Evaluation of three simple hydrosalinity models applied to citrus orchards in the Lower Coerney River irrigation area, Eastern Cape, South Africa.

THESIS

Submitted in Fulfilment
of the Requirements for the Degree of

MASTER OF SCIENCE

of Rhodes University

by

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February 1992

ABSTRACT

Three hydrosalinity models of different complexity were evaluated against data from selected citrus orchards in the Lower Coerney River irrigation area. These models were statistically compared with field data, and found to vary in accuracy of output predictions. The simplest model, the LEACHING REQUIREMENT (LR) model, has the lowest data input requirements and produces output predictions that correlate with up to 93% of the variance in measured data. SODICS, which is theoretically more detailed and requires a greater level of detail in input, produces predictions of an accuracy equivalent to the LR model. The PEAK model was assessed in two parts, the PEAKM module simulating soil moisture and soil moisture movement was able to predict variations in moisture up to 99% of the time. The PEAKD module, which predicts solute concentrations was less effective in replicating real world conditions.

ACKNOWLEDGEMENTS

This research was conducted as part of the Sundays River Project, funded by the Water Research Commission. The owner of Daisy Dell farm on which most of the field data was gathered, Mr J. Hannah, is thanked for giving permission to trample through his orchards. Dr John Herald supervised this study, and provided valuable criticism and guidance.

This thesis would not have been possible without the continual encouragement, motivation and support of Professor Franco Pirajno - even from a distance. Thank you.

CONTENTS

Page

CHAPTER ONE

CHAPTER TWO

CHAPTER SIX

CHAPTER SEVEN

CHAPTER EIGHT

CHAPTER NINE

APPENDICES

LIST OF FIGURES

Page

LIST OF TABLES

CHAPTER ONE

1.1. INTRODUCTION

Limited available water resources must be shared by different competing user groups. Irrigated agriculture is the greatest user of surface water both worldwide and within South Africa, so it is essential that techniques for the control and monitoring of this practise be developed. There are many problems associated with irrigation most notable being the accumulation of salts within the soil system from where they may move into receiving groundwater systems and eventually into downstream surface water. This renders the water resource less valuable to other downstream users.

The long term success of irrigation schemes can only be assured through careful management of conditions in the root zone. Solute transport models can be used to understand the effects of irrigation practises. Such models are useful tools in attempting to resolve the problems of sustaining long term yields while maximising crop output, balancing competing user demands, minimising damage to aquatic ecosystems, and the monitoring and control of soil salinity under irrigation systems.

The purpose of this research is to assess the application of three hydrosalinity models for irrigation management. Useful management models are those which have practical application, requiring data that is easily obtainable while generating information that has direct relevance for the management of an irrigation scheme. The models to be investigated by this study are management tools that have produced useful predictions when applied to problems under non-test conditions subsequent to their development. They have also been applied in varying environments, but not in Southern Africa.

These models have been designed for different uses, and hence have different levels of data input requirements and accuracy of output prediction. The simplest model, the Leaching Requirement (LR), is used widely by the USDA for irrigation scheduling. This model is depth integrating, spatially lumped and assumes steady-state conditions within the soil profile. It is based on solute mass balance and has low data requirements from which the leaching flux at the base of the root zone is calculated. Although simple, it has been widely used for the management of many irrigation schemes (Frenkel, 1984; Oster, 1984).

A more detailed model is that developed by Rose et. al. (1979), the SODICS model, which attempts to account for variable field conditions. SODICS is depth incremental and allows for transient-state field conditions.

The PEAK model (Rose et. al., 1982) considers both the movement of a solute peak through the soil, and the dispersion of solute about that peak. This more closely approximates field conditions within the soil, and hence the output generated has been found more accurate than the other two models.

These three solute transport models are evaluated using data from fields in the Lower Coerney irrigation area. The utility of the models is assessed on the basis of predictive accuracy, and also in terms of management applicability. The effect of spatial variability of field conditions on the model performance is also considered.

1.2. AIMS AND OBJECTIVES

The aim of this study is to evaluate the application of three hydrosalinity models to the management of irrigated lands within the Lower Coerney River Valley. Initially the study determines the sensitivity of all the model parameters, and then the ability of each model to simulate actual soil moisture and solute movement over time is evaluated.

The specific objectives are to:

1. Determine which parameters each model is most sensitive to.

2. Determine the likely range of input parameters for the study area from available data.

3. Gather all input data required by each model, and present predictive results.

4. Assess model predictions using a statistical comparison between actual field data, measured independently of the model input requirements. This provides a quantitative measure of the accuracy of the model predictions.

5. Evaluation of each model as a management tool, in the light of findings presented in both the sensitivity analyses and accuracy of prediction.

1.3. THE STUDY AREA

The study area is located 40 km north of Port Elizabeth, between the latitudes 33°26' and 33°31' south and longitudes 25°37' and 25°41' east (Figure 1.1). Selected orchards and adjacent areas of natural vegetation within the Lower Coerney River irrigation area were investigated. The Coerney River is a tributary of the Sundays River, part of the interbasin transfer scheme bringing water from the Orange River for the purpose of irrigation in the Sundays River Valley. The area presently under irrigation will be expanded in the near future with the construction of a new storage dam and canal at the upstream end of the catchment.

1.3.1. Climate

This area falls within the transitional belt between the spring and winter rainfall maxima that exist to the north and south of the area respectively (Stone, 1988). Consequently, rainfall occurs fairly evenly throughout the year, with slight maxima in spring and autumn. Average annual rainfall is between 300-400mm, although extreme values ranging from 162mm to 735mm have been recorded (Bekker, 1968). Rainfall is mainly cyclonic in origin associated with the onshore air advected behind passing frontal systems. Orographic effects result in localisation of events, which seldom fall uniformly over the entire valley.

Mean maximum daily temperatures range from 26°C in January to 19°C in July, and minima range from 15°C in January to 7°C in July. Extreme temperatures range from -4°C in winter to 42°C in summer (Schulze, 1965). On average berg winds occur one to three times a month and elevate temperature above 38°C (Pearce, 1987). In the valley, moisture loss by evaporation is high, with a mean monthly pan evaporation of 118mm during the study period.

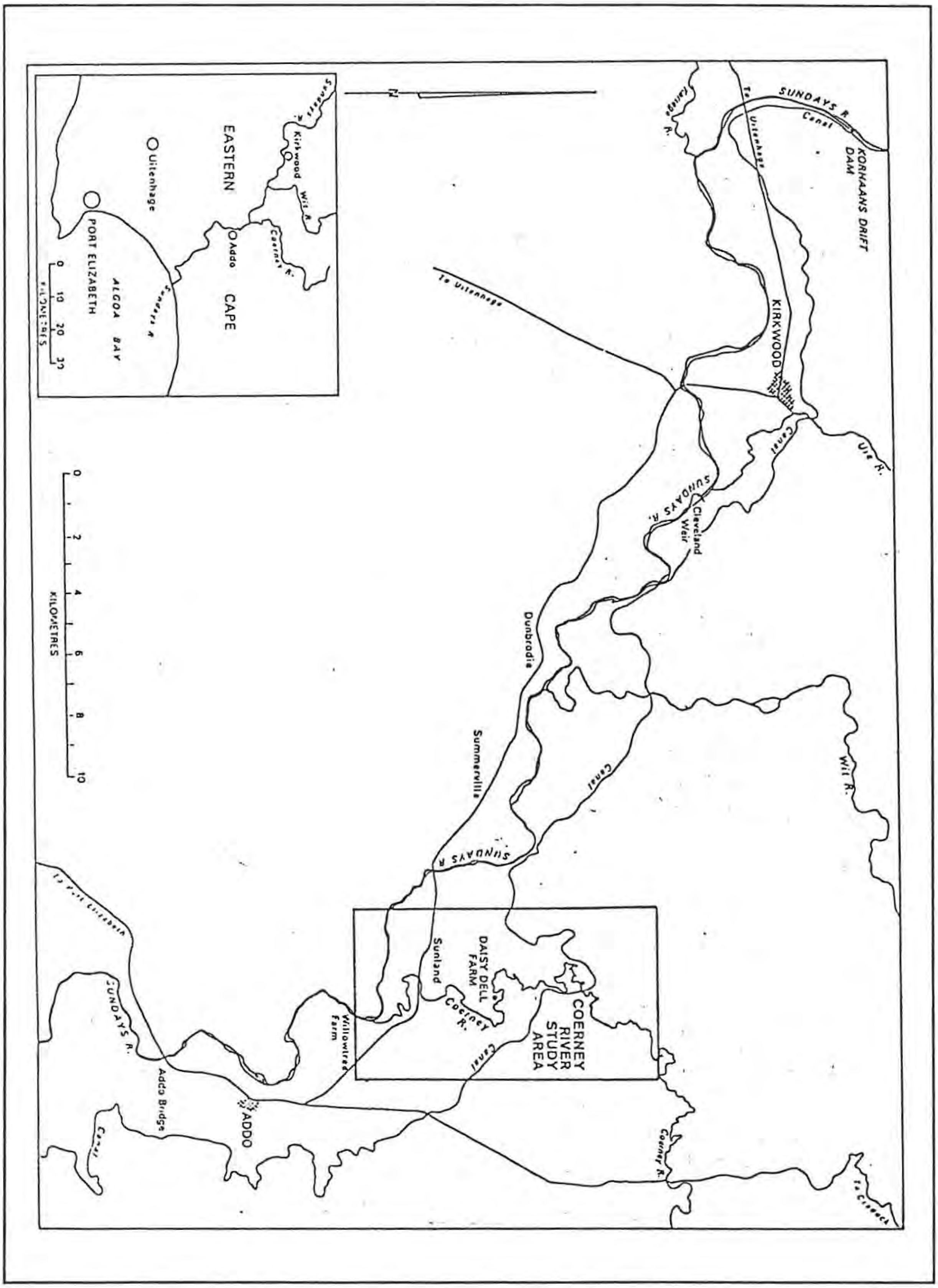


Figure 1.1. Location of the Study Area

1.3.2. Landuse

Natural vegetation in the area is limited in extent by the intensive agricultural practises. Although sparse, the existing patches of indigenous vegetation may be classified as Valley Bushveld according to Acocks (1988). Most of the lower Coerney River valley is now under cultivation, with the major crop being citrus. Lucerne and pasture are irrigated to provide fodder and grazing for commercial dairy cattle, and vegetables are grown as cash crops.

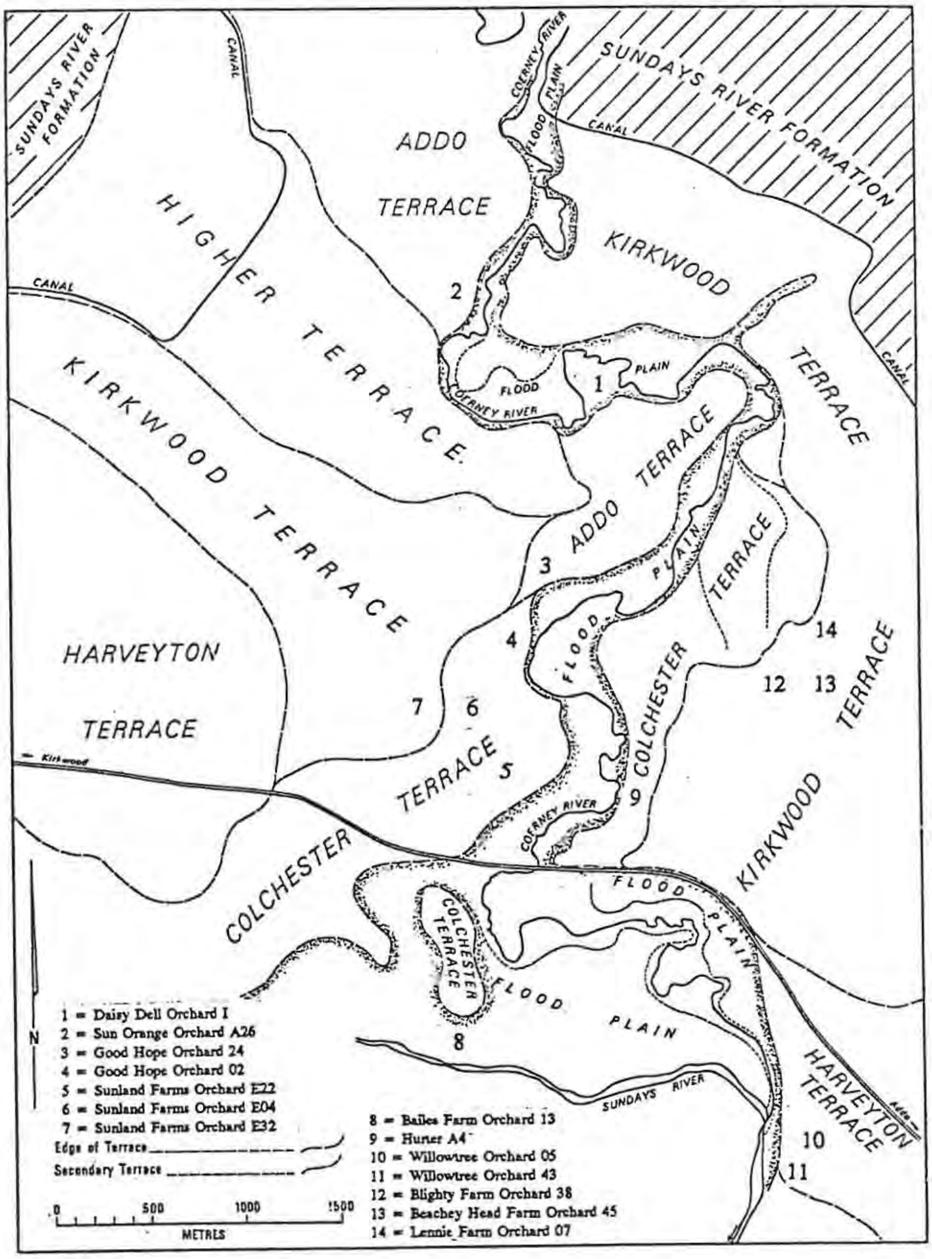


Figure 1.2. Geomorphology of the Study Area

1.3.3. Topography

The morphology of the Sundays River valley area has been determined by the tectonic and drainage history of the region, which has resulted in a series of terraces developing in the Cretaceous rocks and river alluvium (Figure 1.2). Four terraces have been recognised, each consisting of an alluvial deposit overlying a boulder bed, which is thought to represent a former stream channel subsequently infilled by finer alluvium as the river migrated laterally (Ruddock, 1947). The present bed of the Coerney River consists of a conglomerate layer, with a silty matrix (Shone, 1976). It dissects the terraces and forms a flood plain which becomes broader and more complex in the downstream direction. It is on these terraces that the orchards are located, as they provide naturally horizontal surfaces requiring little levelling for development.

The Cape Supergroup underlies the area, comprising the Witteberg, Bokkeveld and Table Mountain Sandstone Groups which are sedimentary units that were extensively tectonically deformed during the Palaeozoic period (330-450 M bp). The resultant east-west trending ridges and associated faults led to the development of several small fault-controlled basins. The Algoa Basin is the largest of these, and consists of a series of grabens which have been filled by three clastic formations, the Enon Conglomerate, the Kirkwood Formation and the Sundays River Formation (Tankard et. al., 1982). The Sundays River Formation directly underlies the study area, consisting of thinly interbedded mudstone and siltstone. Evidence for the environment of deposition is provided by the thick bioturbation and marine fossils, from which it can be inferred that this formation accumulated in estuarine and interdistributary conditions (Tankard, 1982; South African Committee for Stratigraphy, 1980).

Recent alluvium consisting of semi-consolidated, interbedded clays, sands and gravels overlies all geological formations.

1.3.4. Soils

A soil map was produced by Shone (1976), from which four main soil types can be distinguished.

a.) Silty soils, known as Coerney River alluvium are located adjacent to the Coerney river channel.

b.) Soils developed on the coarse textured grey sandy alluvium and covered with a thin fine textured aeolian deposit are found on the lower terraces, particularly the Colchester and upper Addo terraces.

c.) A similar soil to b.) is found in the northern part of the Kirkwood terrace. This is distinguished by the existence of a 3m thick layer of coarse sand, pebbles and boulders which underlies the alluvium. The top soil is also of fine textured aeolian origin.

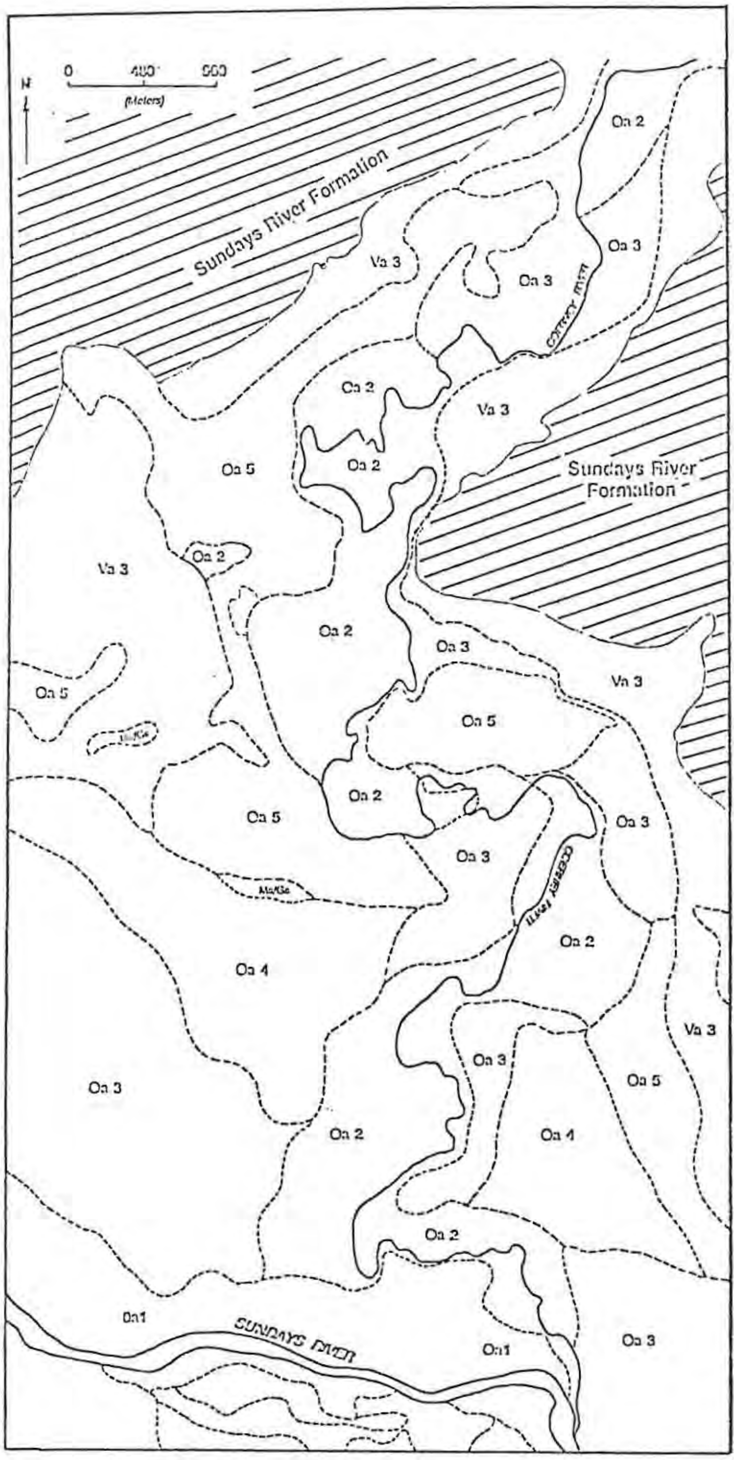
d.) Colluvial soils derived from the Sundays River Formation occur along the outer margins of the Kirkwood terrace.

Figure 1.3 shows the results of more recent soil mapping, undertaken by the Department of Agriculture in 1977 according to the Binomial Classification System developed by MacVicar et. al. (1977). Most of the soils were found to be of the Oakleaf Form interspersed with small areas of Valsrivier Form, and both these forms are developed on unconsolidated alluvial material.

Oakleaf Form

Oakleaf Form soils consist of an orthic A horizon overlying a neocutanic B horizon (MacVicar et. al. 1977). All the Oakleaf soils in the Coerney River area belong to the Calcareous division, and have apedal to weak blocky structure in the B horizon.

Soils on the flood plain, Addo and Colchester terraces are classified as Limpopo series with non-red B horizons and fine sandy-loam to sandy clay textures. Soils developed on the Kirkwood, Harveyton and Higher terrace are classified as Letaba/Shigalo series with red B horizons. Textures are similar to the Limpopo series, with the clay content increasing on the Higher terrace, and the outer areas of the Kirkwood terrace.



KEY TO SOIL CLASSIFICATION

SYM BOL	SOIL DESCRIPTION
Oa1	Deep (>1200mm) grey apedal fine sandy loam with pebbles, calcareous.
Oa2	Deep (>1200mm) non-red apedal to heavy block structured fine sandy loam, calcareous.
Oa3	Deep (>1200mm) non-red apedal to heavy block structured fine sandy clay loam to sandy clay, calcareous.
Oa4	Deep (>1200mm) red apedal to heavy block structured fine sandy loam to fine sandy clay loam, calcareous.
Oa5	Deep (>1200mm) red apedal to heavy block structured fine sandy clay loam to sandy clay, calcareous.
Va3	Red weak to strong blocky structure, fine sandy clay loam to sandy clay. Calcareous, depth to structured B-horizon <450mm
Ms/Gs	Shallow (<450mm) grey apedal calcareous fine sands, overlying rock and/or calcrete.

Figure 1.3. Soils of the Study Area

Valsrivier Form

This form is defined as an A horizon overlying a pedocutanic B horizon, having a moderate to strong blocky structure and a fine sandy-clay-loam to sandy-clay texture. The soil series is Zuiderzee, having a predominantly red B horizon which is calcareous and has a clay content of 15-35%.

1.3.5. Irrigation

The Coerney River area forms part of the Sundays River Valley intensive agricultural region producing mainly citrus and lucerne, with minor crops including potatoes, pumpkins, maize, vines with some dairy farming carried out. The sampled orchards are planted with citrus and lucerne, and were established at dates varying from 1955 to 1981. Methods of irrigation include flood, basin and micro-jet.

1.4. SIGNIFICANCE OF THE STUDY

The natural streamflow and groundwater in the Sundays River Valley region are too highly saline for either irrigation or human consumption. Water is imported from the Orange river through a diversion into the Little Fish River. It is then stored in Korhaans Drift Dam and distributed under gravity throughout the Lower Sundays river valley by means of a network of lined canals.

The Sundays River irrigation area has been subject to the problems of salinisation and waterlogging of the soil under irrigation from as early as 1930. As far back as 1927 farm mismanagement was blamed for impaired drainage and declining soil quality (Shone, 1976). In 1981 the problems of chlorosis, defoliation, die-back, unseasonal fruit set, root disease, varying yields and quality deterioration among others led to an attempt to establish the causal factors. Physical characteristics of the soil were identified as responsible for poor soil drainage. Management practises such as orchard traffic and extensive levelling increase soil compaction, and heavy irrigations then exacerbate the problem and retard gas exchange. These conditions need light frequent irrigation applications, and hence a finer resolution of control over the amount and timing of water applied.

This greater level of control required by farmers is intended to steer a course between waterlogging the soil and excessive salt accumulation. There must however be a basis for management decisions. Simple leaching models with low data requirements and easy application such as those used in this study are a method whereby irrigation managers can effectively schedule water applications, while optimising conditions in the soil.

Another factor to be considered is the scheduled expansion of the irrigation area in the Lower Coerney river valley from the current extent of approximately 792 hectares by over 50% to 1 702 hectares (Tylcoat, 1985). The present water demand is 85 million cubic meters per annum, which is approximately 1 073 cubic meters per hectare annually. The average salinity of this water is 120 mS/m, which represents approximately 24 meq/L total ion concentration. The load coming is thus approximately 680 tonnes every year, which may double with the extended area. It is important for the success of the entire irrigation scheme to monitor the fate of this load, to identify any localised zones of salt accumulation, and to determine whether there is a net build up throughout the area over the long term.

Few cases of local model application, and still fewer validation exercises have been reported in the literature. Van Rooyen (1977) considered the effect of drainage water on downstream irrigation water quality using the steady state solute model of Oster and Rhoades (1975), Van Rooyen and Moolman (1980) predicted the effect of water table depth and irrigation frequency during the season on soil salinisation and Moolman et. al (1983) used a solute transport model to describe the effect of irrigation return flow on the mean monthly baseflow salinity. Meyer and Green (1981) report that the "USDA-Irrigation Scheduling Model" was tested on a wheat crop at Roodeplaat near Pretoria in 1979. The model was calibrated using data from weighing lysimeters prior to its application. The model uses meteorological data and a crop water use coefficient to predict the rate of evapotranspiration and a soil water balance is then calculated and irrigations are forecast. The model was found to overpredict actual evapotranspiration by about 15%.

CHAPTER TWO

2. THEORETICAL BACKGROUND

To integrate soil properties, soil processes and the impact of different management practises, each must be understood in turn. An overview of the soil properties which affect the processes involved in soil moisture movement through the soil is given. This is followed by a discussion of solute flux which is dependent on moisture movement. Mathematical representations of both moisture and solute flux are also presented.

2.1. PHYSICAL PROPERTIES OF THE SOIL

Weathering of parent rock material through physical disintegration and chemical alteration over time leads to the formation of mineral particles, which in combination with the effects of biological activity make up the soil. Thus, primary physico-chemical properties of the soil are determined by the geology, climate, vegetation and biological activity of the area (Foth, 1978). Soil is composed of approximately 45% mineral matter, which is the basic framework of the soil (Steila and Pond, 1989). These minerals strongly influence the physical character of the soil, as well as providing a nutrient reservoir for plants. The physical and chemical characteristics of the soil will be discussed, as these determine the soil's hydraulic properties and chemical behaviour.

2.1.1. Texture

As weathering proceeds, a group of mineral fragments is produced from the original parent rock. These fragments may be classified into size categories (Table 2.1.), which make up the soil texture. Each size category imparts certain characteristics to the soil, and depending on the relative amount of each size, the characteristics will be more or less dominant.

Sand is composed mostly of quartz (SiO_2) although coarser sand contains rock fragments as well. The relatively large particle size increases pore size and permeability but reduces the soil water holding capacity. Sand acts as a framework for the smaller, more reactive components such as silt and clay, but as quartz is chemically unreactive, it provides few nutrients for plant uptake.

Silt produces smaller pores due to its smaller particle size, so more available water is retained by silt than sand. The lower particle size results in a greater surface area to volume ratio than sand. This means silt has a higher weathering rate, releasing nutrients for plant growth more readily than sand.

Clay is made up of small mineral particles formed from the breakdown of parent material and weathering products (Steila and Pond, 1989). The extremely small size results in a high surface area to volume ratio which allows clay particles to behave as chemical agents. Most clay particles are plate-like in structure, with a net negative charge on the wide surface and a positive charge on the narrow edges.

Chemical reactions between clay particles and water are facilitated by the dipolar nature of the water molecule and the electrically charged surfaces of the clay particles. Small pores associated with clay particles increase the soil water holding capacity of the soil as the surface tension of the films of water increases with reduction in particle size. These water films are therefore held with both surface and molecular tensions.

Table 2.1. Particle Size Classification of Soil Textures

TEXTURAL CATEGORY	PARTICLE SIZE
Very Coarse Sand	2000 - 1000 μ
Coarse Sand	1000 - 500 μ
Medium Sand	500 - 250 μ
Fine Sand	250 - 100 μ
Very Fine Sand	100 - 50 μ
Silt	50 - 2 μ
Clay	> 2 μ

(after Steila and Pond, 1989)

Due to electrostatic charges, clay platelets may clump together, forming aggregates of the same size as silt or sand. These aggregates will then result in similar properties to those imparted by the sand particles, acting to increase pore sizes, increase permeability and reduce soil water holding capacity. The ability of clay particles to form aggregates within the soil through adhesive and cohesive forces determines the consistence of the soil. Clay minerals also have the capacity to absorb water, thus expanding their volume considerably. During alternating wet and dry conditions the clay will swell and shrink, creating cracks and structural features within the soil.

Most soils are made up of a combination of textural classes with a variety of interacting properties. These properties are now discussed in turn.

2.1.2. Soil Structure

The arrangement of soil particles into aggregates is determined by the soil texture. Sand and silt have little tendency to aggregate, except when bound by clay particles or organic matter. Chemical bonding between clay particles is possible as the broad negatively charged surfaces may form a clump with the narrow positively charged surface of another platelet. Soil structure determines the porosity, permeability and hence the infiltration rate of water. The path taken by infiltrating water is also influenced by the soil structure, as preferential flow will be concentrated in the inter-aggregate areas. Soil moisture movement can be divided into rapid macropore flow between aggregates, and slower flow within aggregates. Mineralogical, chemical and biological factors are all involved in the stability of aggregates (Thompson and Troeh, 1978). If the clumps readily break down under wetting or interference by farming, porosity will be reduced along with permeability and infiltration rates.

2.1.3. Particle and Bulk Density

The weight per unit volume of the solid fraction of the soil constitutes the particle density. This is determined by the density of the minerals making up the soil, and as these are dominated by silicates, the particle density of most soils on average is similar to that of quatrz, i.e. 2.65 g/cm^3 (Steila and Pond, 1989).

$$\text{Particle Density} = \frac{\text{Weight of soil solids (grams)}}{\text{Volume of soil solids (cm}^3\text{)}}$$

The weight of a dry soil sample divided by its volume gives its bulk density. This includes the empty spaces between soil particles, so in general the greater the bulk density, the less pore space.

$$\text{Bulk Density} = \frac{\text{Weight (grams)}}{\text{Volume (cm}^3\text{)}}$$

With increasing depth down the profile, bulk density may increase due to the compaction of the weight of overlying soil. Farming activities such as traffic and stock trampling can increase bulk density at the surface as well.

2.1.4. Soil Porosity

The space between soil particles contains water and vapour, the total volume of which is the porosity.

$$\text{Porosity} = 100 - \frac{[(\text{Dry bulk density})] \text{ x } 100}{[(\text{Particle density})]}$$

Increasing bulk density leads to decreased porosity. In general, a highly aggregated clay textured soil will have low bulk density and therefore high porosity, while a poorly aggregated soil will have high bulk density and low porosity. As porosity is a measure of the available space within the soil, it is indicative of the movement and retention of moisture within the soil, as well as soil aeration. Large voids or macropores allow rapid infiltration and drainage, while small pores restrict infiltration and drainage, thus enhancing soil water retention. Porosity generally decreases with depth as the bulk density increases, leading to a gradual decrease in pore sizes and infiltration rate down the profile.

2.1.5. Permeability

The ease with which water can flow through a soil, expressed as a rate of movement, is the soil permeability. Pore size and interconnectivity determine the permeability, which is a measure of the effectiveness of the links between the pores. A soil may have high porosity but poor permeability if the pores are not connected, or joined by very narrow pathways. Over time, preferential flow through slightly larger pores will lead to a gradual enlarging of the pore and its links to the next pore. This will further encourage preferential flow through the soil, so rapid flow may occur in one zone while slow or non-existent flow may dominate in another area. This heterogeneity of flow may become entrenched in the profile over time, resulting in very different behaviour and properties over a short distance within the same soil. Together, the porosity and permeability determine the infiltration rate of incoming moisture. As both usually decrease with depth, the rate of infiltration will also decrease.

2.1.6. Organic Matter

The decomposition of vegetation and biological matter into a number of organic compounds within the soil constitutes the humus component. Humus is insoluble in water, although some may go into colloidal suspension (Foth, 1978), and has a high cation exchange capacity. Humus can adsorb cations onto the cation exchange sites, and can also adsorb approximately 8 to 9 times their volume of water (Tivy, 1982). These properties lead to similar behaviour between organic matter and clay particles. A correlation between clay and organic matter content in a soil has also been found (Foth, 1978) implying both similar behaviour and occurrence. Together, the clay and organic matter ensure greater availability of water and nutrients. Organic compounds contain reactive chemical groups that can develop electrical charges and effectively flocculate clay particles into aggregates depending on the number of reaction sites within the compounds (Chang and Anderson, 1968).

2.1.7. Cation Exchange Capacity

As clay platelets and some organic particles carry a net negative charge on the flat surfaces. There is a tendency for these particles to form a chemical bond with positively charged cations that are carried in the soil solution. In this way a neutral particle is formed. The charge on the particle determines the amount of positive ions that can be attached to its surface. As the soil solution is continually carrying new cations past the clay particle, the cations on the clay surface may be replaced by other cations with a higher affinity for the clay particle, depending on relative ionic concentrations and ionic reactions. The clay sites where cations attach themselves are therefore known as exchangeable sites, and the amount of cations that can be accommodated in this way as the cation exchange capacity (CEC) of the soil. The CEC controls to a large degree the solute content of the soil water. Indirectly it also controls the physical structure of the soil, as if all exchangeable sites are filled and the clay particle neutral, it cannot form an aggregate with other clay particles, thus reducing the potential porosity, permeability and infiltration rate of the soil.

Soil physical and chemical properties are interdependent, resulting in a three dimensional heterogeneity within the soil that is difficult to quantify. All act together to determine the hydraulic properties of the soil. Naturally derived soil properties affect and are often modified by landuse practises, especially farming and irrigated agriculture over the long term.

2.2. SOIL MOISTURE

Water and air are found in the interstitial spaces between soil particles. The supply of water, its rate of movement and the availability of oxygen are all determined by the amount and size of soil pores (Steila and Pond, 1989). However, before rain or irrigation water enters the soil pores, it must infiltrate beneath the soil surface.

Infiltration is the process whereby water enters the soil through surface void spaces and then percolates downward into the soil. The amount of water that a soil can absorb within a period of time is its infiltration capacity, which is unique to each soil. Many factors influence the infiltration capacity, resulting in temporal and spatial variation in this property.

The antecedent conditions in the soil influence infiltration capacity and rate. If the soil is dry before infiltration begins, wetting the surface generates a strong capillary potential immediately below the soil surface which supplements the gravitational force to increase infiltration (Steila and Pond, 1989). If the soil is already wet the amount of water that can be absorbed by the soil is reduced which inhibits infiltration. Under these conditions, ponding of water will occur on the soil surface, and eventually surface runoff will result. Clay minerals occupy less space when dry than wet, leaving cracks within the soil. If the soil is initially dry, infiltrating water will move rapidly under macropore flow. If the soil is initially wet, or as infiltration proceeds and water is absorbed by the these minerals, they begin to swell and block the macropores. Thus flow rates will decrease rapidly if clay minerals are present.

Raindrop impact and agricultural activities such as traffic and livestock trampling can compress soil particles and break down soil aggregates. This increases surface bulk density, thus reducing porosity and hence reducing infiltration rates. Interstitial spaces may also become blocked by the inwash of fine particles released from the aggregates, reducing permeability and further inhibiting infiltration.

2.3. SOIL MOISTURE RETENTION

Once water has entered the soil profile it is acted on by two main forces. Capillary forces act in all directions to hold a layer of water around each soil particle. Gravitational forces act downwards to draw the water out of the profile into receiving groundwater. The moisture film immediately in contact with the soil particle is rigidly held by adhesive electrostatic forces between the dipolar water molecule and the electrically charged soil surfaces. These molecular forces are so strong the water is considered to be part of the particle crystal lattice, and exhibits little or no movement. This water can only be removed from the soil by heating to temperatures of up to 500°C which breaks down the soil minerals and releases the water molecules. Hygroscopic water results from the affinity of soil particles for water vapour in the soil atmosphere and only accounts for a small percentage of the soil water (Ross, 1989).

2.3.1. Capillary Forces

Further out from the soil particle surface but still within micropore space, with an approximate thickness of fifteen molecular layers is a liquid envelope held in position by capillary forces (Steila and Pond, 1989). These are created by the surface tension of water and thus act equally in all directions to hold a layer of water around soil particles. Capillary forces exceed the gravitational force until a critical pore radius (r) is reached, when the capillary forces are overcome by gravity, and the water drains out of the soil. The strength of the capillary force (Φ) holding this water is determined by:

$$\Phi = (2¥\cos\tau)/g(q_l - q_g)R \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (2.1)$$

where ¥ = surface tension of water
τ = contact angle of water
q_l = density of the liquid
q_g = density of gas
R = pore radius

(after Hillel, 1980)

Larger pores have greater menisci, so the force with which water is retained is less than for smaller pores. Overlying the water table is a layer of soil at capillary saturation where capillary forces dominate. The moisture films separate into discrete menisci and there is a systematic decrease in the amount of moisture in the soil in the upwards direction. The depth of the capillary fringe depends on the size of the pores - the theoretical extent in clay with small pores is very great, whereas the depth is negligible in a sandy soil (Equation 2.1).

The capillary forces exert an attractive force on water within the soil, which can be measured by the matric potential of the soil. When both macro- and micropores are saturated, the soil particles are surrounded by the maximum thickness of water and the matric potential is zero. At this point the capillary forces are also equal to zero, and any increase in soil water will now drain under the influence of gravity. Conversely as the soil dries out the moisture is held with increasing force, as would be expected according to Equation 2.1.

2.3.2. Gravitational Forces

Gravity exerts a constant downward force on the soil water and leads to drainage out of the soil, imparting a uni-directional vector to soil moisture flow. Water affected by gravity is usually contained in macropore space which have low capillary potential as shown by Equation 2.1. Such water is only temporarily held within the soil and drains rapidly, so is of limited use for extraction by plants.

2.3.3. Plant Available Water

Plants obtain most of their water from capillary water. As the soil dries out the matric potential increases until a force of approximately -15 MPa is reached when the plant can no longer extract water from around the soil particle (Lesk, 1982). This tension is termed wilting point, and if the soil dries out further permanent wilting point is reached, from which plants can no longer recover. Once all gravitational water is removed and the maximum amount of water is retained in the soil, the soil water content is at field capacity. This is dependent on the number of small pores and makes up on average 30% by volume for a clay soil, and less than 10% for sandy soils (Foth, 1978).

Plant available water is the difference between the field capacity and the wilting point of plants. Fine particles increase the field capacity and thus also the available water content.

2.4. HYDRAULIC CONDUCTIVITY

Soil hydraulic conductivity is determined by the permeability of the soil, which in turn is the product of the porosity and the interconnectivity of the pores. The size of pores also influences conductivity as macropores allow rapid flow while narrow links between macropores, and micropores inhibit rapid throughflow. Macropores can become preferential routes of movement bypassing areas with lower conductivity. Hydraulic conductivity is affected by the phenomenon of hysteresis and air encapsulation.

2.4.1. Hysteresis Phenomena and Hydraulic Conductivity

Hysteresis is the phenomenon whereby the relationship between two variables differs depending on the direction of change in one or both variables. This is illustrated in Figure 2.1 where the relationship between matric potential and soil moisture is shown to be hysteretic. As soil moisture increases (broken line) the matric tension decreases rapidly until at saturation the tension is at zero. Conversely, as water content decreases (solid line) the matric tension increases rapidly to a level higher than at the same moisture content in the increasing direction.

Many hydraulic properties of the soil exhibit hysteresis, as the most fundamental relationship between matric potential and soil moisture is hysteretic (Hillel, 1980). A number of explanations for this have been given:

* Individual pores are geometrically non-uniform, so for moisture to fill a pore of greater radius requires a more soil water than a pore of smaller radius (Equation 2.1). The converse is true for water draining out of pores.

