H^+ release and Me consumption
Dissolution and precipitation of sulphates	Me, H^+ release and consumption
Dissolution of hydroxides, carbonates, silicates	H^+ consumption
Co-precipitation	Me consumption

Geochemical Control on contaminant release:

kinetic vs equilibrium

- kinetic control

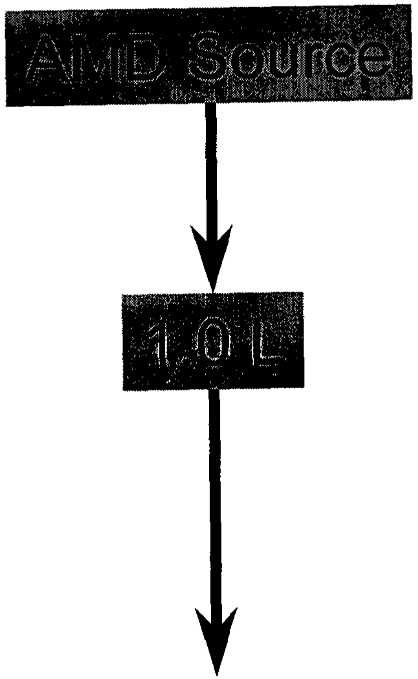


10 mg/d AMD Source

1.0 L

Concentration after 1 d = 10 mg/L
after 2 d = 20 mg/L

- equilibrium control



Concentration after 1 d = 10 mg/L
after 2 d = 10 mg/L

Geochemical Reactions - Governing Principles

- Thermodynamics (Equilibrium)
    - determination of whether a reaction has sufficient energy to proceed
    - calculation of “effective” concentrations - activities
    - use of experimentally-determined thermodynamic constants

Geochemical Reactions - Governing Principles

- Kinetics
  - determination of reaction rates
  - use of experimentally-determined kinetic rate equations and constants

Geochemical Processes

Mass-transfer processes	Rate-controlling processes	Rate-modifying factors
DISSOLUTION / PRECIPITATION by: acid-base reactions hydrolysis redox reactions co-precipitation gas release/capture Wetting-drying ION EXCHANGE / SORPTION RADIOACTIVE DECAY	DIFFUSION - macroscopic - microscopic - atomic-scale NUCLEATION SURFACE REACTION ADSORPTION/ DESORPTION	CATALYSIS bacterial galvanic abiotic TEMPERATURE PRESSURE SURFACE AREA

Models for AMD Prediction

Definitions

- Model: a theoretical or physical construct that simulates a system
- Geochemical model: ...for geochemical systems
- Computer model: computer program incorporating theoretical or physical construct

Classification of Geochemical Models

- Equilibrium thermodynamic models
- Mass transfer models
- Coupled mass transfer-flow models
- Empirical and engineering models

Equilibrium thermodynamic models

- Solve the equilibrium distribution of mass among various solid or dissolved species and complexes
- Results reported as saturation indexes (SI) for minerals
- examples: MINTEQ, PHREEQE

Mass transfer models

- Simulate the kinetic evolution of solution chemistry as the system progresses towards equilibrium
- Results give aqueous concentrations and solid masses vs time
- examples: EQ6, PATHARC

Coupled mass transfer-flow models

- Simulate the evolution of solution chemistry in open fluid-rock systems
- Consider flow and solute transport
- examples: MINTRAN, PHREEQM

Empirical and Engineering models

- Simulate solution chemistry by using simplifying assumptions
- Focus on comparison of containment conditions
- examples: WATAIL, ACIDROCK

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Data Requirements

MODEL	CLASS ---->	EQUIL.	M.T.	M.T./FLOW	EMP/ENG
Input	Parameters				
Field	Water Chem.	+++	++	++	+
Data	Mineralogy	+	+++	++	+
	Surface Area	0	+++	+++	+
	Temperature	+	+	+	+
	Oxygen	+	++	++	++
	Water Balance	0	+	++	++
	Pile Structure	0	0	0	++
Lab Data	Column Test	0	0	0	+
	Humidity Cell	0	0	0	+
Database	Thermodynamic	+++	+++	+++	++
	Kinetic	0	+++	+++	+

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Model Applicability vs Prediction Objectives

Model	**Class ---->**	**Equil.**	**M.T.**	**MT/Flow**	**Emp/Eng**
Prediction Objective	I.D. Species	+++	++	+	0
	Max. Conc.	+	++	+	0
	Max. Loads	+	++	++	+
	Duration	0	++	+++	++
	Conc. - Time	0	+	++	+
	Decomm. Option	0	0	++	+++

Relative applicability of models
0 = none or not used
+ = the least
++ = intermediate
+++ = the most

Summary

- Physical, geochemical systems described
- Incorporation in computer models
- Computer model classification - levels
- Data requirements
- Applicability vs prediction objectives

Summary (cont'd)

1) Identify objectives
2) Characterize processes
3) Select model
4) Interpret results

Recommendations (1)

- Field dataset collection
- Better determination of reaction mechanisms
- Collect thermodynamic equilibrium constants
- Develop kinetic rate equations

Recommendations (2)

- Do not expect existing geochemical models to accurately predict water chemistry with time
- Encourage the application of mass transfer models to well-defined systems
- Use empirical models

Recommendations (3)

- Coordinate model development to follow developments in the understanding of geochemical and physical processes

MODELING ACIDIC DRAINAGE

(with emphasis on waste rock)

Daryl Hockley

Steffen Robertson & Kirsten (Canada) Inc.

Outline

Survey of available models

Conclusions from review

Recommendations for ARD modeling

Examples

Survey of Available Models

"critical review and discussion of mathematical models of acidic drainage from waste rock piles ..."

"emphasis on engineering models..."

"reference to ... physical and conceptual modelling"

Topics covered

Terminology

Process - specific models

Engineering models

Recommendations

Terminology

"... discussions about modeling are often confused by imprecise or inconsistent terminology"

conceptual vs. physical vs. mathematical models

empirical vs. mechanistic

deterministic vs. stochastic

comprehensive vs. process specific

Process - Specific Models

"models of individual processes,

or groups of coupled processes,

that contribute to, influence or are influenced by

acidic drainage in waste rock"

See Figure 1 of Background Material

Process - Specific Models

1. External processes and variables

- *site geology & mine planning*
- *site hydrogeology*
- *site meteorology*

Process - Specific Models

2. Construction of waste rock piles

- *pile geometry*
- *distribution of material*
- *mixing of material during construction*
- *effects on physical characteristics*

See Figure 2 of Background Material

Process - Specific Models

3. Infiltration and water flow within waste rock piles

- *infiltration*
- *unsaturated flow*
- *channel flow*
- *saturated flow*

See Figure 3 of Background Material

Process - Specific Models

4. Oxygen and heat transport

- *advection*
- *thermal convection*
- *air phase diffusion*

See Figure 4 of Background Material

Process - Specific Models

5. Geochemical processes

- *oxidation of sulphide minerals*
- *dissolution of carbonates, hydroxides, silicates*
- *precipitation of oxy-hydroxides*
- *precipitation and dissolution of sulphates*
- *co-precipitation, ion exchange, sorption*

See Figure 5 of Background Material

Process - Specific Models

6. **Contaminant transport within waste rock piles**
7. **Downstream impacts**
8. **Remediation measures**
   - *covers*
   - *geochemical controls*
   - *collection and treatment*

Engineering Models

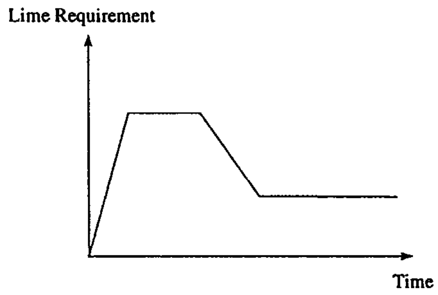
"models that are intended to support practical decisions about real systems"

Engineering Models

Empirical models

Equity Silver Technical Committee (1991)

SRK (1995)



Engineering Models

Semi-empirical models

ACIDROCK - Senes (1991)

QROCK - SRK (1993)

FIDHELM - ANSTO (1994)

Conclusions from Review

Process - Specific Models

- *surprising number & diversity*
- *some processes well understood & modeled*
- *other (important) processes neglected*
- *current approach is "bottom up"*

Conclusions from Review

Engineering Models

- *all are at least partly empirical*
- *empirical models are more transparent*
- *poor documentation*
- *lack of consideration of uncertainty*
- *lack of validation*
- *"bottom up"*

Conclusions from Review

Current State of the Art

- *Mechanistic models of some processes are available. They are reliable if used in appropriate circumstances and with appropriate input parameters.*
- *Understanding of other important processes is not sufficient to allow mechanistic modeling. Empirical models are available but reliability is very dependent on data availability.*

Conclusions from Review

Current State of the Art

- *It's relatively easy to create comprehensive models by coupling process-specific models. Several examples exist in the literature and in the consulting community.*
- *A good alternative is to make judicious selection of process specific models, and use them appropriately.*

Conclusions from Review

Given the current state of the art, we need to:

- *be aware of weaknesses in fundamental understanding*
- *appreciate difficulty and expense associated with measuring model inputs*
- *know which processes can be modeled easily, and which can be more easily measured in the field or laboratory*
- *understand the context, and carefully select the appropriate level of precision*

Recommended Approach to ARD Modeling

(1) clearly define the question

(2) determine information needs

(3) review available information

(4) select appropriate combination of modeling, field measurement and laboratory testing

(5) consider uncertainty and present "conclusions" rather than "results"

Start simple!

Example 1
Selecting remediation measures for fourteen waste rock piles

Example 1
Define the question

Fourteen waste rock piles resulting from uranium mining
- acid generating material present in all piles
- remediation coupled by lack of space in pit

For each waste rock pile, only three realistic options existed:
- relocation to pit
- cover in situ
- collect and treat

Example 1
Determine information needs

In selecting among the realistic option, ten factors were identified as potentially important:

Cost: implementation
future water treatment
land values
Risk: radiological
conventional
long term environmental
institutional
Acceptance: local public
regulations
existing permits

Example 1
Review available information

Of the ten factors, the following could be adequately characterized using existing information:

- land values
- radiological risks
- conventional risks
- long term environmental risks
- institutional risks
- local public acceptance
- regulatory acceptance
- conformance with existing permits

Example 1
Select appropriate methods

Further information required about:
- implimentation costs
- long term water treatment

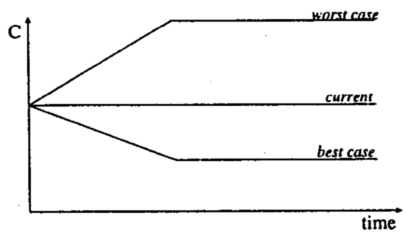
Implimentation costs estimated using normal methods

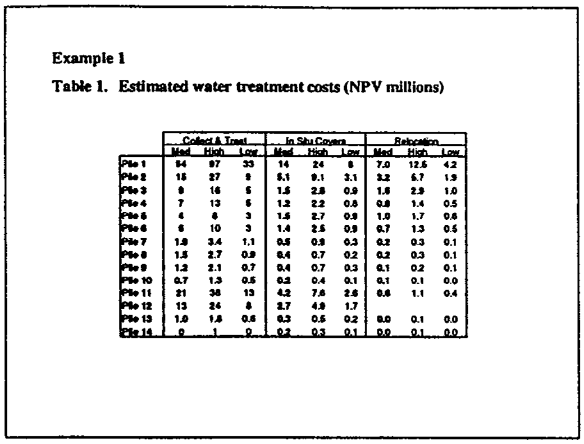
Detailed relationships between water treatment costs, flowrates, and water quality could be developed relatively easily.

Estimates of long term water quality under each remediation option would be much more difficult.

Example 1
Select appropriate methods

"Start simple" approach used to estimate water quality:

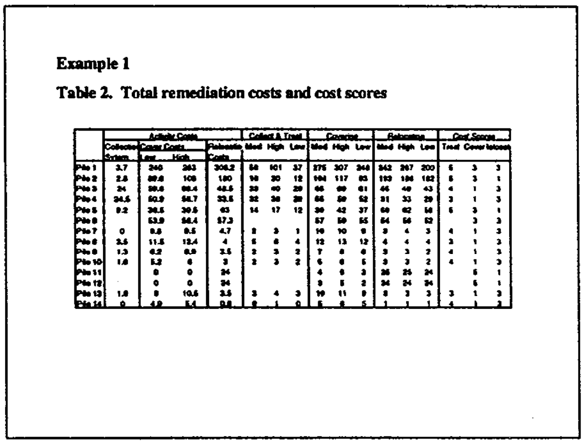




Example 1

Table 1. Estimated water treatment costs (NPV millions)

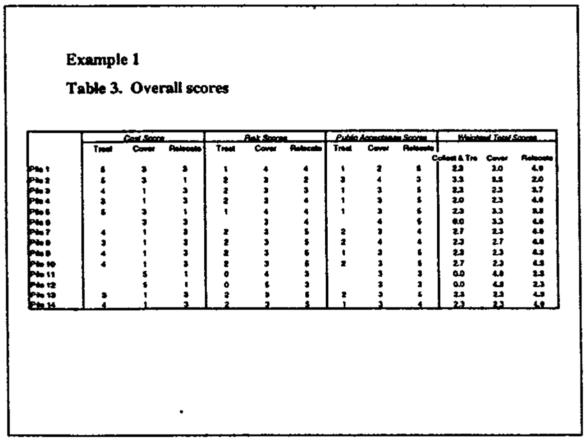
	Collect & Treat			In Situ Covers			Relocation		
	Med	High	Low	Med	High	Low	Med	High	Low
Pile 1	54	97	33	14	24	8	7.0	12.6	4.2
Pile 2	15	27	9	5.1	9.1	3.1	3.2	5.7	1.9
Pile 3	9	16	5	1.5	2.8	0.9	1.6	2.9	1.0
Pile 4	7	13	5	1.2	2.2	0.8	0.8	1.4	0.5
Pile 5	4	8	3	1.5	2.7	0.9	1.0	1.7	0.6
Pile 6	6	10	3	1.4	2.5	0.9	0.7	1.3	0.5
Pile 7	1.9	3.4	1.1	0.5	0.9	0.3	0.2	0.3	0.1
Pile 8	1.5	2.7	0.9	0.4	0.7	0.2	0.2	0.3	0.1
Pile 9	1.2	2.1	0.7	0.4	0.7	0.3	0.1	0.2	0.1
Pile 10	0.7	1.3	0.5	0.2	0.4	0.1	0.1	0.1	0.0
Pile 11	21	38	13	4.2	7.6	2.6	0.6	1.1	0.4
Pile 12	13	24	8	2.7	4.9	1.7			
Pile 13	1.0	1.8	0.6	0.3	0.5	0.2	0.0	0.1	0.0
Pile 14	0	1	0	0.2	0.3	0.1	0.0	0.1	0.0



Example 1

Table 2. Total remediation costs and cost scores

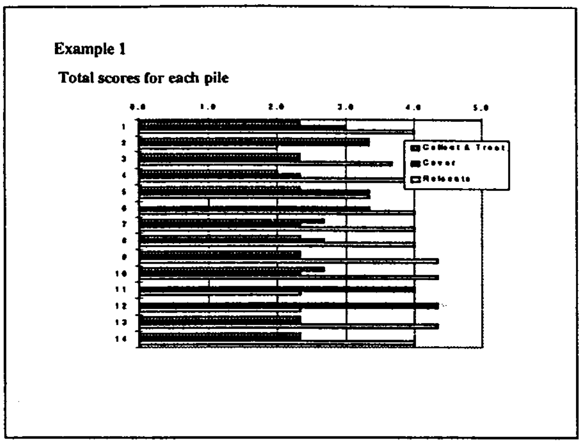
	Activity Costs				Collect & Treat			Coverage			Relocation			Cost Scores		
	Collection System	Cover Costs		Relocate Costs	Med	High	Low	Med	High	Low	Med	High	Low	Treat	Cover	Relocate
		Low	High													
Pile 1	3.7	240	263	306.2	58	101	37	275	307	248	342	267	200	5	3	3
Pile 2	2.8	89.6	108	180	18	30	12	104	117	83	193	196	182	5	3	1
Pile 3	24	30.6	60.4	48.5	33	40	29	66	69	61	46	48	43	4	1	3
Pile 4	34.5	50.9	54.7	33.5	32	38	29	66	59	52	31	33	29	3	1	3
Pile 5	9.2	36.5	39.5	63	14	17	12	39	42	37	60	62	58	5	3	1
Pile 6		53.9	56.4	57.3				57	59	55	54	56	52		3	3
Pile 7	0	9.8	9.5	4.7	2	3	1	10	10	9	3	4	3	4	1	3
Pile 8	3.5	11.5	12.4	4	5	6	4	12	13	12	4	4	4	3	1	3
Pile 9	1.3	6.2	6.9	3.5	2	3	2	7	8	6	3	3	2	4	1	3
Pile 10	1.8	5.2	6	3	2	3	2	6	6	5	3	3	2	4	1	3
Pile 11		0	0	24				4	6	3	26	25	24		5	1
Pile 12		0	0	24				3	5	2	24	24	24		5	1
Pile 13	1.8	9	10.6	3.5	3	4	3	10	11	9	3	3	3	3	1	3
Pile 14	0	4.9	5.4	0.8	0	1	0	6	6	5	1	1	1	4	1	3



Example 1

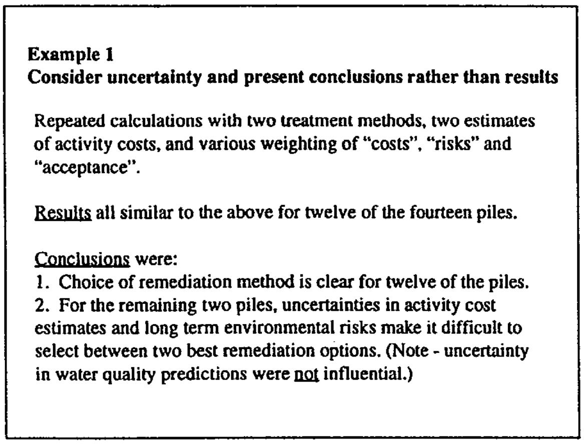
Table 3. Overall scores

	Cost Score			*Risk Scores*			*Public Acceptance Scores*			*Weighted Total Scores*		
	Treat	Cover	Relocate	Treat	Cover	Relocate	Treat	Cover	Relocate	Collect & Tre	Cover	Relocate
Pile 1	5	3	3	1	4	4	1	2	5	2.3	3.0	4.0
Pile 2	5	3	1	2	3	2	3	4	3	3.3	3.5	2.0
Pile 3	4	1	3	2	3	3	1	3	5	2.3	2.3	3.7
Pile 4	3	1	3	2	3	4	1	3	5	2.0	2.3	4.0
Pile 5	5	3	1	1	4	4	1	3	6	2.3	3.3	3.5
Pile 6		3	3		3	4		4	6	0.0	3.3	4.0
Pile 7	4	1	3	2	3	5	2	3	4	2.7	2.3	4.0
Pile 8	3	1	3	2	3	5	2	4	4	2.3	2.7	4.0
Pile 9	4	1	3	2	3	6	1	3	5	2.3	2.3	4.3
Pile 10	4	1	3	2	3	5	2	3	5	2.7	2.3	4.3
Pile 11		5	1	0	4	3		3	3	0.0	4.0	3.3
Pile 12		5	1	0	5	3		3	3	0.0	4.3	2.3
Pile 13	3	1	3	2	3	5	2	3	5	2.3	2.3	4.3
Pile 14	4	1	3	2	2	5	1	3	4	2.3	2.3	4.0



Example 1

Total scores for each pile



Example 1

Consider uncertainty and present conclusions rather than results

Repeated calculations with two treatment methods, two estimates of activity costs, and various weighting of "costs", "risks" and "acceptance".

Results all similar to the above for twelve of the fourteen piles.

Conclusions were:

1. Choice of remediation method is clear for twelve of the piles.
2. For the remaining two piles, uncertainties in activity cost estimates and long term environmental risks make it difficult to select between two best remediation options. (Note - uncertainty in water quality predictions were not influential.)

Example 2
Selecting remediation method for acid generating pile

Example 2
Define the question

Waste rock pile releasing acidic drainage. Pile has been in place for twenty years.

Remediation options that would reduce current oxidation rates have been proposed.

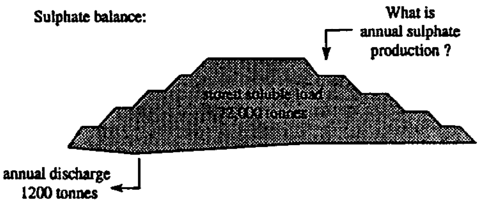
Key questions are whether acid generation will stop on its own and whether active remediation will have significant impact.