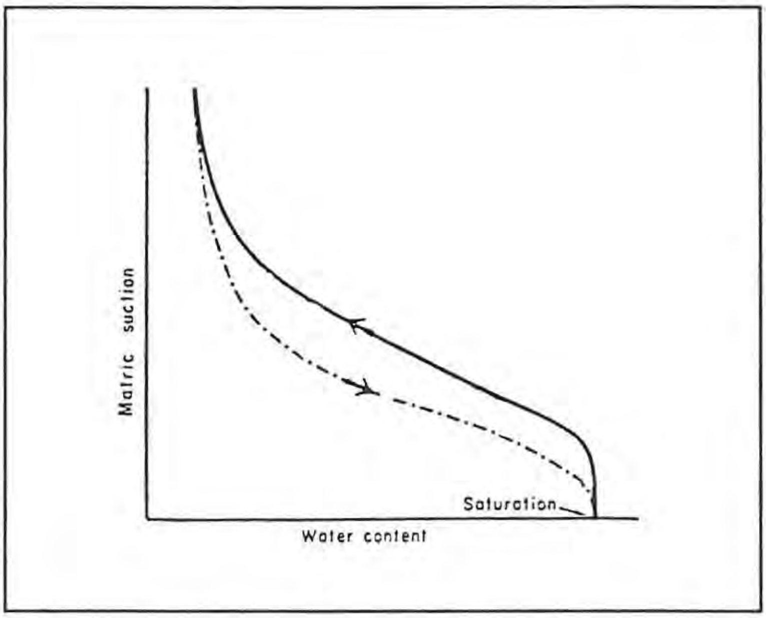


Figure 2.1. Hysteresis results in variation in the relationship between Matric Potential and Soil Moisture, depending on the direction of change in either parameter

- The contact angle of the meniscus of pore water and the pore wall is greater in an advancing meniscus than a receding meniscus. Greater suction will be exhibited during drying than wetting, as the smaller radius of curvature results in greater capillary force (Equation 2.1).

- Swelling, shrinking and changes in soil structure during the wetting and drying phases will lead to differential hydraulic conductivity.

Most unsaturated flow processes include successive cycles of wetting and drying, and the hysteretical nature of the hydraulic properties of the soil must therefore be taken into account. However, hysteresis is rarely considered in hydrological studies as the complexity of the numerical solution of unsaturated flow in the aerated zone is greatly increased with alternating boundary conditions (ie. wetting and drying). Further complications occur when a partially wetted soil begins to drain, or a draining soil becomes re-wetted, as intermediate curves develop within the hysteresis curve. Hysteresis effects are therefore difficult to quantify, and consequently are generally ignored for practical reasons (Mualem, 1979).

Hysteresis has also been reported in saturated conditions. Stauffer and Dracos (1986) found that hysteresis between capillary force and degree of saturation strongly affected the response of capillary forces in the saturated zone. Capillary tension increases were much larger for high degrees of saturation than for low degrees. This means that in the vicinity of the groundwater surface where the degree of saturation is high, small increases in the soil moisture content by infiltration may result in large capillary force changes. This would enable an immediate rise in the water table as the soil would be able to hold water against gravitational forces to a greater height. This rise eventually increases the hydraulic gradient and the whole water body contained in the saturated domain will then move with increased velocity. In this way, hysteresis is the cause of the rapid spreading of capillary force variations without significant mass transport.

The hysteresis effect is greater in coarse textured soils than finer textured. As most soils are composed of a mixture of textures, often with discrete layering, hysteresis becomes more pronounced.

2.4.2. Stratification and Hysteresis within the Soil Profile

As the wetting front moves vertically, it encounters a series of soil layers that were previously dry. Coarse textured soil layers generally inhibit vertical flow as the capillary force they can exert is low, as shown by Equation 2.1 where the greater the pore radius, the lower the capillary force. Conversely, fine textured soil layers are easily wetted. This means water may prefer to move laterally in fine layers rather than vertically through coarser ones (Routson et. al., 1979; Price et. al. 1979; Crosby et. al. 1968,1971).

The hysteresis loops of the vertical and lateral hydraulic conductivities have opposite directions (Mantaglou and Gelhar, 1987). In the wetting front of stratified soils, the vertical hydraulic conductivity is small while the lateral hydraulic conductivity is large. This situation is reversed during drying. Lateral movement is probably due to the fact that at high tensions, or dry conditions, horizontal stratification enhances lateral movement.

The degree of hysteresis of hydraulic conductivity increases as the capillary tension head increases, that is in dry soil. At a given mean capillary force, a large variability in the soil moisture content exists at the wetting front. As the drying part of the plume moves vertically it encounters soil layers that have already been wetted during the passage of the plume. Because of this, the soil layers show less variability in soil moisture and capillary tension head during drying than wetting (Mantaglou and Gelhar, 1987). Capillary tension thus shows hysteresis of variance with wetting and drying phases.

2.4.3. Hysteresis and Irrigation

Hysteresis can be influenced by the irrigation scheduling regime as hydraulic conductivity increases with soil matric potential. More lateral movement occurs as dry layers are encountered, and will thus be common where low application of water and the resultant high capillary tension exist. Greater vertical movement occurs under wet conditions, where applications of water are high and there is a resulting low capillary tension.

2.4.4. Air Encapsulation and Hydraulic Conductivity

It has been recognised for over 50 years that pockets of air remain in some pore spaces after the wetting of soils (Constantz et. al. 1988). Smith and Browning (1942) found that wetted soil cores retained an average of 9.1% air. Even after prolonged saturation some air remains in the transmission zone, resulting in all but the shallowest layers of the soil profile remaining effectively unsaturated. It has been suggested that air remains in soils during wetting because some pore spaces fill before others in response to wide variations in pore water velocities (Peck, 1969; Fayer and Hillel, 1986).

Variation in pore water velocities is common during infiltration, and may cause pockets to form. Partial wetting of soils may also be due to the presence of negative pore water pressures near the wetting front which inhibit the filling of larger soil pores as the wetting front passes. Once air pockets are created the air volume within the transmission zone remains nearly constant, as continued water flow preferentially circumvents these empty pores, taking paths of lower resistance to flow. Once encapsulated, air can persist in the transmission zone even after weeks of continuous infiltration (Bianchi and Haskell, 1966).

A positive correlation exists between infiltration rates and amount of air encapsulated. Higher infiltration rates result in greater variation of pore water flow velocities which promotes greater air encapsulation. In turn, air encapsulation reduces the hydraulic conductivity of the transmission zone as the total volume of interconnected pores available for water flow is reduced. Constantz et. al. (1988) found a 12% air retention caused a 10 - fold decrease in infiltration rate, and a 4% retention caused a 5-fold decrease but the magnitude of decrease in hydraulic conductivity was the same for all soil types. This means the absolute air encapsulation is not directly proportional to the decrease in conductivity. Wilson et. al. (1989) found that air encapsulation increases with increasingly coarse-grained material with an upper limit of approximately 20% encapsulated air as a percentage of total pore space. Air retention is thus dependent on both texture and infiltration rate, and will therefore vary with depth in the soil profile.

2.4.5. Variability in Soil Hydraulic Properties

Considerable differences in hydraulic properties of soils can occur with spatial location, even within a given soil type. Variability occurs on a wide range of scales, from micro- to field-wide fluctuations, and in three dimensions. Lateral variation in hydraulic properties, such as hydraulic conductivity, is not as great as variation in the vertical direction in most soils, which are anisotropic in all directions, especially vertically (Mantaglou and Gelhar, 1987). Temporal changes can be even greater than spatial variation.

Variations in soil properties are usually not completely random, but have structural arrangements. Changes over time are also generally ordered, in seasonal cycles or showing net directional progression. Capillary forces, mean soil moisture content and soil moisture capacity show large scale hysteresis in stratified soils (Mantaglou and Gelhar, 1987). This is due to the spatial variability of the local hydraulic soil properties, rather than to hysteresis in the parameters themselves.

2.5. GROUNDWATER

Once soil water has successfully infiltrated below the root zone, it proceeds to the underlying groundwater system. This input of water from the soil may cause the water table to rise, and if sufficiently shallow, the moisture could move back up into the root zone under capillary forces. If the water table is deep, infiltrated water will be absorbed into the groundwater body, and begin a lateral movement under gravitational and hydraulic potential forces. Eventually, the groundwater may encounter a surface stream, and begin to flow with the surface water body.

Irrigation practises have an important effect on the underlying groundwater of an area. Water applied artificially to the soil through irrigation increases the amount of infiltrating moisture, and hence the volume of water input to groundwater. Drainage through the soil profile is necessary to leach salts which would otherwise accumulate in the root zone. Crop plants extract water from the soil while leaving most of the salt behind. The high evaporation characteristic of arid regions acts to further concentrate salts in the soil especially if the applied water has a high salinity. Unless leached away such salts will eventually begin to inhibit plant growth (Hillel, 1980).

Salt accumulation can only be prevented by application of an amount of water greater than that consumed by evapotranspiration. A significant fraction of applied water must be allowed to flow through the root zone and hence leach away the excess salts. Inevitably this leads to contamination of the receiving groundwater. Unless the groundwater is deep, or lateral drainage rapid, the excess irrigation water can cause a progressive rise in the water table. Once within approximately two meters of the soil surface, the groundwater will reach the root zone by capillary action in the overlying capillary zone. In this way the salts that were previously leached are returned to the soil. Thus, for effective salinity control of the soil the position of the groundwater table must be monitored, along with the amount of water leaching below the root zone.

When groundwater eventually reaches the surface as stream flow, the effects of irrigated agriculture will be extended beyond the field/orchard scale, and if the receiving stream is used for further irrigation the result will be a progressive salinisation of the water in the downstream direction. Thus, the impacts of irrigation on groundwater may be displaced spatially and temporally from the site and time of irrigation.

2.6. MATHEMATICAL REPRESENTATIONS OF SOIL MOISTURE MOVEMENT

An understanding of the factors affecting soil moisture and its movement allows the mathematical or modelled representation of this phenomena. The soil is a highly complex system, exhibiting variability at all scales in both spatial and temporal directions. Attempts to quantify the soil system mathematically usually involve some degree of simplification, as the accurate representation of all factors simultaneously is virtually impossible. Initially, the easiest assumption to make is that the soil is completely saturated.

2.6.1. Saturated Conditions

The water balance of the soil can be used to account for the incoming and outgoing fluxes of a soil compartment. Under saturated conditions where most pores are considered filled, and the hydraulic conductivity constant at maximum rate, the difference between incoming moisture and stored moisture gives the outgoing moisture (Equation 2.2.).

Under saturated conditions:

$$\delta S = I + Qu - E_t \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (2.2)$$

where δS = change in water storage
I = infiltration
Qu = net upward flow
E_t = evapotranspiration

Application of Equation 2.2 is inhibited because it is difficult to quantify the capillary rise (Qu). An alternative approach is described by Darcy's Law, which gives the flow rate (Q) as the product of the matric potential gradient and the hydraulic conductivity of the soil over a period of time. Darcy's Law does not require direct measurement of upward flux as it assumes that a positive change in matric potential indicates wetting conditions, hence downward flux, while a negative change in potential indicates drying (Equation 2.3):

$$q = -Ks.H \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (2.3)$$

where q = moisture flux
Ks = saturated hydraulic conductivity
H = hydraulic gradient = $(\delta(g + c)/\delta z)$
where g = gravity forces
c = capillary forces
z = depth

2.6.2. Unsaturated Conditions

Darcy's Law can also be applied to unsaturated conditions if steady state is assumed

(Richards, 1931) and the unsaturated hydraulic conductivity is measured.

In a partially saturated soil the effective volume in which flow can occur is reduced as the larger pore spaces are filled with air. If these empty pores were filled with impermeable solid material, the conditions of flow would be analogous to those found in saturated media with a reduced hydraulic conductivity. The transition from wet to dry conditions is characterised by a large decrease in hydraulic conductivity which occurs over several orders of magnitude (Hillel, 1980; Remson, et. al., 1971). Assuming steady state:

$$q = -Ku.H \quad \ldots\ldots\ldots\ldots \quad (2.4)$$

where q = moisture flux
Ku = unsaturated hydraulic conductivity
H = hydraulic gradient

Capillary forces act in all directions, while gravitational forces (z) act in the vertical direction only. Equation (2.4) may now be expressed in three dimensions (x, y and z):

$$q = -Ku[\delta(g + c)/\delta z + \delta c/\delta y + \delta c/\delta x] \quad \ldots\ldots\ldots\ldots \quad (2.5)$$

The steady state assumption can be avoided if Equation (2.5) is combined with the continuity equation (Equation 2.2), hence accounting for changes in moisture content with time:

$$D\theta = \delta/\delta z[Ku(\delta c + 1)/\delta z] \quad \ldots\ldots\ldots\ldots \quad \text{vertical direction}$$

$$D\theta = \delta/\delta x[Ku(\delta c)/\delta x] \quad \ldots\ldots\ldots\ldots \quad \text{horizontal direction}$$

where $D\theta$ = $\delta\theta/\delta t$ = change in soil moisture content with time
θ = soil moisture content

This form of Darcy's Law applicable to unsaturated conditions is known as Richards Equation. Unsaturated conductivity varies with moisture content, and Richards Equation assumes that conductivity at a given moisture content is equal in all directions. In field soils, which are largely stratified, layering results in a variable conductivity in the vertical direction, which may also influence movement in the horizontal direction as well. If the wetting front reaches a dry, coarse layer, downward flow is reduced as the hydraulic conductivity of the dry soil will be low. Further infiltration will then depend on the magnitude of the hydraulic gradient, with moisture movement being restricted until the gradient can overcome the forces of water retention in the finer grained layer. A dry fine-grained layer would wet rapidly due to its high matric potential, but would have a smaller hydraulic conductivity and so the speed of infiltration would be reduced. This would also lead to saturation above the impeding layer. This means stratification acts to enhance lateral flow over flow in the downward direction, thus reducing the efficiency of Richards equation in predicting soil moisture movement.

2.6.3. Soil Structure affects Soil Moisture Movement

The influence of macropores in soil water flow is recognised as a mobile inter-aggregate phase within macropores, while an immobile, intra-aggregate phase exists within micropores (Radulovich, et. al., 1989). Soil macropores may allow turbulent flow, whereas the Darcy equation assumes laminar flow only. However, in a study by Radulovich et. al., (1989) the velocity of macropore water movement did not result in a Reynolds number exceeding unity; thus all movement remained laminar.

Although the Darcian requirement of laminar flow is met, there is a further problem introduced by the differentiation of moisture movement into macro- and micro-pore flow. According to Darcy's Law once field capacity is reached, all pre-existing water is displaced by infiltrating water. This does not occur in nature as most micropore water is strongly held by capillary forces and is not displaced, while most macropore water is rapidly replaced by incoming water. Velocities are higher in macropores, so infiltrating water can bypass the micropore water hence reaching greater depths before displacement of immobile soil moisture occurs.

2.7. SOIL WATER CHEMISTRY

All nutrients required by plants other than the gases O_2 and CO_2 are taken up by roots as solutes from the soil solution. The concentration of chemicals within the root zone is controlled by a number of factors including the soil mineralogy which releases ions during the weathering process. Salt inputs through irrigation and rainwater provide further chemical enrichment of the soil solution and climatic factors such as evaporation may concentrate salts in the upper soil layers.

Solutes and nutrients are conveyed to the roots through transport processes, which are also responsible for nutrient loss through drainage and leaching. Opposing the transport processes are storage mechanisms which can retain plant nutrients against drainage and leaching. These storage processes are the mechanisms of cation and anion adsorption and exchange. The distribution and equilibration of solute ions depends on the amount and type of charge generated on the colloid surfaces and the type and concentration of ions present in the soil solution.

2.7.1. Micropore Chemistry

Micropore water is in close contact with the soil surface, and is held in place by molecular and capillary forces. At such small distances, chemical reactions between ions held electrostatically on soil particle surfaces can occur in response to concentration gradients within solution. This interaction takes place slowly and over molecular distances, which means the immediate soil solution may be in chemical equilibrium with the particle surface, but in disequilibrium with more distant soil water. Once cation exchange reactions occur, the released ions move by diffusion in response to the concentration gradient that exists within the laminar zone of micropores (Ross, 1989). These solutes reach larger pores where soil moisture is less tightly held, and flow is more rapid. The micropore water chemistry therefore, is dictated by the mineralogy of the soil particles around which it is held.

2.7.2. Macropore Chemistry

Macropore water moves primarily under gravitational forces, and hence moves more quickly through the soil profile. This rapid movement does not allow the macropore flow to come to a chemical equilibrium with the soil particles, which are largely bypassed. The chemistry of macropore flow therefore is determined by the chemistry of the infiltrating water, irrigation or rainfall. The concentration of non-reacting solutes is fairly uniform across the macropore cross-section due to mixing during turbulent flow (Ross, 1989).

2.8. SOLUTE MOVEMENT

The movement of specific ions through the soil matrix is difficult to describe or predict accurately, as the processes of precipitation, dissolution, reaction, and exchange among others serve to interfere with solute movement (Ross, 1989). Negative ions such as Cl^- and NO_3^- tend to be conservative, resisting interaction with the soil, so are usually selected for modelling solute movement.

Chemicals within the soil may be transported both horizontally and vertically, depending on several major physical processes (Lindstrom and Piver, 1986). Solute movement is dependent on soil moisture and the transport of solute is assumed to be governed by convection, the viscous movement of the soil solution, and dispersion, thermal motion within the soil solution (Bresler et. al. 1982). The transport of solute through the unsaturated zone to the water table is a complex process, the understanding of which is based on laboratory conditions. The extrapolation of laboratory results to actual field conditions is doubtful (Gvirtman et. al., 1988), but most theory is necessarily derived from the controlled conditions possible only in the laboratory. Theories of transport consider the soil as a continuous porous medium, with equations being derived for a representative unit volume which is large enough to express its properties in terms of statistical averages.

Two mechanisms dominate the transport of solutes through the soil. Firstly, water moving through the soil carries solutes with it by means of convective transport or mass flow. Secondly, the dispersion or migration of solutes under osmotic potential from areas of high to low concentrations within soil water occurs continually by means of diffusion.

2.8.1. Convective Transport/Mass Flow

Solute transport is made up of two convective or mass flow components. In larger pores, turbulent flow dominates and fast convection occurs. Slow laminar transport occurs adjacent to particle surfaces and in micropores. Soil water movement occurs when a difference in water potential exists. Flow is determined by pressure gradients, and when changes in soil water occur through infiltration, redistribution and evapotranspiration, the dissolved salts move with the water.

Convective transport depends on the macroscopic flow velocity. Due to the soil porosity, actual porewater velocity is distributed around an average value and is determined by the distribution of pore sizes and pore shapes. Velocity is faster in large pores, and in the centre of the pores. Water and solutes move at different rates through soil and may be acted upon, transformed, or retarded during their movement through the soil. Where conservative solutes are considered no gains or losses and no solute/surface or solute/solute interactions occur (Ross, 1989). Under these conditions, the convective flow of solute associated with water movement is expressed by:

$$Jc = q.C \qquad \ldots\ldots (2.6)$$

where Jc = convective flux of solute

q = volumetric flow rate

C = concentration of solute

To estimate the travel distance of the solute, the average apparent solute velocity is considered. Actual velocities vary over several orders of magnitude within pores and between pores, so the average is at best an approximation. Solute velocity is assumed to be equal to moisture velocity, which is applicable to conservative ions only:

$$v = q/\theta \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (2.7)$$

where θ = volumetric soil moisture
v = average solute velocity
q = volumetric flow rate

Transport of solutes seldom occurs by convection alone as solutes move within flowing water in response to concentration gradients by the processes of diffusion and dispersion.

2.8.2. Diffusion

Solute movement is affected by solute concentrations, so chemical behaviour at the molecular scale must be considered. All solute molecules exhibit random motion which results in the net movement of ions from high to low concentration until the solution is uniform. The speed of equalisation depends on the concentration difference, thus solute transport by molecular diffusion depends on the concentration gradient of the ion. The average macroscopic flow rate of solute molecules in a uniform aqueous medium is proportional to the concentration gradient ($\delta c/\delta x$) and to the cross-sectional area. This is Fick's first law for saturated media.

$$Jd = -Dw.\delta C/\delta z \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (2.8)$$

where Jd = rate of diffusion
Dw = diffusion coefficient for the solute diffusing in water
C = solute concentration
z = distance in direction of flow

Rewriting the equation for unsaturated conditions:

$$Jd = -Ds.\ \theta.\ \delta C/\delta z \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (2.9)$$

where θ = volumetric soil water content
Ds = diffusion coefficient in the soil

Accounting for three dimensional diffusion:

$$Jd \quad = \quad [-Ds.\delta Cx/\delta x] + [-Ds.\delta Cy/\delta y] + [-Ds.\delta Cz/\delta z] \quad \ldots \ (2.10)$$

In unsaturated conditions the volume of water available for diffusion is reduced, so Ds can increase by several orders of magnitude over Dw. The path of diffusion becomes more tortuous when there is less water available to move through, which further reduces the actual value of Ds. Mahtab, et. al. (1971) found Ds to increase linearly with moisture content of the soil. As the moisture content of a soil decreases, the cross sectional area available for diffusion becomes smaller and the ions have to travel a longer distance to reach a given point. Other factors such as viscosity and anion exclusion become more influential as moisture decreases.

According to Ross (1989), diffusion coefficients in soil are controlled by:

- The state of the medium within which diffusion occurs. Diffusion is most rapid in gaseous media, followed by liquids then solids.

- Soil moisture content. A two- to four-fold increase in diffusion of K^+, Ca^{2+} and Mg^{2+} was measured by Schaff and Skogley (1982) when soil moisture content was increased from 10 to 20%. Table 2.2 shows the effect of increasing soil moisture on the diffusion coefficients of Sodium, Chloride and Phosphorous. When soil moisture content increases from 20 to 40%, the coefficients increase by an order of magnitude for Sodium and Phosphorous, and by 3-fold for the Chloride anion.

- Tortuosity of porespaces. Smaller pores, and increased tortuosity of flow paths within the soil matrix decrease ionic diffusion of all ionic species. This was first recognised by Nye and Tinker (1977), who introduced an impedance factor to modify the diffusion coefficient:

$$Ds \quad = \quad -D.\theta.f.\ \delta C/\delta z \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots \ (2.11)$$

where Ds = diffusion coefficient of solute through soil
D = diffusion coefficient of solute in free solution
θ = fraction of the soil volume occupied by solution
f = impedance factor for tortuosity of diffusion pathway
C = concentration of solute in solution
z = depth

(Nye and Tinker, 1971)

Table 2.2. Diffusion Coefficients of Selected Ions, in relation to Soil Moisture

ION	% MOISTURE BY VOLUME	$D cm^2/s$
Na^+	40	2.2×10^{-6}
Na^+	20	0.2×10^{-6}
Cl^-	40	9×10^{-6}
Cl^-	20	2.4×10^{-6}
PO_4^-	40	3.3×10^{-9}
PO_4^-	20	0.3×10^{-9}

(Rowell et. al., 1967)

Empirical expressions have been derived for diffusion governing the movement of a non-consumptive, non-reactive solute, Phosphorous (Mahtab, et. al., 1971). Ds was governed by the amount of solute in solution and the rate at which solid phase solute is released into solution. The available solute increased as the clay content of the soil increased, and therefore as the clay content increased so did the Ds on average 5 fold in a soil with 5 times as much clay. The Ds values were significantly related to clay content at the 1% level of probability. The writers suggest the increase in Ds values with increased clay content is probably due to the "tortuosity" factor, which also becomes larger with clay content.

Equation (2.10) can only describe steady state diffusion processes. To account for transient processes in which rate of diffusion and concentrations vary with time Equation (2.10) must be combined with the continuity equation (Equation 2.2):

$$A.\delta C/\delta t.z \quad = \quad A[Jd + \delta Jd/\delta z.z] - A.Jd \quad \ldots\ldots\ldots\ldots \quad (2.12)$$

where A = cross sectional area of flow
C = solute concentration
t = time
z = distance
A[Jd + δJd/δz.z] = solute diffusing in per unit time
Jd = rate of diffusion

The diffusion rate (Jd) is not generally constant as it is dependent on both soil moisture and solute concentrations. However, where diffusion is uniform, Equation 2.12 reduces to:

$$\delta C/\delta t = -\delta Jd/\delta z \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (2.13)$$

Convective flow changes the distribution of solutes relative to one another, and induces the second process determining soil solute movement, hydrodynamic dispersion.

2.8.3. Dispersion

Mechanical dispersion is due to local variations in microscopic flow velocity. As water moves faster through wide pores than narrow ones, and through the centre of each pore than along the walls, some parts of flow are more rapid than others. This variability of flow causes mixing of solutions - the degree of which depends on the average flow velocity, pore size distribution, degree of saturation and concentration gradients (Hillel, 1980).

When convective velocity is high such as at near-saturation conditions, hydrodynamic dispersion will exceed diffusion. This means diffusion will be negligible in contributing to solute movement. During unsaturated conditions less flow occurs and hydrodynamic dispersion has a weakened effect. Diffusion will then govern solute movement. A similar partitioning occurs under variable flow velocities. Molecular diffusion is obscured by much larger dispersion effects at high water velocities. As porewater velocity decreases the dispersion coefficient (Ds) decreases and molecular diffusion becomes more important in solute mixing and dispersion effects Kirda et. al. (1973).

Mechanical dispersion (Dm) is similar to Ds, and has been found to depend approximately linearly on the average flow velocity. It has also been found that the dispersion coefficient is independent of porewater velocity (v), and is proportional to the water content (Smiles and Philip, 1978; Elrick et. al., 1979; Smiles et. al., 1981). The dispersion coefficient (Dm) can be expressed by the following:

$$Dm = D0 + Ev \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (2.14)$$

where D0 = molecular diffusion coefficient
E = dispersivity
v = pore water velocity

Equation 2.14 is accepted as being applicable to field conditions (De Smedt et. al., 1986, Kirda et. al. 1973; Hildebrand and Himmelbau, 1973; Yule and Gardner, 1978; Beese and Wierenga, 1983), although it remains controversial. Dispersivity (E) ranges from 0.01 to 1 cm under saturated laboratory conditions, but under field conditions, values of up to 100m have been reported (Freeze and Cherry, 1979). This means it is necessary to calibrate the field dispersivity of a selected ion before Equation 2.14 can be used with confidence.

Under unsaturated conditions both mobile and immobile water phases exist (Van Genuchten and Wierenga, 1977; Gaudet et. al., 1977; Rao et. al., 1980; De Smedt and Wierenga, 1984). Differential rates of matrix flow have been modelled by differentiating soil water into mobile, immobile and stagnant phases. A convective-dispersive transfer of solutes occurs through the simultaneous exchange of solutes between the mobile and immobile phases (De Smedt et. al., 1986). The transport of solutes under these conditions is represented by the following:

For the mobile phase:

$$\delta\Theta_m/\delta t.C_m = \delta/\delta z.[\Theta_m.D_m.\delta C_m/\delta z] - \delta q/\delta z.C_m - ar.\Theta_m[C_m - C_{im}] \quad \ldots\ldots\ldots \quad (2.15)$$

For the immobile phase:

$$\delta\theta_{im}/\delta t.C_{im} \quad = \quad ar.\theta_m[C_m - C_{im}] \quad \ldots\ldots\ldots\ldots\ldots\ldots (2.16)$$

where θ = soil moisture content
C = solute concentration
t = time
z = depth
D = dispersion coefficient
q = volumetric flow rate
ar = rate coefficient of solute exchange between two phases
m = mobile water phase
im = immobile water phase

After sufficient time, it has been shown that the mixing between the phases is such that concentration distributions can be described by:

$$D \quad = \quad \theta_m.D_m/\theta + [\theta^2_{im}v^2]/\theta_m.ar \quad \ldots\ldots\ldots\ldots\ldots\ldots (2.17)$$

where the symbols are the same as before.

From Equation (2.17) it can be seen that the overall dispersion coefficient (D) is the sum of two processes: dispersion in the mobile zone and dispersion due to solute exchange between the mobile and immobile phases. This suggests that when immobile water is present in unsaturated conditions, the overall dispersion can increase significantly, up to 78 times greater than when only mobile water is considered (De Smedt et. al., 1986).

It is doubtful whether the convection and dispersion equations can model solute transport in soils containing a wide range of pore diameters and porewater velocities (Ross, 1989) irrespective of the adaptations and additional subroutines included. This is because different processes are involved, other than the simple convection and dispersion which are invoked as the causal factors in solute transport.

2.8.4. Effect of Soil Properties on Solute Transport

Soil solute concentration and flux are calculated as a function of time and space using macroscopic quantities which vary in a deterministic manner, and are expressed as partial differential equations. To solve these equations it is usually assumed that their flow parameters are uniform throughout the entire field - in reality fields are seldom homogeneous.

The most significantly variable soil physical characteristics are water and solute transport parameters measured under field conditions (Jury, et. al., 1986). Solute convective velocities and dispersion coefficients typically show large standard deviations, often exceeding 100% of the field mean (Jury, 1985). Such extreme variability means accurate average values cannot be estimated at field scale. This leads to the assumption that mass transport phenomena in field soils are intrinsically erratic processes for which quantitative characterisation can only be achieved using stochastic approaches at the field scale. Properties of the soil are regarded as continuous functions of the space coordinates, of which the horizontal dimensions are very large compared with the vertical direction. As the spatial variability of field soil characteristics must be expressed in statistical terms, stochastic elements are often used instead of, or in addition to deterministic ones.

Although soil hydraulic properties are highly variable, even within a given small field (Russo and Bresler, 1981b), variations are not completely disordered. Structured variation occurs which often describes a probability distribution of these factors. Using actual field variability data, it is possible to analyse how much inherent spatial variability of the soil hydraulic properties exists, and hence quantify the probability density function (Russo and Bresler, 1981a). Solute movement at field scale distances and times has been found to show variability according to the hydraulic conductivity. This has been successfully described by a single realisation of a stochastic function parameterised by spatial co-ordinates (Sposito, et. al., 1986).

Cameron and Wild (1982) compared the ability of three models to predict chloride leaching in South England, and found the most accurate results were obtained using the convective-dispersion (CD) method of Rose et. al. (1982). Leaching predictions were less accurate for actual rainfall events than regular irrigation applications, and predictions were only possible once estimates of field diffusivity were available. This highlights the problem in applying simple transport models to heterogeneous field conditions. Field measurements have shown that there is considerable spatial and temporal variability in soil water parameters and many attempts to predict field leaching have failed due to the unknown local field variability in soil hydraulic properties (Nielsen, et. al., 1973; Biggar and Nielsen, 1976; Jury et. al., 1976 Van De Pol et. al., 1977).

2.8.5. Miscible Displacement and Breakthrough Curves

If a liquid infiltrating the soil is not soluble in the pre-existing soil moisture then the process of immiscible displacement will occur, whereby the incoming liquid displaces the soil moisture. Most solutions entering the soil are however mutually soluble and mixing will occur with the chemistry of the incoming solution gradually dominating the soil solution. The change in concentration of the outgoing solution over time can be plotted as a breakthrough curve (BTC).

If the pre-existing water were pushed out of the soil without any mixing with the invading solution, the BTC would show an abrupt change in concentration when all initial water had gone. This would result in piston flow through the soil. As most aqueous solutions are miscible mixing is unavoidable, and the shape of the BTC is variable, depending on a number of factors. This provides a useful method for deducing processes occurring between inflow and outflow points. Nielsen and Biggar (1962) first noted that if the area under the breakthrough curve below 1 pore volume is equal to the area above the curve greater than 1 pore volume, then no solute-solid interaction has occurred. This means retention or release of solutes within the soil will be indicated by the shape of the curve (Selim, et. al., 1989).

Two factors cause mixing and dispersion, resulting in the outflow curve varying:

- Increase in the pore size and consequent increase in porewater velocity causes increased dispersion.

- Increase in the concentration of the inflow solution has a similar effect to increasing pore size. Solutes move from high to low concentrations, and the greater the concentration gradient, the more rapidly diffusion will proceed.

2.8.6. Anion Exclusion

Soil clay particles and humus surfaces exhibit negative charges which repel anions electrostatically. These anions are then concentrated in the centre of the pores where the velocity of flow is relatively faster, and the water volume available for transport 10-20% less than that available for cations (Wild, 1981). This means that anions move more rapidly than positive ions, and can also exceed the average velocity of the soil water. Smith (1972) observed that Chloride moved 1.04 - 1.67 times faster than the average water velocity. If the net anion flux exceeds the net water flux forward displacement of the BTC will result.

Ross (1989) identifies the following factors affecting anion exclusion:

- Anion exclusion increases with increasing anion concentration
- Exclusion increases with anion valency. More electronegative ions will be more strongly repelled by the soil particle surfaces, and to a greater distance than less electronegative ions. The following order of repulsion has been reported: $Cl^- = NO_3^- < SO_4^{2-} < Fe(CN)_6^{4-}$ (Mattson, 1929).
- Exclusion decreases with soil pH, since this decreases the net negative charge on soil colloids. At low pH, there are more Hydrogen (H^+) ions in solution, which readily occupy the cation exchange sites, rendering the soil particle neutral. The particles will no longer be able to repel anions, hence reducing the anion exclusion effect.
- Exclusion decreases with increasing cation saturation of the soil. This is a similar effect to increased pH, except the exchange sites are filled with cations other than H^+.
- Exclusion increases with increased density of negative charge on the particle surface. This means the particle can exert a greater repulsive force on the anions.

The effects of anion exclusion result in negative ions being rapidly propagated through the soil, usually at rates faster than the net moisture movement. As negative ions such as Cl^-, and NO_3^- are conservative, and do not readily become involved in soil reactions or cation exchange, these are often selected as tracers for soil solute movement (Ross, 1989). However anion exclusion means the movement of anions is not necessarily representative of the net soil moisture movement, or movement of other solutes. The use of anions may lead to overestimation of movement, conversely the use of cations may lead to underestimation as such ions are readily adsorbed onto exchange sites.

2.8.7. Solute Reaction

Ion adsorption/desorption during solute transport has been incorporated into a number of models (Wagenet, 1984).The problem in incorporating ion exchange into models of transport for reactive solutes is due to the complexity of the soil system and the numerous interactions of competing ions (Ross, 1989). Simple one-dimensional transport models have been developed for solute leaching models using non-reactive ions such as Chloride and Nitrate. Both laboratory and field validation have concentrated overwhelmingly on non-reactive species, but this is inadequate to describe the gross solute distribution within a field soil (Ross, 1989). Therefore there is a clear need for further field validation using a wider range of ionic species, including cations and an examination of the effects of anion exclusion on so-called non-reactive ions.

2.9. HYDROSALINITY MODELLING

The absolute quantity of water available for crop use is only one of the factors controlling agricultural production. Water quality is also extremely important as plants have a limited tolerance to salinity. There is an increasing need within water management and users for a method whereby the application of water and chemicals to soils and crops can be controlled and optimised. The fate of irrigation water, and the solutes dissolved in it, is ideally suited to the use of models (Wagenet and Hutson, 1987; Russo, 1991).

There are few approaches which have been developed to directly measure environmental indices in the field, and generally these methods have given results of questionable value particularly with respect to fluxes (Wagenet, 1988). Most methods have focused on the development of indirect methods of calculating the required parameters, using mathematically simple to complex representations. Different kinds of modelling procedures include simple, mathematical, conceptual and physically based models, the latter being best suited to model dynamic changes in the environment. Under average conditions, the simulation and forecasting of moisture movement is not difficult but under extraordinary conditions, the use of a model is "a matter of luck " (Naef, 1981).

A mathematical model is a set of mathematical equations describing a system, requiring data inputs and producing outputs which describe the system response. A computer is usually required to run a model. Mathematical modelling is an accepted way to describe a natural system, through integrating basic processes. Soil water and the solutes dissolved in it constitute a natural system that has been modelled at varying levels of resolution, with differing degrees of success. These hydrosalinity models vary in conceptual framework and degree of complexity, and although their potential application is wide, little general use is made of such soil solute models beyond their initial development and testing (Wagenet and Hutson, 1986).

2.9.1. Classification of Hydrosalinity Models

There is apparently little recognition that different types of models are developed for different reasons. The quantity of required input data, depth of consideration of basic processes and sensitivity and accuracy of simulations all depend on the perspective and use requirements of the modeller (Wagenet and Hutson, 1987). Recently a variety of approaches to describe solute leaching in field soils have been proposed, often in response to specific problems (Addiscott and Wagenet, 1985).

Deterministic and Stochastic Modelling

Solute and moisture movement occurring in field soils has been explained both deterministically (Bresler, 1973, Childs and Hanks, 1975) and stochastically (Dagan and Bresler, 1979, Jury, et. al., 1982).

There are four main types of models:

- stochastic conceptual
- stochastic empirical
- deterministic conceptual
- deterministic empirical

where stochastic = a variable in expression is a probability distribution
deterministic = all variables are free from random variations
conceptual = functional form derived from understanding of physical processes
empirical = functional form not derived from an understanding of physical processes

The main distinction between these models is the conceptual assumptions made in the model formulation. Deterministic models attempt to describe all processes operating as accurately as possible in a theoretically rigorous way, and have been the most widely used approach in hydrosalinity modelling (Wagenet, 1988). These models assume that soil water and solute displacement processes operate to result in a definable water or solute distribution in the soil profile. Water movement is described by the interaction between the hydraulic gradient and a water content dependent hydraulic conductivity (Richard's Equation). Physical convection and chemical diffusion are assumed to combine to displace a solute in the soil (the Convective-Dispersion Equation).

As previously mentioned, the spatial variability of input parameters such as hydrodynamic dispersion and hydraulic properties of the soil render an accurate deterministic representation of the soil system nearly impossible. The porous media of the soil through which water moves are extremely disordered, so it seems erroneous to represent them by something which is intrinsically ordered (Scheidegger, 1957). Models must therefore have an inbuilt "disordering", which is the principle of stochastic modelling (Dagan and Bresler, 1979, Simmons, 1982, Mantoglou and Gelhar, 1987).

The stochastic approach is based on probability density functions and empirical spatial correlations of soil water and solute transfer properties (Tillotson, et. al., 1988). Determination of stochastic values requires intensive sampling to adequately define the field of statistical variation. For those elements exhibiting extreme field variability, stochastic functions are most appropriate, and these can be used in combination with deterministic functions where less variability occurs.

Research and Management Modelling

Models developed for research or management purposes differ in the quantity of input data required, extent of theoretical detail, and sensitivity and accuracy of simulations. Research models aim to provide quantitative estimates of water and solute movement having comprehensive data demands, computer execution time, and are often non-transferable from the developer to other users (Wagenet and Hutson, 1986). The strength of these research models is they allow the testing in a comprehensive and integrated manner our knowledge about the processes affecting solute movement in the unsaturated zone. Although a number of these reported models are potentially applicable to solute transport and fate of certain ionic species, few applications have been made (Wagenet and Hutson, 1986).

Management models are less data-intensive, but are commensurately less quantitative in their ability to predict solute and water movement under field conditions. Few models of either type have been tested against field data, and little attention has been paid to the use of the management models for the actual purposes of managing applications to soil of saline irrigation water (Addiscott and Wagenet, 1985).

Deterministic research models are generally unsuited for management purposes due to their intensive data requirements, and detailed theoretical knowledge needed to apply and interpret outputs. Stochastic models have therefore been developed to assist managers in quantifying the natural environment, in a manner that provides useful information for irrigation scheduling. Stochastic approaches assume that the natural environment is inherently random, and definable only in statistical terms. However, they are untested for any environment other than the very limited set of field conditions from which they were derived. For management purposes, these models are mathematically demanding, and highly specific to the environment from which the data was derived for their formulation.

Simpler deterministic models of solute and water movement have been developed, which neglect detailed theoretical aspects and require substantially less data collection than their detailed deterministic predecessors (Addiscott and Wagenet, 1985). These models are intended for general management guidance, and give largely qualitative estimates of solute and water movement. However, it is important to evaluate such models against detailed field data before application.

Functional and Mechanistic Modelling

A third model classification is that of mechanistic and functional approaches. Mechanistic models use the most fundamental process mechanisms describing the system to be modelled. Functional models use more simplified expressions to simulate the environment, thus require less detailed data input and computer expertise for their execution. Mechanistic models consist of rate models, which describe the rate of change of solute concentration in terms of the product of a hydraulic gradient and a rate parameter. Functional models use a capacity approach instead of rate parameters, describing solute movement in terms of volumetric water content rather than time dependent rates.

2.9.2. Theoretical Bases for Hydrosalinity Models

Hydrosalinity models must account for the transport and consumptive use of the soil water during both saturated and unsaturated conditions. Water and solute transport can be simulated using the thermodynamic approach in which soil water moves according to differences in potential energy. The capacity approach in which the ability of the soil to retain water has a certain upper limit can also be used. Field capacity for each layer is specified, and where the water content of a layer reaches this amount any excess water is assumed to percolate to the layer beneath (Moolman and de Clercq, 1990). Crop water uptake is simulated through inclusion of a simple sink term that accounts for evapotranspiration, although some models can distinguish between evaporation and transpiration.

Capacity Approach to Moisture Modelling

This is based on a simple water balance, using relationships that are largely empirical. The maximum volume of water that an individual soil layer can hold is defined as a fixed amount. Infiltrating water moves into the soil until this limit (field capacity) is reached, and any excess then moves down into the next layer. Neither saturated conductivity nor hydraulic gradients are needed. Moisture movement is capacity driven and flow in the downward direction only is usually considered. Capillary rise can be incorporated, and evapotranspiration is included as a simple sink term.