Example 2
Review available information

Extensive set of ARD characterization data:
- geological and mineralogicaldescriptions of source rock
- construction history
- extensive drillhole database including static tests
- clear delineation of zones within pile
- five years of reliable water quality monitoring
- column tests

Example 2
Review available information

Sulphate balance:



Example 2
Select appropriate combination of modeling and laboratory or field methods

Comparison of current oxidation rates to current sulphate release rates and to stored sulphate load

Instrumentation of pile to measure oxygen and heat distributions

Oxygen and/or heat transfer modeling to quantify current oxidation rates

Example 2

Figure 1. Example resuts from monitoring installation

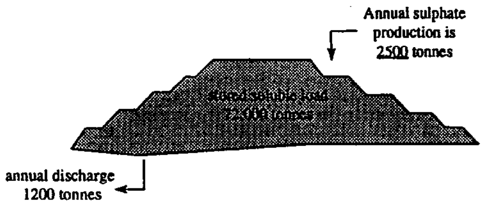
Example 2

Figure 2. Example of heat transfer model

Example 2

Figure 3. Results of heat transfer model

Example 2
Results



Example 2
Present conclusions rather than results

Conclude that rate of sulphate production by continuing oxidation exceeds rate of sulphate removal ... therefore no "self remediation"

However, current rate of oxidation is small in comparison to stored contaminant load ... therefore measures to slow oxidation are unlikely to result in rapid decrease in contaminant discharges

Consideration of detailed cost estimates led to recommendation that pile be covered in situ, with cover design to emphasize reduction of infiltration rather than control of oxidation

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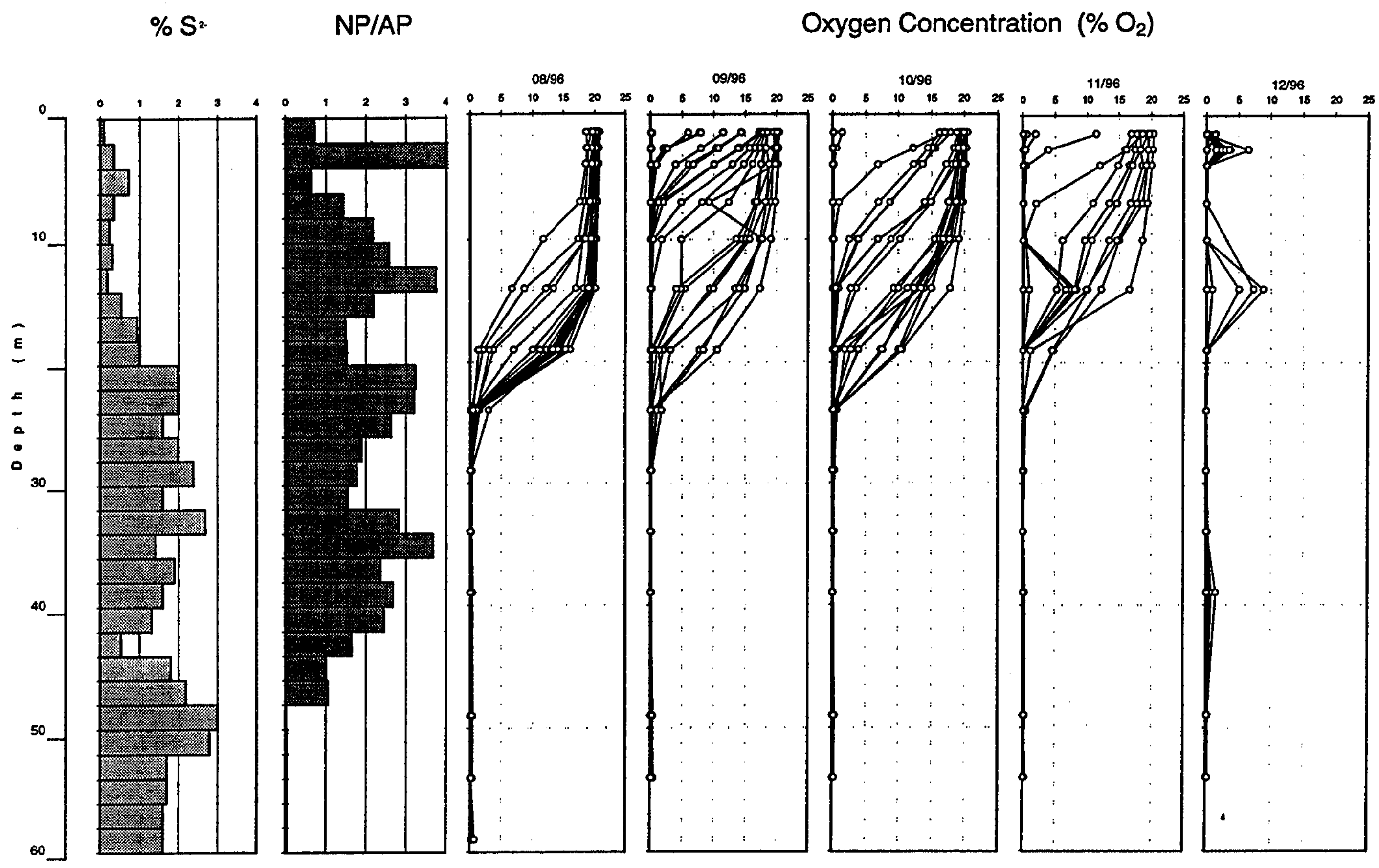
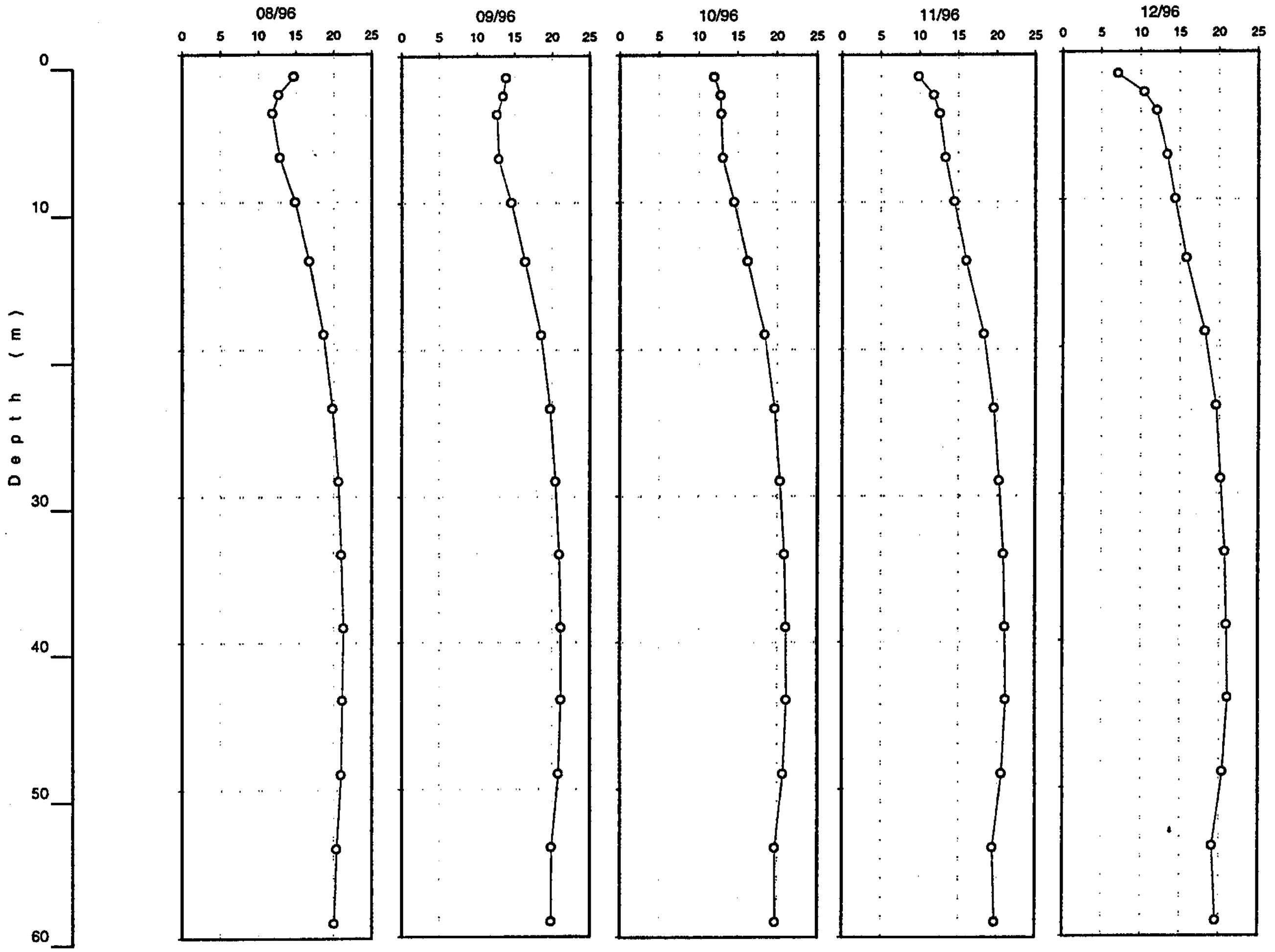
Drill Hole Ro 3 - 40
Data



Example 2
Figure 1A
Steffen, Robertson and Kirsten (Canada) Inc.

Drill Hole Ro 3 - 40
Data

Temperature Profile (C)



Example 2
Figure 1B
Steffen, Robertson and Kirsten (Canada) Inc.

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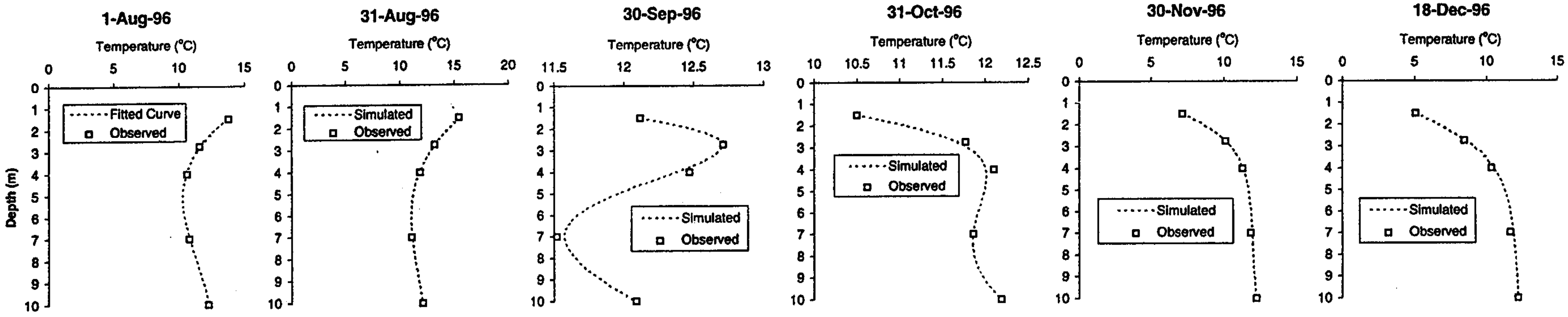
Calibration of Thermal Diffusion Co-efficient