The capacity approach assumes steady state soil salinity conditions exist. Processes included in the models are usually only those of dissolution and precipitation processes in a simple mass balance between incoming and outgoing solute loads from a soil layer. The assumption of steady state conditions is unrealistic as transient conditions where the soil loses/gains salt with time are more common. Thermodynamic models do not have the requirement of steady conditions. As transient conditions are theoretically complex to model and more data intensive than steady state, this approach is not as simple or easily applied as the capacity approach.

Thermodynamic Approach to Moisture Modelling

Water transport is explained as occurring due to potential energy differences within the soil. This arises when an internal matric tension gradient exists across some spatial distance within the soil. Richard's Equation describes water flow in soils, and combines Darcy's equation for saturated flow with the equation of continuity (see Section 2.6).

The saturated conductivity for each soil layer and gradient in matric potential between each layer must be measured in the field. Conductivity varies over orders of magnitude within a single field, and unsaturated conditions are more common than saturation, which complicates the measurement of these parameters. Where evapotranspiration is to be simulated, a sink term is added as in capacity models.

Simple convective-dispersion models have been developed for solute leaching studies of non-reactive solutes. These models have been adapted to account for more realistic field soil conditions - particularly in layered soils and under the influence of macropore flow.

2.9.3. Solute Modelling

Analytic solutions of the classical Convective Dispersion Equation (CDE) have been widely used as models of chemical transport and transformation in soil-water systems, although such models are limited to conditions of steady-state water flow in homogeneous soils (Van Genuchten and Wagenet, 1989). Solute transport according to the miscible displacement theory states that the flux of solute is the result of the combined effects of diffusion and convection:

$$J = Jd + Jc \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2.18)$$

where J = solute flux
Jd = solute transported by diffusion
Jc = solute transported by convection

Convection is the chemical diffusion of solute in response to concentration gradients existing in the soil solution. Fick's first law of diffusion is used to describe the diffusion process.

$$Jd = -Ds.\delta C/\delta z \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2.19)$$

where Ds = the effective diffusion coefficient of the chemical in the soil
C = solute concentration
z = depth

Dispersion is the physical mixing resulting from variations in water flow velocity within each pore and between pores. This is mechanical dispersion and can also be described by using an adapted version of Fick's law.

$$Jc = [-\theta.Dm.v.\delta C/\delta z] + [v.\theta.C] \quad \ldots\ldots\ldots\ldots\ldots (2.20)$$

where Jc = convective flux of solute
Dm = mechanical dispersion coefficient
v = average flow velocity

θ = soil moisture content
C = solute concentration
z = distance

Combining Equations 2.19 and 2.20 gives the convective dispersion equation of solute transport:

$$J = [-\theta.Dv.\theta.\delta C/\delta z] + [q.C] \quad \ldots\ldots\ldots\ldots\ldots\ldots (2.21)$$

where q = volumetric water flux
D = Dm + Ds

The use of Equation 2.21 to represent solute transport in leaching models is subject to large spatial differences in the relationship between water flux, water content and the apparent diffusion coefficient.

2.9.4. Validation of Models

Model predictions must be compared with measured data to prove that the model output is a realistic representation of field processes. To compare model simulations with measured data the model input parameters must be known and field data to compare with model outputs must also be available. According to McLaughlin (1988):

- from a technical or scientific point of view a model is validated when it properly describes physical processes, and
- from a regulatory point of view it is validated when the model yields adequate predictions with the implicit goal being to reduce the risk of use of the model leading to inappropriate decisions.

The criteria for validation are not universally accepted, however. Loague et. al. (1988) suggest that a model is a good representation of reality, and hence valid, if it can be used to predict certain observable phenomenon with acceptable accuracy and precision. These writers do not however define what this precision and accuracy level is.

Statistical measurement of the validity of models is desirable, but data sets of sufficient size to provide a representative range of the model output performance are difficult to provide. Statistical testing and graphical representation are used in model validation, but there is no defined procedure or technique that is widely accepted. A 100% correlation between model output and field data would occur if the model could perfectly simulate actual conditions.

This is extremely unlikely to occur in reality, as field validations of solute transport models have been less successful than laboratory validations (Ross, 1989) which seldom approximate actual data. Modellers must be content with less prefect correlations, and the level of accuracy of prediction that is acceptable will vary between model users. The most important aspect however, is that the modeller is aware of the model's validity, and does not apply it indiscriminately.

The level of acceptable inaccuracy will vary with applications, hence one model may be valid for a situation requiring general trends and qualitative information, such as irrigation management or educational purposes, but invalid for pure scientific research.

2.9.5. Sensitivity Analyses and Model Calibration

Model validation is distinguished from calibration, which is the procedure whereby model output is progressively refined using data specific to the site or area in which it is to be applied. Model parameters are adjusted until the predictions generated are acceptable approximations of these measured data. Validation involves comparison of the model with field data with no alterations made to improve the output performance. Data used for the validation must necessarily be different from that used for calibration, or the validation becomes a meaningless exercise (Moolman and de Clercq, 1990).

The process of obtaining all data requirements for model implementation is expensive and time consuming. Before a sampling and analysis program is embarked upon, a sensitivity analysis should be carried out on the models in order to determine the relative importance of each input parameter in determining the model output. The objective of the sensitivity analysis is to identify those variables having little or no impact on the model predictions; these variables can then be measured with less intensity and accuracy than other, more effective parameters. In this way the user can isolate the most important field variables to the particular model, and focus more attention on obtaining the highest degree of accuracy possible of these variables. Less important parameters can be measured through less intensive, inexpensive means.

The determination of the input requirements to a model is time consuming and expensive, and the necessity for absolute accuracy in field measurements of each parameter must be gauged before the model is applied. Those parameters to which the model is insensitive may then be measured with less accuracy than others which may fundamentally affect the model output. A sensitivity analysis attempts to determine which parameters in the model have the most impact on the output predictions. A small variation in one parameter may lead to a wide variation in the output predicted, whereas variation in another parameter may have negligible effect on the model performance, behaving as a fixed value. Each parameter is varied in turn, holding all others constant, and the effect of this variation on the model output is noted. Different combination of variables may be varied together, ignoring unrealistic combinations, to assess the degree of interaction and interdependence between parameters.

2.9.6. Limitations of Modelling

A realistic attitude to the abilities and achievements of hydrosalinity models must be developed if such models are to be critically applied (Beven, 1989).

Scale of Application

Hydrosalinity models range from high resolution, highly deterministic to low resolution simpler models. There are difficulties in attempting to accurately represent and predict conditions in the root zone, but large scale and widespread irrigated agricultural practises require a means whereby such conditions can be monitored. Long term sustainable use of irrigation techniques in marginal areas requires careful control over root zone conditions, and the lack of such control is reflected in salinisation of previously arable land in many irrigation systems (eg. Fish River Scheme, South Africa; Murray-Darling Scheme, Australia; Aswan High Dam, Egypt).

The scale of application will limit the models that can be usefully applied (Moolman and de Clercq, 1990). Irrigation and other large scale water uses must be modelled at a large scale, which requires low resolution, averaging models rather than the high resolution models more applicable to the small scale. The accuracy of prediction in general declines with simplification in model approach and data inputs, therefore the large scale models lose accuracy over smaller scale approaches.

Spatial Variability

The physics on which most model equations are based are small scale and derived from homogeneous systems under laboratory conditions. It is assumed that the same small scale equations can be applied at the field scale using the same parameter (Beven, 1986). The spatial variability of the hydraulic characteristics of soils has been shown to be structured by experimental studies, where measured values are correlated in space. However, increasing the scale of averaging reduces the derived variance of parameter values. This is because the averaging process is linear, while reality is non-linear; averaging presupposes the model equations are applicable to the field scale while they are derived on a smaller scale; and the random function is assumed stationary, while in reality varies both spatially and temporally (Beven, 1989).

Spatial variability has been accounted for through the incorporation of stochastic parameters into models, which describe variables that are intrinsically random. The parameters chosen are those which represent a probability density function of a range of measured samples of the variable. The stochastic parameter, therefore, must be calibrated for the area on which the model is to be applied, as universal "constants" are highly generalised, and so unlikely to provide acceptable output.

Data Requirements

Data limitations restrict the application of physically based models to a far greater extent than theoretical considerations (Beven, et. al., 1980). Physically based distributed models are expensive in terms of both computing and data requirements. High resolution models may provide a better approximation of reality than the simpler models, but the time and expense required to measure and quantify all model inputs may render the model prohibitively expensive for routine use in management. Very simple models can provide a useful, if not more accurate representation of the system and the benefits from additional complexity may not be warranted by the corresponding increase in cost. Often decisions can be made efficiently without the use of mathematical models, and the time and money needed to do the modelling could be better spent addressing real life problems. Field data with proper interpretation may be more acceptable.

Field Validation of Models

Models of the physical environment have been largely untested (Tillotson et. al., 1988). Simulation models can only simulate a solution, the results of which are predetermined by the input (Hillel, 1985). When a model has faulty premises or data, there is a danger that it will gain a false aura of respectability simply because it was processed on a computer. There is a need therefore to substantiate or refute the results predicted by models, this can only be done through controlled and detailed experimentation of the system which the model aims the simulate. As information on the actual field conditions is generated "it is becoming increasingly clear that, at present, only approximate prediction of water movement and chemical distributions can be made" (Wagenet, 1988). Furthermore, a prerequisite for the validation of a model is that the necessary model parameters be estimated independently. The intrinsic interdependence of many hydraulic parameters, and the problems in measurement makes this ideal difficult to fulfil.

Despite these limitations, models enable complex phenomena to be simulated. Most soil water flow problems cannot be solved or evaluated by any other means, so a computer model which can be operated rapidly using easily obtainable data is an invaluable tool for soil scientists (Hutson, 1983).

2.9.7. Hydrosalinity Models Selected for Evaluation

Three hydrosalinity models were selected for evaluation in the Lower Coerney River Irrigation area. The criteria for selection were their variable levels of theoretical rigour and hence data requirements. These variations lead to differing levels of ease of applicability for managerial purposes as well as the potential absolute accuracy of results generated.

The three models applied in this study can be placed on a continuum of varying complexity and output calibre from the simplest (LR model), through more complex (SODICS model) to the most theoretically intensive (PEAK model). It has been found that the spatial and temporal accuracy of predictions increases with increasing model complexity (Thorburn, 1988), along with the data requirements. A higher level of data is required for more complex models. For the user, detailed data are not always readily available to meet input requirements, so as the model increases in complexity so does the potential limitation to its practical application (Thorburn, 1988).

Detailed predictions of solute movement may not be required in irrigation management, and so the output generated by the PEAK model may be unnecessarily detailed and not cost effective as far as the input information is concerned. Even with the use of field orientated models of low complexity there is a trade off between detail of prediction and data requirements. This situation will have to be resolved by the individual user, who must achieve a compromise between the detail of prediction and practical constraints on data availability.

CHAPTER THREE

3. RESEARCH DESIGN AND METHODS

3.1. CONCEPTUAL FRAMEWORK

Three simple hydrosalinity models for use in irrigation scheduling were selected for evaluation in the Lower Coerney river irrigation area. The models have different levels of theoretical complexity, data input requirements and detail of output predictions. All have been successfully applied in other parts of the world, but not as yet in southern Africa.

Sensitivity analyses were carried out on the models to identify the relative importance of input parameters in controlling model predictions. The results of the sensitivity analyses provided the basis for collection of data from selected sites in the study area. Those model parameters which showed little or no effect on model output were less rigorously measured than those factors to which the model responded more sensitively.

Once the input requirements had been gathered, the models were run and output predictions compared against independently measured field data. The two data sets consisting of predicted and actual information were then statistically compared. The results of this comparison, together with the level of detail of model requirements allowed an assessment of the utility of each model to be made.

3.2. DATA REQUIREMENTS OF SELECTED MODELS

As mentioned, the data input for each model was measured separately from the field measurements used for statistical comparison with model outputs. This means the model outputs can be compared with a data set that is independent of the model inputs. Any artificial relationship between the model output and comparative data is avoided in this way.

3.2.1. Leaching Requirement (LR) Model

Data for the LR model is very simple and consists of irrigation amounts and quality, and the soil solution concentration at a certain depth within the profile. Irrigation water concentration was monitored on a weekly basis throughout the study period. Soil solution concentration was measured on a weekly basis, from the soil extract taken at a suction of -80kPa. From this information, the leaching fraction could be calculated. Infiltration over the study period was assumed to be equivalent to applied irrigation and rainfall, as no runoff was observed. Using infiltration and irrigation water concentration, the leaching flux could then be calculated by the LR model, using the concentrations of all major ions (Cl^-, Na^+, Ca^{2+}, Mg^{2+}, K^+) individually, as these concentrations were available for both the irrigation water and the soil solution.

3.2.2. SODICS

Computer listings of SODICS are included in Appendix A. Data is required for two points in time for the SODICS model to operate, and the conditions at these times must be sufficiently different to allow calculation of the model equations. The SODICS model is designed to predict soil solute profiles and mean leaching flux annually, although it has been successfully applied at shorter intervals. For this reason, two types of time intervals are used in this study. Data were collected at weekly time intervals, and then averaged into monthly and 3-monthly (quarterly) intervals. Data at longer intervals were also collected; namely at the time of Orchard development, 1981 and 1991.

SODICS uses the concentrations of the Chloride anion to trace soil moisture movement as Cl^- is assumed to undergo little adsorption or interaction with other solutes. The irrigation application rate (I) and the Chloride concentration of the irrigation water (Ci) were obtained from irrigation management data and weekly canal sampling respectively. The mass of solute applied through rainfall is disregarded as it is negligible compared to the salts applied in the irrigation water. As the original SODICS Model did not consider the effects of evapotranspiration, a crop factor was applied to the I term.

The rooting depth was found by field inspection, and the depth of model simulation (z) was set at a greater depth to include the entire root zone. SODICS can only be applied above the water table, which is seven metres below surface in the study orchard. Bulk density was found to have no impact on model output during the sensitivity analysis. However, the soil hydraulic properties were taken into account through the field capacity (θ_{fc}) parameter, which did have a significant effect on model predictions. θ_{fc} was taken as the field capacity moisture content of the soil at each depth, derived from the soil moisture content found 48 hours after soil saturation and subsequent free drainage following a prolonged storm event which occurred between 15-17 November, 1989.

3.2.3. The PEAK Model

This model predicts the movement of a solute peak through the soil, and as with SODICS this movement is traced using Chloride concentrations. PEAK is divided into two modules, the first part (PEAKM) simulates soil moisture and soil moisture movement, from which the position of the solute peak within the soil is calculated. The output from PEAKM is read by the second module (PEAKD), together with other data, which then simulates the dispersion of solute about the peak.

PEAKM

Input requirements for this module comprise the depth of irrigation and rainfall (I), and the depth of actual evapotranspiration which is determined from the pan evaporation modified by a crop factor (Et). The proportion of evapotranspiration occurring before infiltration (j) was found to have no effect on model output during the sensitivity analysis. Field capacity (θ_{fc}) used in the SODICS model was also applied to PEAKM.

PEAKD

Values of soil Chloride concentration were simulated at 300mm depths, to coincide with the weekly soil solute measurements. The solute diffusion coefficient (D0) was taken from similar studies reported in the literature (Rose, et. al., 1982; Barry, et. al., 1985; Thorburn, 1988), as it was found to be relatively unimportant in determining model output during the sensitivity analysis. The dispersion coefficient (D) was taken as 20mm after comparison with field data showed the lower dispersivities to give a better indication of soil solute profiles. The determination of D is a calibration exercise, as the measurement of field dispersivity was beyond the scope of this study.

3.3. DATA COLLECTION

A micro-plot situated within an orchard on Daisy Dell Farm in the Lower Coerney River irrigation area was sampled intensively over 24 months (1/7/89 to 30/6/91). Fourteen other orchards were also sampled at conditions representing two separate points in the irrigation history of the orchards. Each orchard was paired with an adjacent unirrigated area, which was considered to be representative of the conditions prevailing before orchard development.

Hydrological Data

Irrigation scheduling data was obtained from the farmers and the Lower Sundays River Irrigation Board for the period of study. Rainfall data was supplied by the Institute for Water Research, Rhodes University, using information recorded by a network of data logging tipping-bucket raingauges in the area, including one on Daisy Dell Farm. Weekly A-pan evaporation data was collected at this station, and daily evaporation data was obtained from the Department of Agriculture's Research Station at Addo, 4km from the farm.

Soil moisture was ascertained from daily tensiometer readings, and at weekly intervals using neutron a probe at depths of 15, 30, 60, 90 and 120cm. Soil moisture measured from the gravimetric samples was used to establish a rating curve between the tensiometer and neutron probe readings. Soil physical parameters including bulk density, porosity and texture were determined for a number of volumetric samples, and hydraulic conductivity was determined by in situ measurement, using the method of Talsma and Hallam (1974).

Soil Chemistry

Weekly soil solution extracts were taken at 15, 30, 60, 90 and 120 cm depths using in situ soil moisture extraction tubes under -80kPa vacuum. These samples were then analysed in the Water Quality Laboratory, Rhodes University for the following parameters:

- electrical conductivity (EC in mS/m)
- chlorides (in mg/L) using silver nitrate precipitation technique
- cations (Ca, Mg, Na, K in mg/L) using AA-1275 series (Varian, 1979) spectroscopy
- total dissolved solids where sufficient sample was obtained

Detailed chemical analyses of gravimetric samples were conducted at the beginning and end of the study period. The cation exchange capacity of one profile was determined by the Department of Soil and Agricultural Water Science, University of Stellenbosch. The solute content of the irrigation water was monitored through sampling of the irrigation canal on a weekly basis.

Crop Data

The study was conducted on mature citrus orchards, which provide a slowly growing canopy cover when fully developed. For the purpose of this investigation the canopy size and rooting network of the orchard is considered constant. The rooting depth required for SODICS and PEAK was measured by inspection. While the crop grown provides continuous cover, times of harvest, flowering and fruit set were noted.

3.4. DATA ANALYSIS

Hydraulic Properties

Porosity was determined from bulked gravimetric samples. Porosity measurements were used to determine the saturated moisture content (Θs) of each sample taken gravimetrically. Actual moisture content (Θ) was then divided by this saturation content and transformed to give

$\log(\theta/\theta s)$. The matric potentials (ϕ) measured by the tensiometers for the same gravimetric samples were also logged, and plotted against $\log(\theta/\theta s)$ to derive the soil water retention curve. The a and b parameters required for Campbell's equation were determined from this curve.

The daily and weekly neutron probe readings were converted to soil moisture values using a conversion factor derived by regressing the neutron probe readings at each depth against a corresponding volumetric moisture measurement.

The field capacity for each soil depth was assumed to be equivalent to the soil moisture at -5kPa (Hutson, 1983). This was confirmed using field data from a storm event which saturated the orchard to the 60cm depth during 15-17 November, 1989. The tensiometer readings at this time were -3 and -5kPa respectively for the 30 and 60 cm depths, thus the field capacity occurred at these potentials.

Solute Concentrations

The weekly solute data set was extended using an interpolation technique for those depths where the soil was too dry for sample extraction. The total number of samples taken was 330, of which 65 were dry. The daily tensiometer data was then edited to correspond with the weekly soil solute data, for the analyses of solute fluxes.

CHAPTER FOUR

4. DATA DESCRIPTION AND ANALYSES

Data required for all model inputs and comparison with model outputs were collected at weekly intervals over a period of 24 months from the micro-plot within an orchard on Daisy Dell Farm. The weekly data were then averaged into monthly and quarterly intervals. The SODICS model was also run using data gathered at longer intervals from a number of sites within the Lower Coerney river irrigation area.

4.1. HYDROLOGICAL AND METEOROLOGICAL DATA

Irrigation Water Quality

Irrigation water is supplied through a network of lined canals from the storage dam, Khorhaans Drift Dam. The water originates in the Orange River, from where it is conducted through a system of tunnels and the channel of the Little Fish River. After storage in the dam, water is allocated to each farmer according to the water rights issued by the Lower Sundays River Irrigation Board. This water is supplied on a quota system, and most farms have a small dam for temporary storage of this water.

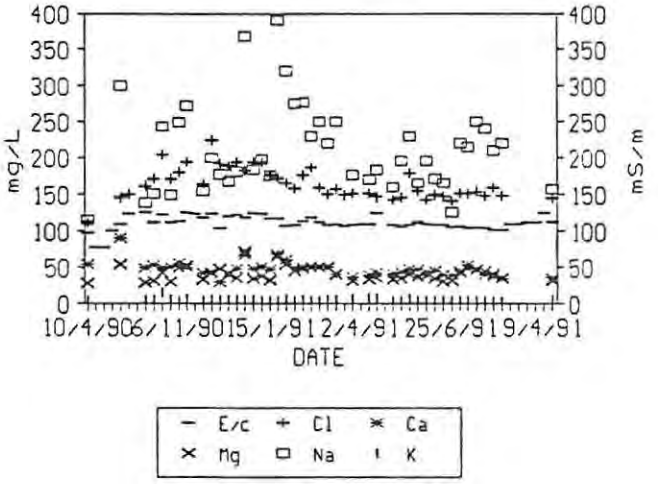


Figure 4.1. Irrigation water quality for the period 10/4/90 to 10/4/91

At all stages along the route from the Orange river to the individual orchard, the process of evaporative losses are active, which result in progressive concentration of the solute load in this water. Irrigation return flow from the irrigated agriculture along the Little Fish River also increases the salinity of the water before it becomes available for irrigation within the study area.

The water quality illustrated in Figure 4.1 shows a relatively constant electrical conductivity (e/c) throughout the seasons, although the Chloride concentrations increase over the period November to February, which is the irrigation season along the Fish River. Figure 4.1 shows the concentrations of major ions in the irrigation water. The greatest concentration, and highest variability is shown by Sodium. Chloride is the second highest concentration, but is much less variable. The Calcium and Magnesium concentrations are lower than Chloride, and similar in magnitude and variability. Potassium has the lowest concentration of all ions, with low variability.

Irrigation Scheduling, Rainfall and Evaporation

Figure 4.2 shows the variation in irrigation, rainfall and actual evaporation in mm/week within the study orchard. Irrigation data was supplied by the farmer at Daisy Dell. Rainfall was obtained from the automatic rain loggers of the Institute for Water Research, Rhodes University, and daily actual evaporation was supplied by the Department of Agriculture Citrus Research Station at Addo.

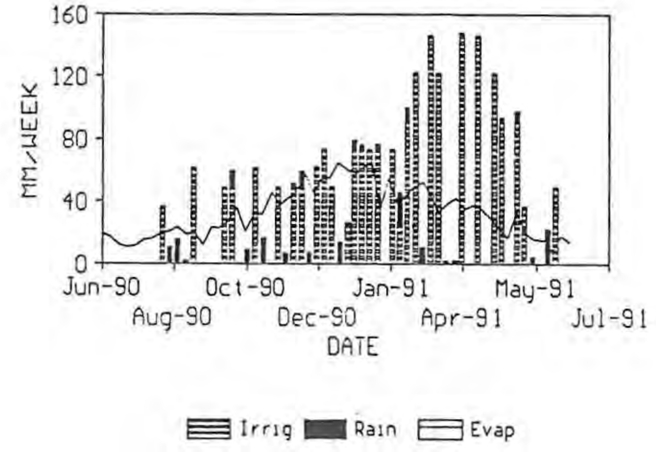


Figure 4.2. Irrigation, Rainfall and Actual Evaporation measured in weekly depths for the study orchard on Daisy Dell farm.

Maximum evaporation rates occur during the summer months from November to February. Irrigation shows highest application rates between January and April. Irrigation and evaporation maxima do not coincide, with highest irrigation applications occurring during the period of fruit growth and ripening. Minimum evaporation rates occur during the winter months from April to August, when there is correspondingly less irrigation.

4.2. DATA FROM SELECTED ORCHARDS FOR USE IN SODICS

Orchards within the Lower Coerney irrigation area that had been previously sampled by Folscher (1982) were sampled at 30, 60, 90 and 120cm depths. These orchards were predominantly flood and basin irrigated until 1980 when microjets were introduced (Folscher, 1982). The older orchards are still irrigated using the former technique, although increasingly farmers are implementing the more capital intensive microjet equipment.

Table 4.1. Crop, Irrigation and Soil Details of Sampled Orchards

Grower	Cultivar	Irrigation method	Soil Type
Bailes	Navels	Basin	Oa1
Beachey Head	Lemons	Basin	Oa3
Blighty	Lemons	Basin	Oa3
Briggs 24	Valencia	Basin	Oa4
Briggs 02	Valencia	Basin	Oa5
Daisy Dell I	Valencia	Microjet	Oa3
Hurter	Lucerne	Basin	Oa4
Lennie	Lemons	Basin	Va1
Sunland 04B	Navels	Microjet	Oa3
Sunland 32	Valencia	Microjet	Oa4
Sunland 22	Lemons	Microjet	Oa3
Sun Orange A26	Navels	Microjet	Oa2
Willowtree 43	Lemons	Basin	Oa1
Willowtree 05	Navels	Basin	Oa1

KEY TO SOIL CLASSIFICATION:

* Oa1: Deep (>1200mm) grey apedal fine sandy loam with pebbles, calcareous.
* Oa2: Deep (>1200mm) non-red apedal to heavy block structured fine sandy loam, calcareous.
* Oa3: Deep (>1200mm) non-red apedal to heavy block structured fine sandy clay loam to sandy clay, calcareous.
* Oa4: Deep (>1200mm) red apedal to heavy block structured fine sandy loam to fine sandy clay loam, calcareous.
* Oa5: Deep (>1200mm) red apedal to heavy block structured fine sandy clay loam to sandy clay, calcareous.
* Va1: <450mm non-red weak to strong blocky structured fine sandy clay loam to sandy clay overlying structured B horizon, calcareous.

The irrigation methods, crops grown and soil types for the study orchards are summarised in Table 4.1. The predominant soil type in the Lower Coerney irrigation area is the Oakleaf Form, with small isolated patches of Valsrivier Form. Characteristics of the Oakleaf soil series found in the orchards under study, are very similar, with variation in colour and texture. Thirteen of the orchards sampled were on this soil type with only one, Lennie Farm, on Valsrivier Form.

Data used in the assessment of SODICS is shown in Table 4.2. Each sampling site within an orchard was paired with a sample taken from adjacent unirrigated land. It was assumed that the unirrigated land represented the soil salinity conditions that would have prevailed in the irrigated orchard prior to development (Thorburn, 1988). All these orchards were previously analysed by Folscher (1982), thus information from three times during the irrigation history of each orchard was obtained: the time of development, the 1981 analyses (Folscher, 1982) and the 1991 analyses (this study). The model was run using the unirrigated soil status as the initial time (T0), and the 1991 conditions for the final time (T1). The 1981 data was then statistically compared with the model predictions for that year.

Table 4.2. Summary of relevant data presented by Folscher (1982) and measured in 1991.

Owner + Orchard	Depth (cm)	Root Depth (cm)	Year Developed	Bulk Density g/cm^3	CEC meq/100g	Cl 1981 mg/L	Cl 1991 mg/L
Bailes 13	0-30	90	1974	1.4	8.6	25	
	30-90			1.5	8.3	5	
	90-120			1.68	6.8	5	
Fenix G	0-30	100	1972	1.85	9.2	40	470
	30-60			1.43	10.4	120	430
	60-120			1.50	9.5	280	350
Briggs 02	0-30	45	1973	1.64	12.1	60	790
	30-60				11.5	70	950
	60-100			1.60	20.6	60	1060
Briggs 24	0-30	80	1974	1.51	9.2	30	510
	30-90			1.66	8.9	360	500
HannahDD	0-30	90	1977	1.30	8.6	5	380
	30-60			1.42	5.4	80	220
	60-100			1.61	10.6	660	260

Table 4.2. (Contd.)

Owner + Orchard	Depth (cm)	Root Depth (cm)	Year Developed	Bulk Density g/cm^3	CEC meq/100g	Cl 1981 mg/L	Cl 1991 mg/L
Hurter A4	0-45	100	1955	1.29	12.0	5	520
	45-120			1.41	12.4	40	770
Sunland 04	0-30	45	1960	1.67	5.4	5	250
	30-90			1.90	8.2	70	690
	90-150			1.42	11.0	540	580
Sunland 22	0-15	60	1957	1.42	6.8	5	490
	15-60			1.40	6.7	5	320
	60-120			1.73	10.2	105	620
Sunland 32	0-30	60	1976	1.41	12.6	35	520
	30-60			1.46	17.1	155	950
Hannah A26	0-30	60	1980	1.55	16.4	25	450
	30-90			1.57	8.5	70	720
	90-150			1.50	9.9	47	450
Willowtree 43	0-30	60	1972	1.70	7.4	46	380
	30-120			1.65	7.4	150	370
Willowtree 05	0-30	100	1960	1.63	5.9	5	260
	30-60			1.43	4.6	5	360
	60-120			1.54	5.2	70	320
Willowtree 45	0-30	100	1974	1.83	12.4	270	550
	30-60			1.73	20.8	910	1020
	60-120			1.43	15.0	1200	1260
Willowtree 38	0-30	60	1956	1.42	11.9	5	510
	30-90			1.43	16.8	200	990
	90-150			1.65	12.0	130	770
Lennie 07	0-30	30	1973	1.33	8.5	5	
	30-60			1.67	12.1	5	
	60-120			1.80	18.8	5	

4.3. MICRO-PLOT FIELD DATA

A micro-plot was set up within orchard M on Daisy Dell Farm, containing four tensiometers, four neutron access tubes and a set of soil extraction tubes all at depths of 15, 30, 60, 90 and 120cm. Mature valencia oranges have been grown in this orchard since 1977. Selected soil physical properties for Daisy Dell orchard M are summarised in Table 4.3.

Table 4.3. Selected soil physical properties measured at DDM03

Depth (cm)	Bulk Density g/cm^3	Porosity (%)	% Sand	% Silt	% Clay	CEC meq/100g	Field Capacity (%)	Organic Carbon (%)
0-15	1.58	39.42						
15-30	1.59	38.53	66	9	25	8.5	35	42
30-60	1.64	42.24	60	13	27	8.0	30	14
60-90	1.49	45.24	65	12	23	7.0	29	8
90-120	1.71	34.49	74	9	17	7.2	20	6

4.3.1. Soil Moisture

Soil moisture was derived from weekly tensiometer readings taken in the orchard DDM03, through a conversion factor obtained from simultaneous gravimetric and tensiometer readings. Figure 4.3 shows soil moisture over the study period at depths of 30, 60, 90 and 120 cm. The 30cm layer is on average more moist than the other layers and exhibits the greatest variability, indicated by the highest standard deviation of 1.49 (Table 4.4). This variability is expected as this layer forms the soil surface, and is thus affected by the boundary effects of evaporation, irrigation and rainfall to a much greater extent than the underlying layers. With increasing depth, the soil moisture decreases, and becomes more uniform through time.

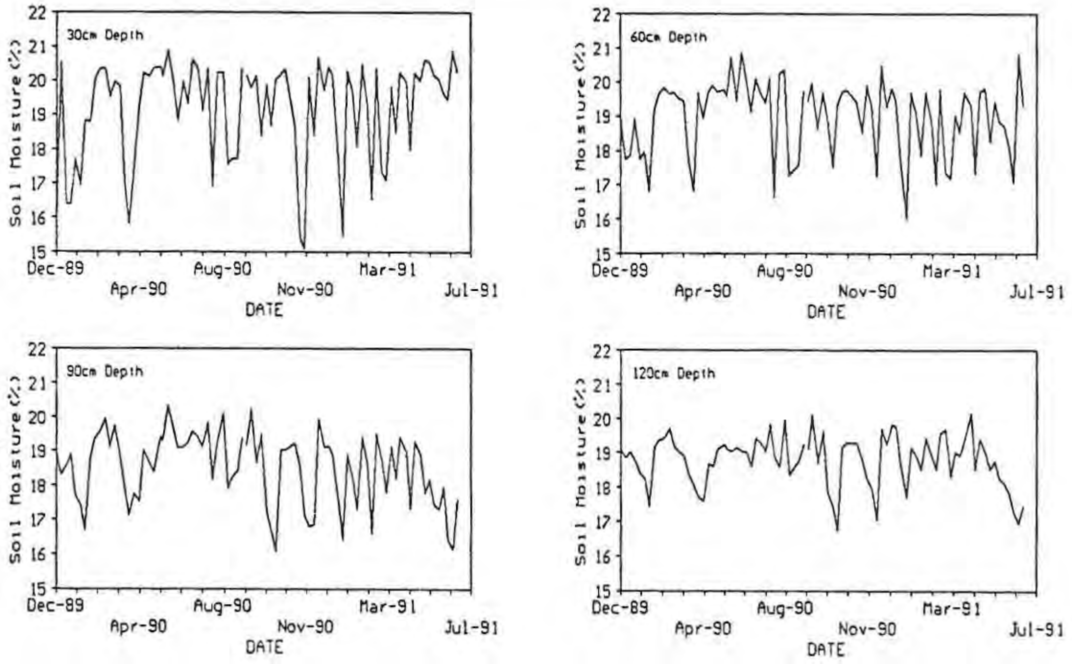


Figure 4.3. Soil Moisture at DDM03

Table 4.4. Summary of soil moisture percentages by volume at DDM03 for the study period

	30 CM	60 CM	90 CM	120 CM
MEAN	19.14	18.94	18.51	18.79
MINIMUM	15.08	16.00	16.07	16.73
MAXIMUM	20.89	20.89	20.36	20.16
STD. DEV.	1.49	1.10	1.05	0.73

4.3.2. Determination of Soil Moisture Flux

Three methods of calculation were used for the calculation of moisture flux. Each technique was based on different physical processes, and produced results which varied accordingly.

Determination of Soil Moisture Flux using Darcy's Law

The first technique of flux determination uses the matric potential of the soil at two points in time in combination with the hydraulic conductivity of the soil to find the movement of moisture. This is Darcy's Law:

$$q = -K.\mathrm{grad}H \qquad (4.1)$$

where q = moisture flux
K = soil hydraulic conductivity
gradH = hydraulic gradient

(Vauchaud and Vauclin, 1990)

All fluxes are extremely low according to this technique, with a maximum of 30mm/week at the 60cm depth. Hydraulic conductivities determined using the method of Talsma and Hallam (1974) ranged from 12.5mm/day at 30cm depth, 9.76mm/day at 60cm depth and 5.0mm/day at 90 and 120cm depths. Figure 4.2 shows inputs of over 150mm/week through the irrigation and rainfall combined, which are not accounted for by Equation 4.1. Moisture flux at the 60 and 90cm depths is much greater and more variable than the 30 and 120cm layers. This finding does not reflect the trends expected from the soil moisture, as the 30cm layer should show the most variability in flux, due to the same factors influencing soil moisture.

Determination of Soil Moisture Flux using the Water Budget Approach

An alternative calculation of soil moisture flux was made using the water budget approach:

$$q = I + R - Et - dS \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4.2)$$

where q = moisture flux (mm/day)

I = depth of irrigation (mm delivered through emitter to wetted area)

Et = depth of evapotranspiration (Pan Evaporation assumed to occur evenly over study orchard x Crop Factor of 0.7)

dS = change in soil moisture storage within wetted area (mm)

Fluxes generated by this method are illustrated in Figure 4.5. The irrigation season is clearly reflected at all depths by the high fluxes, both positive and negative, from January to April. Fluxes at all depths are similar in both magnitude and variability (Figure 4.5).

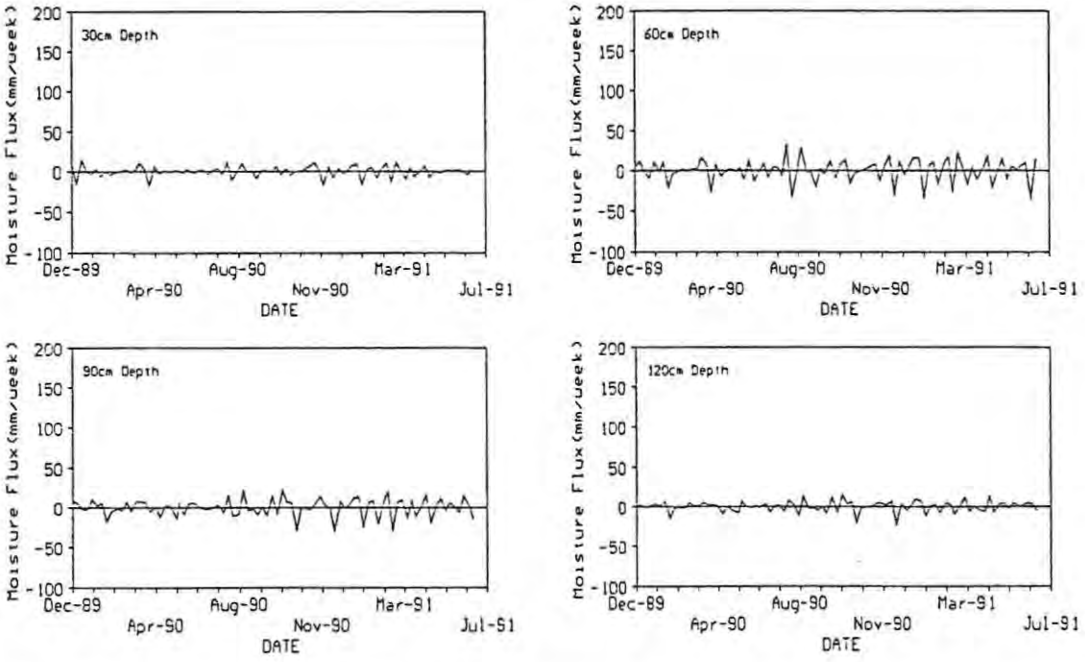


Figure 4.4. Soil Moisture Fluxes determined using differences in matric potentials

These findings are unrealistic because moisture movement through the soil profile will decrease with depth, as root uptake reduces the absolute amount of water available to move and the hydraulic conductivity of the soil decreases through compaction and increased bulk density. The positive fluxes shown in Figure 4.5 are mirrored by negative fluxes of similar proportions. This means there is upward movement of water through the soil at rates of up to 100 mm/week, immediately preceded and followed by net downward movements at even greater rates of 100 to 150 mm/week. Under natural conditions it is extremely unlikely that such rapid reversals of flow occur, especially of such magnitude. Furthermore the water table is more than 7m below the soil surface, which is too deep to provide a source of moisture for upward capillary movement.

Determination of Soil Moisture Flux using a Chloride Mass Balance

A volumetric mass balance approach was applied to an area of 10cm^2 in which the soil moisture occupying each 30cm depth was translated into a volume of water that would occupy a representative cube of soil occupying 3000cm^3. The solute load for each ion in this

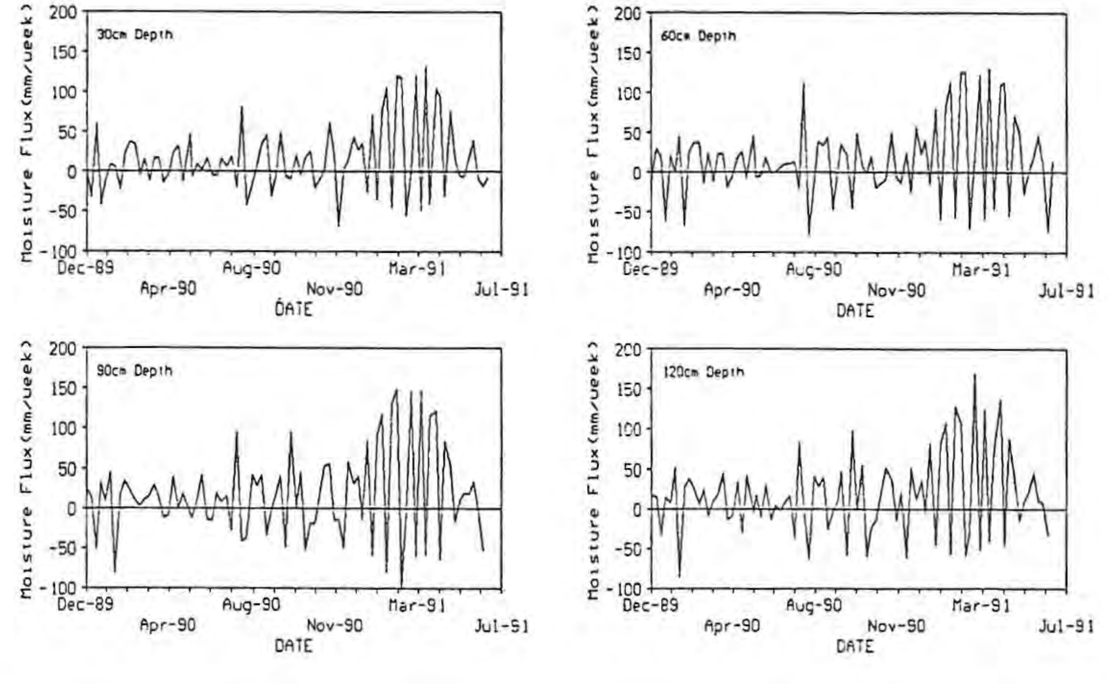


Figure 4.5. Water Budget measurement of flux through the Root Zone at DDM03

moisture was calculated from the soil solution concentrations measured at weekly intervals. The net solute loss from each 30cm layer was then determined for each ion, and compared with the incoming irrigation salt load (Table 4.5). The close approximation between the load of each ion within each layer and the net incoming load of that ion in the irrigation water suggests that this technique is accounting for most of the moisture movement within the profile.

The difference between the irrigation input load and the load determined using the mass balance was calculated from:

$$\text{Difference} = \frac{\underline{(\text{irrigation input - load in the layer most different to the irrigation input})}}{(\text{Irrigation input})} * 100$$

eg. the difference calculated using Cl^-:

$$\text{Difference} = \frac{\underline{(4680 - 4285) * 100}}{4680}$$

$$= 8.42\%$$

The similarity between the solute load input through irrigation and the solute loads lost from each 30cm soil layer is shown by the differences in Table 4.5. Potassium has the greatest difference between incoming irrigation load and outgoing load in the soil solution. This may be due to plant uptake, as K^+ is a constituent of fertiliser and hence a plant requirement. Cation exchange processes will also affect K^+, leading to its preferential adsorption over hydrogen ions. It is likely however, that the extremely low concentrations of this ion result in a proportionately greater error margin in field collection and laboratory analysis. Calcium shows the second greatest disparity between incoming load and calculated outgoing load. This may also be due to cation exchange processes, especially as Ca^{2+} is added to the soil as an ameliorant for dispersed soils.

Chloride shows an unexpectedly high difference of 8.42%. As a conservative ion, Cl^- is less likely to become involved in adsorption onto soil exchange sites or react with other ions

Table 4.5. Solute loads lost from each $3000cm^3$ soil layer down the profile at the microplot at DDM03, over the study period

ION	30 CM MG/L	60 CM MG/L	90 CM MG/L	120 CM MG/L	IRRIGATION INPUT MG/L	DIFFERENCE (%)
CHLORIDE	4660	4544	4285	4285	4680	8.42
CALCIUM	1572	1503	1453	1414	1622	12.85
MAGNESIUM	1174	1160	1144	1127	1184	4.8
SODIUM	5899	5825	5716	5995	5995	4.64
POTASSIUM	136	111	98	93	149	37.43

present in the soil solution. For this reason, Cl^- is commonly used as a tracer for soil moisture movement in hydrosalinity modelling. The difference indicates approximately 8.42% of the load coming into the soil through the irrigation water is not accounted for by the load calculated by the mass balance technique. This percentage is low relative to the uncertainty in measurement, and variability problems in the unsaturated zone. However, two cations show smaller differences, and thus a closer correlation between irrigation and calculated loads.

Magnesium shows an unexpectedly low value of 4.8%, which means all but 4.8% of the incoming Magnesium also leaves the soil. Divalent cations are susceptible to cation exchange processes and reactions within the soil solution. Mg^{2+} is therefore not considered to move freely through the soil in response to gravitational and capillary forces alone. The low difference indicates that this is occurring, which can be explained if the soil is saturated with Mg^{2+}. Such a situation is unlikely, and a further possible explanation is that errors in measurement were able to counteract each other, and result in a unusually low difference.

Sodium results in the lowest difference between irrigation input and calculated loads, of 4.64%. The high concentrations of this ion in the soil have been cited as causal factors in poor drainage experienced in parts of the Lower Coerney irrigation area (Folscher, 1981). Remedial measures including the application of Calcium in the form of gypsum ($CaSO_4.2H_2O$) to displace the Na^+ ions from the cation exchange sites and encourage flocculation have been routinely applied throughout the entire Sundays River valley. It is feasible therefore that the soil system may be saturated with Na^+ ions, and these can then move as freely through the soil as a non-reactive species.

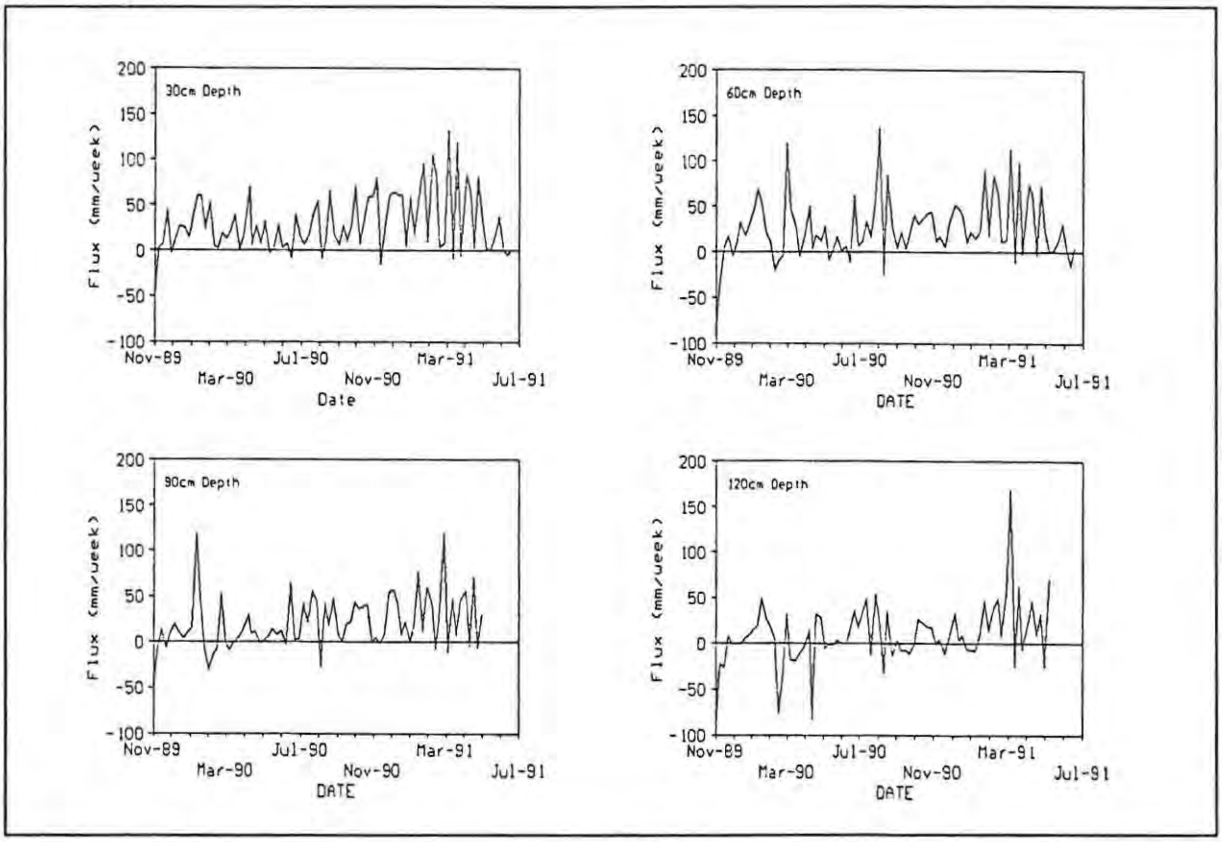


Figure 4.6. Soil Moisture fluxes generated using the Chloride Mass Balance technique

Although lower differences were obtained using Magnesium and Sodium loads, Chloride was considered to be the most likely to portray soil moisture fluxes without interference effects of cation exchange and solute interactions. Soil Chloride concentrations determined each week (mg/L) were divided by the load calculated each week (mg), to give the weekly moisture flux in litres. This amount was then converted to millimeters, to allow comparison with the other methods of flux calculation.

The fluxes illustrated by Figure 4.6 are more realistic than shown in Figures 4.4 or 4.5. The mass balance generated fluxes are of an acceptable order of magnitude, considering the inputs from irrigation and rainfall shown in Figure 4.2, unlike the fluxes generated using differences in matric potentials (Figure 4.4). There are less extreme negative fluxes in Figure 4.6, and a discernible reduction in flux with depth from 30 to 120cm, unlike the flux determined using the water balance technique (Figure 4.5).

4.3.3. Evaluation of methods of Soil Moisture Flux determination

A summary of the soil moisture fluxes generated using each technique is presented in Table 4.6. Any short term erroneous fluctuations are less influential when an average rate for the entire period is considered. The method of flux determination using differences in matric potential (MATRIC) shows upward movement above 60 cm, below which downward movement predominates. As the upper layers provide the moisture which moves into the lower layers, this data seems erroneous.

Both the water balance (WATBAL) and Chloride mass balance (MASSBAL) approaches show more sensible results than the MATRIC method. Overall flux determined using these two techniques decreases with depth, as is expected due to the losses of evapotranspiration, and potential lateral flow within the soil matrix. All fluxes are positive, which is also to be expected under conditions of frequent irrigation (Figure 4.2).

The confidence in the MASSBAL method of flux determination led to a statistical comparison with the fluxes generated by the other techniques. Variation in flux determined using the water balance (MATRIC) only accounts for 54% of the variation in the flux determined using the MASSBAL method, while the WATBAL method accounts for 59% of the variation in flux generated using MASSBAL. This means that the MATRIC method is unable to replicate more than 54% of the variability, as well as the absolute amount of flux generated by the MASSBAL method.

The water balance method (WATBAL) may have more realistic overall fluxes, but the variability in flux determined using WATBAL only replicates 59% of the variability in flux determined using MASSBAL.

The failure of the matric potential technique to account for more than 54% (Table 4.6) of the soil moisture movement determined using the MASSBAL method may be explained in terms of the physical processes operating within the soil and the different theoretical bases underlying each technique. Differences in matric potential do not account for absolute moisture movement, as rapid throughflow of the mobile phase may occur too quickly for the tensiometer to register the correct soil potential.

Table 4.6. Total Moisture Flux in Litres derived using different methods for the study period (1/7/89 to 30/6/91).

	30 CM	60 CM	90 CM	120 CM	R^2 AGAINST MASSBAL METHOD
MATRIC	-7.7	-6.2	12.81	4.55	54%
WATBAL	1.17	1.11	1.07	1.01	59%
MASSBAL	2.47	2.09	1.42	0.70	

where MATRIC = flux generated by matric potential differences
WATBAL = flux generated by the water balance
MASSBAL = flux generated by the mass balance

The moisture held in the soil by capillary forces that results in the tension measured is largely micropore water. Water in macro-pores is governed by gravitational forces, which result in rapid draining of water. As the tensiometer adjusts to ambient soil moisture over a period of several hours, in that time a considerable amount of soil moisture could have moved through the macropores within the soil. The unsaturated conductivity of the soil ranges from 5-12 mm/day movement within the soil matrix is slow enough to be gauged by the tensiometer. On the basis of these results it is suggested that the matric potential technique measures micropore flow.

Lateral flow is not accounted for by any of the three techniques considered. Although the MASSBAL mass balance method considers a small 10cm^2 area, which together with the depth of 30cm constitutes the 3000cm^3 volume, the measurement taken by the tensiometer is considered constant over the area. Lateral variations in soil moisture or concentration are not taken into account. The process of lateral flow is to be expected, although no evidence has been collected to support the occurrence of this phenomenon. Lateral flow would account for the systematic underestimation of load lost by the MASSBAL method against irrigation input with depth for all ions. With depth, soil physical properties such as bulk density, compaction and permeability will change to inhibit vertical movement in favour of lateral flow.

Under a microjet irrigation situation in the orchard, there will be wetted areas immediately under irrigation emmitters and dry areas between the tree rows. The matric potential in the dry soil will be higher than the wet soil, so moisture will be drawn towards the dry areas by the hydraulic gradient set up in this way. Thus the irrigation technique further encourages lateral flow within the soil.

4.4. SOLUTE CONCENTRATIONS

Soil solute concentrations were measured at each depth (Figure 4.7), and are summarised in Table 4.7. Chloride (Figure 4.7a) and Sodium (Figure 4.7c) vary sympathetically over time, and exhibit similar variability at all depths. The concentration of these ions increases with depth to 120cm. This suggests the soil peak of Sodium and Chloride lies below the root zone, and beyond the depth investigated.

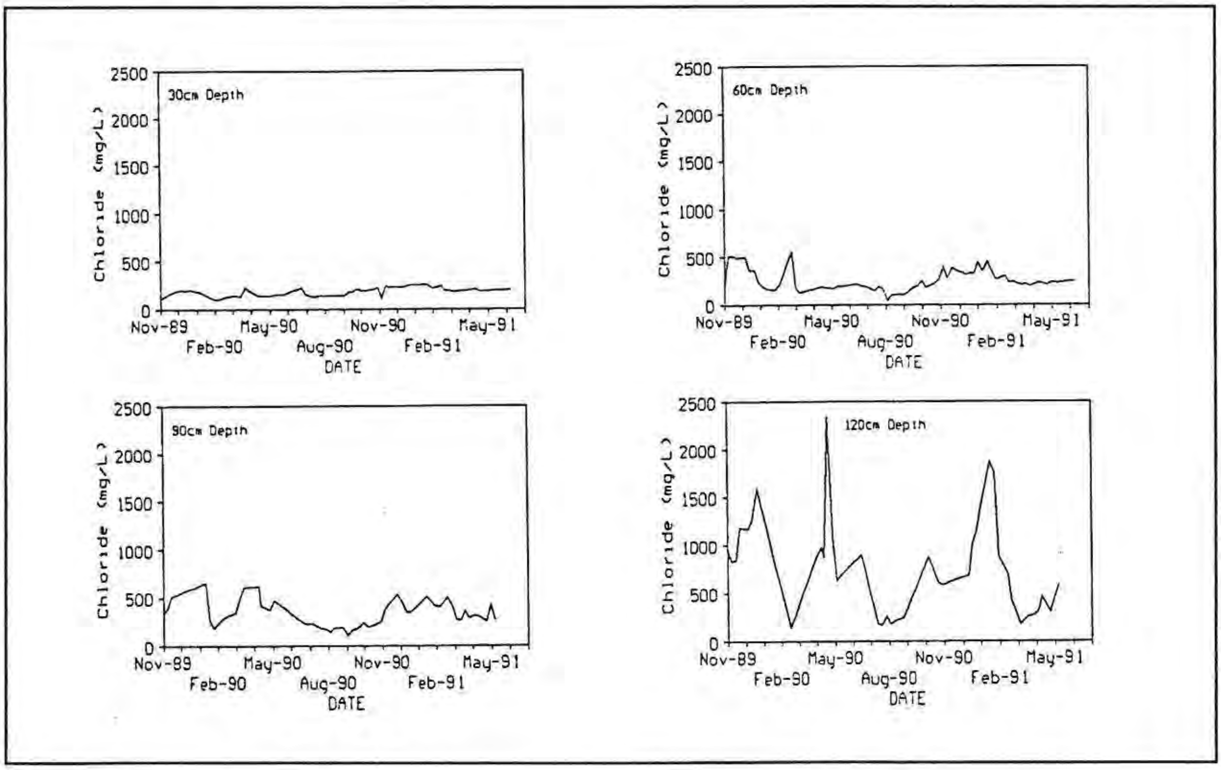


Figure 4.7a.) Weekly Chloride concentrations in the soil solution at DDM03

Chloride is a conservative ion, unreactive and unlikely to take part in exchange processes. The Cl^- ion concentration in the irrigation water shown in Figure 4.1 is approximately constant. Given that the amount of irrigation varies over time, the concentrations of Chloride in the soil are expected to show less variability than the other ions, which are susceptible to cation exchange processes, and also show variability in the irrigation water before entering the soil.

Table 4.7 shows that there is no significant difference in the variability between the depths and ionic concentrations, as the coefficients of variation (CV) are similar for all values. Calcium and Magnesium are closely related in both variability and absolute concentration (Figure 4.7b). The concentration peaks of these cations occur at the 60cm depth, below which there is a gradual decline in concentration. The Potassium cation shows a lower absolute variability than all other ions and also exhibits a concentration peak at 60cm, with a marked decrease in concentration below this level (Figure 4.7c).

The Orchard rooting depth was observed to average 60cm, which may be significant in influencing the concentration profiles shown in Figure 4.7, especially Ca^{2+}, Mg^{2+} and K^+. Selective uptake of soil moisture and nutrients by plant roots serves to concentrate the remaining soil solution, and this may be more significant where concentrations are low, as with Potassium.

Table 4.7. Summary of Soil Solutes measured at DDM03 over the study period

Solute	Maximum	Minimum	Mean	Standard Deviation	Coefficient of Variation (CV)
Chloride					
30cm	259	89	175	42	0.24
60cm	558	35	247	113	0.46
90cm	657	106	367	142	0.39
120cm	2351	139	723	433	0.60
Calcium					
30cm	174	51	104	29	0.28
60cm	380	69	147	66	0.45
90cm	136	42	88	21	0.24
120cm	629	36	152	90	0.59
Magnesium					
30cm	102	38	58	15	0.26
60cm	213	47	89	36	0.40
90cm	100	29	60	16	0.27
120cm	355	28	97	48	0.50
Sodium					
30cm	400	115	185	49	0.27
60cm	640	151	278	107	0.39
90cm	914	262	553	146	0.26
120cm	2160	250	1094	508	0.46
Potassium					
30cm	205	0	35	21	0.60
60cm	113	4	57	21	0.37
90cm	30	6	21	4	0.19
120cm	49	3	14	9	0.64

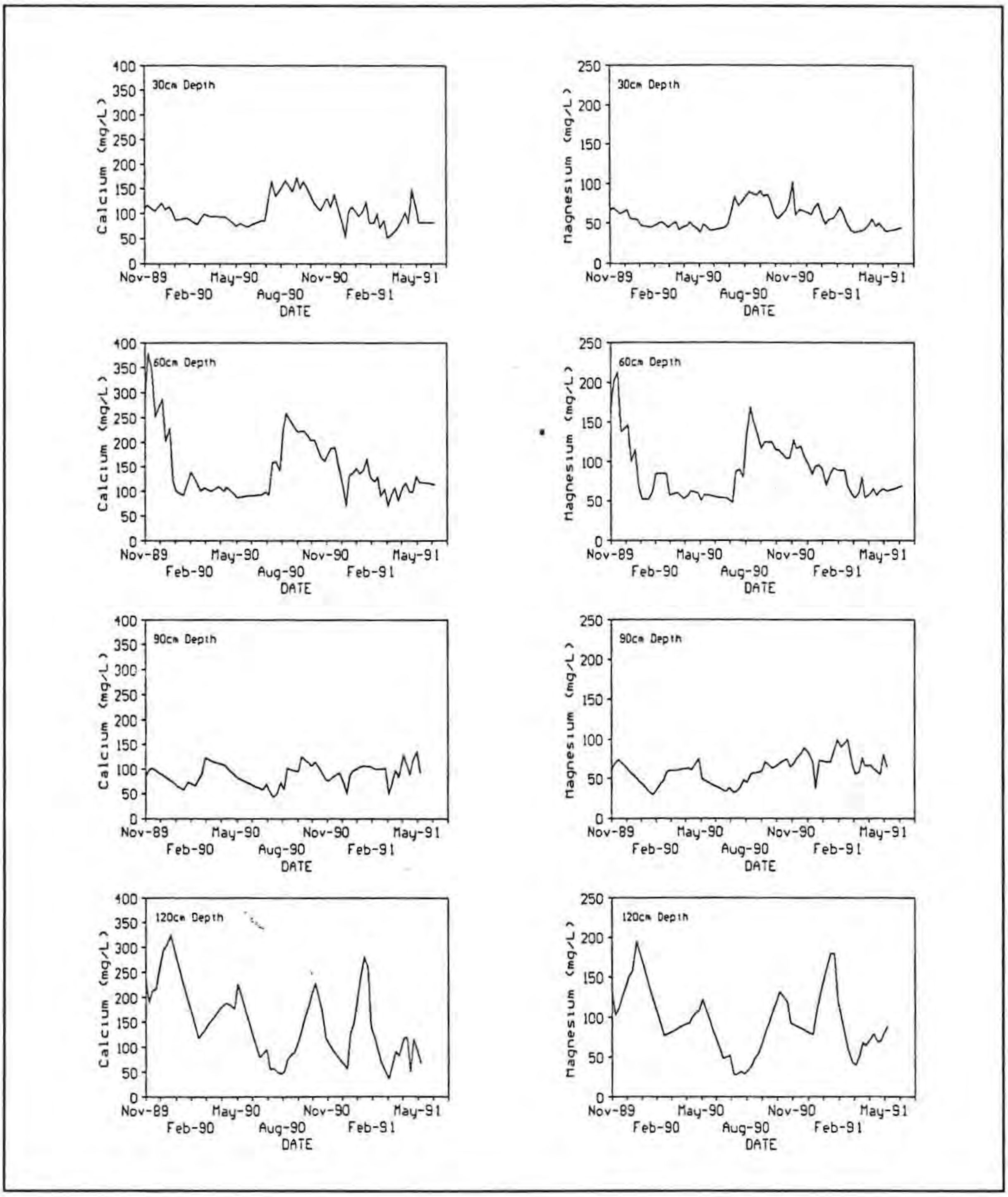


Figure 4.7b.) Weekly Calcium and Magnesium concentrations in the soil solution at DDM03

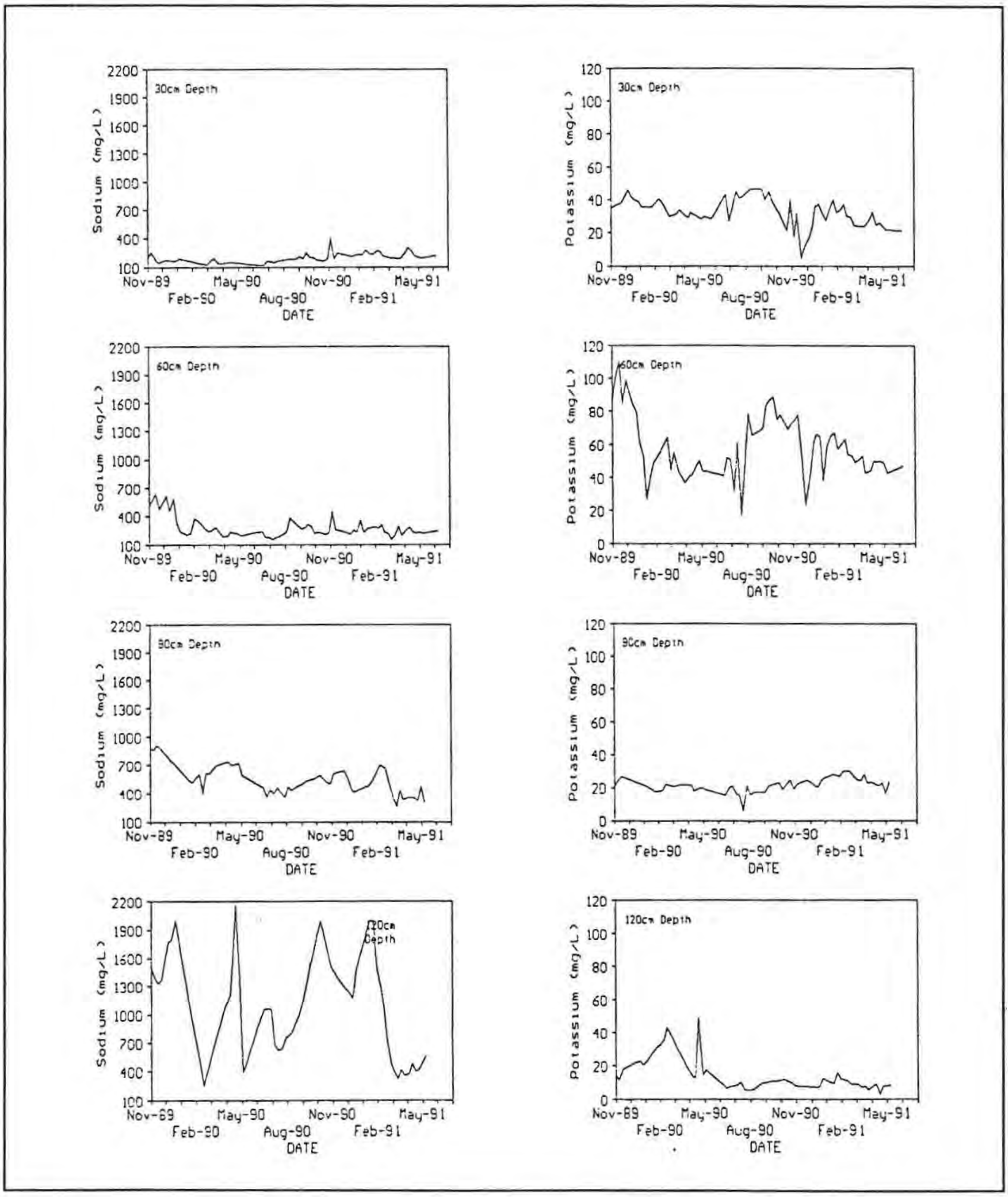


Figure 4.7c.) Weekly Sodium and Potassium concentrations in the soil solution at DDM03

4.5. SOLUTE FLUX

The convective loss of ionic species was determined from:

$$Li = Ci.q.t \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (4.3)$$

where Li = leaching of ionic species i

Ci = concentration of species in the soil solution

q = moisture flux (mm/week according to the mass balance technique)

t = time interval (week)

Solute fluxes of Chloride, Calcium, Magnesium, Sodium and Potassium are illustrated in Figure 4.8. The Cl^- fluxes are consistently greater than those for the analysed cations. This is due to its overall higher absolute concentration (shown in Figure 4.7a.), higher solubility and hence mobility. Cl^- is the least reactive ion considered, and so less likely to be taken up in exchange reactions within the soil. Sodium flux is the next highest, which is also due to its high natural concentration.

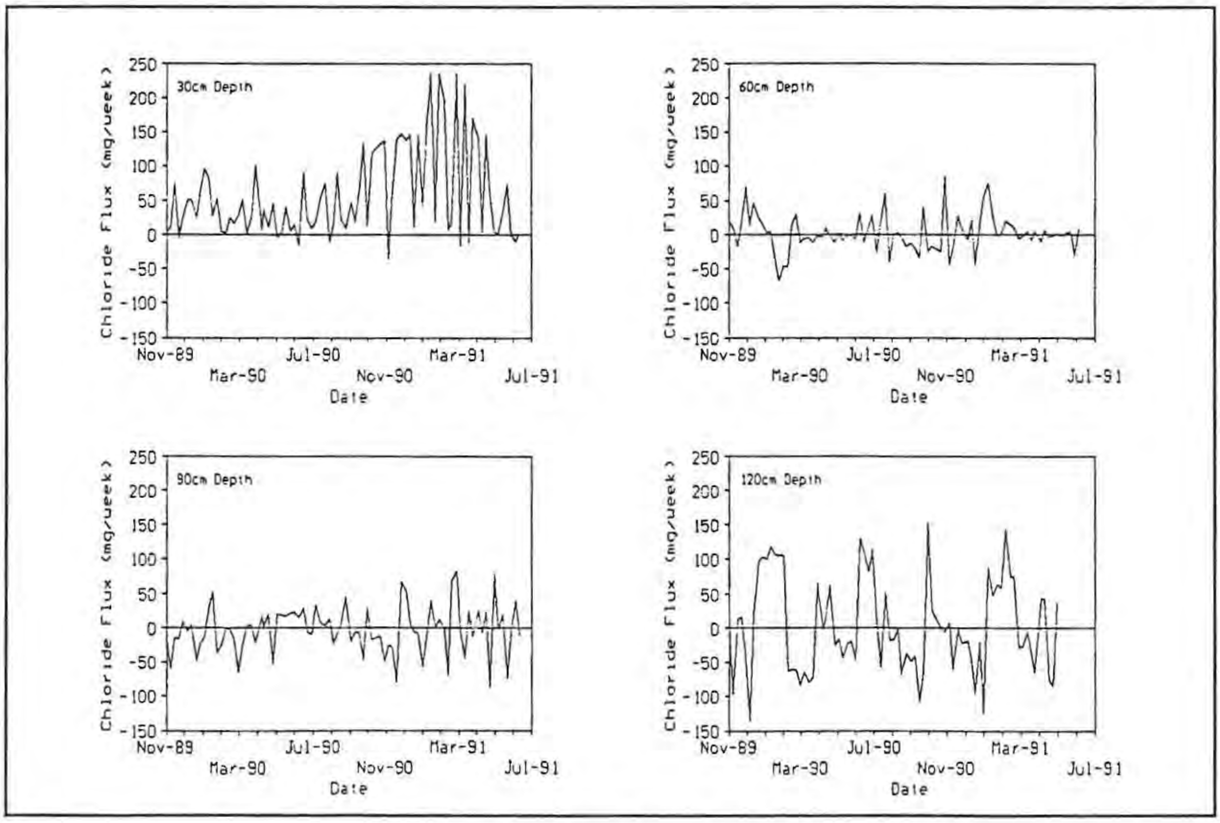


Figure 4.8a.) Chloride Flux at DDM03

The Calcium concentration may be artificially elevated due to the history of gypsum ($CaSO_4.2H_2O$) application in the orchard, although none was added during the study period. Previous applications were at a rate of 4 and 2 tonnes per hectare annually in 1985 and 1986 respectively. This action is intended to saturate the soil with the divalent cation Ca^{2+} in the soil exchange sites previously occupied by monovalent ions. Ca^{2+} increases the flocculation ability of the soil particles, and is applied as a remedy for dispersed saline soil.

The maximum Magnesium flux (Figure 4.8c) is 1.4 mg/week, while the greatest Ca^{2+} flux is 3.9 mg/week. Figure 4.7b shows the similarity in variation between these divalent cations, although the concentrations of Calcium are higher than those of Magnesium. This accounts for the lower fluxes measured for Mg^{2+}. Potassium flux is low, except for 4 peaks, which do not correspond with any concentration peaks in Figure 4.7c, and are regarded as anomalous.

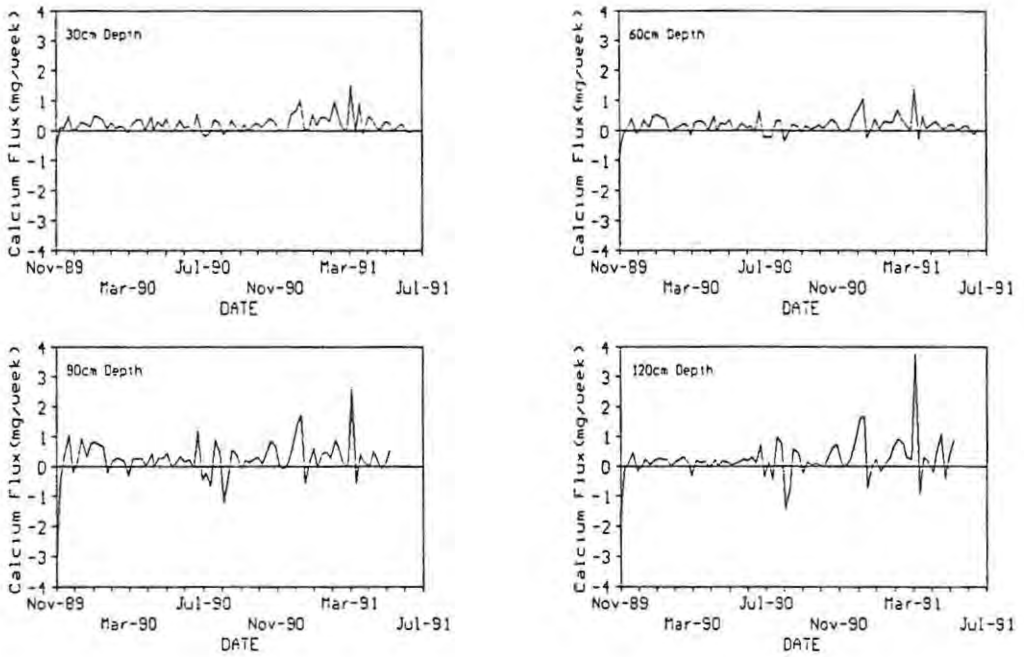


Figure 4.8b.) Calcium Flux at DDM03

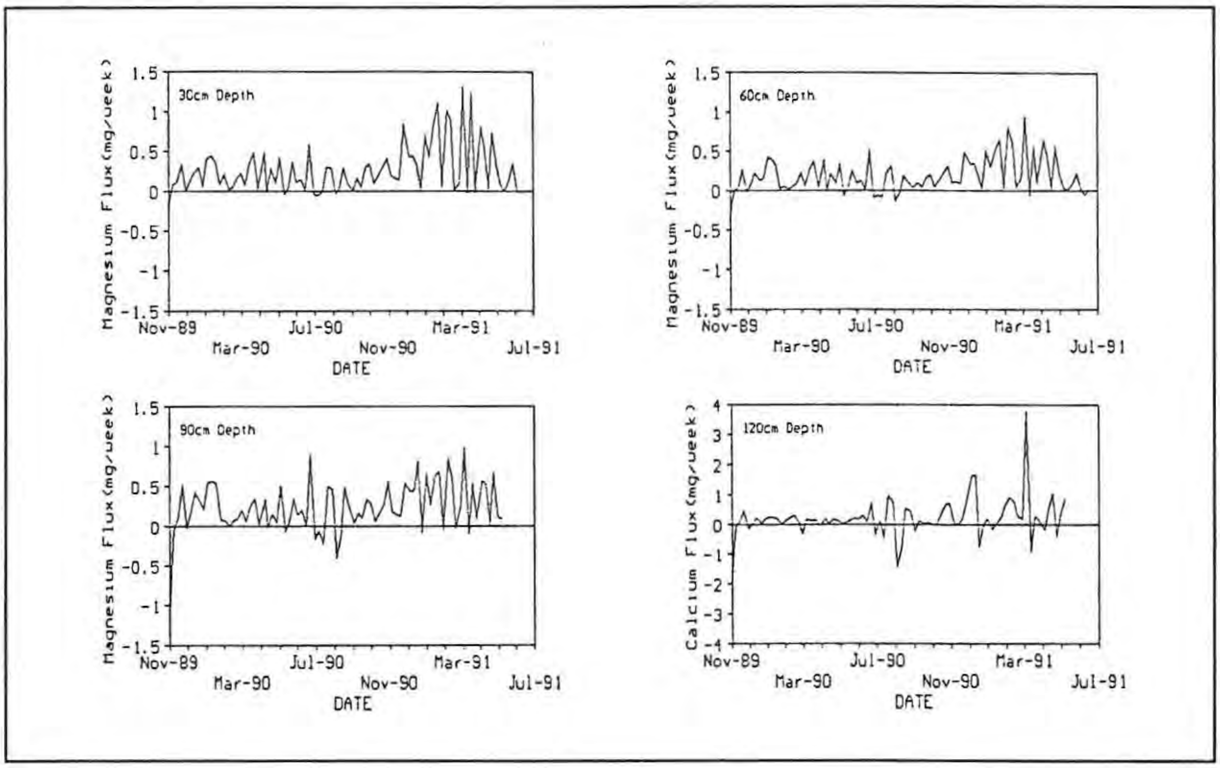


Figure 4.8c.) Magnesium Flux at DDM03

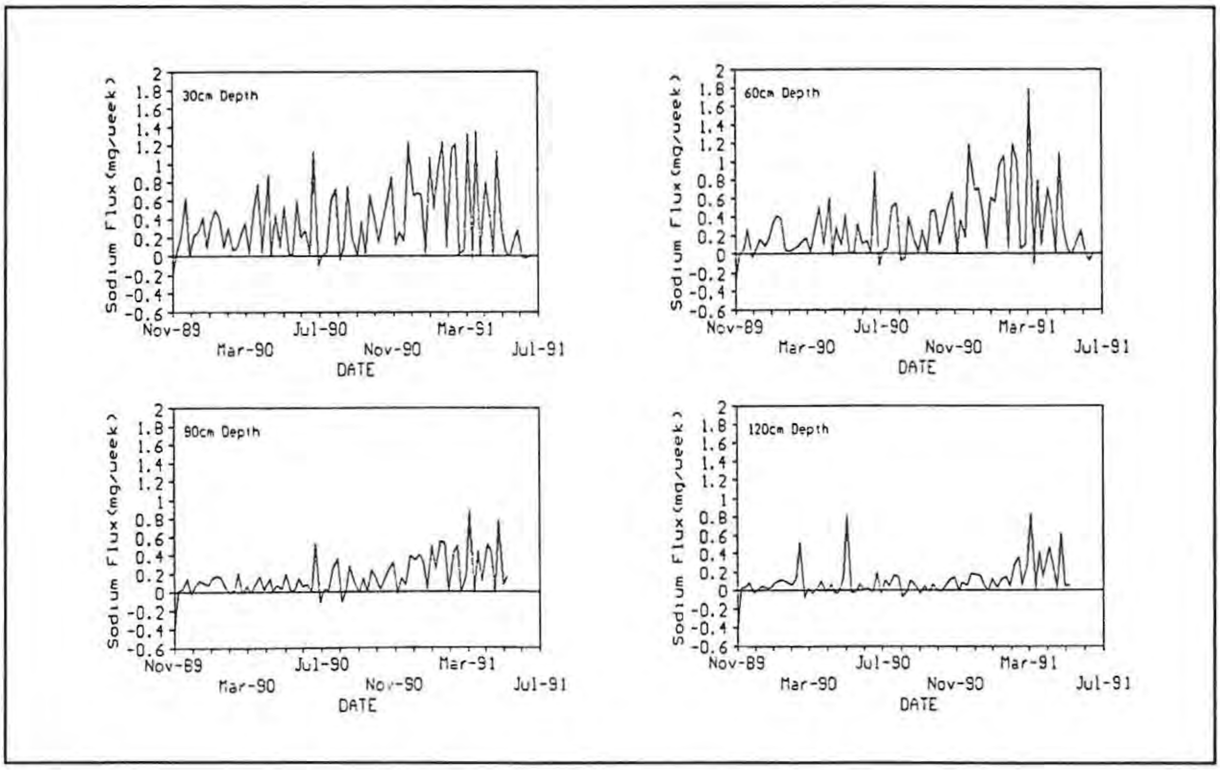


Figure 4.8d.) Sodium Flux at DDM03

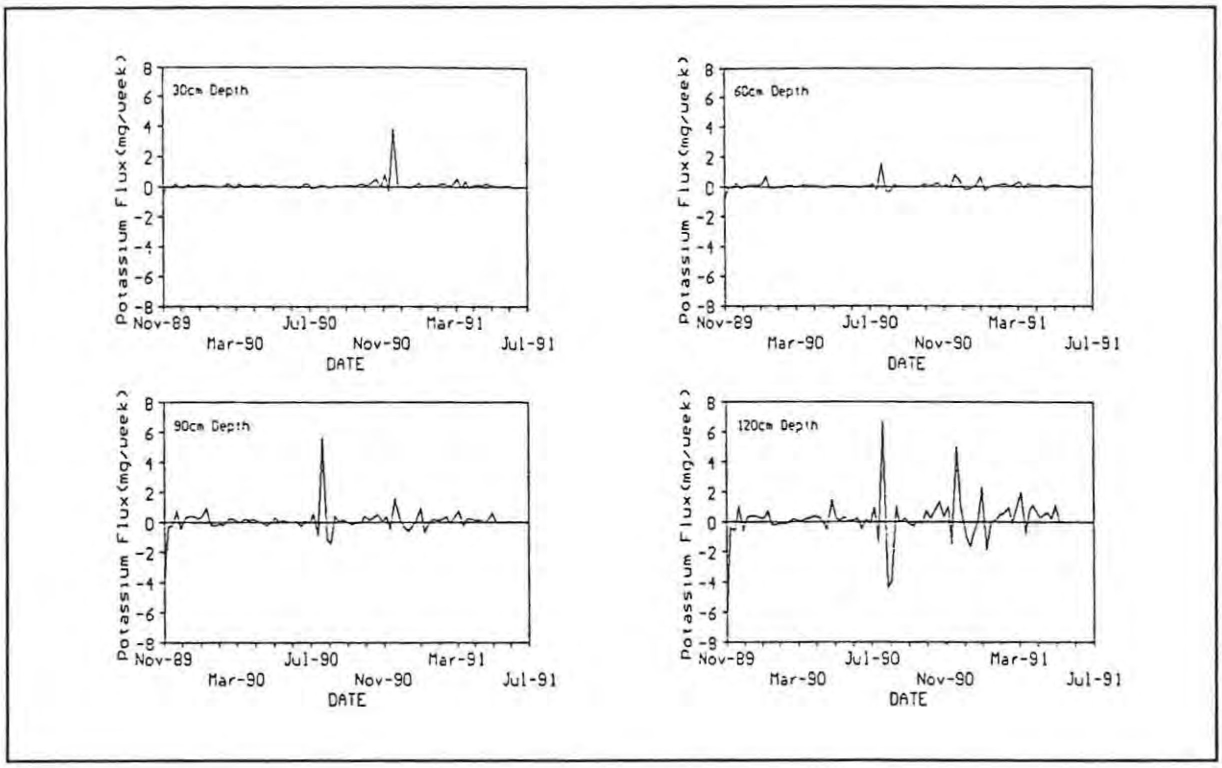


Figure 4.8e.) Potassium Flux at DDM03

CHAPTER 5

5. THE LEACHING REQUIREMENT MODEL DERIVED USING THE LEACHING REQUIREMENT APPROACH

5.1. MODEL DESCRIPTION

The concept of the leaching requirement (LR) was developed by the U.S. Salinity Laboratory (USSL, 1954), and defines LR as the fraction of irrigation water that must drain through the root zone to keep root zone salinity below the limit that can be tolerated by the crop. This salinity limit is crop specific, with selected crop tolerances identified by the USSL (1954) as follows:

low salinity tolerance: <40mS/m (eg. citrus)
moderate salinity tolerance: <80mS/m (eg. beets, alfalfa, cotton)
high salinity tolerance: ≤ 120mS/m (eg. barley)

The Leaching Requirement (LR) model is a simple lumped parameter representation of the mass balance. The amount and quality of applied irrigation water is assumed to determine the amount and quality of soil moisture flux leaving the root zone. The LR model does not account for the effects of soil physical properties, or any chemical interactions that may take place within the soil, thus steady state conditions are assumed.