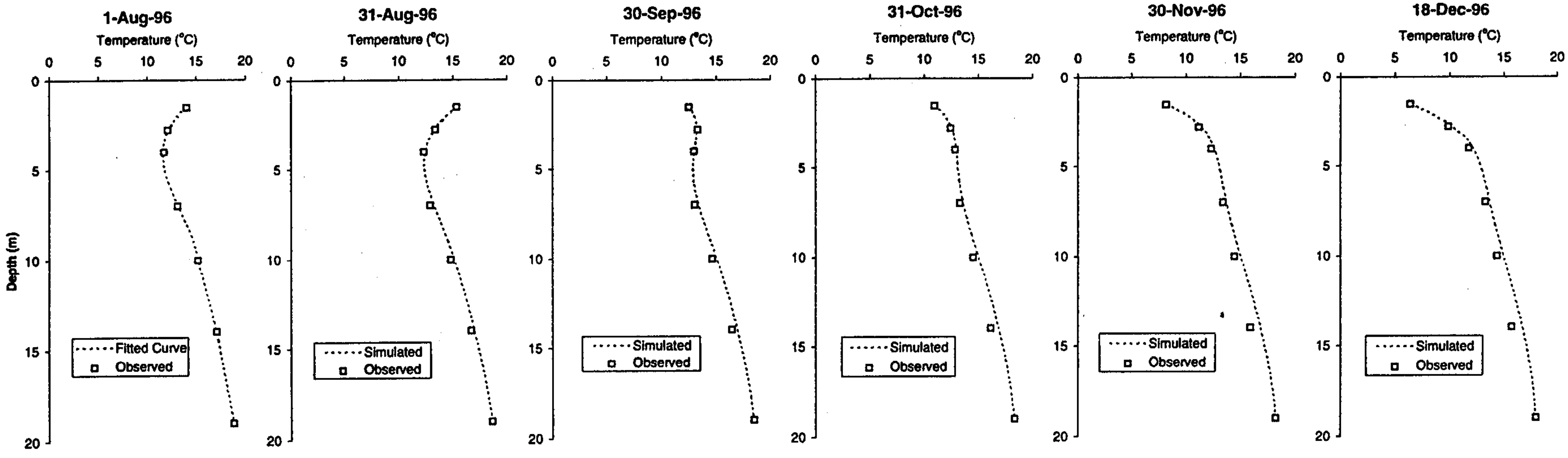
Borehole 36

Diffusion Co-efficient: 8×10^{-7} m^2/s



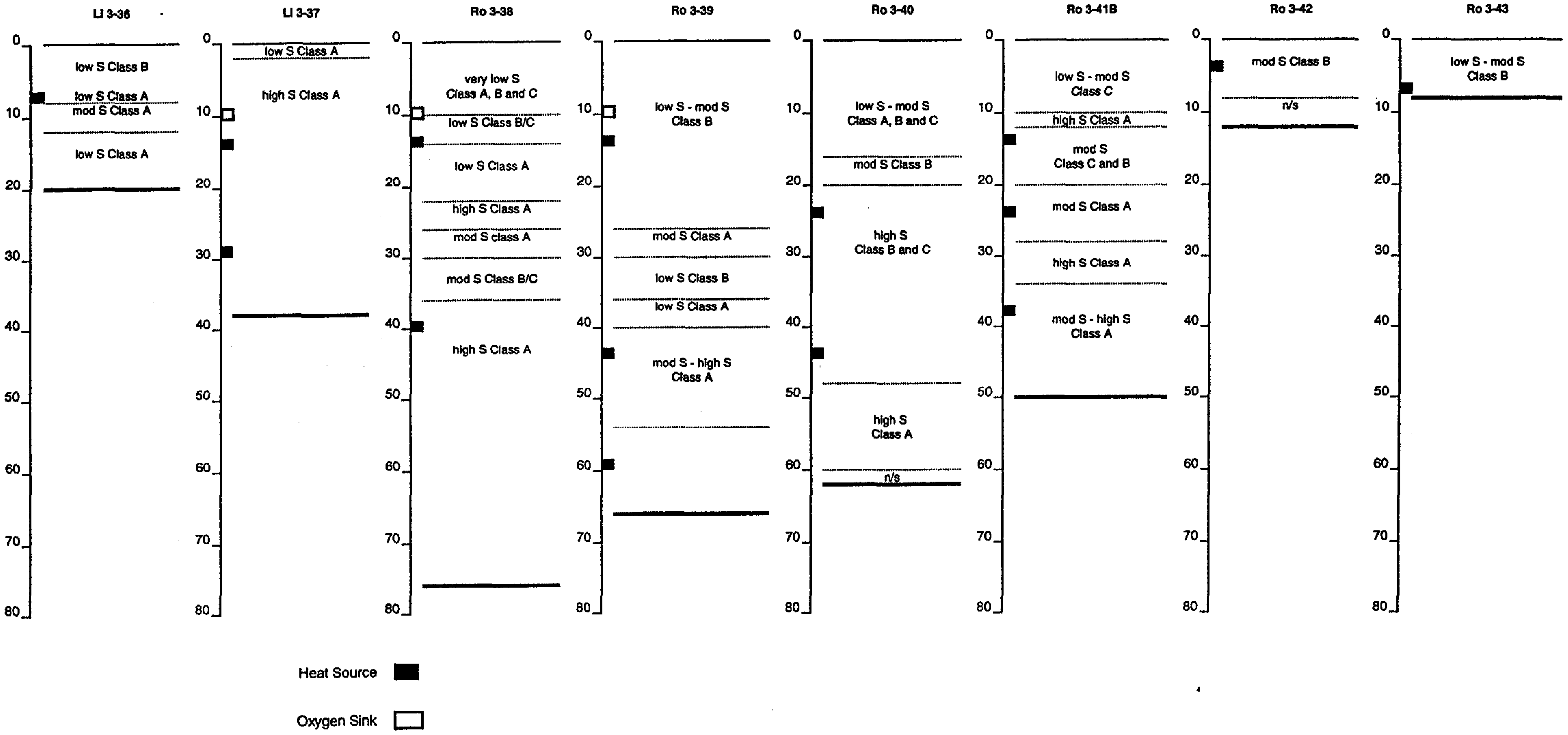
Borehole 40

Diffusion Co-efficient: 5×10^{-7} m^2/s



Example 2
Figure 2
Steffen, Robertson and Kirsten (Canada) Inc.

Summary Logs



Example 2
Figure 3
Steffen Robertson Kirsten (Canada) Inc.

Example 3
Selecting remediation method for neutral pH pile

Example 3
Define the question

Waste rock pile releasing drainage with high sulphate concentrations (to 35,000 ppm) at neutral pH

Uranium discharges also a concern

Need to estimate uranium and sulphate concentrations if pile were to be covered with oxygen consuming material and/or engineered soil cover

---

Example 3
Review available information

Extensive set of ARD characterization data

Used "diagnostic modeling"to estimate:
- historical oxidation rates
- channelization of flow through pile
- nature of buffering minerals - influence of dolomite
- controls on contaminant solubility

Example 3
Review available information

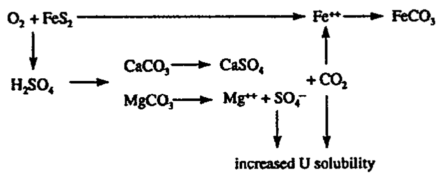
Use of geochemical equilibrium models
MINTEQA2, PHREEQ-C, EQ3

input measured concentrations
allow program to calculate aqueous speciation
compare estimated concentrations to mineral solubilities

select probable solubility controlling phases
use model to predict equilibrium cocentrations

Example 3
Review available information

Identified key chemical reactions


$O_2 + FeS_2$
Fe^{++}
$FeCO_3$
H_2SO_4
$CaCO_3$
$CaSO_4$
$+ CO_2$
$MgCO_3$
$Mg^{++} + SO_4^{--}$
increased U solubility

Example 3
Select appropriate model

Two-way coupled processes determines major element chemistry:

- O2 transport
- Pyrite oxidation
- Carbonate dissolution
- CO2 transport

Need one model of these processes

Output of first model used to predict trace element concentrations, including U

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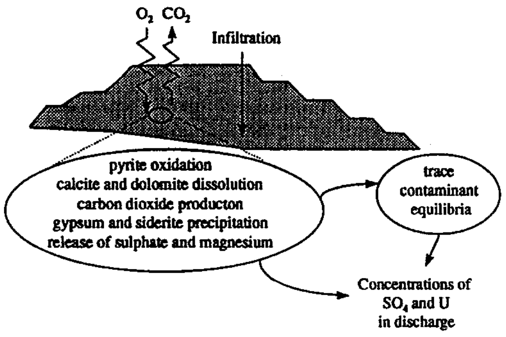
Example 3



O_2 CO_2

Infiltration

pyrite oxidation
calcite and dolomite dissolution
carbon dioxide producton
gypsum and siderite precipitation
release of sulphate and magnesium

trace
contaminant
equilibria

Concentrations of
SO_4 and U
in discharge

Example 3
Present conclusions rather than results

Conclude that cover and oxygen consuming material will lead to significant long term decrease in sulphate concentrations

Expect short term increase in uranium concentrations, but difficult to quantify

Uncertainties in flow patterns through cover lead to uncertainties in prediction of short term loads

Example 4
Reality check on estimates of sulphate concentrations

Example 4
Define the question

Proposed expansion of tailings impoundment

Tailings are 5% sulphide

Earlier prediction is sulphate concentrations of 1500 ppm in groundwater, decreasing to 300 ppm

Example 4
Review available information

Very limited ARD characterization data

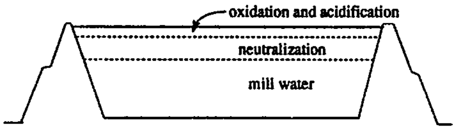
Some field data from existing site, but only under operating conditions

No possibility to get further data at this time

Conclude that prediction will need to be based largely on literature data

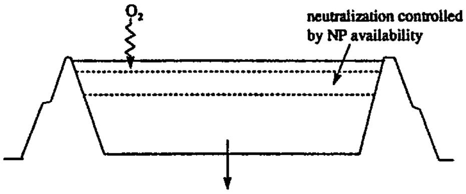
Example 4
Review available information

Literature indicates reaction path



Example 4
Review available information

rate of oxidation and acidification controlled by
oxygen diffusion through unsaturated pores



neutralization controlled
by NP availability

short term discharge water quality
controlled by mill water composition

Example 4
Select appropriate model

Key question is long term discharge water quality

Need to consider:

- O2 transport - controlled by tailings water content
- Overall oxidation rate controlled by oxygen transport
- Oxidation of sulphide minerals at different rates
- Dilution and downwards transport of acidity by infiltration
- Consumpion of NP
- Secondary mineralization of trace metals