The solute concentration of soil moisture in the root zone is determined by the balance between incoming solutes (Ci) and outgoing solutes (Cd). The LR model implies that by varying the amount of applied water it is possible to control the concentration of salts in the drainage water, and hence to maintain the concentration of the soil solution in the root zone at some level between the irrigation and drainage water concentrations.

The relationship between volumes and salinities of the irrigation, soil and drainage waters can be expressed by the following:

$$Vd.Cd = Vi.Ci \quad \ldots\ldots\ldots\ldots \quad (5.1)$$

where Vd = volume of drainage water
Vi = volume of irrigation water
Cd = concentration of drainage water
Ci = concentration of irrigation water

Thus the Leaching Fraction (LF) = Vd/Vi = Ci/Cd. When the maximum permissible drainage water concentration (Cd) for a specific crop is specified, the minimum permissible Leaching Fraction is fixed if the irrigation water concentration is also fixed (Ci). This is the leaching requirement (LR).

Using this model, Bernstein and Francois (1971) found that yields of alfalfa were relatively unaffected when the soil solution concentration was allowed to approach the limits of the plant capacities. This showed that much greater efficiency in water use may be possible without significant reductions in yield. These authors conclude that leaching requirements may be reduced to 25% of the level previously thought essential for crops of low to moderate salt tolerance.

The input requirements of the LR model are very simple, consisting of irrigation quantity and quality, and the soil solution concentration at a specified depth. Irrigation managers will generally have information available on the irrigation water quality and quantity applied. The quality of the soil solution at a specified depth is obtainable through a simple sampling procedure. This means the LR model can readily be applied without extensive sampling or expensive laboratory analyses. The equation is linear and can be calculated on a pocket calculator, without the necessity for computer time. Although simple in concept, the LR model can be applied in a number of ways:

- Given the irrigation water concentration and the desired soil solution concentration, the amount of irrigation to be applied can be determined.
- Given the irrigation water concentration and actual soil solution concentration, the leaching flux necessary to reduce salt build up can be calculated.
- If over-irrigation is suspected, the effects of reduction in irrigation water of known

concentration on the concentration of soil solution can be assessed before any change in scheduling is attempted.

The simplicity and small data requirements of the LR model allow its application without the need for highly trained personnel, specialised equipment or detailed analyses. However, the theoretical simplicity of the model may lead to problems for application. The assumption of steady state conditions may not be met, as steady state salinity may be approached very slowly when the leaching fraction is less than 10%, and in most soils steady state conditions rarely exist. The LR model cannot account for such non-steady conditions.

The LR concept cannot account for the distribution of salts within the root zone, and the spatial and temporal variation of root zone salinity. These aspects are dependent on irrigation management, as infrequent irrigation often leads to a buildup of salts between irrigations. With high frequency irrigation it is possible to maintain a zone of soil with a soil water concentration approximately equal to the irrigation water concentration.

Temporal variations in soil solute concentrations occur at a range of scales from localised short term effects between irrigations to long term field-wide changes over several years or decades. It is to quantify and predict such short to long, and localised to wide-spread changes in soil salinity that leaching models are required. As the LR model is applicable only in situations where steady-state is assumed to exist, or reached very rapidly, it cannot be used with confidence in the majority of field situations. Where steady state has not been reached, or where the solute balance is changing with landuse development and other human impacts, the model assumptions limit the application of the LR model.

The effects of soil macropore flow and lateral soil moisture movement cannot be modelled by the LR approach, which does not incorporate any soil physical parameters. The soil parcel is regarded as a black box through which moisture moves in a constant manner. This seldom occurs in reality as most soils are structured and preferential flow can be expected to occur.

5.2. SENSITIVITY ANALYSIS OF THE LEACHING REQUIREMENT MODEL (LR)

This model consists of the following equation:

$$F = L/I = Ci/Sz \quad (5.2)$$

where F = leaching fraction
L = leaching flux (L/week)
I = applied irrigation and rainfall (L/week)
Ci = solute concentration of irrigation water (meq/L)
Sz = solute concentration of soil water at depth z (meq/L)

All factors are directly related and hence equally important in determining the output of the model. It is not appropriate to carry out a sensitivity analysis.

5.3. ASSESSMENT OF THE LR MODEL USING FIELD DATA

The leaching requirement is the fractional volume of applied water that must drain below the root zone to keep the root zone salinity within the tolerance limit of the crop grown (Equation 5.2). In this assessment, the LR model was used to predict the leaching flux at one site for which intensive data was available, and fourteen other sites where less detailed information was obtained. The intensive data allows a rigorous comparison between model output and actual conditions, and the results of this procedure provide the validation of the model. Once accepted as valid, the model is then applied to orchards where less information is available, with the confidence obtained from the initial exercise.

Data were collected over a period of 24 months at weekly intervals from a site within Orchard M on Daisy Dell farm. The model input requirements are very simple consisting of the irrigation water concentrations which were collected from the supply canal, and soil solute concentrations which were extracted through in situ soil moisture extraction tubes. All samples were analysed in the Water Quality laboratory, Rhodes University. Although the LR model is not intended for short term fluctuations in soil salinity (Jury et. al., 1978; Rose et.

al., 1979) it has been successfully used to model soil solutes at the level of 4 to 6 irrigation episodes (Bernstein and Francois, 1973).

A spreadsheet was set up on the QUATTRO PRO statistical package, consisting of the model equations. Concentrations of the major cations Ca^{2+}, Mg^{2+}, Na^+, K^+, and the Cl^- anion in the incoming irrigation water and the outgoing soil solution from each 30cm depth increment were entered to determine the leaching flux at each depth. Thus both the incoming and outgoing water associated with each parcel of soil was known. The LR output was statistically compared with the values of moisture flux derived using differences in matric potential, the water balance and the Chloride mass balance. These methods are described in Chapter 4.

The data was then organised into increasing time increments, from weekly to monthly and quarterly intervals. The R^2 values of the correlation between predicted leaching flux and flux determined using the three techniques are shown in Table 5.1.

5.3.1. Weekly time increments

The weekly interval input data results show very low correlations between the moisture fluxes predicted using the model and flux determined using the difference in matric tension (MATRIC) technique at all depths. The R^2 values range from 0% for Potassium at 120cm to a maximum of 6.5% for Sodium at 90cm, with a mean of 2.5% (Table 5.1).

The water balance method of flux measurement (WATBAL) produces higher correlations at all depths, ranging from 1.1% for Potassium at 30cm to 72.7% for Magnesium at 30cm depth. Potassium is not expected to represent a good tracer of water movement through the soil, especially as it is artificially added to the system in the form of fertiliser. The high correlation shown by the LR flux derived from Magnesium concentrations is unexpected, as a divalent cation is more likely to become involved in cation exchange processes than monovalent ions. However, the low cation exchange capacity (CEC) summarised in Table 4.3 means these processes are unlikely to be important in inhibiting ionic movement.

All the R^2 values for Chloride, Calcium and Sodium are very close to the Magnesium correlation, which means the Mg^{2+} concentration is not significantly more effective than the other major ions in representing moisture flux. This is further illustrated by the overall mean of 51.9%, which shows an improvement of more than an order of magnitude over the mean of the correlation between the MATRIC method and LR output.

Table 5.1. R-Squared values (%) of the correlation between LR generated leaching flux and 3 methods of determining soil moisture flux

	WEEKLY INCREMENTS			MONTHLY INCREMENTS			QUARTERLY INCREMENTS		
	MATRIC	WATBAL	MASSBAL	MATRIC	WATBAL	MASSBAL	MATRIC	WATBAL	MASSBAL
30CM									
Cl	1.4	69.9	78.6	3.4	34.9	60.5	10.9	24.9	65.0
Ca	2.1	66.2	63.4	4.7	46.2	52.4	19.0	43.3	66.2
Mg	1.9	72.7	64.8	10.5	42.6	48.8	23.6	40.3	60.5
Na	2.3	69.8	62.9	11.1	25.5	55.9	12.5	28.1	67.4
K	1.0	1.1	59.5	19.9	20.9	30.4	21.0	48.4	69.3
60CM									
Cl	1.0	53.8	52.1	16.4	42.2	56.6	6.3	66.3	92.9
Ca	1.5	55.4	46.9	11.7	57.4	38.0	28.4	23.5	0.0
Mg	1.6	58.5	48.8	19.2	52.5	40.1	24.5	61.9	46.7
Na	1.4	55.2	48.2	11.5	61.2	45.8	6.5	71.2	67.7
K	0.3	45.9	39.6	6.7	47.0	36.1	3.0	57.0	54.7
90CM									
Cl	6.3	53.8	40.6	0.0	44.4	48.4	0.3	50.7	83.4
Ca	4.8	49.7	39.7	10.1	32.3	66.3	10.0	27.1	44.2
Mg	4.4	51.5	37.2	13.5	22.1	62.4	12.1	20.3	34.8
Na	6.5	59.5	39.1	3.4	67.6	50.1	12.2	60.7	72.1
K	4.8	58.5	34.5	7.8	40.9	66.5	2.7	34.9	60.0
120CM									
Cl	2.3	41.4	33.3	0.1	50.3	42.0	0.2	58.8	29.1
Ca	2.2	40.5	37.6	0.0	58.2	50.7	1.4	65.9	52.7
Ma	2.0	49.9	34.7	0.2	55.5	52.4	2.1	68.5	50.5
Na	2.2	47.4	27.9	0.0	61.5	38.1	19.7	69.9	49.9
K	0.0	36.2	8.2	1.9	21.0	10.7	7.5	24.8	25.9

where
MATRIC = Matric Potential Flux measurement
WATBAL = Water Balance Flux measurement
MASSBAL = Volumetric Mass Balance Flux measurements

The mass balance method of moisture flux determination (MASSBAL) produces the highest correlation against predicted flux at the weekly time interval, of 78.6% for Chloride at 30cm, as both MASSBAL and the LR input use the same Cl^- concentrations. This is not the case for the MATRIC and WATBAL methods. The minimum value is 8.2%, for Potassium at 120cm. The overall mean correlation is 44.9%, which is lower than that found between the LR flux and the WATBAL method.

Of the ionic concentrations used in the model, Chloride concentrations result in fluxes most similar to those determined using the three techniques, with the other ions showing a decrease in accuracy from $Na^+ > Mg^{2+} > Ca^{2+} > K^+$. Chloride flux is shown in Figure 5.1, and the cations are illustrated in Appendix D. For all ions the discrepancy between determined and predicted flux decreases with depth. As the methods of determining moisture flux do not account for lateral and macropore flow, the increasing similarity between predicted and determined flux with depth means the model is varying in the same direction as the moisture fluxes determined using the different methods.

The Chloride anion is affected by anion exclusion, which forces the Cl^- into the centre of pores due to electrostatic repulsion. Chloride therefore moves more rapidly than other ions, and can exceed the movement of the wetting front (Smith, 1973). The results show the relatively faster movement of Cl^- with respect to the other ions, although in this investigation, Chloride under-estimates the moisture movement. This means Cl^- must be lost to the system, either through macropore flow, plant uptake or reaction processes within the soil.

As a conservative ion, Cl^- is regarded as ideal for monitoring soil moisture movement because it is not likely to become involved in chemical processes such as cation exchange within the soil (Ross, 1989). These results indicate that although the Cl^- concentration is the best tracer of soil moisture movement of all ions considered, it is not completely conservative. A limitation of the LR model is that it cannot predict upward moisture flux. Table 5.2 shows the minimum fluxes using all ions to be zero, whereas in reality negative flux occurs at all depths.

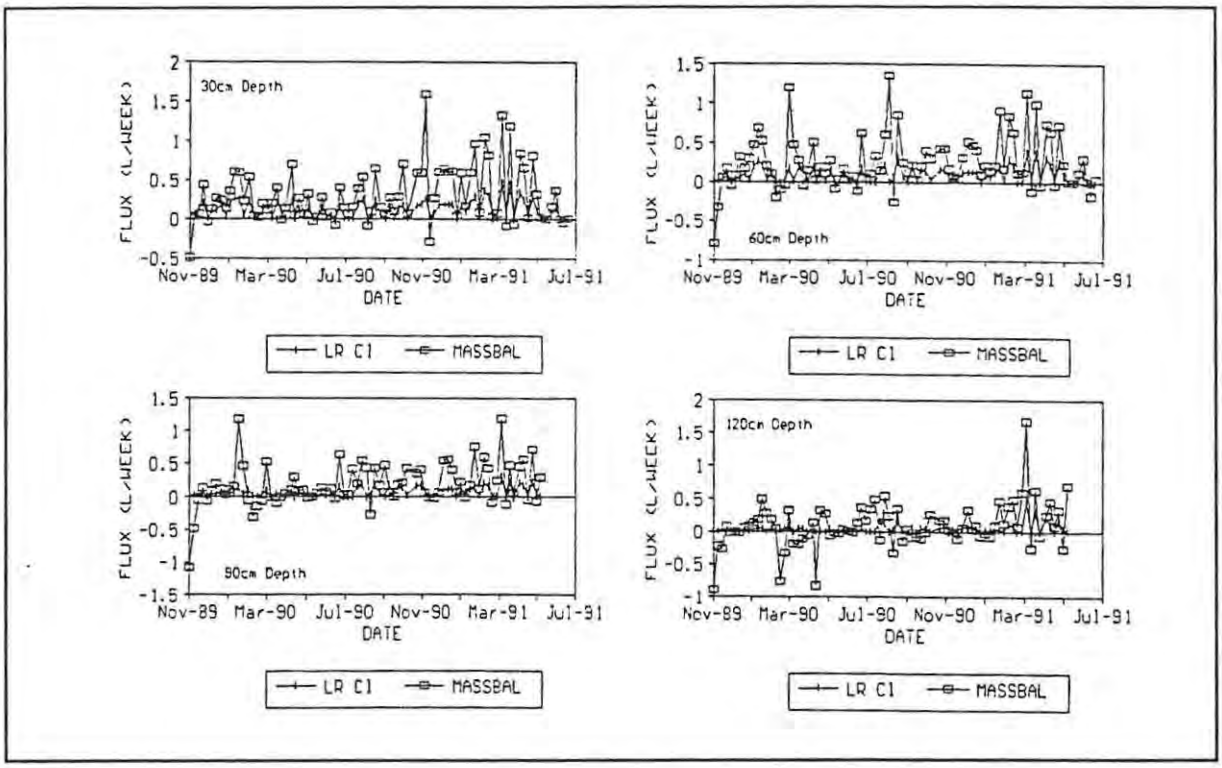


Figure 5.1. Comparison of Leaching Flux determined using the LR model based on Chloride concentrations (LR Cl) and the Chloride mass balance approach (MASSBAL) at weekly intervals.

Upward capillary movement of moisture within the soil is associated with high evaporation and consequent precipitation of salts is more likely to occur under such drying conditions. This means the inability to account for upward flux, especially in the Coerney River area where the climate is semi-arid, is a potentially inhibiting factor to the successful application of the LR model.

It must be noted that the variation in flux determination is greater than all mean predicted fluxes, and all maximum predicted fluxes except Cl^- (Table 5.2). It should also be noted that the variation in soil moisture flux determined by the mass balance is very great at all depths, rising to a maximum of 0.36 litres per week at the 30cm depth within the micro-plot area. This variability is 6% greater than the mean determined flux at this depth (0.30 litres per week), rising to 40%, 83% and an extreme of 278% at 60cm, 90cm and 120cm respectively. This indicates the variability within the methods of flux determination is so great that the average value is not strictly indicative of actual flux.

Table 5.2. Summary of weekly leaching flux (Litres) determined using the LR Model for the micro-plot area

	MAXIMUM	MINIMUM	MEAN	STD. DEV.
30CM Cl	0.48	0	0.12	0.11
Ca	0.19	0	0.03	0.03
Mg	0.30	0	0.05	0.06
Na	0.28	0	0.07	0.07
K	0.04	0	0.01	0.01
MASSBAL	1.59	-0.50	0.30	0.36
60CM Cl	0.39	0	0.09	0.10
Ca	0.14	0	0.02	0.02
Mg	0.21	0	0.04	0.04
Na	0.35	0	0.05	0.06
K	0.02	0	0.00	0.00
MASSBAL	1.35	-0.80	0.25	0.35
90CM Cl	0.31	0	0.07	0.07
Ca	0.19	0	0.03	0.03
Mg	0.20	0	0.05	0.05
Na	0.15	0	0.03	0.03
K	0.03	0	0.01	0.01
MASSBAL	1.19	-1.08	0.18	0.33
120CM Cl	0.48	0	0.05	0.07
Ca	0.26	0	0.02	0.04
Mg	0.28	0	0.04	0.05
Na	0.13	0	0.02	0.03
K	0.09	0	0.02	0.02
MASSBAL	1.69	-0.09	0.09	0.34

where MASSBAL = moisture flux determined from the volumetric mass balance

5.3.2. Monthly time increments

As the time interval increases, the relation between predicted flux and flux determined using the MATRIC and MASSBAL methods improves. Predicted flux shows a decrease in correlation at this interval against the water balance method of flux determination (WATBAL), but this is followed by an increase in correlation at the quarterly interval. This trend is to be expected because irrigation in the study microplot Orchard M is carried out on average four times per month, and the minimum number of irrigation events to which the model has been successfully applied is four (Bernstein and Francois, 1971). It seems that a monthly time step is the minimum increment that should be used on in this study.

The correlations between predicted flux and flux determined using the MATRIC method range from 0% for Calcium at 120cm to 19.9% for Potassium at 30cm. The overall correlation is 7.6%, more than double the value obtained at the weekly interval, but is still too low to have any significance.

Table 5.3. Monthly leaching flux in Litres determined using the LR Model for the micro-plot area.

	MAXIMUM	MINIMUM	MEAN	STD. DEV.
30CM DEPTH				
CHLORIDE	0.92	0.20	0.47	0.18
CALCIUM	0.31	0.03	0.10	0.07
MAGNESIUM	0.56	0.07	0.21	0.12
SODIUM	0.56	0.14	0.28	0.11
POTASSIUM	0.06	0.01	0.02	0.02
MASSBAL	2.83	0.04	1.18	0.69
60CM DEPTH				
CHLORIDE	0.80	0.12	0.37	0.18
CALCIUM	0.22	0.02	0.08	0.05
MAGNESIUM	0.36	0.05	0.14	0.08
SODIUM	0.49	0.07	0.21	0.12
POTASSIUM	0.03	0.01	0.01	0.01
MASSBAL	2.44	-0.90	1.00	0.77
90CM DEPTH				
CHLORIDE	0.56	0.10	0.25	0.13
CALCIUM	0.25	0.05	0.11	0.06
MAGNESIUM	0.40	0.10	0.19	0.08
SODIUM	0.30	0.04	0.10	0.06
POTASSIUM	0.06	0.02	0.03	0.01
MASSBAL	1.62	-0.04	0.77	0.49
120CM DEPTH				
CHLORIDE	0.71	0.04	0.16	0.15
CALCIUM	0.28	0.02	0.08	0.07
MAGNESIUM	0.40	0.03	0.14	0.09
SODIUM	0.30	0.02	0.06	0.06
POTASSIUM	0.14	0.01	0.07	0.04
MASSBAL	2.00	-0.86	0.39	0.69

where MASSBAL = moisture flux determined from the volumetric mass balance

The average residual values obtained between flux determined using the WATBAL method and the LR model of 44.2% are much greater than those obtained between the modelled flux and flux determined by the MATRIC method, with a maximum of 67.3% for flux predicted using Sodium concentration. The minimum correlation of 20.9% is obtained using LR predicted flux based on Potassium concentration, although this value is higher than any found using the MATRIC method.

The MASSBAL method results in a mean R^2 of 47.6% although the range is lower than the WATBAL method, with a minimum of 10.7% and a maximum of 66.5% for Potassium at 120cm and 90cm respectively. This extreme variability in predictive accuracy shown by using K^+ concentrations is evidence for its erratic movement through the soil, and potential involvement in plant uptake or soil process interactions.

Table 5.3 shows that the difference between predicted and determined fluxes decreases with depth but the variability within the determined flux remains high, ranging from 42% to 23%, 36% and 77% at 30, 60, 90 and 120cm. This variability is less than that found with the weekly data, due to the averaging effects of the increased time increment. Accuracy of prediction follows the same trend from $Cl^- > Na^+ > Mg^{2+} > Ca^{2+} > K^+$. Predicted Chloride flux is shown in Figure 5.2.

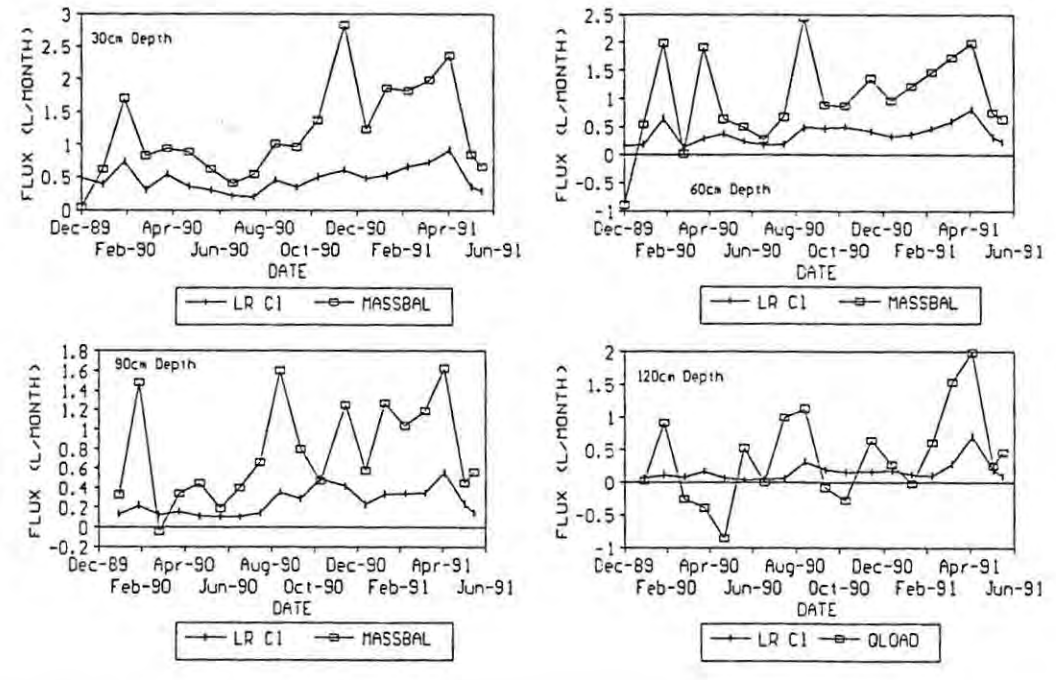


Figure 5.2. Leaching flux determined using the LR model based on Chloride concentrations (LR Cl) and the Chloride mass balance approach MASSBAL, (= QLOAD) at monthly intervals.

5.3.3. Quarterly time increments

Correlations between predicted flux and flux determined using the MATRIC method range from 0.2% for Chloride at 120cm to 28.4% for Calcium at 60cm. The mean R^2 found is 11.2%, and although this shows an increase over the same correlation at the monthly time step, it remains too low to be of any significance.

The flux determined using the WATBAL method shows a maximum correlation of 71.2% with the flux generated using Sodium concentration at 60cm, and a minimum of 20.3% with Magnesium concentration at 90cm. The mean R^2 of 47.6% is lower than the mean for the weekly interval, but the range is smaller which means that for all depths and concentrations the correlation is less variable.

The flux determined using the MASSBAL method shows the highest correlation with predicted flux, with maximum R^2 values of 92.9% and 83.4% using Chloride concentrations at the 60cm and 90cm depths respectively. A minimum correlation of 0% occurs at the 60cm depth, for Calcium concentration, but the overall mean correlation remains the highest of all flux determination methods against LR predictions, at 54.6%.

5.3.4. Summary of LR soil moisture flux predictions assessed against three methods of field moisture flux measurement

The leaching flux generated by the LR model using all ions is lower than the fluxes determined using the three methods, at all depths. The highest correlations between moisture movement determined by all techniques and predicted using all ionic concentrations are found at the quarterly level of time resolution. This trend conforms to the findings of other researchers (Jury, et. al., 1978; Rose, et. al., 1979; Bernstein and Francois, 1973) and is explained as the result of the averaging effects of increasing the time interval.

Short term fluctuations cannot be accurately predicted by this model because variability in solute concentrations over the short term is much greater than the long term, where averaging effects tend to ameliorate temporary extreme values. Model output is dependent on these solute concentrations, and it is therefore anticipated that longer term application will be more accurate.

The method of flux measurement which the LR predictions conform to most accurately is the volumetric mass balance, based on the calculation of solute load movement through the profile. This method is described in Chapter 4, where it was indicated that a discrepancy occurs with increasing depth between incoming irrigation and rainfall and the outgoing moisture flux determined by the mass balance. This finding can be used to explain the trend shown by the results of the LR model.

Correlation accuracy decreases with depth consistently down the profile between LR generated flux and moisture flux determined using the mass balance. This phenomenon is attributed to the technique used for measuring soil moisture flux rather than discrepancies in the LR model, which does not take depth into account at all. The volumetric mass balance measurement of flux under the micro-plot assumes vertical redistribution of all soil moisture, in both up and downward directions. In reality, a greater proportion of lateral flow occurs with depth as the soil moisture plume becomes more diffuse through reduced hydraulic conductivity. This would account for the difference between determined and predicted flux with increasing depth in the profile.

As Chloride is a conservative anion, and less reactive than cations (Ross, 1989; Rose et. al., 1982), it is expected that prediction of flux using Cl^- concentrations will be more accurate than cationic concentrations. However, it must be noted that the correlation between flux generated using Na^+ concentrations and flux determined using all methods is in many instances higher than the correlation using the Cl^- ion. At both 30cm and 120cm over the quarterly interval the R^2 value for Na^+ is greater than the Cl^- correlation, using all soil moisture measurement techniques. At the weekly and monthly time steps the correlations for Na^+ and Cl^- are similar, as can be seen in Table 5.1.

The low cation exchange capacity (CEC) of the soil at all depths, summarised in Table 4.3, may provide an explanation for this phenomenon. The low CEC will result in a low level of interaction between all ions in solution and those in the exchange sites. Thus the exchange processes commonly cited as responsible for inhibiting the movement of ions, especially divalent cations, may be of less importance in this environment. The result is that all cations, notably Na^+, provide a better tracer of soil moisture movement than anticipated.

The explanation for the high mobility of Sodium may also be the nature of the physical environment and historical genesis of the soils within the area. As the underlying geology consists of marine sediments, there is a concentrated source of both Chloride and Sodium ions available within the groundwater associated with these rocks. During the drought periods that naturally occur within the valley, capillary rise of groundwater may have resulted in the mobilisation of these ions upwards within the soil.

Over many cycles this process would result in near saturation of the cation exchange sites by Sodium, resulting in the alkali soils currently found within the valley. The problems associated with high Na^+ concentrations in the soil have been recognised within the Sundays River Valley since the 1930's (Folscher, 1982), including salinisation associated with the irrigation of such dispersed soils.

A further contributing factor is the long history of irrigation in the Valley, often using water having a high salinity. With continuous addition of Na^+ through irrigation the exchange sites would become saturated with the monovalent cation. Although Calcium has been artificially applied in the form of gypsum ($CaSO_4.2H_2O$), it seems that the levels of Na^+ remain high enough to prevent any adsorption into cation exchange sites. Thus Na^+ is effectively "conservative", and hence gives good estimates of soil moisture flux.

5.4. MODEL EVALUATION

Under the highly variable conditions within the unsaturated zone of the soil where many factors affect the movement of moisture into and within the soil, the correlation of almost 93% (Table 5.1) is significant. Detailed data was not available to statistically test fluxes generated by the model for greater time increments but if the trend evident in Table 5.1 continues with increasing intervals, annual outputs from the LR model may well be sufficiently accurate for the scheduling of irrigation on an annual basis. Data requirements are low, and the output accuracy against determined data is relatively good, especially in the light of the simplistic approach made by this model to a highly complex natural system.

If soil moisture was measured by spatial gravimetric sampling at all depths the problems encountered with obtaining accurate soil moisture movement measurements could be solved. A sampling program in three dimensions would attempt to measure lateral flow. Investigation of macropore movement would require the installation of underground drains. However, the expense involved in increasing accuracy of soil moisture movement measurements does not seem warranted in view of the high correlations obtained with the methods of flux determination used in this study. The results indicate that for practical purposes it would not be necessary to sample continuously or at short time intervals, as the accuracy of results increases when data over longer time is used. It is suggested that gravimetric sampling of the soil twice annually would be more cost effective than installing, maintaining, reading and interpreting permanent in situ tensiometers.

As an accessible management tool, the Leaching Requirement model has potential application for irrigation scheduling at the orchard or farm scale. Wider applicability remains to be assessed, but indications from other studies are that this simple leaching model continues to be used for a variety of situations.

The LR model can be used for the assessment of minimum irrigation requirements for different crops (eg. Bernstein and Francois, 1973). If soil salinity and irrigation water quality is known, the minimum amount of irrigation water that must be applied to maintain soil solute concentrations at a certain level is also set. This level is determined by plant tolerance, and the relationship between soil salinity and production.

Irrigation potential of land has been evaluated using the LR model (Shaw and Thorburn, 1985; Shaw et. al., 1987; Hansen and Thorburn, 1987). Again, if the soil salinity and available irrigation water are known, then the required amount of water for the intended crops will also be known. In this way the crops most suited to the specific conditions can be selected. If irrigation water supply is limited it may not be possible to meet the leaching requirements of certain crops, and if irrigation practises have resulted in an accumulation of salts in the soil profile, the LR model can be used to derive remedial measures whereby the leaching fraction is sufficiently high to result in flushing of the solutes below the root zone-zone.

Loss of water below the root zone is assumed to constitute irrigation return flow, so the LR model can be used to assess the proportion of irrigation water entering the groundwater. The quality of this return flow is also predicted by the model, which enables the net load of salts into and out of the system to be monitored. Effects of massive salt input to natural streams and lotic systems are detrimental, resulting in eutrophication and ecological imbalance. As irrigation represents a non-point source of salts, the only way inputs can be gauged is through the use of indirect means such as the LR model.

The LR model can be applied in a predictive manner in which various irrigation scenarios can be set up, and the long term effects on the soil indicated. Theoretically any time step is possible for this type of application, although short term fluctuations are not well represented. The LR model has been successfully used at the irrigation event level (Bernstein and Francois, 1973) and over the long term, ie. decades (Rose et. al., 1979).

CHAPTER 6

6. THE SODICS MODEL

6.1. MODEL DESCRIPTION

The SODICS model is derived in a similar way to the Leaching Requirement (LR) model as it is also based on a simple mass balance of inputs and outputs within the soil. However, SODICS allows for changes in soil moisture and solute concentration with time through the use of a differential function, and this allows transience (or change with time and space) to be included. SODICS was developed by Rose et. al. (1979) and uses Chloride as a tracer of soil moisture movement. Listings of the model are included in Appendix B. The change in mean soil solute concentration (Cs) with time to a given soil depth is expressed according to the principle of conservation of mass:

$$Cz.\Theta.\delta Cs/\delta t \quad = \quad ICi - LCz \quad \ldots\ldots\ldots\ldots \quad (6.1)$$

where Ci = solute concentration of the irrigation water (meq/L)
Cz = solute concentration of the soil at depth z (meq/L)
Cs = soil solute concentration (meq/L)
I = irrigation application rate (mm/year)
L = leaching rate at depth z (mm/year)
Θ = soil water content at and above which leaching occurs (cm^3/cm^3)
t = time (years)
z = depth (mm)

To enable Equation 6.1 to be solved simply, a non-dimensional parameter P is defined as:

$$P \quad = \quad Cz/Cs \quad \ldots\ldots\ldots\ldots \quad (6.2)$$

Combining Equations 6.1 and 6.2 gives:

$$Cs_t = Cs_o + (I.Ci/LP)\underset{[\,z.\theta\,]}{(1-\exp[-L.P.t])} \ldots\ldots\ldots\ldots (6.3)$$

where Cs_t and Cs_o = mean solute concentrations to depth z at times t and o.

If downward leaching occurs, that is $L > 0$, Cs increases with time to a final steady state value (Cf), which can be calculated from:

$$Cf = I.Ci/LP \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6.4)$$

If $L < 0$, that is upward leaching has occurred, Cs continually increases with time. The values of L and Cf can be used to assess the long term fate of an irrigation management practise. A Newton-Raphson iteration is used to find the first approximation for L, by successively solving Equation 6.3 with increasing values of L until the calculated value of Cs_t is less than the measured one. A correction term (H) is added to L. As the calculated L approaches the real value H gets smaller, and L is accepted when H reaches some acceptable level close to zero:

$$H = -f(L)/f'(L) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6.5)$$

where f = function

f' = derivative of f

(after Bellamy and Whitehouse, 1980)

An initial value for L can be specified by the user, providing it is lower than the actual L. In this study the initial value for L is taken as -305 mm/year after Thorburn, et. al. (1987). L is increased by 10 mm/year from the starting value of -305 mm/year for each iteration, to ensure that at no stage does $L = 0$. Equation 6.4 is undefined at $L = 0$. The first approximation of L is improved until the value of H is less than 0.001.

The leaching flux (L) can be calculated if values of Cs are known for two points in time. The difference in concentration between Cs_o and Cs_t must be sufficient to allow Equation 6.3 to be calculated. This period is usually 1 to 2 years, although any time interval may be used (Thorburn, et. al., 1987).

The data requirements of this model are simple and easily obtainable so it can be used where more detailed information is not available. Values for I and Ci are obtained from irrigation management data, and soil salinity profiles at two times must be measured. Each salinity measurement must have a corresponding air dry moisture content. Field capacity can be measured in the field, or taken as the saturation moisture content of the soil (Rose, et. al., 1979).

Bulk density measurements are also required. Soil Chloride concentrations are calculated for each year until steady state is reached, or until 200 years have been simulated. The model output consists of a table containing mean leaching flux, annual soil Chloride concentrations, steady state soil Chloride and the time to reach steady state conditions.

Table 6.1. Range in Parameter values for use in the Sensitivity Analysis of SODICS

	MAXIMUM	MEAN	MINIMUM
Rooting Depth (mm)	1200	600	200
Profile Cl at Time = 0 (meq/L)	10.0	0.5	0.01
Profile Cl at Time = 1 (meq/L)	10.0	0.5	0.01
Cl at Time = 1 and depth = z (meq/L)	10.0	0.5	0.01
Air Dry Moisture at Time = 0 (%)	50	30	10
Air Dry Moisture at Time = 1 (%)	50	30	10
Air Dry Moisture at Time = 1 and depth = z (%)	50	30	10
Field Capacity (cm^3/cm^3)	0.5	0.3	0.1
Bulk Density (g/cm^3)	2.0	1.5	1.0
Annual Irrigation (mm)	2000	1300	700
Irrigation concentration (meq/L)	15	10	5
Time Interval (years)	100	20	1

6.2. SENSITIVITY ANALYSIS OF THE SODICS MODEL

The SODICS model has 12 input parameters each of which was varied in turn while all others were held at their mean values (Table 6.1). The ranges over which the values are varied were determined by the range in field data collected by the Institute for Water Research and the results published by Folscher (1982), both obtained from the Lower Coerney irrigation area. The data used in the sensitivity analysis are realistic extreme values for this environment and soil types within the Coerney Valley.

The leaching flux determined using the mean values for all model parameters is 213 mm/year. Under these conditions, the final Chloride concentration within the soil profile is 0.65 meq/L and the time taken to reach steady state concentration is less than one year. The effects of variation in parameters must therefore be viewed against these results, which constitute the mean. SODICS output can be considered according to the mean leaching flux predicted over the simulation period, the Cl^- concentrations at which the soil will attain steady state and the time taken to reach steady state, given a certain set of input parameter values.

6.2.1. Determination of Leaching Flux

The effects of varying the input parameters for SODICS on the mean leaching flux predicted over the simulation period are summarised in Table 6.2. Mean leaching flux under mean values for all parameters is calculated by SODICS to be 213 mm/year. The leaching flux output is most sensitive to variation in profile Chloride concentration, where the maximum T_1 concentration produced a negative leaching flux of -14 897 mm/year. The minimum soil solute concentration for the profile at depth z resulted in a positive leaching flux of 10 638 mm/year, which is almost 10 times the combined annual total for both irrigation and rainfall (1300mm).

Air dry moisture (ADM) at and T_1 also affected the leaching flux, but to a lesser extent than the profile Chloride concentrations. Maximum ADM at and minimum ADM at T_1 both resulted in an increase in mean leaching flux, to 239mm/year and 279 mm/year respectively. Minimum ADM at T_0 and maximum ADM at T_1 led to the opposite effect, with the mean leaching flux depressed to 184mm/year and 158 mm/year respectively. Depth z had no effect on the leaching flux.

Field capacity (FC) had a greater effect on the mean leaching flux than variation of air dry moisture. The maximum FC resulted in a leaching flux of 355mm/year, with the minimum FC reducing the flux to 71mm/year. This is an unexpected result, as a greater field capacity means the soil has a greater capacity to hold water, leaving less water free to move through the soil than at a lower field capacity.

It is suggested that as the SODICS model is capacity-driven, the field capacity is a measure of the soil's ability to transmit water through the root zone. A greater value of field capacity may indicate the soil to be correspondingly more porous than a lower field capacity, thus allowing more water to penetrate below the root zone depth (1 200mm), and hence result in a greater leaching flux. The lower field capacity would act as a barrier to infiltration, and the soil would not be able to conduct as much soil water through the 1 200mm depth as the greater field capacity.

The only other parameter describing the soil physical state in bulk density, which had no effect at all on the leaching flux.

Table 6.2. Variation in parameters and mean leaching flux predicted by SODICS

	MAXIMUM	LEACHING FLUX (mm/year)	MINIMUM	LEACHING FLUX (mm/year)
Rooting Depth (mm)	1200	L=213	200	L=213
Profile Cl at Time = 0	10.0	L=880	0.01	L=-109
Profile Cl at Time = 1	10.0	L=-14897	0.01	L=213
Cl at Time = 1 and depth = z	10.0	L=10.64	0.01	L=10638
Air Dry Moisture at Time = 0	50	L=239	10	L=184
Air Dry Moisture at Time = 1	50	L=158	10	L=279
Air Dry Moisture at Time = 1 and depth=z	50	L=213	10	L=213
Field Capacity	0.5	L=355	0.1	L=71
Bulk Density (g/cm^3)	2.0	L=213	1.0	L=213
Annual Irrigation (mm)	2000	L=327	700	L=115
Irrigation concentration (meq/L)	15	L=319	5	L=106
Time Interval	100	L=213	1	L=213

Variation in the amount of irrigation applied was expected to have a major impact on the predicted mean leaching flux, but this is not shown by the sensitivity analysis results (Table 6.2). Maximum irrigation resulted in a leaching flux of just over 100mm more than the mean of 213mm/year, while the minimum irrigation resulted in approximately 100mm less than the mean.

Irrigation concentration influenced the leaching flux, but to a lesser extent than the irrigation amount. Maximum irrigation water concentration (15 meq/L) elevated the leaching flux to 319 mm/year, while the minimum concentration (5 meq/L) led to a decrease in flux to 106 mm/year.

The most important parameter in determining the prediction of mean leaching flux by SODICS for this range of data is shown to be the profile soil Chloride concentrations.

6.2.2. Determination of Soil Chloride Concentration

The effects of variation in input parameters on the steady state Cl^- concentrations are shown in Table 6.3. The soil Chloride concentration predictions are most sensitive to changes in the mean profile soil Cl^- concentration values for time T_1 and T_0. The minimum profile concentration at T_0 and the maximum concentration entered for time T_1 both result in an almost infinitely high solute concentration at steady state. Minimum concentration of T_1 results in a concentration of 0.013 meq/L, which is the lowest level reached for any parameter variation. The maximum Cl^- concentration for T_0 produced the second lowest steady state concentration of 0.157 meq/L.

The only other parameter that has any impact on the soil Cl^- concentration at steady state is air dry moisture (ADM) content of the profile. Minimum ADM at T_0 and all moisture contents at T_1, depth z, had no effect on the steady state concentration which remained at 0.65 meq/L. Maximum ADM at T_0 and minimum ADM at T_1 both led to a reduction in the steady state concentration, to 0.579 meq/L and 0.495 meq/L respectively. Maximum ADM at T_1 resulted in an increase in concentration to 0.876 meq/L.

Variation in all other parameters had no effect on the predicted Cl^- concentration of the soil at steady state, apart from a slight decrease from 0.65 meq/L to 0.649 meq/L for the minimum field capacity.

Table 6.3. SODICS predictions of soil Chloride concentration at steady state.

	MAXIMUM	Cl (meq/L)	MINIMUM	Cl (meq/L)
Rooting Depth (mm)	1200	c=0.65	200	c=0.65
Profile Cl at Time = 0 (meq/L)	10.0	c=0.157	.01	c=****
Profile Cl at Time = 1 (meq/L)	10.0	c=****	.01	c=0.013
Cl at Time = 1 and depth = z (meq/L)	10.0	c=0.649	.01	c=0.65
Air Dry Moisture at Time = 0 (%)	50	c=0.579	10	c=0.65
Air Dry Moisture at Time = 1 (%)	50	c=0.876	10	c=0.495
Air Dry Moisture at Time = 1 and depth = z (%)	50	c=0.65	10	c=0.65
Field Capacity (cm^3/cm^3)	0.5	c=0.65	0.1	c=0.649
Bulk Density (g/cm^3)	2.0	c=0.65	1.0	c=0.65
Annual Irrigation (mm)	2000	c=0.65	700	c=0.65
Irrigation concentration (meq/L)	15	c=0.65	5	c=0.65
Time Interval (years)	100	c=0.65	1	c=0.65

6.2.3. Time to reach Steady State

The model output table shows soil Chloride values, which reach an equilibrium or steady state after sufficient time has elapsed. Once constant soil chloride concentrations are reached over 10 successive time increments, it is assumed that steady state conditions have been reached for the parameters defined. The model listing does not continue simulation after 200 time increments, as any simulation of this length is beyond the potential applications for irrigation management. However, the listing can be modified for simulations over longer time intervals. For the purpose of this study, which aims to evaluate the model as a management tool, it was decided to limit the simulation to 200 years.

The profile solute concentration inputs had the greatest effect on the predicted time taken to reach steady state salinity in the soil. Both the minimum T_0 and maximum T_1 concentrations resulted in over 200 years before steady state is reached. This time is limited by the model listing (Appendix A) in which the number of time period iterations is limited to 200 years as the maximum length of time considered reasonable to model for the purpose of this study. The minimum time to steady state determined during the sensitivity analysis is 0 years, which is the time required to reach steady state when all parameters were set to their mean values. This is also obtained for a number of other input variations (Table 6.4).

Air dry moisture (ADM) at T_0 and T_1 all resulted in times to steady state of more than 10 years. However the ADM for depth z at T_1 had no effect on the time to reach steady state which remained at 0 years. Maximum field capacity (FC) had no impact on the time to steady state, although minimum FC increased the mean time to 3 years. Bulk density had no effect on the time taken.

Table 6.4. Results of the sensitivity analysis for SODICS model

	MAXIMUM	Time to Steady State (years)	MINIMUM	Time to Steady State (years)
Rooting Depth (mm)	1200	Y=1	200	Y=0
Profile Cl at Time = 0 (meq/L)	10.0	Y=5	0.01	Y=>200
Profile Cl at Time = 1 (meq/L)	10.0	Y=>200	0.01	Y=1
Cl at Time = 1 and depth = z (meq/L)	10.0	Y=4	0.01	Y=1
Air Dry Moisture at Time = 0 (%)	50	Y=11	10	Y=15
Air Dry Moisture at Time = 1 (%)	50	Y=18	10	Y=10
Air Dry Moisture at Time = 1 and (%) depth = z	50	Y=0	10	Y=0
Field Capacity (cm^3/cm^3)	0.5	Y=0	0.1	Y=3
Bulk Density (g/cm^3)	2.0	Y=0	1.0	Y=0
Annual Irrigation (mm)	2000	Y=0	700	Y=2
Irrigation concentration (meq/L)	15	Y=0	5	Y=3
Time Interval (years)	100	Y=0	1	Y=0

Irrigation amount and concentration had a slight impact on the time to steady state, with the minimum values leading to an increase of 2 and 3 years respectively over the mean time taken. The factor most influential in determining time to steady state is the soil profile Chloride concentration.

6.2.4. Summary of SODICS Sensitivity Analysis

Overall the most influential input parameters affecting the predictions of leaching flux, steady state soil concentration, and time to reach steady state were the soil solute concentration values. Soil physical properties were less important in determining output variability, for example the bulk density had no effect on the model output at any value. The input from the crop grown, consisting of the rooting depth, also had no effect on model performance. It is concluded therefore that the accuracy in field measurement of the soil Chlorides is the most important factor in obtaining the input requirements necessary to run this model. Focus on the soil physical properties need not be as detailed as the soil chemistry.

6.3. ASSESSMENT OF THE SODICS MODEL USING FIELD DATA

The input requirements for the Sodics model are not intensive, which means that it can be used in areas where detailed information is not available. However, accuracy of the model predictions must be measured before application is possible. The accuracy of predictions from Sodics can be assessed in terms of the mean leaching flux predicted, as well as the solute concentration predictions over time. As the solute concentrations are dependent on the leaching flux, this will be analysed first, before detailed assessment of solute concentration profiles are attempted.

In this study, detailed verification of the model's ability to predict leaching flux and soil salinity could only be provided for the microplot site, within Daisy Dell Farm. At a further fourteen orchards within the study area samples were taken from paired sites of irrigated and adjacent unirrigated areas. The unirrigated areas are assumed to be representative of soil conditions prior to orchard development. Samples from these sites were previously analysed by Folscher (1981). Information from three times during the irrigation history of each orchard is available, namely the time of orchard development, the 1981 sampling by Folscher, and the 1991 sampling during this study. The model was run using the unirrigated soil status as the initial time (T^0), and the 1991 conditions for the final time (T_1). The 1981 data were then statistically compared with the model predictions for this year.

6.3.1. Mean Leaching Flux predicted by SODICS

The Sodics model is initially applied to the Daisy Dell Orchard M where detailed information is available. The simulation period is the same as previously described (Chapter 4), namely 1/7/89 to 30/6/91. Data is arranged in the format required by the model with each parameter averaged to each depth considered. Thorburn et. al. (1987) state that this model can be applied over any time increment, providing that sufficient change has occurred in the soil salinity to allow the calculation of the decay curve (Equation 6.4).

Table 6.5. Summary of weekly leaching fluxes (mm/week) determined using three methods, and that predicted by the SODICS model. The maxima, minima, mean and standard deviations were calculated for all values obtained over the study period, and are summarised below.

	MAXIMUM	MINIMUM	MEAN	STD.DEV.
30CM				
SODICS	193.37	-82.92	4.01	40.16
MASSBAL	70.71	-49.99	21.66	24.51
MATRIC	14.83	-18.59	0.11	6.83
WATBAL	80.85	-191.77	2.63	38.68
60CM				
SODICS	205.10	-85.02	3.40	43.90
MASSBAL	135.37	-79.91	25.77	35.55
MATRIC	32.83	-34.89	-0.12	13.63
WATBAL	137.38	-366.07	8.51	66.10
90CM				
SODICS	152.00	-74.31	7.15	42.85
MASSBAL	118.64	-48.37	15.57	26.30
MATRIC	22.40	-30.96	0.18	10.61
WATBAL	112.15	-76.00	8.15	35.16
120CM				
SODICS	148.78	-69.57	4.75	44.79
MASSBAL	53.77	-89.55	3.61	26.59
MATRIC	15.36	-21.05	0.07	6.45
WATBAL	135.59	-719.43	-6.07	107.47

where MATRIC = Matric Potential Flux measurement
WATBAL = Water Balance Flux measurement
MASSBAL = Volumetric Mass Balance Flux measurements

In this evaluation, as with the LR Model evaluation, variable time intervals were used and the results of these are presented in Tables 6.5 to 6.7. The output from SODICS were then statistically compared with measured values (Table 6.8).

Weekly Time Interval

Correlations between leaching flux predicted using SODICS and the flux determined using the three methods are low at this time interval as shown by the residual (R^2) values which range from 0 to 22.56%, with a mean of 5.52% (Table 6.8). The highest correlations occur between predicted flux and that calculated using the MASSBAL method, followed by the

WATBAL and MATRIC methods. Table 6.5 shows the mean SODICS fluxes which range from 4.01 to 3.40, 7.15 and 4.75mm/week at 30, 60, 90 and 120cm respectively. The corresponding MASSBAL fluxes are approximately 5 times greater above 90cm, although the 120cm depth shows less than 1mm difference at 3.61mm/week.

Flux determined using the WATBAL method above 90cm is much closer to the predicted value than flux determined using the MASSBAL technique, but drops to a negative flux of -6.07mm/week at the 120cm level. Thus the variability of prediction is most closely matched by the flux generated using the MASSBAL method, but the absolute values of predicted flux are more similar to the WATBAL flux. Flux determined using the MATRIC method is very low, less than 1mm per week on average, with a negative flux at 60cm.

The correlations between all determined fluxes and the flux predicted using SODICS are too weak to be considered significant. It is suggested that this is due to the small time interval adopted. The difference in soil salinity over one week is too slight to allow an accurate solution to Equation 6.4, thus the output results do not match the field data.

Monthly Time Interval

There is an improvement in the predictive accuracy at this time increment over the weekly period, to a mean R^2 of 17.2%. The highest correlations occur between predicted flux and that determined using the MASSBAL method, to a maximum of 54.24% at 120cm depth (Table 6.8). The correlation between predicted flux and that determined using the MATRIC method is more significant than the relation between predicted flux and that determined using the WATBAL technique, in contrast to the weekly data, having a maximum of 36.21% at 120cm.

However Table 6.6 shows the same trend as the weekly data illustrated by Table 6.5. While variability in predicted output is most closely correlated with the MASSBAL measured flux, in absolute terms the predicted data is more similar to the WATBAL measured flux. MATRIC, while accounting more closely for variability, is 4 to 10 times lower than predicted flux.

Table 6.6. Summary of monthly leaching fluxes (mm/month) determined using three methods, and predicted by the SODICS model

	MAXIMUM	MINIMUM	MEAN	STD.DEV.
30CM				
SODICS	177.12	-82.34	11.09	68.64
MASSBAL	204.67	3.79	111.68	58.53
MATRIC	18.12	-17.89	0.22	10.50
WATBAL	185.31	-161.74	36.81	70.33
60CM				
SODICS	185.81	-66.02	24.61	62.64
MASSBAL	244.36	-89.57	98.02	81.44
MATRIC	30.53	-34.89	0.81	17.50
WATBAL	178.68	-215.76	34.29	79.45
90CM				
SODICS	99.53	-97.60	12.04	60.97
MASSBAL	160.05	-149.09	61.73	70.28
MATRIC	27.01	-30.30	0.41	15.60
WATBAL	158.77	-224.47	32.77	76.67
120CM				
SODICS	241.94	-58.47	66.12	100.30
MASSBAL	153.91	-131.34	22.04	73.33
MATRIC	13.65	-19.34	0.01	9.23
WATBAL	147.70	-230.02	32.87	80.17

Quarterly Time Interval

The maximum correlations are obtained from predicted flux and flux determined using all methods when SODICS is applied to data of this time interval. The combined mean correlation between predicted flux and that determined using all techniques is 57.11%, a 3-fold increase over the monthly mean correlation of 17.2% (Table 6.8). The fluxes generated from all 3 measurement techniques together with those predicted by SODICS are illustrated in Figure 6.1. Greatest R^2 values are obtained from the correlation between predicted flux and that determined using the WATBAL method, with a maximum of 93.22% at the 30cm depth, and the overall mean using this measurement technique is 76.25%.

Table 6.7. Summary of quarterly leaching fluxes (mm/quarter) determined using three methods, and predicted by the SODICS model

	MAXIMUM	MINIMUM	MEAN	STD.DEV.
30CM				
SODICS	165.94	43.26	77.20	43.73
MASSBAL	616.55	156.74	366.74	175.86
MATRIC	16.71	-16.95	-1.10	9.90
WATBAL	494.24	60.94	183.02	160.38
60CM				
SODICS	208.80	33.26	94.27	57.68
MASSBAL	517.68	144.31	309.24	134.76
MATRIC	34.89	-34.89	-1.45	21.48
WATBAL	498.46	60.49	183.68	162.02
90CM				
SODICS	154.42	28.29	67.38	44.81
MASSBAL	384.44	31.45	201.94	131.38
MATRIC	26.35	-30.30	0.05	17.46
WATBAL	497.73	59.14	184.06	161.48
120CM				
SODICS	220.90	-23.05	58.35	88.34
MASSBAL	412.96	-151.23	90.44	174.75
MATRIC	12.51	-14.22	0.10	9.07
WATBAL	497.48	59.38	184.06	161.15

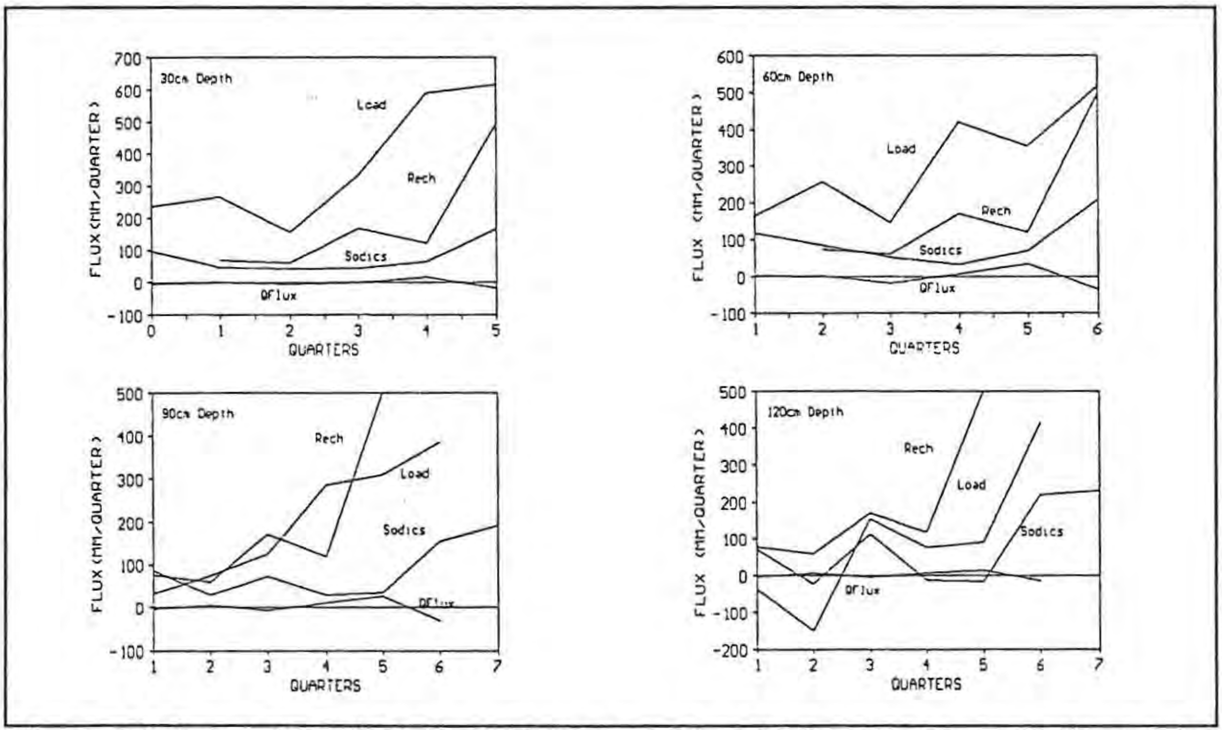


Figure 6.1. Quarterly Soil Moisture Fluxes determined by 3 methods and predicted using Sodics where LOAD = MASSBAL; RECH = WATBAL; FLUX = MATRIC; SODICS = model predictions

Absolute flux values are not as similar as this high correlation suggests, for example, the 30cm depth SODICS flux of 77.2mm/quarter is less than half the WATBAL flux of 183mm/quarter (Figure 6.1). Although the importance of a discrepancy in prediction of the magnitude of 10cm over a 3 month period may not be great in management terms, the ability of the model to replicate the absolute leaching flux measured using this technique is not as good as the model's ability to replicate the variability of the measured flux.

Comparison between predicted flux and that determined using the MATRIC method gives the second most significant relationship, with a mean of 62.6%. However, Figure 6.1. shows fluxes determined using the MATRIC method to be consistently lower than the SODICS leaching flux output, as seen at both weekly and monthly time intervals (Tables 6.5 and 6.6). So while variability between predicted flux and flux determined using the MATRIC technique is accounted for 63% of the time, absolute values are highly disparate.

Flux determined using the MASSBAL method only accounts for 32.50% of the variation in predicted leaching flux, which is an unexpected finding (Table 6.8). At both the weekly and monthly increments, the MASSBAL determined fluxes provided the best mean R^2 values when correlated against SODICS predicted flux. This trend is also observed using the LR Model output. Table 6.8 provides an indication as to why this low correlation is obtained.

At all depths the flux determined using the MASSBAL method is much greater than the SODICS output, although the discrepancy decreases with depth (Table 6.8). At the 30cm depth, MASSBAL flux is approximately 5 times greater than SODICS, this difference reduces to less than 2-fold at 120cm (Figure 6.1).

It has been suggested previously (CHAPTER 5) that the MASSBAL method of leaching flux measurement is less reliable with increasing depth, due to its failure to account for lateral and macropore flow. The SODICS output more closely approximates the MASSBAL flux at depth than at the surface. As the model contains no equations representing macropore or lateral flow, these results support the contention that such processes may be operating.

Table 6.8. Residual values (%) of SODICS leaching flux compared with 3 different methods flux measurement

	MATRIC	WATBAL	MASSBAL
WEEKLY			
30CM	0.01	16.18	22.56
60CM	0.27	0.00	1.33
90CM	0.31	0.84	3.48
120CM	0.22	4.55	16.57
MEAN	0.20	5.39	10.98
MONTHLY			
30CM	4.21	32.52	24.90
60CM	0.03	3.04	0.53
90CM	20.76	6.16	6.25
120CM	36.21	17.68	54.24
MEAN	15.30	14.85	21.48
QUARTERLY			
30CM	42.01	93.22	37.28
60CM	36.11	79.46	18.60
90CM	82.02	74.67	8.83
120CM	90.27	57.65	65.31
MEAN	62.60	76.25	32.51

Table 6.9. Correlation between leaching flux predicted using the LR and SODICS models summarised as residuals (%)

ION	30CM	60CM	90CM	120CM
CHLORIDE	0.00	36.55	10.37	63.30
CALCIUM	0.66	6.31	6.00	33.36
MAGNESIUM	1.11	15.49	8.60	0.17
SODIUM	21.76	2.13	17.99	58.94
POTASSIUM	1.33	0.60	3.49	1.31

Output from the Sodics model at quarterly intervals is compared with LR generated fluxes, using all ionic concentrations (Table 6.9). The correlations, as represented by the resudual values, between SODICS flux and the LR fluxes using Cl^- and Na^+ concentrations are the highest, at 63.3% and 58.94% respectively. The Na^+ concentration results in the greatest correlation at 30 and 90cm depths, while the Cl^- concentration results in greatest correlation at 60 and 120cm.

6.3.2. Soil Chloride Concentrations predicted by SODICS

Solute concentration is dependent on leaching flux, which is determined to be most accurately modelled at the quarterly interval. Each quarterly time period is independently modelled, and the predicted soil chloride concentrations for the consecutive increments are presented in Figure 6.2. Once steady state is reached, after 10 identical consecutive concentration values are obtained, the modelling process is terminated.

At the 30cm depth, steady state conditions exist for both the first and third quarters, at 0.18mg/L Chloride. Quarters 2, 4 and 5 show an increase in steady state concentrations to 0.25, 0.32 and 0.37 mg/L respectively. Throughout the data period there is a net increase in Cl^- at the 30cm depth, with steady state conditions attained within 4 years.

At the 60cm depth the opposite trend occurs. All quarters show a decrease in concentration, with steady state reached in under three years. The first, third and sixth quarters reach the same steady state concentration of 0.2 mg/L, while the second quarter shows a decrease to 0.17mg/L.

The 90cm soil chloride concentrations are less uniform than the shallower depths. Steady states over all quarters are reached after around 5 years, but the first, third and sixth quarters show a decrease to 0.12 and 0.23 mg/L, while the second, fourth and fifth quarters show an increase in concentration to 0.4, 0.53 and 0.75 mg/L respectively.

The 120cm depth is less ordered than the overlying layers, with quarters 1, 3 and 6 decreasing to reach steady state very rapidly at 0.3, 0.05 and 0.08 mg/L respectively. In contrast quarters 2, 4 and 5 increase in concentration to over 1000mg/L within 20, 33 and 26 years.

6.3.3. SODICS applied to other sites

Fourteen sites within selected orchards and matched samples from adjacent unirrigated lands were sampled at 30, 60, 90 and 120cm depths. These sites were previously unsampled, except for a survey conducted in 1981. The samples were analysed for the data required by the SODICS model, and then a simulation is performed for each site over a period of 200 years, or until steady state is reached.

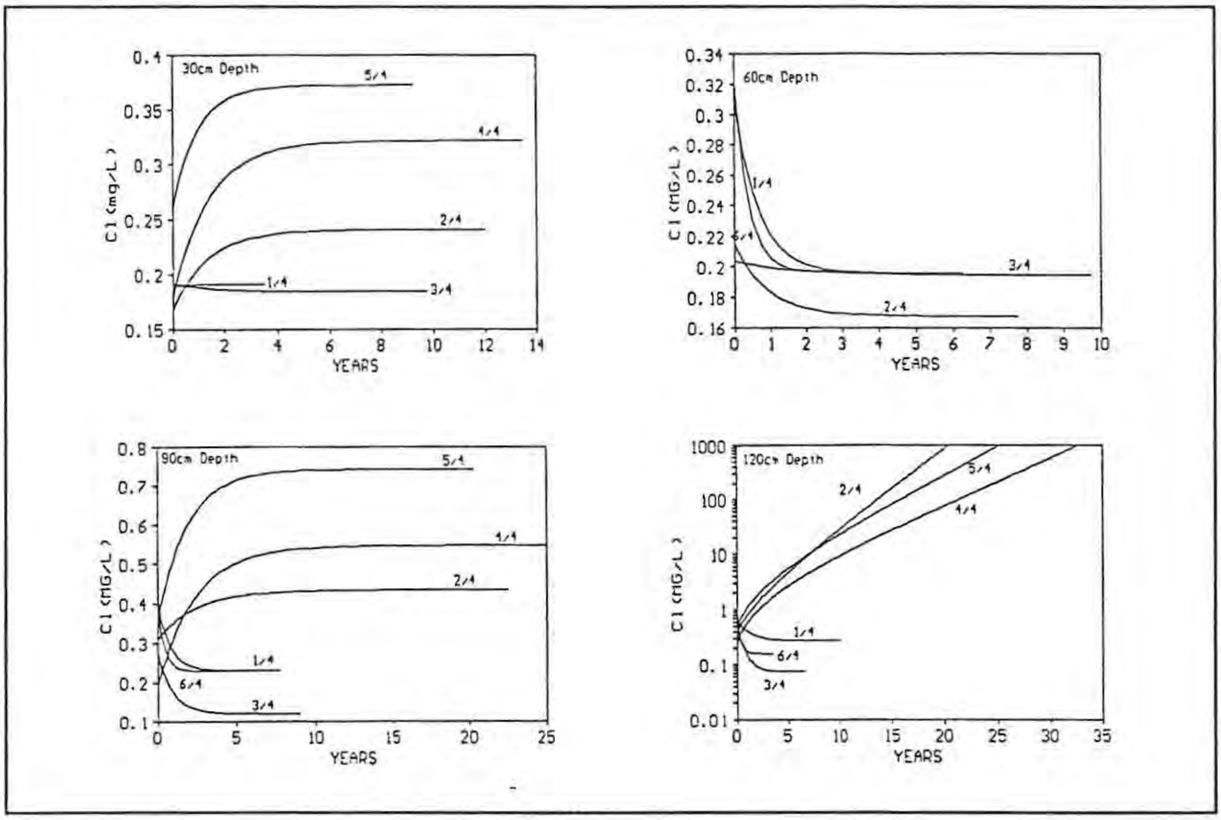


Figure 6.2. Soil Chloride concentrations predicted using Sodics at 30, 60, 90 and 120cm depths for the respective quarterly time periods. Predictions are terminated once steady state is reached.

Mean Leaching Flux

The mean leaching flux predicted by the SODICS model could not be validated against measured field data for these sites, as the necessary data for comparison is not available. The SODICS output from the undocumented sites is compared with LR output for the same sites. This is justified on the basis of the level of confidence in the accuracy of LR Model predictions (Chapter 5) and the correlations between SODICS and LR illustrated in Table 6.9.

Results illustrated in Table 6.9 show the maximum correlation of 63.3% between the SODICS output and the LR generated leaching flux using soil Chloride concentration occurs at 120cm depth. For the same depth using Sodium concentrations, a correlation of 58.95% is obtained. While the LR predicted leaching flux cannot be assumed to represent actual field conditions, the similarity between the flux generated using both models supports the validity of SODICS.

Soil Solute Profiles

For the fourteen selected sample sites, data from adjacent unirrigated land is used for the input, and T_1 data is determined from the irrigated land. The length of time since orchard development is noted (Table 4.2), and this is used to work out the number of years prior to 1981 for each orchard. The output for number of iterations since development is compared with the data measured in 1981. The results of these simulations are presented in Appendix E, two examples of which have been selected as representative (Figures 6.3 and 6.4).

Figure 6.3. illustrates a trend towards steady state at all soil depths. Initial soil Cl^- concentrations are around 150mg/L below the 30cm depth, and with irrigation this concentration decreases rapidly to less than 10mg/L, which is less than the concentration of the irrigation water (14.3meq/L). It appears in this example that irrigation is having a flushing effect on the accumulation of salts naturally occurring within the soil. If the current irrigation conditions continue, steady state concentration will be attained in the soil after about 40 years, at a concentration of approximately 10mg/L throughout the profile.

In contrast, Figure 6.4. shows a different scenario where soil chloride concentrations are steadily increasing at all depths, particularly below 30cm. Above 30cm there appears to be a trend towards steady state, although this is not attained within the 200 years over which the simulation is carried out. For the depths below 30cm the model predicts a rapid increase in soil chloride concentrations, reaching levels greater than 10 000 mg/L in about 80 years if the current irrigation regime is sustained. Figure 6.4. is an example of a salinisation trend, which is also seen in 5 of the profiles investigated by this study. It may be advisable for the irrigation managers of these lands to examine the irrigation scheduling and attempt to reverse this trend.

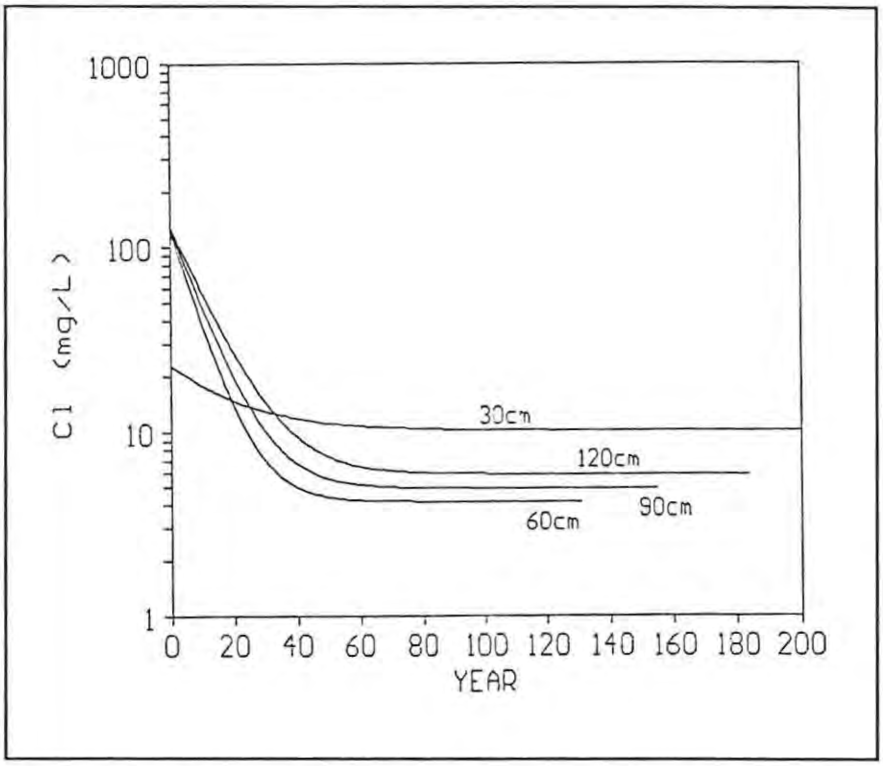


Figure 6.3. Soil Chloride profiles predicted by the SODICS model at Goodhope Farm Orchard 02.

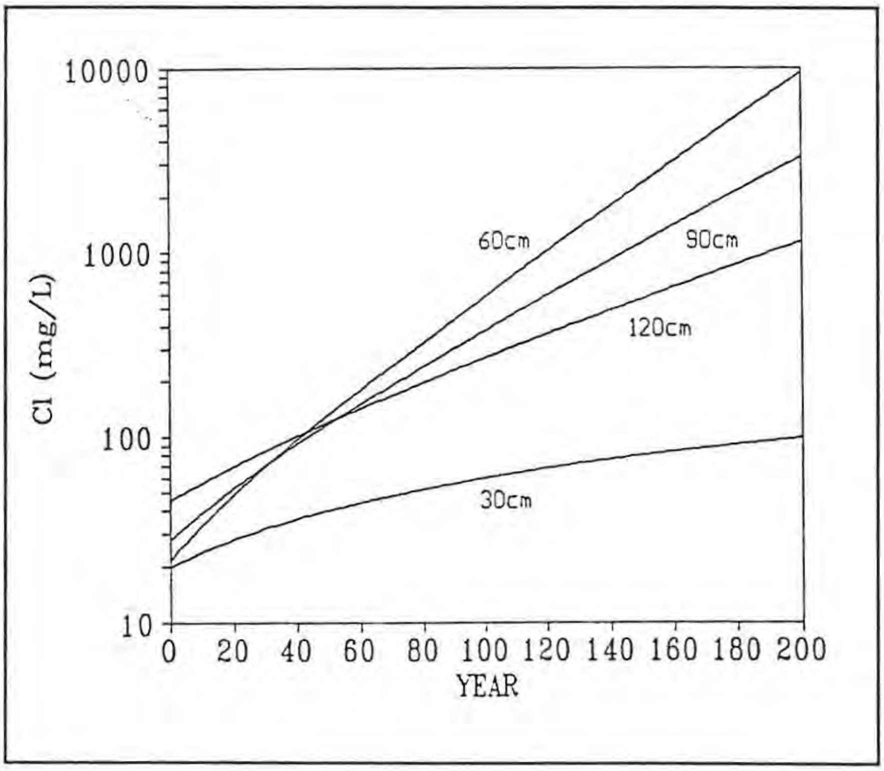


Figure 6.4. Soil Chloride profiles predicted by the SODICS model at Goodhope Farm Orchard 02.

The residual values were then determined by correlating simulated Cl^- concentrations with data obtained in 1981 for all sites at 30, 60, 90 and 120cm depth. The R^2 values are 4.07%, 1.36%, 3.06% and 2.83% for each depth respectively. These correlations are too low to have any significance. A possible explanation for the failure of the SODICS model to replicate actual Chloride concentrations is that the exact 1981 sampling site is not known, so while the 1991 sites were located in the same Orchards, they were not in the exact spot previously sampled.

Secondly, the SODICS model considers mean application rates and water quality throughout the simulation period, which results in unrealistic predictions. Irrigation management has varied throughout the simulation period. Some orchards are 36 years old (Table 4.3), over which time the amount and timing of irrigation application, as well as technique of irrigation and irrigation water quality have changed. The measurement of soil Cl^- at and T_1 is the basis for the calculation of the decay curve (Equation 6.4), which is then used to calculate model predictions. Soil Cl^- at T_1 and must be relatively accurate, as the simulated mean leaching flux shows a high degree of similarity to the LR flux.

The erroneous Chloride predictions must be due to parameters other than the soil chloride concentrations at T_0 and T_1. The only other parameters representing Cl^- input are the irrigation water quality and the amount of irrigation water applied which determines the incoming Chloride load. The model uses mean values for these parameters, which is unrealistic, and this is therefore a potential explanation for the model's failure to predict Cl^- concentrations.

6.4. MODEL EVALUATION

The correlation between leaching flux predicted by SODICS and the three methods of flux measurement improves as the time increment of input data increases, from a maximum R^2 of 22.56% at the weekly interval to a maximum of 54.24% at the monthly interval and 93.22% at the quarterly interval. The variability is well replicated by the SODICS model, and the absolute values for flux are also close approximations of the WATBAL and MASSBAL moisture flux measurement techniques. SODICS is also able to simulate negative fluxes, which match those shown by the WATBAL method.

The soil chloride concentrations predicted by SODICS and the time taken to attain steady state conditions could not be statistically tested against field data, as this was not available. The soil profile concentrations show a build up of Chloride in the upper 30cm layer, a loss of Cl^- from the 60cm layer, and both accumulation and loss below 60cm.

The data requirements for SODICS are simple, but not routinely available. The necessity for air dry moisture contents of each soil Chloride concentration measurement prohibited the application of this model to a wider area, where soil solution concentrations were available. The computer listings are easy to install and operate, so the applicability of SODICS is limited by the data requirements rather than computer complexity.

CHAPTER SEVEN

7. THE PEAK MODEL

7.1. MODEL DESCRIPTION

The PEAK model is based on the convective-dispersion equation for solute and moisture movement through porous media. It is a transient mass balance model, developed in response to the limitations of the steady state models. It is of a similar order of simplicity to the steady state SODICS model, but has been demonstrated to give better predictions of recharge rates (Thorburn, et. al., 1991).

The movement of a peak of non-adsorbed, non-reactive solute through a soil under constant moisture flux was modelled by De Smedt and Wierenga (1978). The peak was modelled in two parts: the first section predicts the movement of a solute peak through a soil profile (PEAKM), and the second predicts the dispersion of the solute about the peak (PEAKD). Listings of PEAKM and PEAKD are included in Appendices B and C, respectively.

7.1.1. PEAKM

The original requirement for constant moisture flux (De Smedt and Wierenga, 1978) was alleviated by Rose et. al (1982) using a mass balance approach. The movement of the peak solute concentration through uniform soil is described by:

$$J = qC - Ds.\theta.\delta/\delta z \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (7.1)$$

where J = solute flux

q = volumetric flow rate

Ds = diffusion coefficient in soil

θ = soil water content

C = solute concentration

z = soil depth

The model assumes:

- there is no preferential movement of water through the soil, such as macropore flow, lateral flow, soil cracking or other instability effects (Thorburn, 1988).
- the soil drains to a constant water content after each infiltration. This is termed field capacity.
- no significant soil-solute interactions or chemical transformations occur.
- crop water uptake is uniform with depth to the base of the root zone.
- the profile is at field capacity below the root zone.

Equation 7.1 was then modified by Rose et. al., (1982) to account for plant solute uptake:

$$\Theta \delta C/\delta t = C.\delta q_r/\delta z - q\delta C/\delta z \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (7.2)$$

where q_r = volumetric water uptake by plant roots.

q = volumetric flow rate

Θ = soil water content

C = solute concentration

Water input to and loss from the soil profile is considered separately as an infiltration event and an evapotranspiration event respectively. During infiltration, q_r is much less than the water flux, so Equation 7.2 reduces to Equation 7.1. During evapotranspiration, the reverse occurs, with q_r much greater than the water flux which is approximately zero. In this phase there is a negligible change in the position of the concentration peak but an overall increase in solute concentration.

The depth beneath the soil surface of the solute concentration peak is defined as the depth at which the solute flux, $\delta C/\delta z$, = 0. This equation neglects the effect of dispersion, which has been shown to result in an overestimation of approximately 10% of the depth predicted (Rose et. al., 1982). This error is considered acceptable within the context of the model application.

During an infiltration event the depth of a solute peak (a) can be represented by:

$$\delta a/\delta t = q/\Theta_{(z=a)} \quad \dots\dots\dots\dots \quad (7.3)$$

where a = depth beneath the soil surface of the solute peak
z = soil depth
q = volumetric flow rate
Θ = soil moisture content

During an evapotranspiration event $\delta a/\delta t = 0$. Equation 7.3 has been shown to generate an acceptable approximation of solute peak movement in laboratory studies (Warwick et. al., 1971; Ghuman et. al., 1975; De Smedt and Wierenga, 1978).

Equation 7.3 was then presented in discontinuous form. The solute peak movement within a profile is calculated by assuming that the solute is displaced by the wetting front of successive water applications, between which evapotranspiration occurs (Rose et. al., 1982). The depth below the soil surface of the solute peak is calculated in finite time intervals:

$$a_n = a_{(n-1)}/\Theta_{fc} + \Sigma_W \quad \dots\dots\dots\dots \quad (7.4)$$

where a = depth of solute peak
n = number of time element
Θ_{fc} = soil moisture content at field capacity
Σ_W = equivalent ponded depth of water which passed below previous peak position

A general expression for Σ_W is:

$$\Sigma_W = I.n.t - g(\Theta_{fc} - \Theta_{(n-1)} + j.E_t.t/r) \quad \dots\dots\dots\dots \quad (7.5)$$

where I = infiltration rate over the period of simulation
n = number of event
t = time interval
g = depth of water required to bring soil moisture to field capacity
Θ_{fc} = soil moisture at field capacity
$\Theta_{(n-1)}$ = soil moisture content at the end of the previous time increment
j = proportion of evapotranspiration occurring before infiltration
E_t = evapotranspiration rate over the period
r = depth of rooting

If peak movement occurs, two extreme boundary condition are possible: either infiltration is complete before evapotranspiration begins ($j = 1$), or evapotranspiration ends before infiltration begins ($j = 0$). If values for j cannot be determined with confidence from irrigation scheduling data, the extreme values can be used to define envelope curves encompassing the uncertainty in prediction of peak movement.