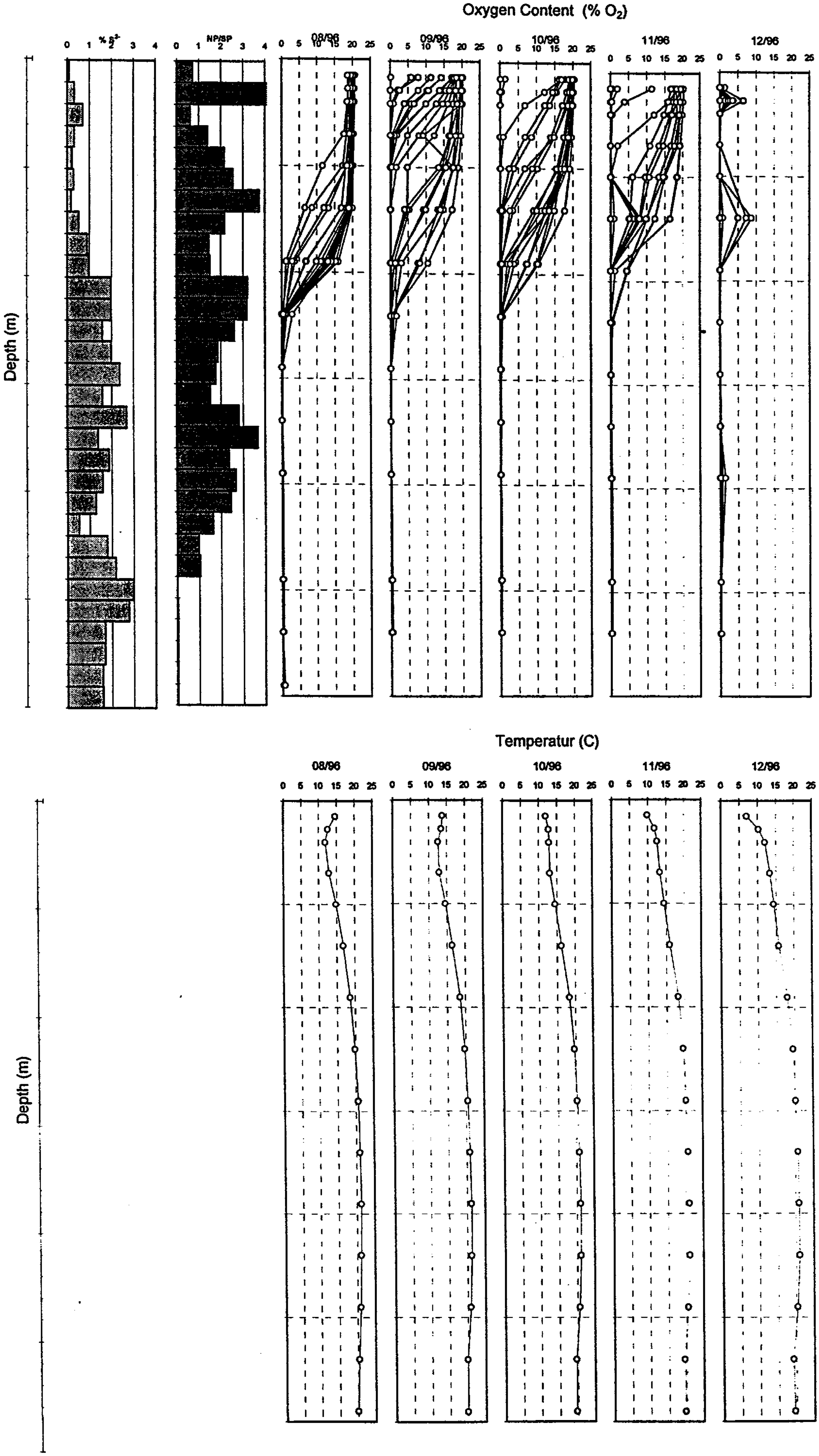

Oxygen Content (% O2)
% S2-
0 1 2 3 4
NP/SP
0 1 2 3 4
08/96
09/96
10/96
11/96
12/96
0 5 10 15 20 25
Depth (m)
Temperatur (C)
08/96
09/96
10/96
11/96
12/96
0 5 10 15 20 25
Depth (m)

Figure 4

Example 4
Select appropriate model

Used series of simple models

- Uniform unsaturated flow model to estimate water contents
- Literature model to relate water content to oxygen diffusion coeficient
- One dimensional oxygen diffusion and consumption model
- Relative oxidation rates (of various metal sulphides) from literature
- Dilution by infiltration rate to estimate concentrations in acidic zone
- MINTEQA2 to estimate concentrations after secondary precipitation
- NP mass balance to estimate time of arrival of acidic front

All calculations were implemented in an EXCEL spreadsheet to allow for easy sensititivty analyses

Example 4
Present conclusions but be clear how (in)conclusive they are

"Calculations completed using simple models and literature data indicate that the earlier work is correct in concluding that acidic conditions are unlikely to develop."

"The sulphate concentrations estimated by the earlier work are within the range obtained from our calculations. However, the upper end of our range is 2500 ppm, higher than estimated earlier."

"The prediction that sulphate concentrations will decline to 300 ppm shortly after closure is not supported by our calculations."

Reiterate uncertainties caused by lack of site specific data.

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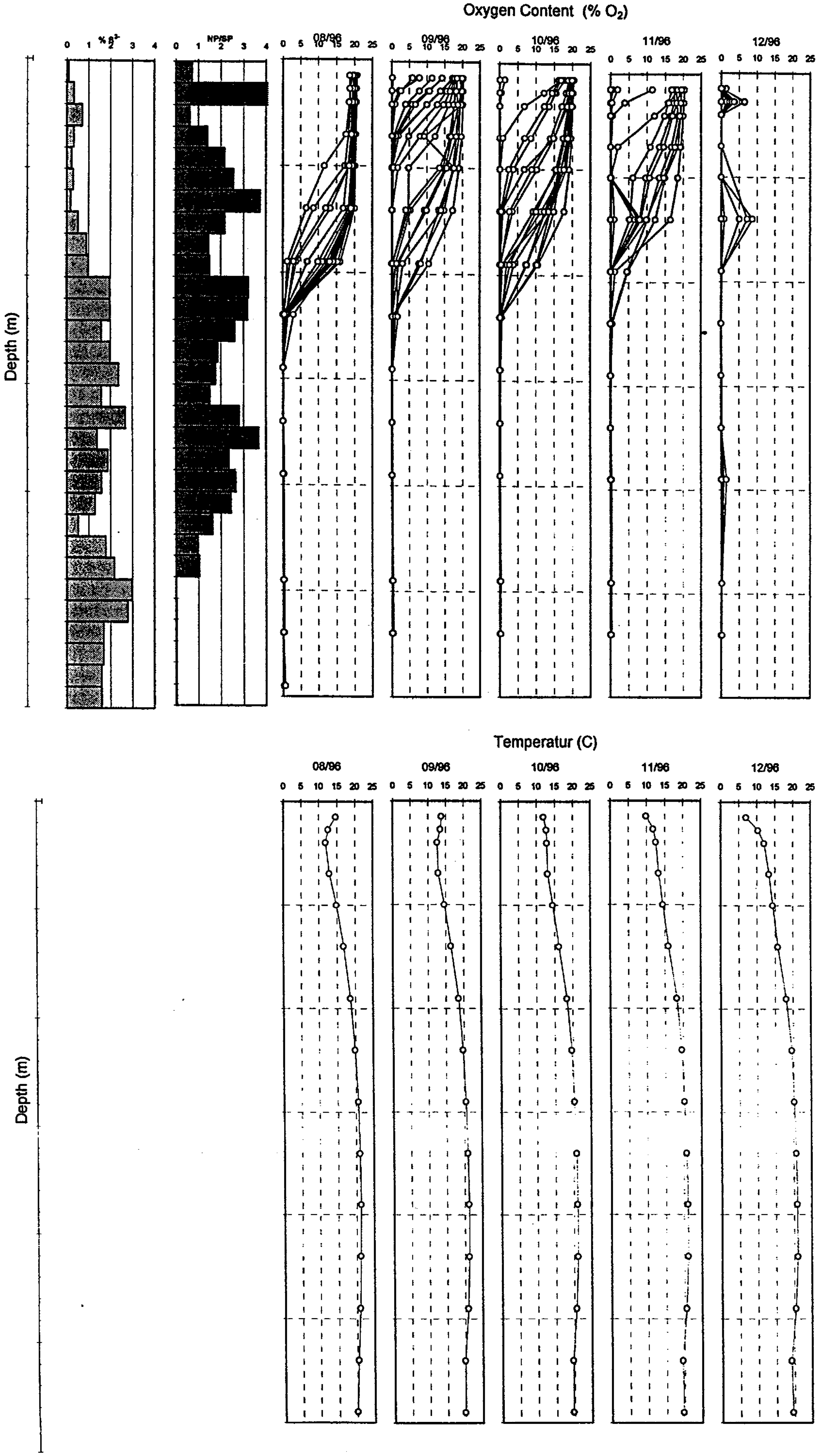

Oxygen Content (% O_2)

Temperatur (C)