The value of g is constrained by the previous depth of the peak and the rooting depth. If the previous depth to peak lies above the rooting depth, g is equal to the previous depth. Conversely, if the previous depth to peak lies below the rooting depth then g is taken as equal to the rooting depth.

The previous profile water content must be known to determine $\Theta_{(n-1)}$, which is calculated by:

$$\Theta_{(n-1)} = \Theta_{(n-2)} + (I_{(n-1)} - E_{(n-1)}.\delta r/\delta t) \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (7.6)$$

Soil moisture content during the previous time period ($\Theta_{(n-1)}$) is constrained by the field capacity of the soil considered and the wilting point of the crop grown. If $\Theta_{(n-1)}$ is greater than the field capacity then the soil moisture content is assumed to have been equal to field capacity. Conversely, if $\Theta_{(n-1)}$ is less than wilting point, then the soil moisture is assumed to have been equal to the wilting point.

The data required to run the PEAKM model comprises details about irrigation scheduling events, rainfall, evapotranspiration and variation in crop rooting depths.

7.1.2. PEAKD

The convective dispersion equation based on the mass conservation of a non-adsorbed, non reactive solute requires that:

$$\delta.\theta C/\delta t = -\delta J/\delta z \quad \text{(7.7)}$$

where θC = mass of solute per unit soil volume
J = flux of solute
z = depth

Mass movement of water will give a convective flux of solute (Jc) which can also be described as qC. Water movement will also result in a diffusion like flux of solute (Jd) proportional to the concentration gradient. According to Fick's first law:

$$Jd = -Ds.\theta.\delta C/\delta z \quad \text{(7.8)}$$

where Ds = diffusion coefficient in soil
θ = soil moisture content
C = concentration of solute
z = depth

The total contribution of both convective (Jc) and diffusive (Jd) fluxes constitutes the convective dispersion equation:

$$\begin{aligned} J &= Jc + Jd \quad \text{(7.9)} \\ &= qC - Ds.\theta.\delta C/\delta z \end{aligned}$$

Substituting Equation 7.9 into Equation 7.8 gives:

$$\delta C/\delta t = D.\delta^2 C/\delta z^2 - (q/\Theta).\delta C/\delta z \tag{7.10}$$

$$= D.\delta^2 C/\delta z^2 - v.\delta C/\delta z \tag{7.11}$$

where $q/\Theta = v$ = pore water velocity

De Smedt and Wierenga (1978) solved Equation 7.11 for constant flux boundary conditions, using values for the depth of the solute peak (a) from Equation 7.4:

$$C/C_o = 0.5\ \mathrm{erfc}[(z-a)/2(Ds.t + a.E)^{0.5}] \tag{7.12}$$

where C_o = initial solute concentration

C = solute concentration

erfc = error function term (Carslaw and Jaeger, 1959)

z = depth of soil

a = depth of solute peak below surface

Ds = molecular diffusion coefficient in soil

E = solute dispersivity coefficient

Equation 7.12 calculates the leading edge of the dispersed solute pulse. The trailing edge (b) is given by:

$$b = a - L \tag{7.13}$$

where b = depth of the step decrease in solute concentration (trailing edge)

a = depth of solute peak below surface

L = depth of the solute pulse (leading edge)

When b is used to solve Equation 7.11:

$$C/C_o = 0.5\ \mathrm{erfc}[(z-b)/2(Ds.t + b.E)^{0.5}] \tag{7.14}$$

As the solute pulse depth is given by a - b, Equation 7.14 is taken from Equation 7.12:

$$C/C_o = 0.5\ \mathrm{erfc}[(z-a)/2(Ds.t + a.E)^{0.5}] - 0.5\ \mathrm{erfc}[(z-b)/2(Ds.t + b.E)^{0.5}] \quad \ldots (7.15)$$

Values for L, E and Ds are required to solve Equation 7.15. Where the solute applied is through the irrigation water:

$$L = I.t/\theta_{fc} \quad \ldots \ldots \ldots \ldots \ldots \ldots (7.16)$$

where I = infiltration rate

t = time

θ_{fc} = field capacity

E must be determined through calibration of predicted output with measured data. Ds is taken as approximately 60mm^2/day (Rowell et. al., 1967).

7.2. SENSITIVITY ANALYSIS OF THE PEAK MODEL

The PEAK model is divided into two parts, the first (PEAKM) predicts the movement of a solute peak through the soil and the second (PEAKD) uses the output from PEAKM to predict the dispersion of a solute about the peak. These modules will be analysed separately for the purpose of determining the sensitivity of model output to variations of input.

7.2.1. Sensitivity Analysis of PEAKM

This model has six input parameters, each of which was varied in turn between the extremes used in the SODICS sensitivity analysis (Table 7.1). The effect of variation in each parameter on the model output is shown in the following graphs.

Table 7.1. Parameter values used for the sensitivity analysis of the PEAKM model

	MAXIMUM	MEAN	MINIMUM
I (rainfall + irrigation MM/MONTH)	250	100	50
E (evaporation MM/MONTH)	300	130	30
Crop Factor	0.95	0.7	0.45
Rooting Depth (MM)	1200	600	200
J (proportion of evapotranspiration occurring before infiltration)	1.0	0.5	0.0
Field Capacity (kg/kg)	0.5	0.3	0.1

Depth of infiltrating water (irrigation and rainfall): (I)

This parameter was varied between the extremes of 250 and 50mm per month (Figure 7.1). The maximum and minimum values selected for I were compiled from the irrigation scheduling data and measured rainfall. The model output shows no peak movement with the lowest I value, a migration to 1000mm depth with the mean I of 100mm per month, and a 10 fold greater distance travelled, using the highest I value. I is instrumental in determining peak movement. Only when I exceeds E can movement occur, which is whenever I is equal to, or greater than 70mm. The minimum I is 50mm, so no movement occurs. When the mean value of I is used, the modelled peak moves to a depth of 4000mm over 12 time intervals, and the maximum I results in a depth of 10 000mm.

Depth of evaporation: (E)

The original model listings were modified to allow pan evaporation and a crop factor to be used, instead of a combined value for E which is difficult to quantify. E was varied between 30mm and 300mm/month (Figure 7.2), with a mean of 130mm/month, and the crop factor held constant at 0.7. The extremes for E were realistically derived from evaporation data obtained from the Department of Agriculture Citrus Research Station at Addo, located approximately 4km from the microplot on Daisy Dell farm.

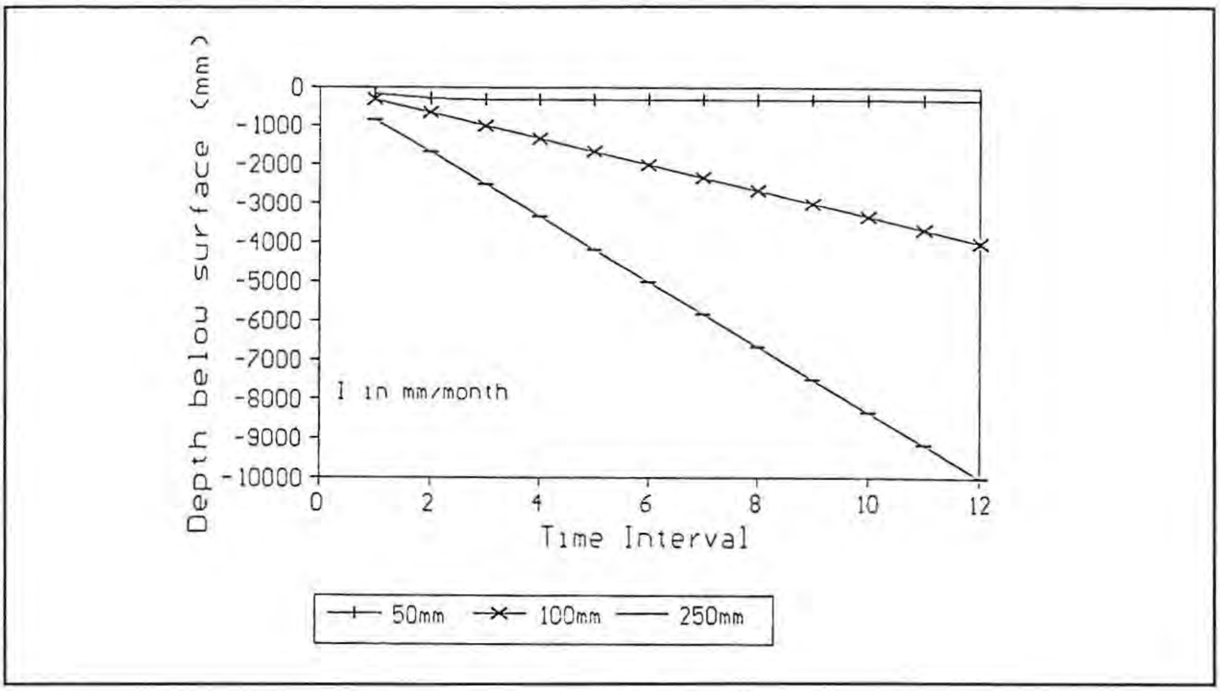


Figure 7.1. Effects of variation in irrigation and rainfall (I) on the peak depth predicted using PEAKM

As with I, the E parameter is instrumental in determining peak movement. E interacts with I to control the amount of water available for downward movement within the soil. The maximum E value of 300mm/month produced no peak movement at all over the simulation period. This is because maximum E exceeded the mean I of 100mm/month. The peak would not be expected to move unless actual evapotranspiration (E x Crop Factor) is less than the depth of irrigation and rainfall (I).

The mean E of 130 mm/month is greater than mean I of 100mm/month, but peak movement occurs due to the reduction in E through the use of the crop factor (the mean value of which is 0.7). The crop factor reduces the evaporation and only when E = 143 mm/month will peak movement be zero. Any value of E below this results in peak movement with no variation in rate of movement. Once E falls below 143mm/month the peak produced is identical to that produced using total mean conditions. The parameter E affects model output in an all or nothing manner, with no movement at all above E = 143 mm/month, and a constant movement rate and depth below E = 143 mm/month.

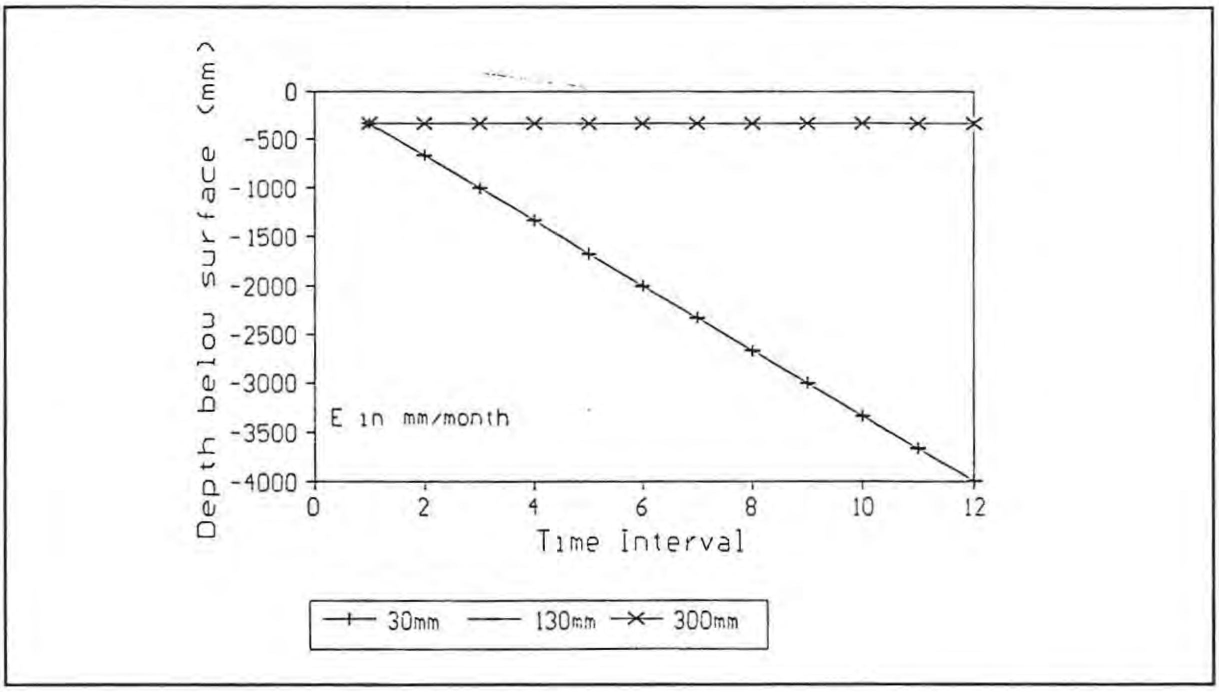


Figure 7.2. Effects of variation in depth of evaporation (E) on the peak depth predicted using PEAKM

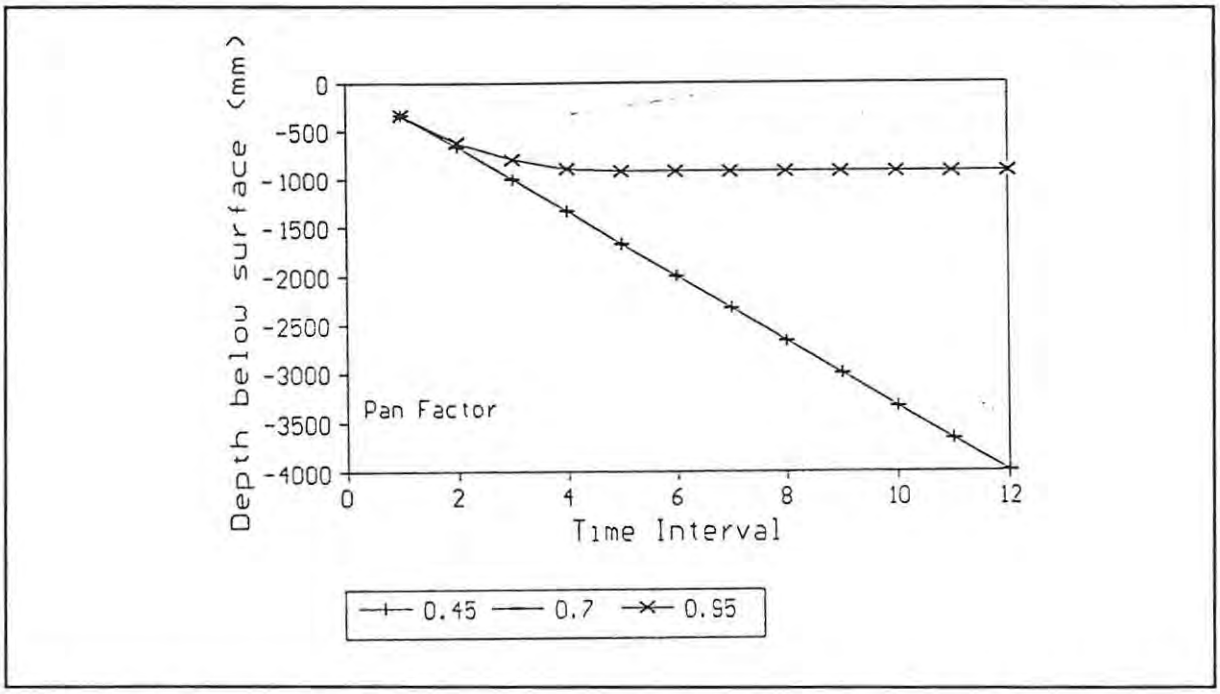


Figure 7.3. Effects of variation in the Crop Factor on the peak depth predicted using PEAKM

Crop Factor: (CF)

This parameter was varied between 0.95 and 0.01, with a mean of 0.7 as shown in Figure 7.3. All values less than 0.7 produced peak movement equivalent to that of total mean conditions. Values greater than 0.7 result in a systematic decrease in peak movement, which is to be expected: as the PF value approaches one, the model output will approach the straight line, with no change in depth, as was calculated when E exceeds 143mm/month.

Rooting Depth

Maximum and minimum rooting depths of 1200mm and 200mm respectively were taken from Folscher's (1982) extensive survey of the entire Sundays River Valley. The mean rooting depth of 600mm was the depth determined by inspection of the orchard sampled. The rooting depth had no effect whatsoever on the peak movement predicted by the model (Figure 7.4).

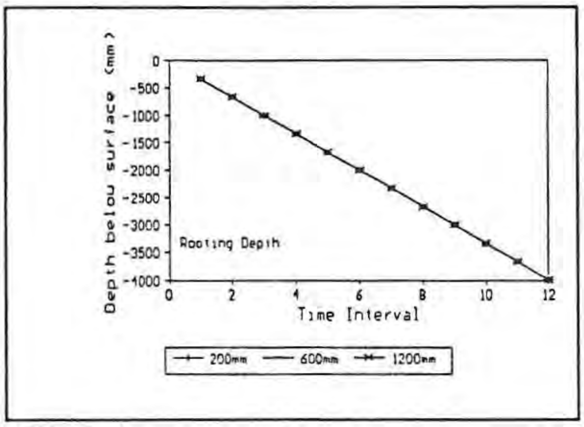


Figure 7.4. Effect of variation in rooting depth on predicted peak depth

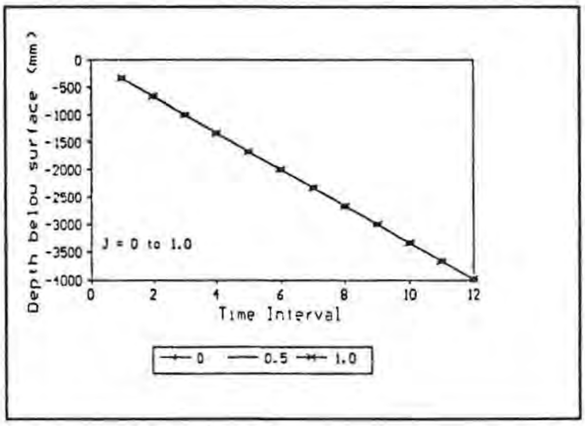


Figure 7.5. Effect of variation in J on on predicted peak depth

Proportion of evaporation occurring before infiltration: (J)

The proportion of evaporation occurring before infiltration (J) is a subjective parameter, requiring interpretation of the irrigation management data. The value of J lies between 0 and 1 that must be estimated from irrigation scheduling information, or calibration of the model against measured data. As this parameter had no effect on model output in this study, it was not considered an important model parameter (Figure 7.5).

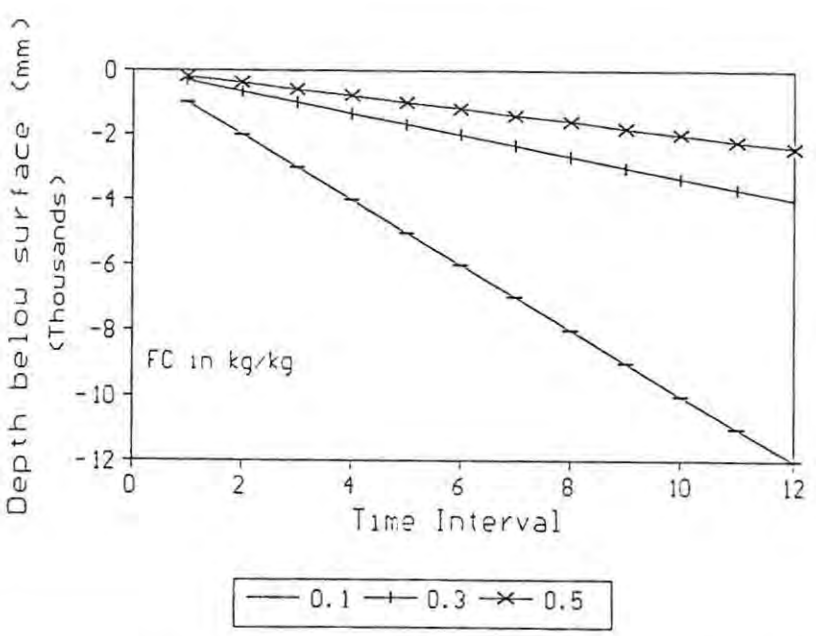


Figure 7.6. Effect of variation in Field Capacity on PEAKM model output

Field Capacity: (FC)

This parameter was varied between 0.5 and 0.1 kg/kg, which are the extreme values for a clay-rich soil and a sand respectively (Figure 7.6). Of the soil physical properties accounted for in this model, FC is shown to have the most impact on the output peak movement. Although difficult to quantify in the field, FC was taken to be equivalent to the soil moisture content measured after saturation (matric potential = 0kPa) was reached during a three day storm event during November 1989. After the soil was saturated, it drained naturally over a period of 48hours, at which point the soil was assumed to be at field capacity (Hutson, 1983).

The FC down the study profile varied between 0.28 and 0.35, with 0.3 taken as the mean. Peak movement occurring when FC equalled 0.1 was approximately 2 500mm, and the mean FC produced a movement to 4 000mm, an increase of only 1 500mm. However between 0.3 and 0.5 the distance travelled by the peak was 8 000mm, which illustrates that at high field capacities, the effect of this parameter on model output becomes more crucial than at low field capacities.

7.2.2. Sensitivity Analysis of PEAKD

The PEAKD model requires an input table generated by PEAKM, as well as other parameters, and uses the concentration of Chloride to trace the movement of a solute peak through the soil. As the most influential soil hydraulic parameter affecting PEAKM output was the field capacity, the sensitivity analysis on PEAKD was performed using the maximum, mean and minimum field capacity output tables from PEAKM. The other parameters are summarised in Table 7.2.

Table 7.2. Variation in parameters for the sensitivity analysis of the PEAKD model

	MAXIMUM	MEAN	MINIMUM1	MINIMUM2
PEAKM INPUT using variable FC	0.5	0.3	0.1	
Maximum calculated depth(mm)	1200	1200	1200	
Depth Increment(mm)	50	50	50	
Diffusion coefficient (mm^2/month)	300	100	10	
Dispersion coefficient(mm)	150	100	50	5
Initial depth of infiltrating water(mm)	27	9	1	
Irrigation concentration of Cl^-(meq/L)	15	10	5	

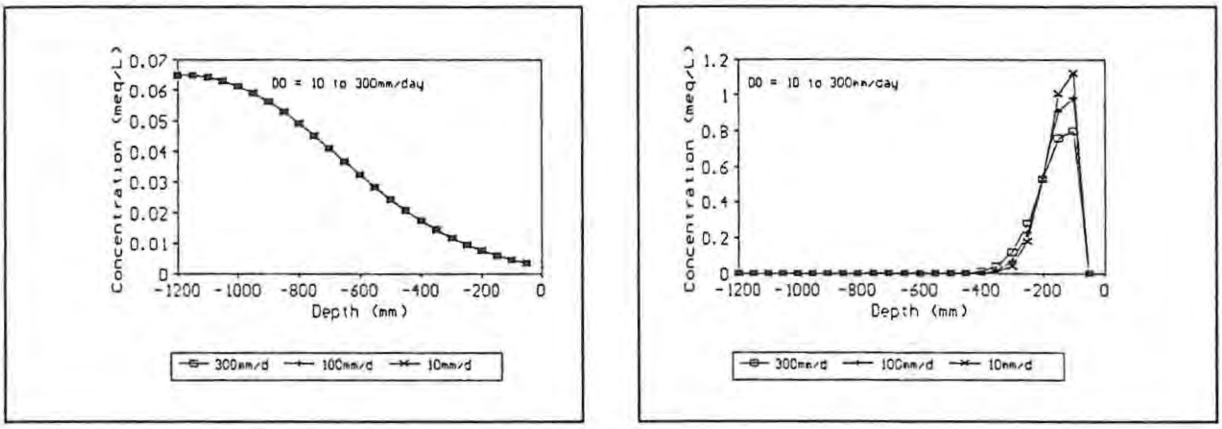
Neither the maximum calculated depth, nor the depth increment are intended to have any effect on the model output. The depth increment allows greater detail to be obtained for smaller depths, but for the purpose of the sensitivity analysis, this was unnecessary.

Diffusion Coefficient: (D0)

Variation in this parameter had no effect on the model performance (Figure 7.7). Output variations were due to differences in the input from PEAKM. The input table resulted in altering the output concentration curve slightly between the maximum FC and mean FC, with peak concentrations of 0.0555 to 0.0557 meq/L for the maximum and mean FC respectively. The minimum FC PEAKM input table produced more noticeable results altering the shape of the concentration curve, and elevating the peak concentration to 0.065 meq/L.

Minimum Field Capacity input from PEAKM

Maximum Field Capacity input from PEAKM



Mean Field Capacity input from PEAKM

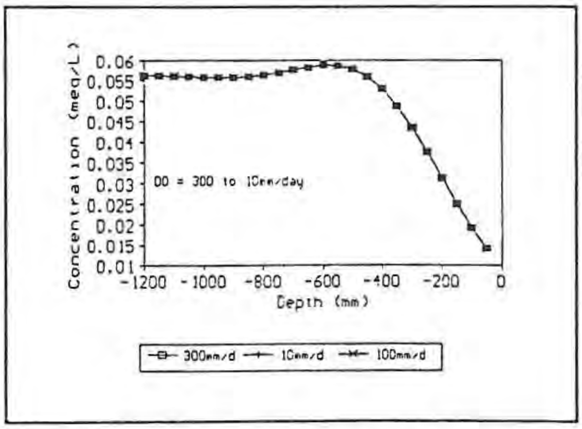


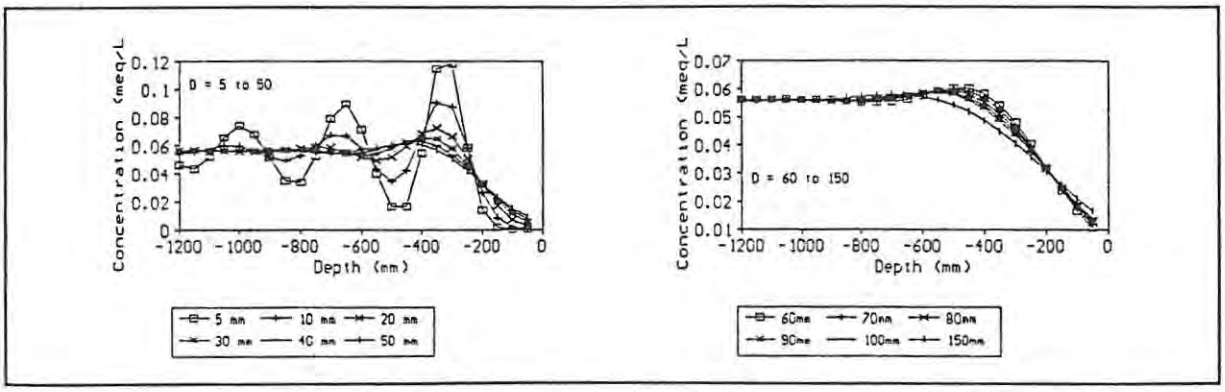
Figure 7.7. The effects of variation in Diffusion Coefficient on predicted peak depth and concentration using maximum, minimum and mean Field Capacity to determine PEAKM inputs

Dispersion Coefficient: (D)

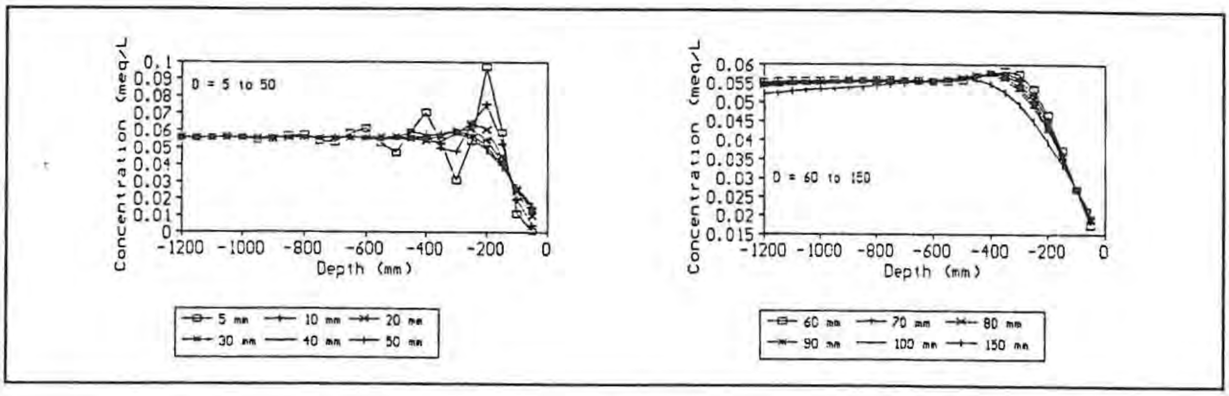
Variation in dispersion coefficient (D) between the range published in the literature (Rowell, et. al., 1967; Barry, et. al., 1985; Cameron and Wild, 1982; Rose, et. al., 1982) of 30mm to 120mm produced extremely variable model results. Incremental values for D were then entered to determine the direction and magnitude of change in output resulting from smaller changes in D. Values entered were from 10mm at intervals of 10 to 100mm, with a minimum of 5mm and maximum of 150mm (Figure 7.8). The impact of variations in low levels of D, ranging from 5 to 50 mm is high, but D becomes less effective between 60 and 150mm in influencing the peak curve. The range of D that has been determined for Chloride movement in sandy clays and clay rich soils is between 60 and 100mm (Rowell, et. al., 1967). This range has a lower effect on model predictions, so 60mm was chosen as the most appropriate for use in this study.

When the maximum field capacity (FC in kg/kg) input from PEAKM was used, the final concentration curve was less variable than with the mean FC input, and the range in concentrations of the peak reduced from 0.12 meq/L at 300mm depth below surface to 0.1 meq/L at 200mm. However, the minimum FC table produced a concentration curve unlike either the mean or maximum FC. Minimum FC resulted in peak concentrations generally higher than the mean or maximum FC, at around 0.22 meq/L, and the depth of peak is much greater, at 1000mm. Thus at low FC values, choice of D is more influential in determining the output from PEAKD than intermediate or high FC.

Mean Field Capacity PEAKM input



Maximum Field Capacity PEAKM inputs



Minimum Field Capacity PEAKM input

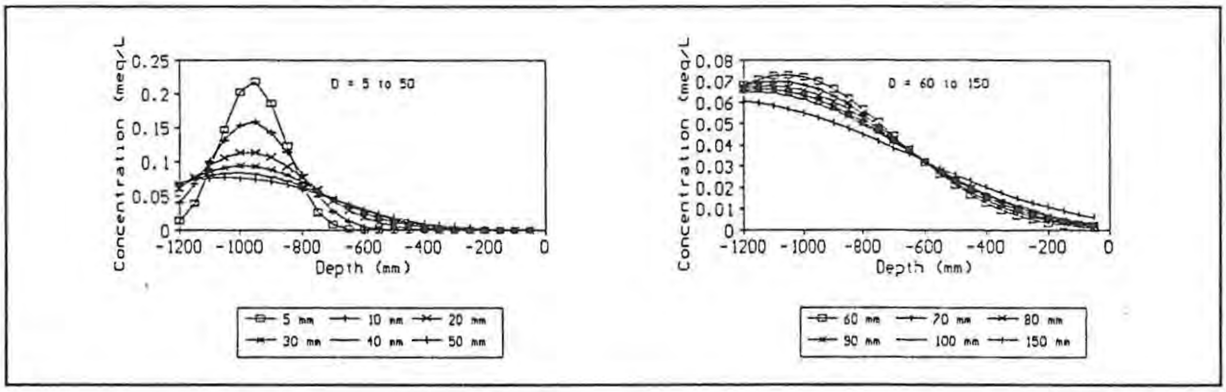
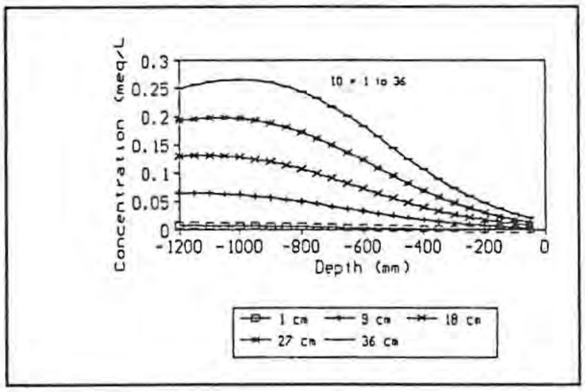


Figure 7.8. Effect of variation in Dispersion Coefficient on predicted peak depth and concentration, using maximum, minimum and mean Field Capacity to determine PEAKM inputs

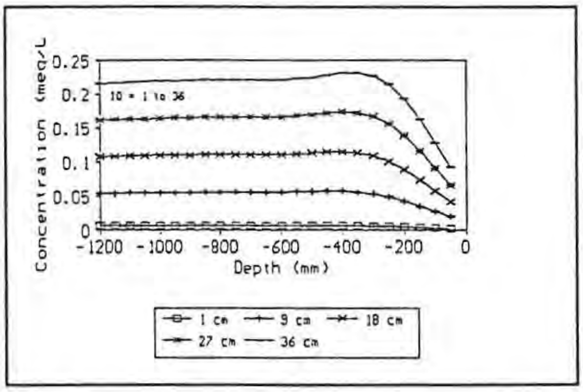
Initial depth of infiltrating water: (IO)

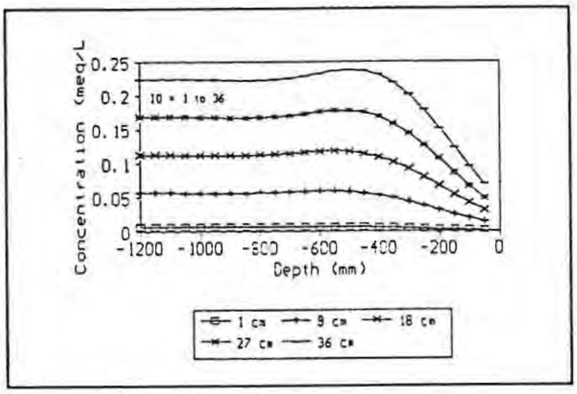
Given a field capacity of 0.3, the depth of moisture required to raise the soil moisture to field capacity within a 300mm layer was calculated to be 90mm. IO was then varied by factors of 9, so that the initial conditions would be such that 300, 600, 900 and 1200 were at field capacity. The concentration curves generated in this way using the PEAKM input table for mean FC have a similar shape, with the peak occurring at the same depth of 450mm, but are all displaced by approximately 0.05 meq/L for peak concentration (Figure 7.9). Maximum FC produces almost identical peak concentration curves, with the peak slightly shallower, at around 350mm. The minimum FC input has peak concentrations higher at all IO values, and the depth to the peak is greater, at around 1000mm.

Minimum Field Capacity input from PEAKM



Maximum Field Capacity input from PEAKM





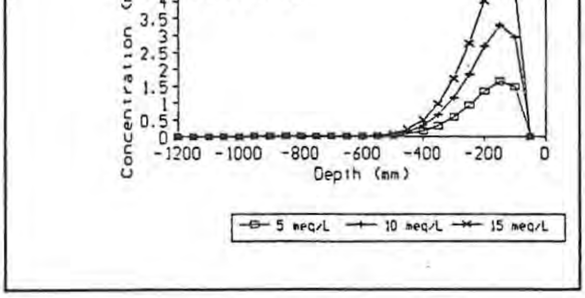
Mean Field Capacity input from PEAKM

Figure 7.9. Effect of variation in initial profile moisture on peak depth and concentration, using maximum, minimum and mean Field Capacity to determine PEAKM input

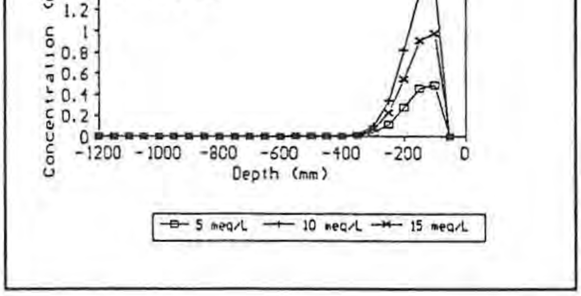
Irrigation concentration: (CO)

Figure 7.10 shows that this is an important input variable in determining the concentration of the peak. The shape of the soil concentration curve follows a similar trend for all PEAKM inputs and all irrigation concentrations (CO). However, the concentrations of the solute peaks vary between 5 and 0 meq/L.

Peak concentrations vary between 0.09 and 0.03 meq/L for the irrigation concentrations (IO) of 15 and 5 meq/L respectively when mean field capacity (FC) input from PEAKM is used. The depth of peak is similar for all concentrations of irrigation water, occurring at 550mm depth. The maximum FC input results in peak concentrations slightly lower than the mean FC input, ranging from 0.085 to 0.028 meq/L for the maximum and minimum concentrations respectively. The peak depth is slightly shallower, at around 425mm. Minimum FC input produces a concentration peak curve, with higher concentrations, ranging from 0.098 to 0.033, and a deeper peak at around 1200mm.



Minimum Field Capacity input from PEAKM



Maximum Field Capacity input from PEAKM

Mean Field Capacity input from PEAKM

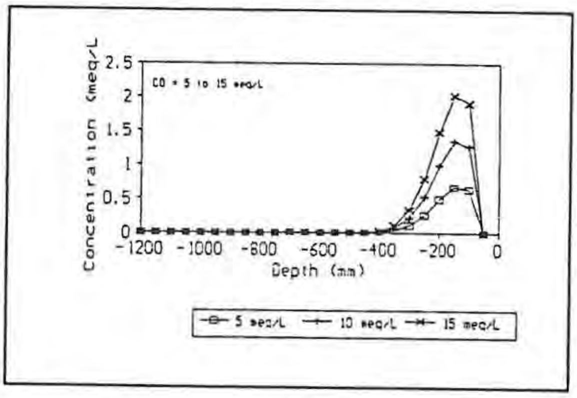


Figure 7.10. Effect of variation in irrigation concentration on peak depth and concentration, using maximum, minimum and mean Field Capacity to determine PEAKM inputs

7.3. ASSESSMENT OF THE PEAK MODEL USING FIELD DATA

The PEAK model has been applied to daily data (Barry, et. al., 1985), monthly data (Rose, et. al., 1982), and annual data (Thorburn, 1988). In this study, weekly, monthly and quarterly intervals are used to allow comparison with the LR and SODICS models.

7.3.1. PEAKM

PEAKM predictions of soil moisture will be discussed for each time increment of data entered, followed by the predicted fluxes.

Soil Moisture predicted by PEAKM

Soil moisture predicted by the model and determined from in-situ tensiometers readings are illustrated in Figure 7.11. The upper limit in PEAKM moisture is determined by the field capacity, which was set at 21% moisture by volume. PEAKM is a capacity driven model, in which the soil moisture must reach field capacity before moisture movement can occur. Above 21% moisture content, any more incoming water will move downwards, thus the soil can hold no more than 21% moisture by volume.

Figure 7.11 reflects the limit set on soil moisture content by the field capacity, where a flattening of the predicted soil moisture curve occurs at 21% soil moisture. This effect becomes more marked with increased time intervals, as indicated in Figure 7.11. The monthly time step shows that after 5 months of simulation soil moisture is constantly at field capacity, and the entire quarterly increment is at field capacity. Conditions in the soil are unlikely to remain at field capacity continuously as indicated, which implies that the field capacity of 0.21 is too low. However, under frequent irrigation the averaging effect of longer time intervals may result in soil moistures at or near field capacity.

Table 7.5. shows the decrease in accuracy of PEAKM predicted soil moisture over increasing time increments. The weekly mean simulated moisture and field moisture differ by less than 0.1%, the monthly means differ by 1.63%, and the quarterly difference is 2.12%. In practical terms these differences may be insignificant, but the trend of increasing disparity over greater times could limit the utility of the model at longer intervals. This trend is also unexpected, as the other models all showed an improvement in accuracy of prediction with increasing time intervals.