Figure 4

Welcome Screen Search Report List

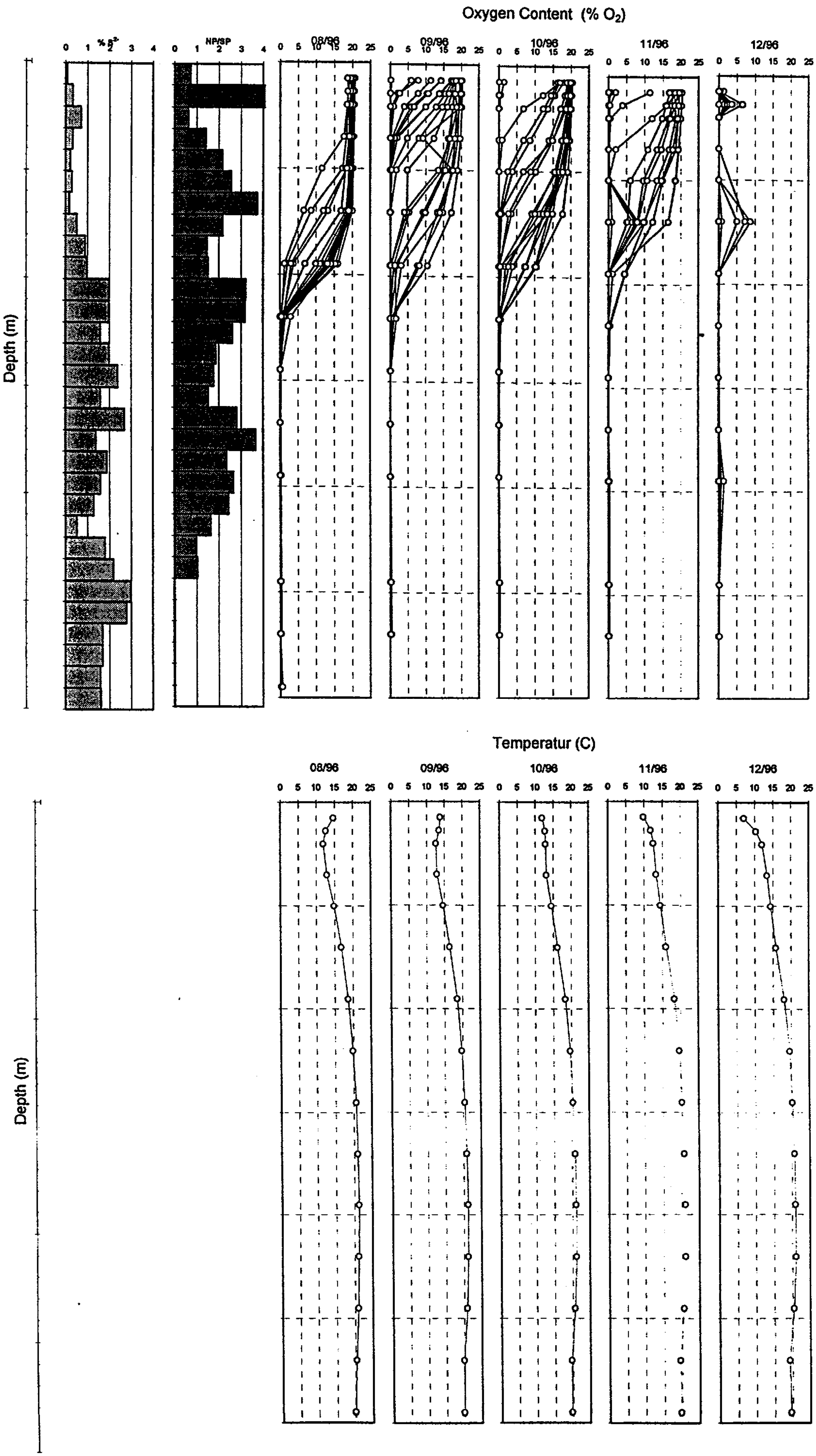

Figure 4

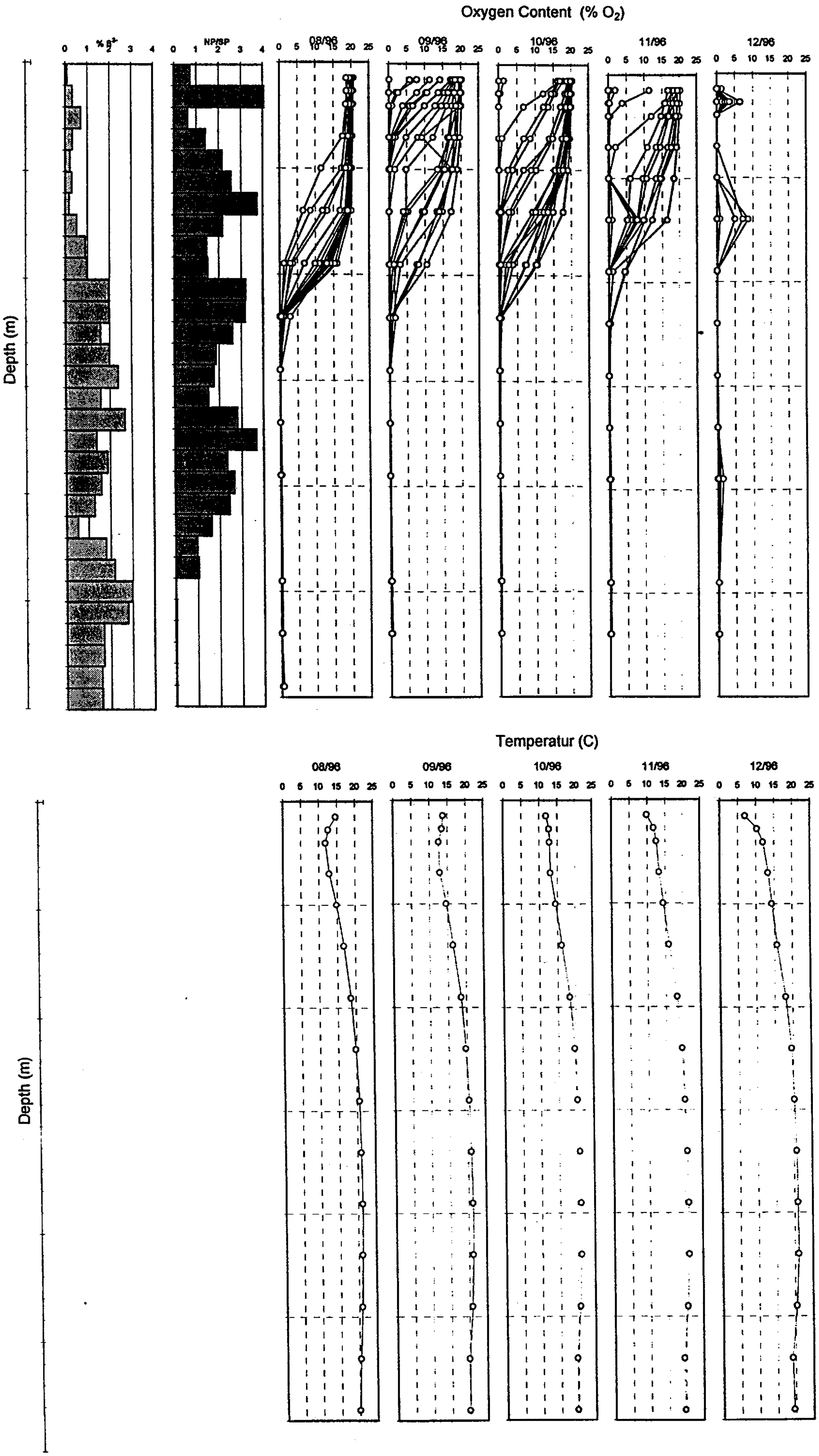
Oxygen Content (% O_2)
% S^{2-}
0 1 2 3 4
NP/SP
0 1 2 3 4
08/96
09/96
10/96
11/96
12/96
0 5 10 15 20 25
Depth (m)
Temperatur (C)
08/96
09/96
10/96
11/96
12/96
0 5 10 15 20 25
Depth (m)

Figure 4

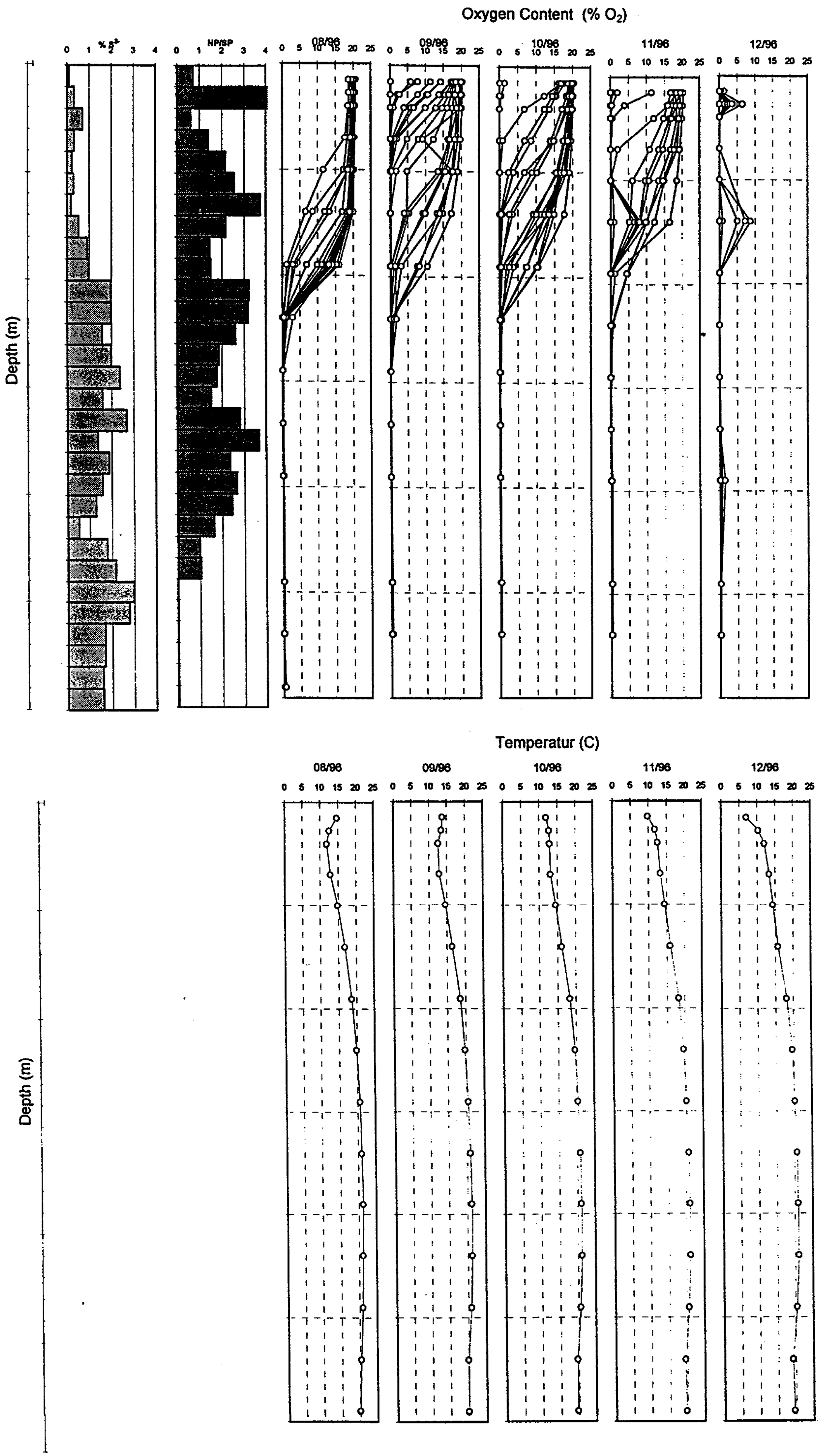
Oxygen Content (% O2)
Depth (m)
% S²⁻
0 1 2 3 4
NP/SP
0 1 2 3 4
08/96
09/96
10/96
11/96
12/96
0 5 10 15 20 25
Temperatur (C)
08/96
09/96
10/96
11/96
12/96
0 5 10 15 20 25
Depth (m)

Figure 4

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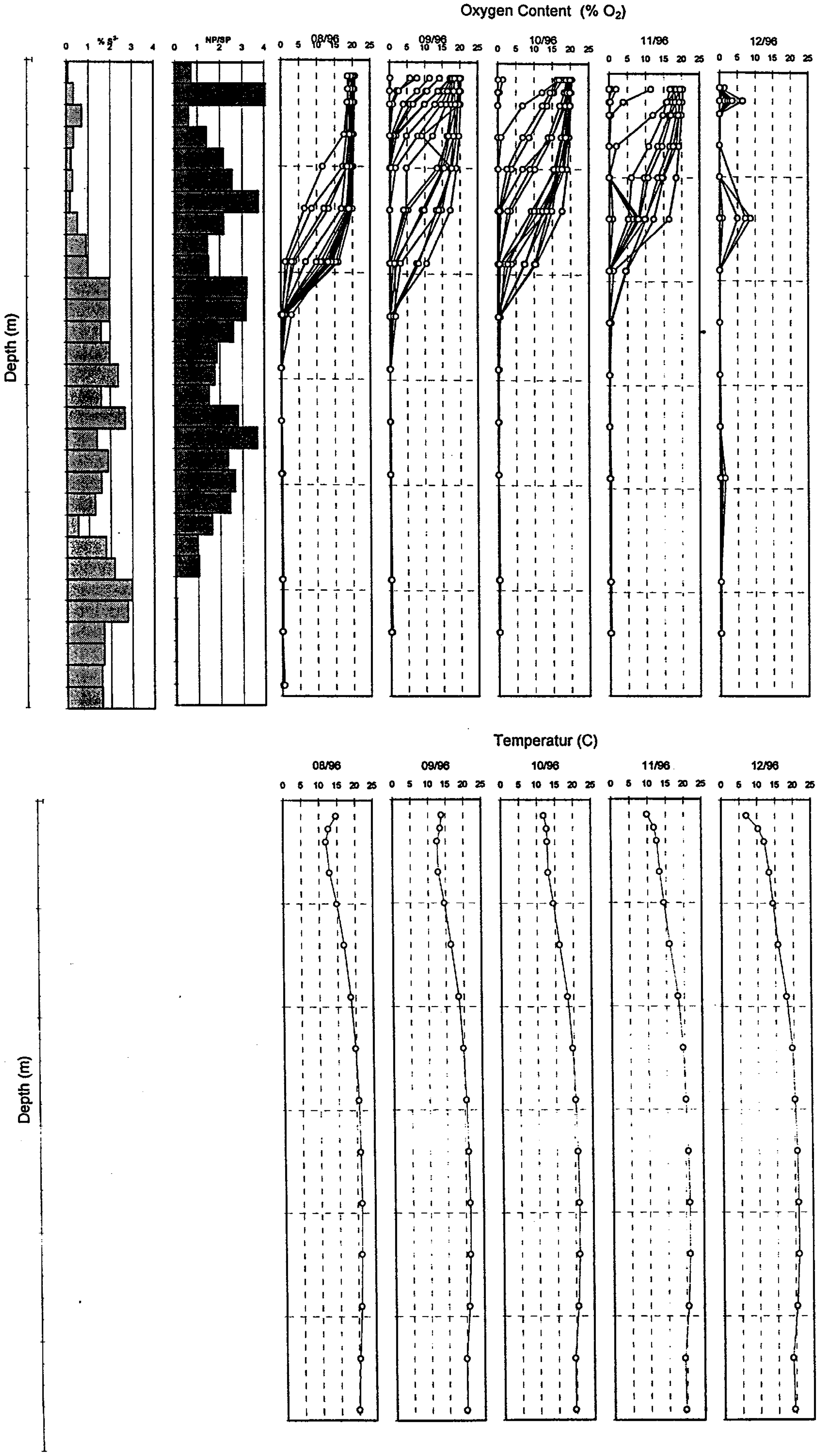
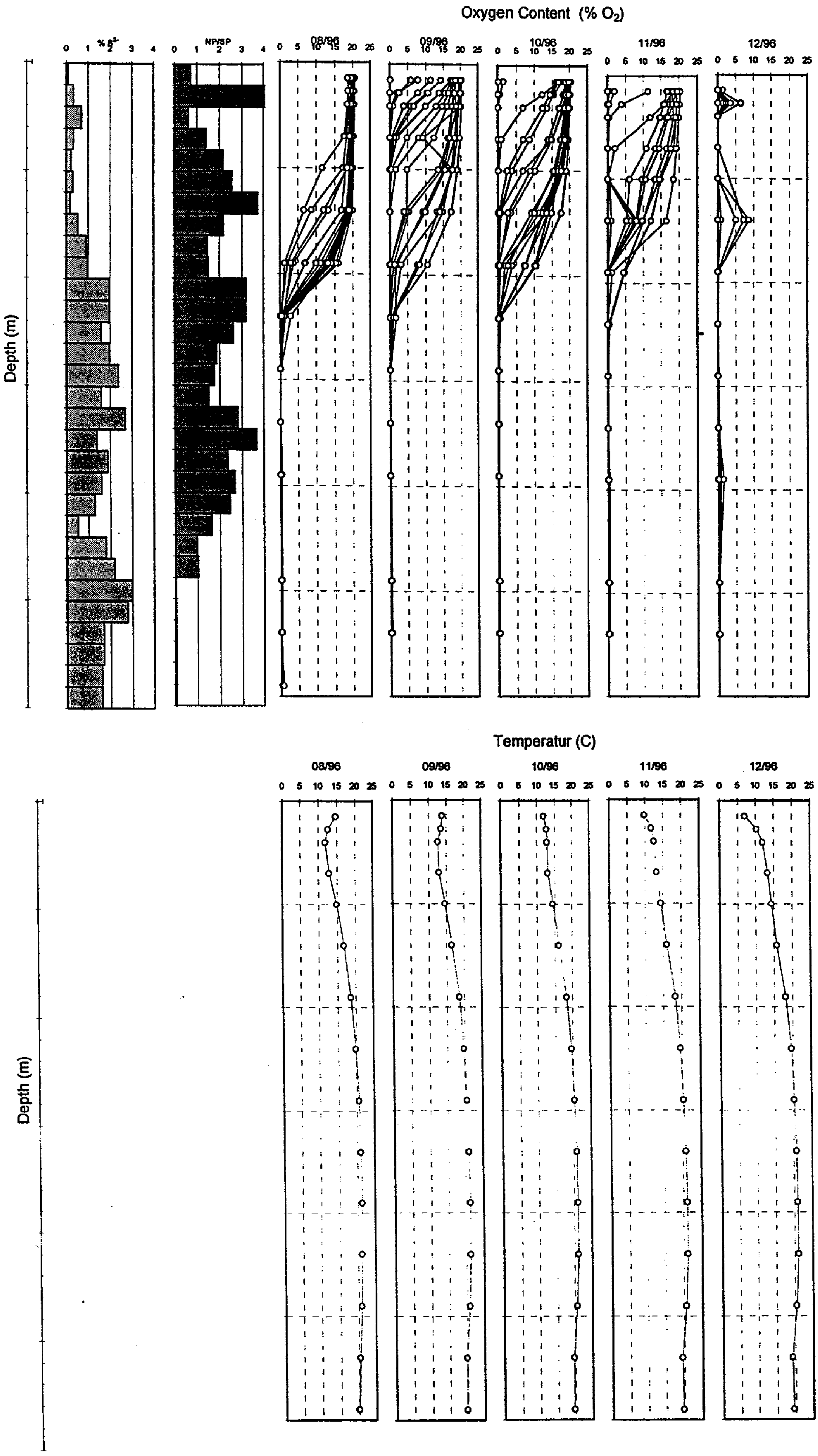


Oxygen Content (% O_2)

Temperatur (C)

Figure 4


Oxygen Content (% O_2)
Depth (m)
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NP/SP
0 1 2 3 4
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10/96
11/96
12/96
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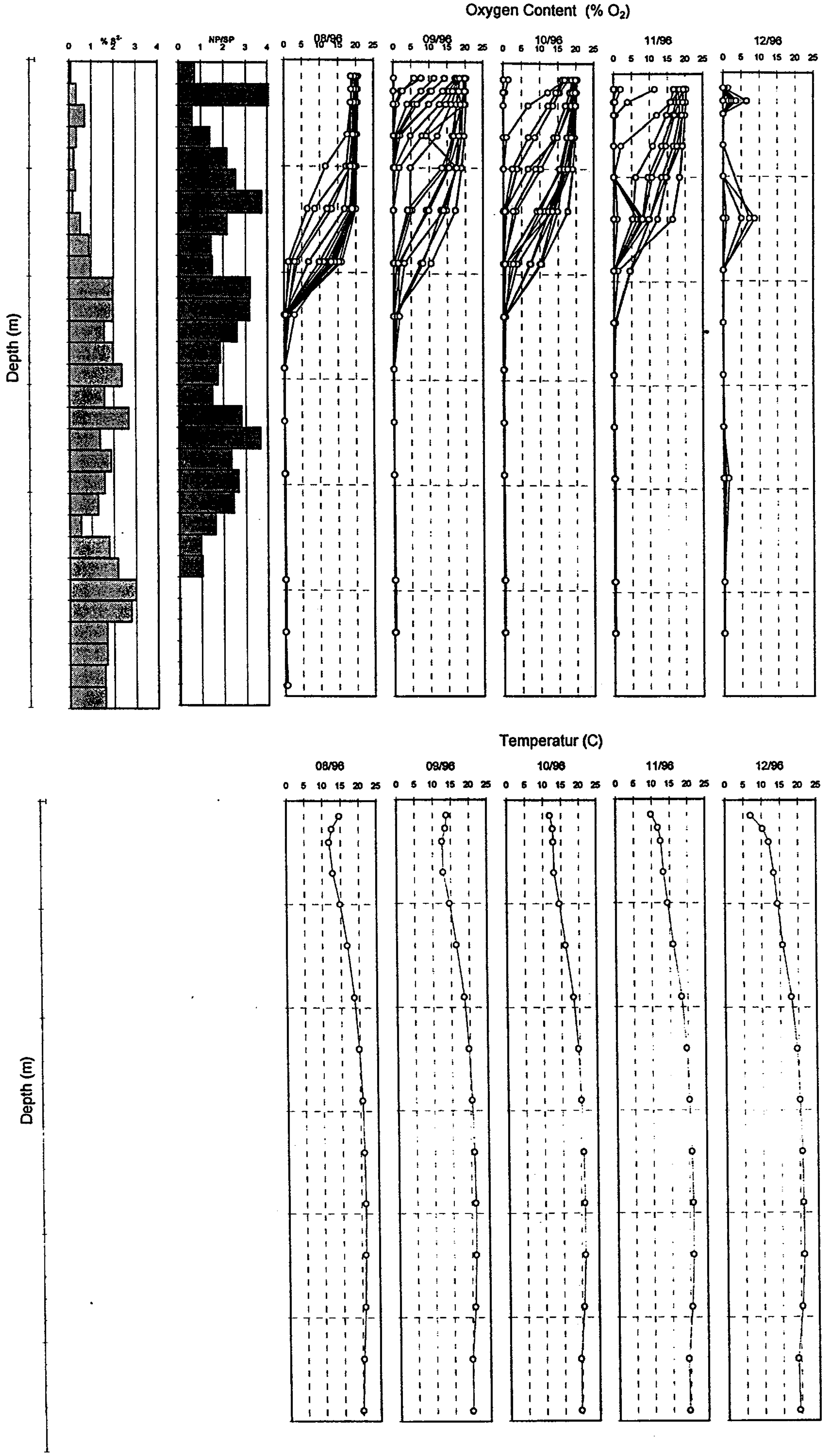
Depth (m)
08/96
09/96
10/96
11/96
12/96
0 5 10 15 20 25

Figure 4


Oxygen Content (% O$_2$)
Depth (m)
% S^{2-}
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NP/SP
0 1 2 3 4
08/96
09/96
10/96
11/96
12/96
0 5 10 15 20 25
Temperatur (C)
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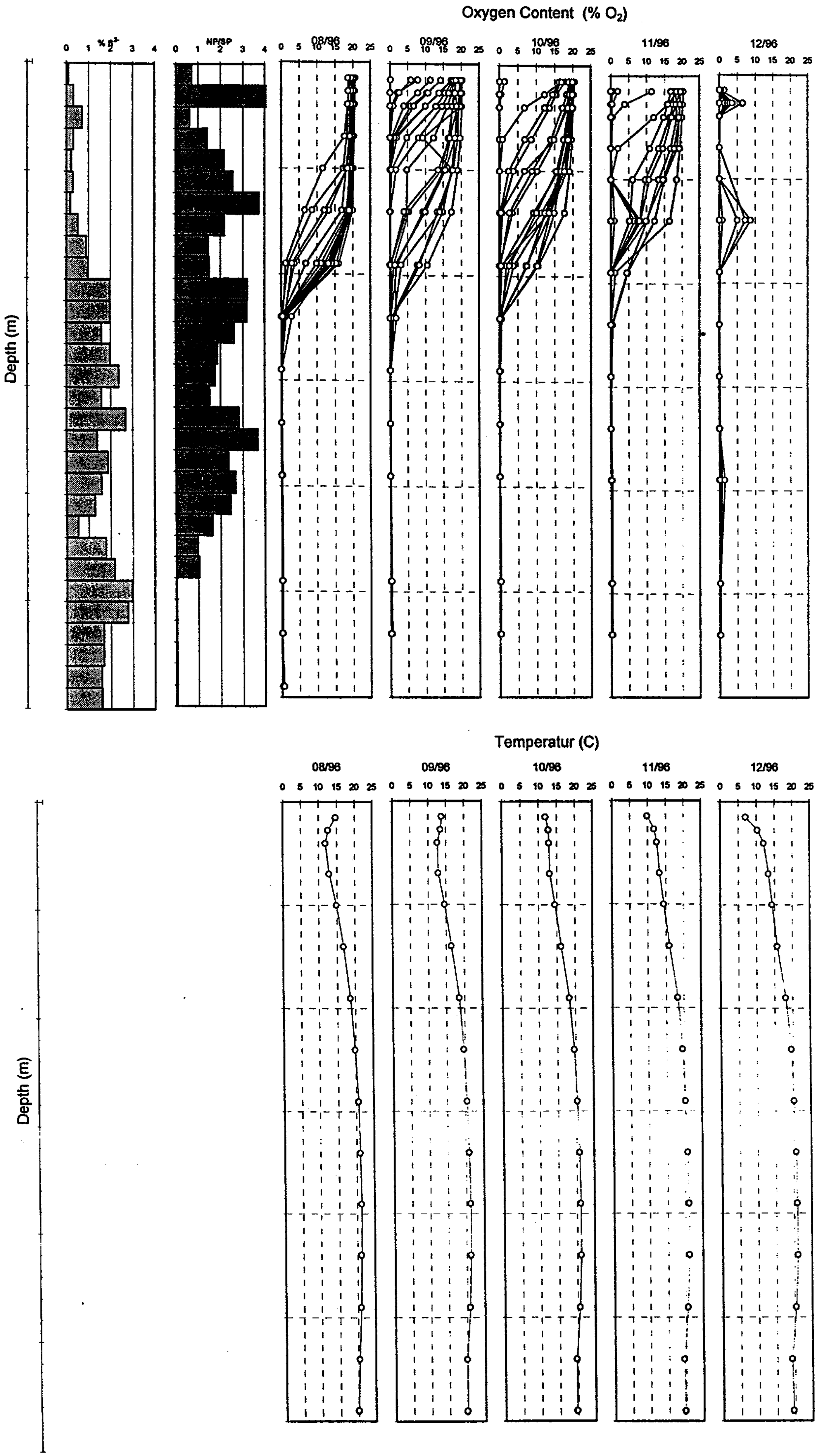
09/96
10/96
11/96
12/96
0 5 10 15 20 25
Depth (m)

Figure 4


Oxygen Content (% O2)
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12/96
0 5 10 15 20 25
Depth (m)
Temperatur (C)
08/96
09/96
10/96
11/96
12/96
0 5 10 15 20 25
Depth (m)

Figure 4

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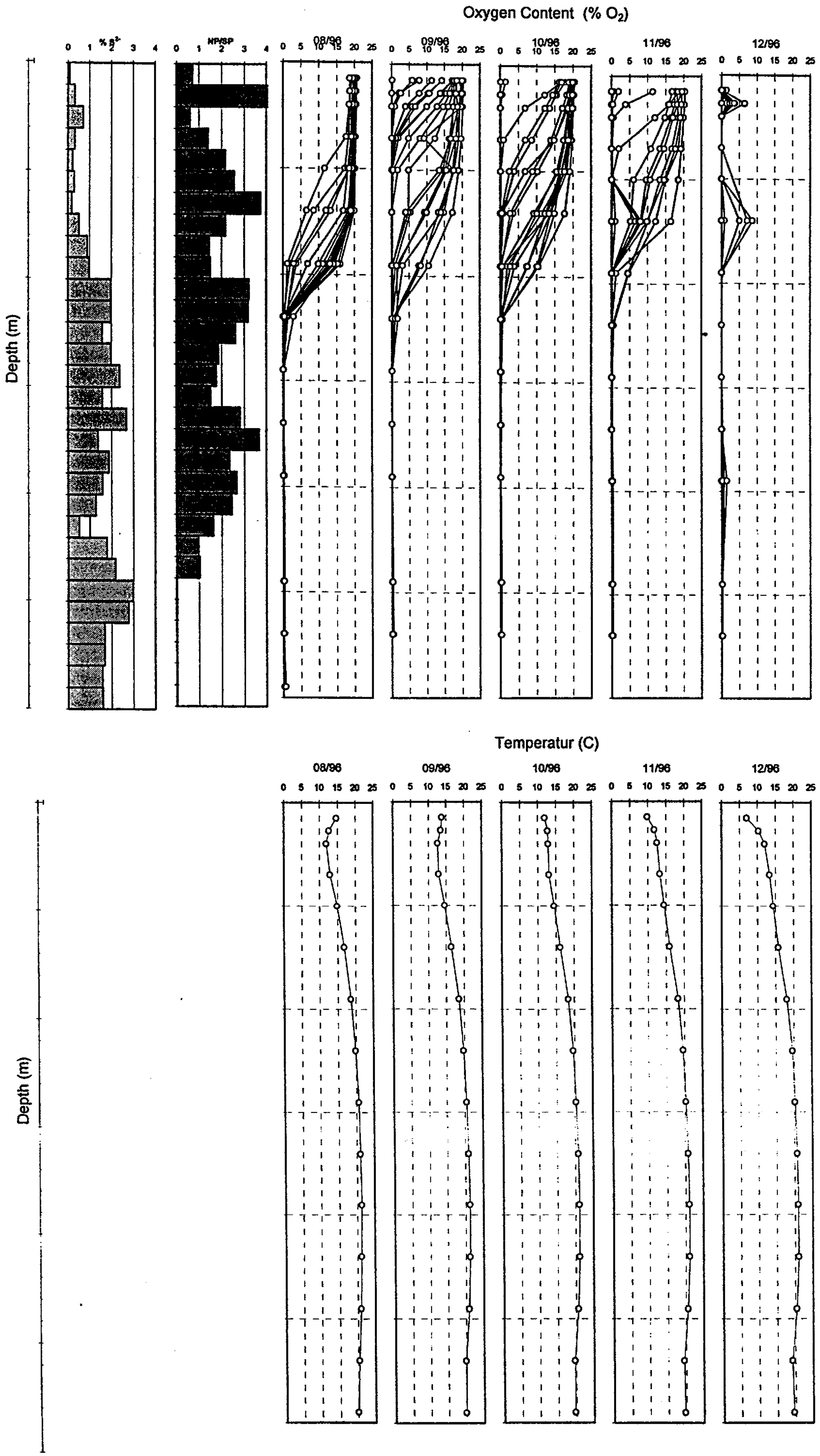
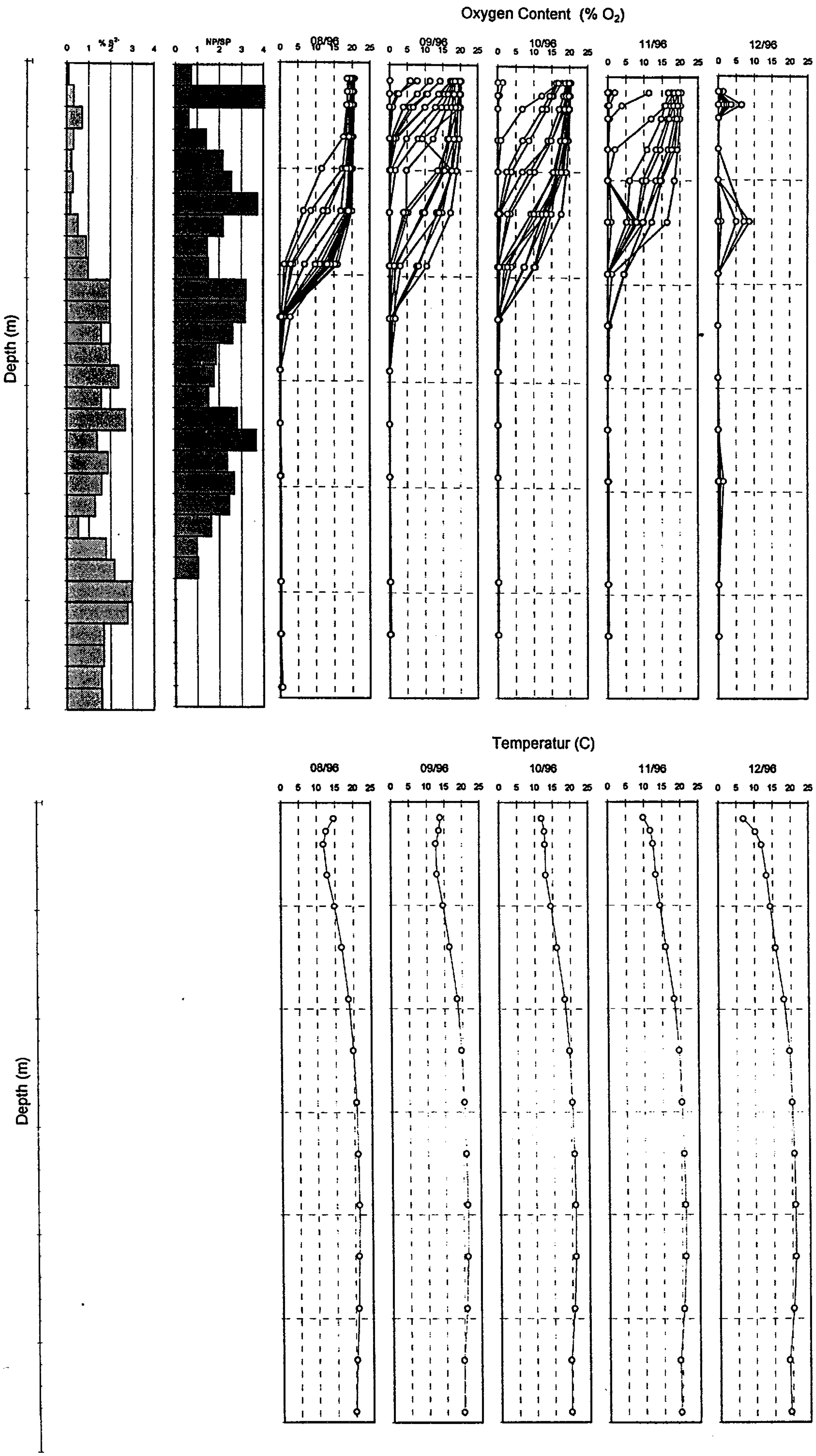


Figure 4


Oxygen Content (% O2)
% S2-
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10/96
11/96
12/96
0 5 10 15 20 25
Depth (m)

Figure 4