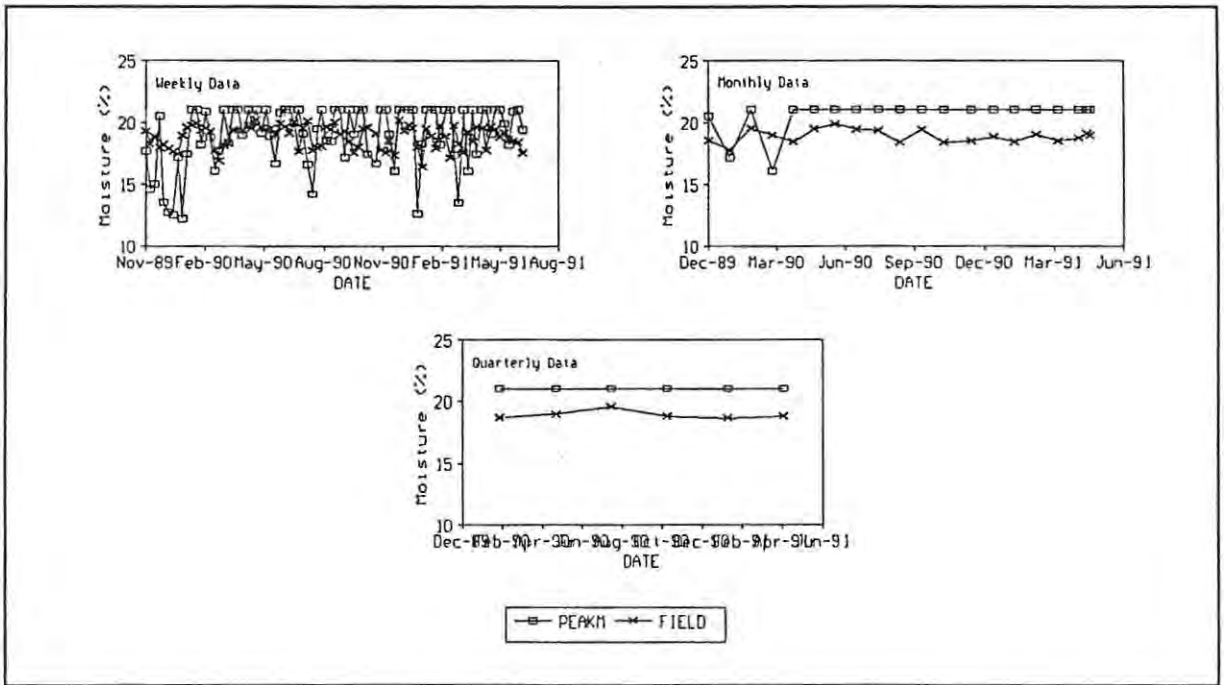


Figure 7.11. PEAKM soil moisture predictions using weekly, monthly and quarterly input data for the soil profile between 0 and 1 200mm

Soil Moisture Movement predicted by PEAKM.

The predicted leaching flux data show the opposite trend to PEAKM soil moistures. Soil moisture movement predicted by PEAKM was compared with three methods of flux determination at weekly, monthly and quarterly levels of time resolution. Results of correlations between predicted and measured flux are presented in Table 7.6.

Correlations of PEAKM flux against all determination techniques show an improvement as the time interval increases, in contrast to the trend observed between predicted and actual soil moisture. So although the ability of PEAKM to predict soil moisture is limited with greater time increments, the flux predictions seem to be enhanced.

At all time increments the lowest correlations occur between PEAKM flux predictions and flux determined using the MATRIC method, which range from 6.24% to 8.03% and 40.23% at weekly, monthly and quarterly intervals respectively (Table 7.6). This is also evident from Figures 7.12 and 7.13, where neither the variability nor the absolute rates of flux determined using the MATRIC method and PEAKM predictions are alike. PEAKM leaching flux rates are consistently higher than those obtained using MATRIC, and more variable.

Soil moisture flux determined using the MASSBAL method correlate with PEAKM flux by more than double the correlations determined between flux determined using MATRIC and predicted using PEAKM, at 26.53%, 33.50% and 70.72% for the increasing time periods. There is a similar variability in flux direction between PEAKM and the MASSBAL determined flux (Figure 7.12), although PEAKM flux is also consistently higher than that determined using the MASSBAL method. Figure 7.13 shows less compatibility in variation between PEAKM and MASSBAL determined fluxes, with a major reversal in direction of flux occurring in October, 1990.

Table 7.5. Soil Moisture (% by volume) predicted by PEAKM and measured in the field

	MAXIMUM	MINIMUM	MEAN	STD. DEV.
Weekly Data				
PEAKM	21.00	12.20	18.98	2.49
FIELD	20.26	16.40	18.86	0.89
Monthly Data				
PEAKM	21.00	16.10	20.54	1.31
FIELD	19.86	17.80	18.91	0.51
Quarterly Data				
PEAKM	21.00	21.00	21.00	0.00
FIELD	19.56	18.61	18.89	0.32

Table 7.6. Residual values (%) for predicted soil moisture flux against three methods of flux measurement

	MATRIC	WATBAL	MASSBAL
Weekly Data	6.24	50.97	26.53
Monthly Data	8.03	95.06	33.50
Quarterly Data	40.23	99.85	70.72

where
MATRIC = flux measured using differences in matric potentials
WATBAL = flux generated from the water balance approach
MASSBAL = flux generated from the mass balance approach

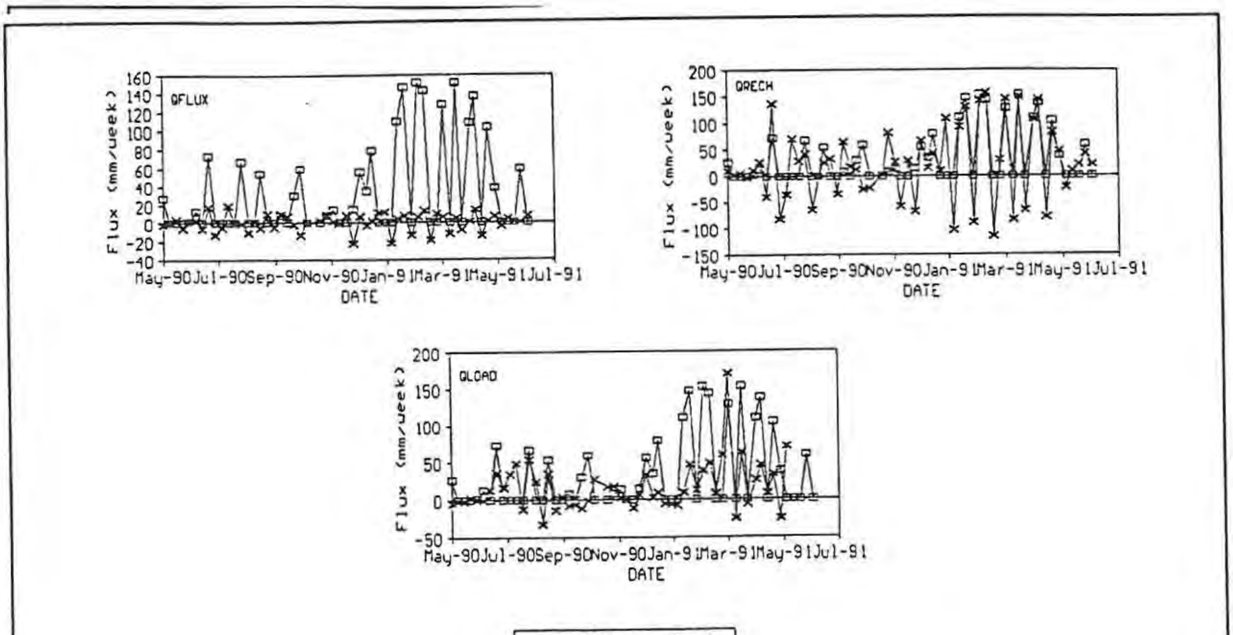


Figure 7.12. Flux predicted using PEAKM and determined using the MATRIC, WATBAL and MASSBAL methods at weekly data intervals

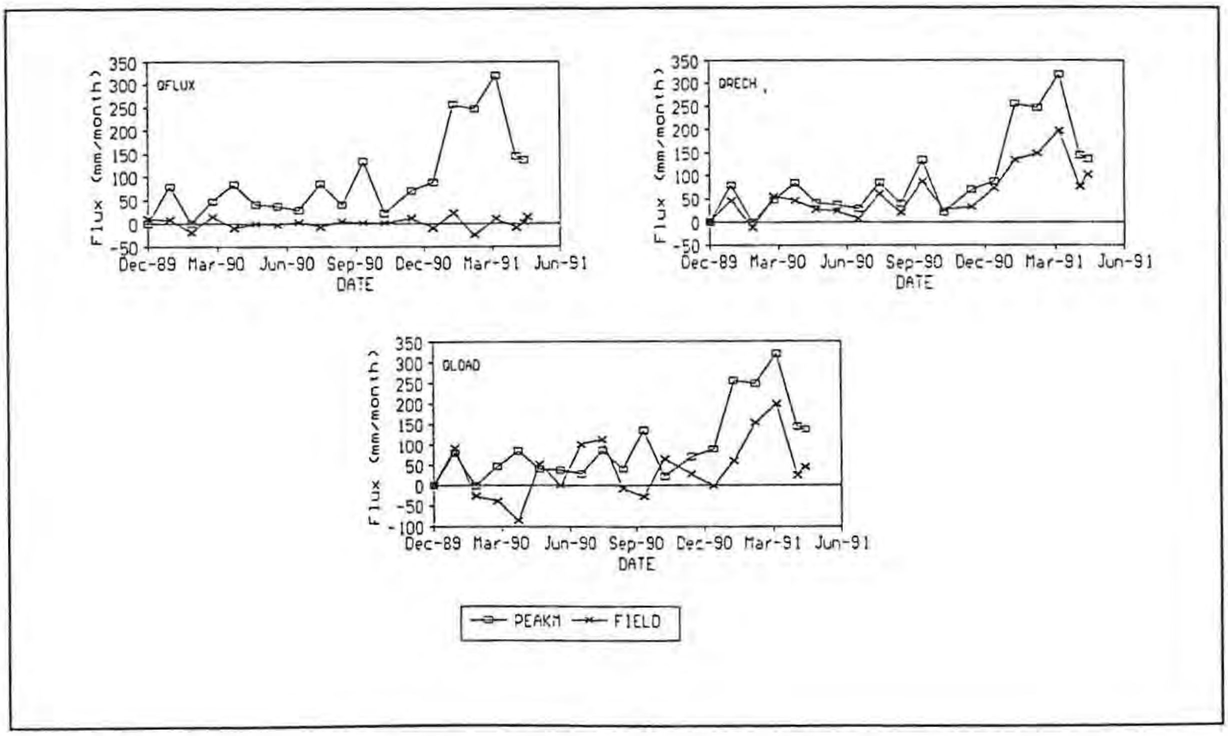


Figure 7.13. Flux predicted using PEAKM and determined using the three methods of determination at monthly data intervals, where QFLUX = MATRIC; QRECH = WATBAL and QLOAD = MASSBAL.

Flux calculated using the WATBAL method showed the highest correlations against the PEAKM flux for all time steps, with a R^2 value of 50.97% correlation at the weekly increment, 95.06% with monthly data, and a near perfect correlation of 99.86% at the quarterly interval. Both Figures 7.12 and 7.13 reflect this relationship. Figure 7.12 shows the extreme negative fluxes obtained by the WATBAL approach, which are not replicated by PEAKM. The averaging effect of increasing the time increment from weekly to monthly results in a better correlation in Figure 7.13 The consistently greater fluxes predicted by PEAKM over WATBAL are attributed to the effect of these negative fluxes on the average leaching flux measured by WATBAL. These variable levels of correlation with each technique of flux measurement must be attributed to the theoretical bases underlying each method of flux calculation.

The calculated soil moisture flux using Darcy's Law (MATRIC) is based on thermodynamic differences in the soil. These energy gradients then determine moisture movement, in combination with the hydraulic conductivity of the soil. It is been suggested that MATRIC estimates micropore water movement as the speed of adjustment of the tensiometer is too slow to detect rapid macropore flow. The low correlation between MATRIC and PEAKM flux indicates that PEAKM is not measuring micropore movement

Soil moisture flux determined using the chloride mass balance approach (MASSBAL) does not show as high a correlation with the flux predicted by PEAKM as was determined between MASSBAL and the fluxes predicted using the LR and SODICS models. This is attributed to the mechanisms represented by MASSBAL and PEAKM. MASSBAL is based of a balance of solute mass entering, leaving and stored within the soil. PEAKM uses an adapted form of water budget, where water inputs to the soil are known, and through knowledge of certain soil physical parameters, the storage of water can be estimated. The output of water is then the difference between inputs and storage. Although based on slightly different approaches, MASSBAL and PEAKM should give similar results, as they are both dependent on the capacity of the soil to retain moisture. The maximum correlation obtained of 70.71% at quarterly time intervals must not be disregarded.

The correlations between soil moisture flux measured by the water balance technique (WATBAL) and PEAKM are highest, up to 99.85% at quarterly intervals. The monthly fluxes illustrated in Figure 7.13 are closely related in absolute terms as well as showing mutual variation. The reason for the close correlation between the fluxes determined using the WATBAL method and those predicted using PEAKM is that they are both forms of the water budget. This does not necessarily prove that flux predicted by PEAKM is 99.85% accurate. It simply indicates that both methods replicate one another very well.

7.3.2. PEAKD

Output from PEAKM (Table 7.4) forms the initial input to PEAKD. The PEAKM module predicts the movement of a peak of soil moisture through the soil. The PEAKD module uses the PEAKM output to locate the solute peak, and then applies the molecular diffusion (D0) and dispersion (D) coefficients to simulate the dispersion about the peak. As both D0 and D are very difficult to quantify in the field, Rose, et. al., (1982) suggest the model must be calibrated against measured data by varying D0 and D until the best fit between simulated and measured data is determined. However, it is then difficult to evaluate the model independently, by comparing model output with data that the model has already been calibrated against.

In this study, the sensitivity analysis showed variability in the diffusion coefficient (D0) was not as influential on model results as the dispersion coefficient (D). D0 was taken to be 300cm^2/month, as in several other studies (Barry, et. al., 1985; Cameron and Wild, 1982; Rose et. al., 1982; Thorburn et. al., 1987). D was determined to have more impact on the model output, so the initial selection of D between 30 and 50mm (Cameron and Wild, 1982) was varied slightly during the application of the weekly input data. Solute concentrations in the same order of magnitude as field data were only obtained for very low values of D, between 5 and 20mm. It was then decided that 20mm would be taken for D at all time increments. The other input requirements are entered manually and listed in Table 7.7.

Table 7.7. Input parameters entered manually to PEAKD

Diffusion coefficient (D0)	Dispersion coefficient (D)	Irrigation concentration (C0)	Initial profile moisture depth (I0)	Maximum depth modelled (z)
75cm^2/week 300cm^2/month 900cm^2/quarter	20mm	143meq/L	233mm	1200mm

Input data from PEAKM at weekly, monthly and quarterly increments were read into PEAKD, together with the parameters in Table 7.7.

Soil Chloride Profiles predicted using Weekly Input Data

All correlations are weak for this time increment (Table 7.8). There is no correlation between predicted and measured Cl$^-$ concentrations at the 60 and 120 cm depths, and effectively no relationship at 90cm either, as the R^2 value of 1.04% is insignificantly low. At 30cm a correlation of 13.57% was obtained, which is much greater than at deeper levels, although too low to be considered significant.

Table 7.8. Residual values (%) of predicted against measured soil Chloride concentrations

DEPTH	WEEKLY DATA	MONTHLY DATA	QUARTERLY DATA
30CM	13.57	0.91	0.00
60CM	0.00	1.37	37.63
90CM	1.04	12.40	41.87
120CM	0.00	5.66	50.69

Variation in actual soil chloride concentrations are not reflected by the model predictions (Figure 7.14). PEAKD is designed to predict the dispersion of a solute about a peak, the depth of which is determined by PEAKM. However, actual soil concentrations at the weekly interval show no indication of a peak within the soil. Therefore it may be inappropriate to use PEAKD in conditions where there is no clear peak, as it has failed to simulate the conditions in this study where no concrentation peak exists.

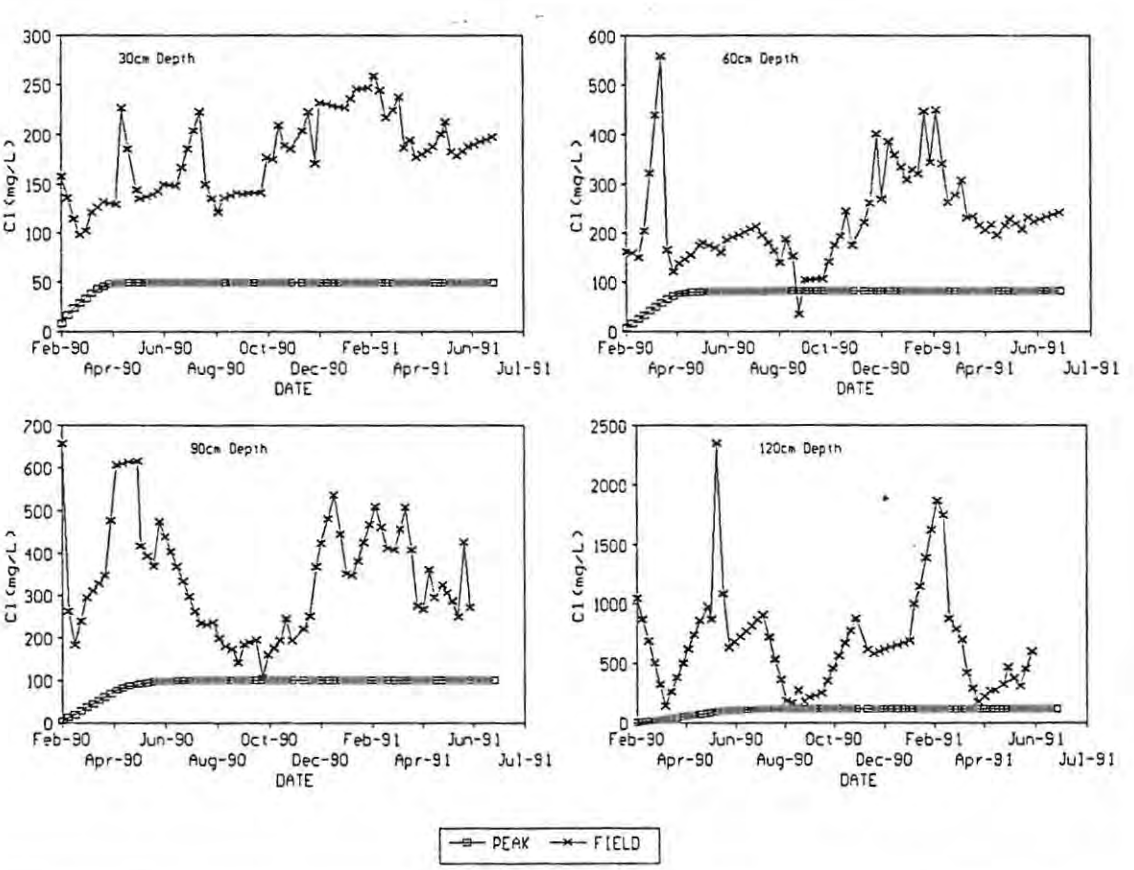


Figure 7.14. Weekly Soil Solute concentrations predicted by PEAKD and measured in situ.

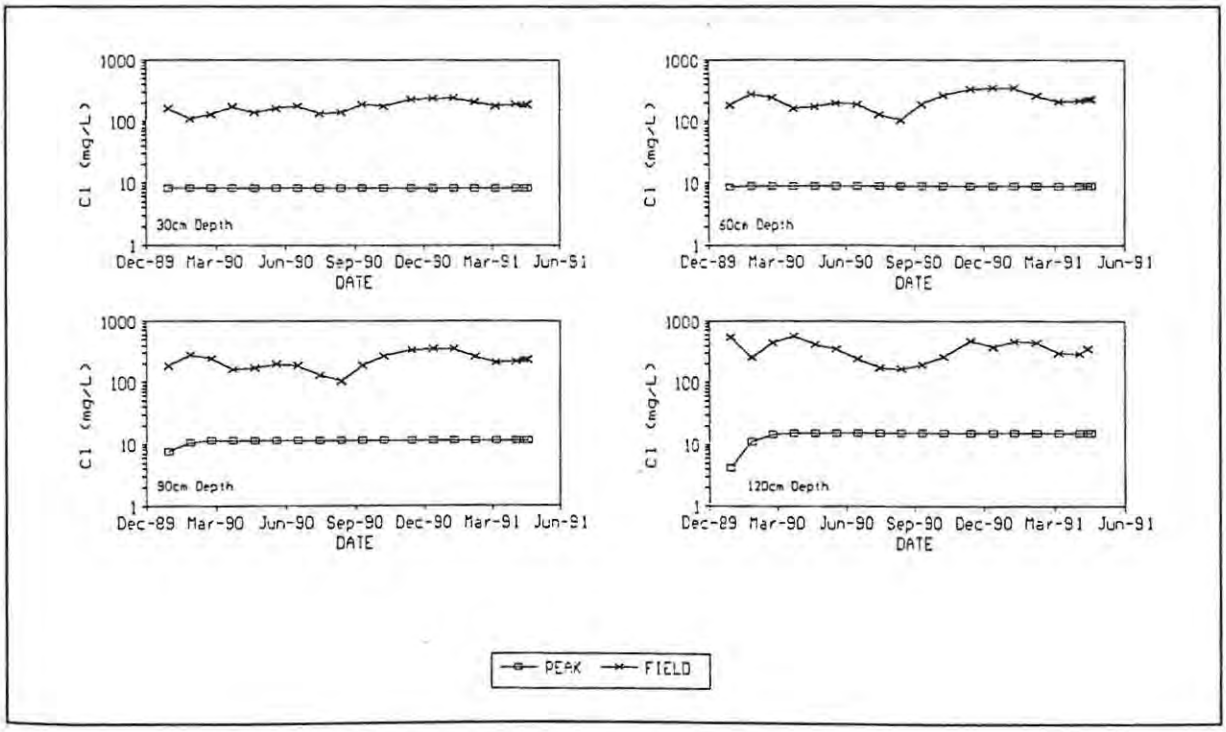


Figure 7.15. Monthly Soil Solute concentrations predicted by PEAKD and measured in situ

Monthly Input Data

The correlations obtained when PEAKD is applied to the monthly data between predicted and measured soil chloride concentrations are slightly greater than those obtained for the weekly increments, at all depths except 30cm (Table 7.8). Maximum correlation of 12.4% occurs at 90cm, followed by 5.66% and 1.37% at 120cm and 60cm respectively. As with the weekly data, these correlations remain too low for any significance.

Quarterly Input Data

According to Table 7.8, correlations between predicted and measured soil Chloride concentrations show a great improvement at this interval, except for the 30cm depth which shows no relationship at all. The 60cm depth shows a 27-fold increase in correlation over the monthly data, to a R^2 of 37.63%. A smaller increase of 3-fold occurs at 90cm to 41.87% and an order of magnitude improvement in correlation occurs at 120cm, where the R^2 reaches 50.69%.

The average correlation for the profile is 32.55%, which is not a high degree of similarity. Even the greatest R^2 achieved indicates that only 50% of the variability in field soil concentrations is accounted for by the PEAKD output. However, considering the difficulty in measuring the model chemical inputs of D, and the high inherent field variability in soil solute parameters, a 50% maximum may be the best estimate obtainable using the PEAKD module.

A graphical representation of the Quarterly solute profiles reveals the correlations given in Table 7.8 are misleading (Figure 7.16). PEAKD does not predict any variation in concentration at all for any depth over the study period. Field data shows an increase in concentration with depth from 30cm to 120cm, and this trend is also followed by the PEAKD output. However, the range of concentration predicted by the model is far greater than reality, with the 30cm concentrations underpredicted by more than an order of magnitude. The 60cm depth is the closest in absolute terms to field conditions but both the 90cm and 120cm depths are greatly overpredicted, by approximately 5-fold.

The results suggest that PEAKD is less successful in predicting soil Chloride concentrations than PEAKM is in predicting moisture flux.

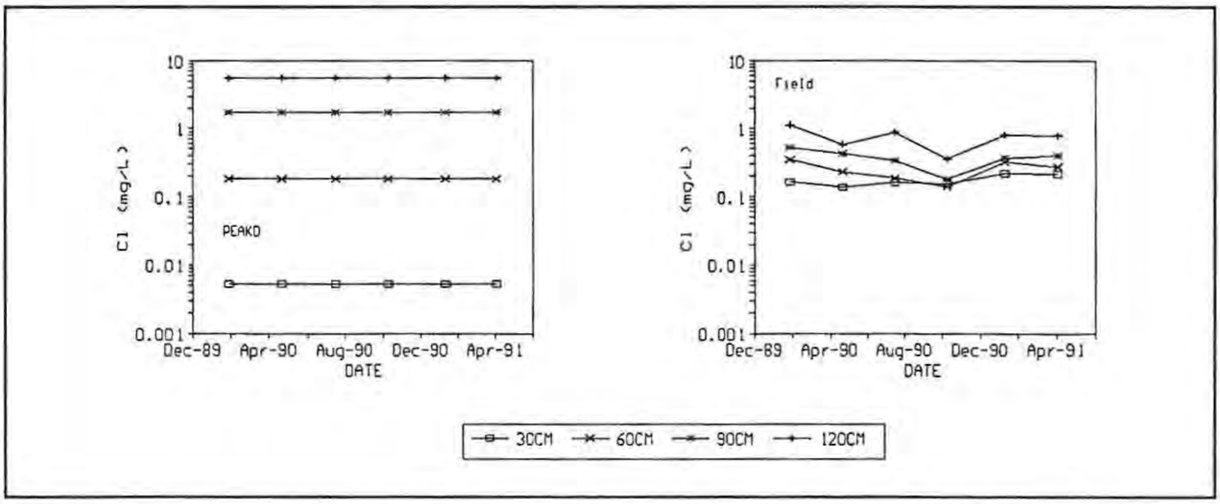


Figure 7.16. Quarterly Soil Solute concentrations predicted by PEAKD and measured in situ

7.4. MODEL EVALUATION

The PEAK model was evaluated in two parts, as the first section (PEAKM) provides the input for the second (PEAKD). Results from PEAKM indicate a high correlation between predicted and soil moisture movement measured using the mass balance and water budget approaches. As the PEAK model is derived from the water budget approach it is NOT surprising that the best correlations occur with field data measured using this technique as well. It is concluded that the processes describing the water budget as calculated by WATBAL in the field soil investigated were simulated by PEAKM at a high degree of accuracy.

The PEAKD section of the PEAK model is less successful in predicting soil solute concentrations. As the agreement between PEAKM and field data has already been established, the input from the PEAKM module cannot be accepted as the source of this error. It must be concluded that either soil solute processes described by PEAKD are not sufficient to account for solute movement, or the choice of input parameters for PEAKD was inadequate. In the case of the latter, further field measurements of such variable and elusive soil properties such as the diffusion and dispersion coefficients would render the model unacceptable for routine management use, and limited as a research tool.

The input requirements of the PEAK model are intensive, and computer time and expertise are required to run the model. PEAKM was able to simulate temporal trends in soil moisture and moisture flux at a satisfactory degree of accuracy, reaching 99.85% correlation with flux measured using the water balance technique. However, PEAKD was unable to replicate soil solute concentrations. While the PEAKM section may be used as a management tool where detailed data are available, the utility of PEAKD is inhibited by the low predictive accuracy, and the need for expensive field measurement of chemical parameters that are not easily quantified.

CHAPTER EIGHT

8. CONCLUSION

Increasingly, irrigation managers are requiring readily accessible, and easily applicable tools to assist in optimal scheduling of irrigation water. Maximum crop production and long term sustainable yields are the aims of irrigated agriculture, together with the optimal use of finite water resources. A tool that can assist in attaining these goals is the hydrosalinity model, which permits the testing of different irrigation scenarios. A management strategy may be assessed in this manner, without the need for potentially expensive trial and error.

A number of hydrosalinity models have been derived for use in irrigation management with varying levels of theoretical complexity, input data requirements and detail of output predictions. Accuracy of prediction also varies between models, so choice of model must depend on the requirements of the manager and available data and technology.

The hydrosalinity models evaluated in this study are all developed for the purpose of irrigation management, and can be applied in a number of contexts. Irrigation timing and amounts required can be determined using the LR (Leaching Requirement) model if the concentration of the irrigation water is known along with the soil solute concentration at a specified depth within the profile, usually the lowest root depth.

The Leaching Requirement concept is a simple relationship between incoming and outgoing water and solutes, and can be applied without the need for computer technology. The soil system is considered to be in steady state, and chemical interactions are not accounted for. The model was originally intended to ameliorate problems associated with salinised soils. If the soil salinity required by the crop grown is known, then the amount of irrigation water of known quality that must leach below the root zone to retain the soil at this optimal salinity can be determined. As results obtained from this model do not need detailed interpretation it is directly amenable to the extension officer, irrigation manager or other user without specialised training.

The assessment of the LR model against field data shows a high degree of correspondence between predicted and measured values. The steady state restriction appears to have little affect on the accuracy of this model to the area of application, which is due to the continuous crop cover and long term history of irrigation in the Lower Coerney river valley. Steady state conditions are likely to predominate in older irrigation schemes, and the use of the LR model may thus be best for such schemes. Where new areas are irrigated, and where changing cropping practises are used, transient conditions will render the LR model less accurate than was found in this study.

Effects of long term irrigation on the accumulation of salts within the soil can be predicted using the SODICS model, if soil moisture and solute concentrations are known at two separate times. SODICS also requires information about the physical characteristics of the soil, irrigation water quality and application amounts. This model is based on a mass balance approach, as with the LR model, of incoming and outgoing water and solutes. Unlike the LR model, SODICS incorporates the continuity equation which allows changes through time to be considered, and hence relieves the steady state restriction of the simpler model.

The accuracy of prediction of SODICS when compared with field data is high, and almost identical to that shown by the LR model. The greater input data requirements and computing expertise necessary for the use of SODICS is not warranted in this area, where the simpler model produces an equivalent degree of accuracy of results. However as SODICS is not restricted by steady state conditions this model may be applied to newly irrigated areas, and where variable crops are grown, with greater confidence than the steady state LR model.

The PEAK model is intended to provide predictive information about the soil moisture, soil moisture flux and solute concentration within the soil profile, to a depth specified by the user. This model consists of two parts, PEAKM predicts the soil moisture regime and PEAKD predicts the diffusion and dispersion of a solute within the soil moisture output from PEAKM. The theoretical basis of the PEAK model is the convective-dispersion equation, and the data requirements are correspondingly high. Computing time and expertise are essential for the use of this model.

The accuracy of prediction of PEAK was assessed against field data in two parts. PEAKM predictions of soil moisture showed a high degree of correspondence with field measurements, and soil moisture flux was even more accurately predicted than either the LR model or SODICS. For detailed information of soil moisture and its movement, PEAKM gave the best results in this study. However, the PEAKD predictions of soil solute concentrations were less accurate. Data requirements were such that values for dispersivity and diffusion coefficients from previous studies were applied as these could not be measured within the scope of this study. Soil solute concentration results compared poorly with field data, which detracted from the high correlations obtained from PEAKM. PEAKM may be used independently of PEAKD, but although a high level of detail is predicted the amount of input data required restricts the application of this model to areas having intensive sampling programs.

Overall the LR model is considered the most useful for management of irrigation scheduling as it requires the least amount of input information, a low level of interpretation of results and computing time is not necessary. The predictions from SODICS are similar to the LR model, and thus the greater input requirements are not warranted except where transient conditions may exist. SODICS further requires a computer for operation. Although the PEAKM module of the PEAK model successfully predicted up to 99% of field soil moisture variability, the inability of the second module PEAKD to accurately predict solute dispersion and diffusion is a disadvantage in the application of this model. PEAK also requires the most detailed information of all models assessed, and cannot be used without a computer.

8.1 FUTURE RESEARCH

The scope and detail of this study are constrained by both time and resource restrictions. Besides an overall extension of the evaluation to consider different models and other localities, a number of aspects which could provide potentially valuable information were identified. These areas could not be investigated in the present study, and are suggested for further research.

* Measurement of chemical parameters not routinely available, including molecular diffusion and dispersion coefficients on different soil types and under different soil physical characteristics such as texture, bulk density, porosity, etc.

* Investigate the occurrence of macropore and lateral flow in more detail, possibly using dyes to trace moisture movement through the soil.

* Quantify evapotranspiration rates through the use of lysimeters.

* Verify the existence of steady state conditions in the soil under older orchards, as opposed to newly developed fields and areas where variable cropping is carried out.

* Adapt SODICS to read variable irrigation inputs, and adapt both SODICS and PEAKD to incorporate variable irrigation water quality inputs.

* Apply all models over a wider area, initially including the entire Sundays River Irrigation area, and then other irrigation schemes throughout Southern Africa.

* Apply the models to the new area currently being developed. This will provide an ideal testing opportunity, as the soil can be sampled before any irrigation whatsoever occurs. Model predictions under rapidly changing conditions will then be tested, as there will be a marked adjustment to the new irrigation water inputs during the expansion of the irrigation scheme into new land.

* Use the models, especially the LR model, as intended to be applied, in a prescriptive manner for treating problems in the soil. Over-irrigation, salinisation and drainage problems can be addressed using these models, especially in the surrounding area of the Lower Coerney River where this evaluation has been carried out.

The primary aim of this study is to evaluate three selected hydrosalinity models for use in irrigation management within the Lower Coerney River Valley. The results of sensitivity analyses conducted on the model parameters are presented, followed by an assessment of model predictions against field data. Each model is then evaluated in terms of its data requirements, ease of application and accuracy of output predictions. Of the three models it is concluded that the Leaching Requirement (LR) model is the most useful in terms of theoretical simplicity, data accessibility, ready applicability and prediction accuracy against the data in this study. The level of accuracy attained can not be generalised to other areas with confidence, however, as the characteristics of the study area are not universal. The Lower Coerney River area is an established irrigation scheme where irrigated agriculture has been carried out for more than 30 years. It is reasonable to expect that steady state or near steady state conditions prevail, under which the Leaching Requirement approach is applicable. In newly developed irrigation schemes or under changing agricultural land use, such steady conditions are unlikely to occur, and the LR model may have less utility.

9. REFERENCES

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APPENDIX A

```
C                     PROGRAM SODICS
C
C       Fortran version of program SODICS developed by Peter Thorburn
C       of the Soil Conservation Research Branch of the
C       Queensland Department of Primary Industries
C
C       A program to model Solute Dymnamics in Irrigated Clay Soils.
C       Based on a model of Rose et. al.(1979), Irrig. Sci. 1:77-87.
C
C... VARIABLE LIST
C   =============
C
C      Z     = rooting depth.
C      I     = annual depth of irrigation water applied.
C      C     = chloride conc. of irrigation water.
C      T     = time from initial chloride measurement.
C      L     = leaching flux.
C      CL0   = profile Cl conc. mean to Z,time = T0.
C      CLT   = profile Cl conc. mean to Z,time = T1.
C      CLZ   = profile Cl conc. at Z,time = T1.
C      S0    = profile Cl conc. at 'field capacity',time = T0.
C      ST    = profile Cl conc. at 'field capacity',time = T1.
C      SF    = profile Cl conc. at 'field capacity',at steady state.
C      ADM   = air dry moisture (%).
C      WM0   = profile 'field capacity' (g/g) mean to Z,time = T0.
C      WMT   = profile 'field capacity' (g/g) mean to Z,time = T1.
C      THE   = profile 'field capacity' (cm^3/cm^3) mean to Z.
C      BD    = bulk density (g/cm^3), mean to Z.
C      P     = non-dimensional parameter, eqn. 2.
C      C1    = calculated constant.
C      C2    = calculated constant.
C      C3    = calculation constants.
C      H     = Newton - Raphson approximation term.
C      FNLE  = f(L), eqn. 3.
C      FNDLE = f'(L).
C      FNS   = f(T), eqn. 3.
C
C
C
C... VARIABLE DEFINITIONS
C   ====================
C
      INTEGER*4  LINNO,T,Z,UNITS,I,Err_stat

C
       REAL*8 C,L,CL0,CLT,CLZ,S0,ST,SF,WM0,WMT,THE,BD,P,C1,C2,C3,
     +     H,CX,ADM0,ADMT,ADMZ,FL,DL
C
```

```
      CHARACTER* 1 OPT1,OPT2,OPT3,OPT4
C
      CHARACTER*20 SITE
C
      DATA OPT1/'Y'/
C
C... SETTING UP FILES
C    =================
C
      OPEN (UNIT = 6)
C
10    PRINT*,'Enter name for output file'
      PRINT*,' '
      PRINT*,' '
      READ (5,'(A1)'),END=10) FILE_OUT
      CALL u_cls
      OPEN (7,FILE='FILE_OUT ',FORM='FORMATTED',STATUS='NEW',
     +          IOSTAT = Err_stat, ERR = 20)
      GOTO 40
C
20    CALL ERR_LST (Err_stat)
      GOTO 10
C
C... PARAMETER INPUT
C    ================
C
40    PRINT *,' '
      PRINT *,'Please enter site idensifier'
      READ (5,'(A30)',END= 40,ERR=40) SITE
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
50    PRINT *,' '
      PRINT*,' What units are soil Cl values expressed as: '
      PRINT *,'       1/ gm NaCl/gm soil'
      PRINT *,'       2/ ugm Cl/gm soil'
      PRINT *,'       3/ gm Cl/100 gm soil'
      PRINT *,'       4/ mg Cl/ml'
      PRINT *,' '
      PRINT *,'Enter the correct option number'
      READ (5,*,END=50,ERR=50) UNITS
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
60    PRINT *,' '
      PRINT *,'Enter rooting depth (mm) '
      READ (5,*,END=60,ERR=60) Z
      CALL u_cls
```

```
      IF (OPT.NE.'Y') GOTO 200
C
70     PRINT *,' '
      PRINT *,' Enter mean Cl at time zero'
      READ (5,*,END = 70,ERR=70) CL0
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
80     PRINT *,' '
      PRINT *,' Enter percent ADM at time zero '
      READ (5,*,END=80,ERR=80) ADM0
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
90     PRINT*,' '
      PRINT*,' Enter mean profile Cl at time T '
      READ (5,*,END =90,ERR=90) CLT
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
100    PRINT *,' '
      PRINT *,'Enter mean profile ADM at time T'
      READ (5,*,END =100,ERR=100) ADMT
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
110    PRINT *,' '
      PRINT *,'Enter Cl conc. at depth Z for time T'
      READ (5,*,END=110,ERR=110) CLZ
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
120    PRINT *,' '
      PRINT *,'Enter ADM at depth Z for time T'
      READ (5,*,END=120,ERR=120) ADMZ
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
130    PRINT *,' '
      PRINT *,' Enter mean profile field capacity at time 0 (G/G)'
      READ (5,*,END=130,ERR=130) WM0
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
140    PRINT *,' '
      PRINT *,' Enter mean profile field capacity at time T (G/G)'
      READ (5,*,END=140,ERR=140) WMT
      CALL u_cls
```

```
      IF (OPT.NE.'Y') GOTO 200
C
150   PRINT *,' '
      PRINT *,' Enter mean profile bulk density'
      READ (5,*,END=150,ERR=150) BD
      call u_cls
      IF (OPT.NE.'Y') GOTO 200
C
160   PRINT *,' '
      PRINT *,' Enter annual water application '
      READ (5,*,END=160,ERR=160) I
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
170   PRINT *,' '
      PRINT *,'Enter Cl concentration of water (meq/l)'
      READ (5,*,END=170,ERR=170) C
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
180   PRINT *,' '
      PRINT *,' Enter time period of trial (years)'
      READ (5,*,END=180,ERR=180) T
      CALL u_cls
      IF (OPT.NE.'Y') GOTO 200
C
C
200   OPT3 = 'Y'
      PRINT *,' '
      PRINT *,' '
      PRINT *,' 1/ Site identifier                          : ',SITE
      PRINT *,' 2/ Chemistry units                           : ',UNITS
      PRINT *,' 3/ Rooting depth (mm)                         : ',Z
      PRINT *,' 4/ Mean profile Cl at time zero                 : ',CL0
      PRINT *,' 5/ Mean profile percent ADM at time 0       : ',ADM0
      PRINT *,' 6/ Mean profile Cl at time T                    : ',CLT
      PRINT *,' 7/ Mean profile percent ADM at time T        : ',ADMT
      PRINT *,' 8/ Cl conc at time T and depth Z             : ',CLZ
      PRINT *,' 9/ ADM at time T and depth Z                  : ',ADMZ
      PRINT *,'10/ Mean prof. field capacity at T = 0 (G/G)  : ',WM0
      PRINT *,'11/ Mean prof. field capacity at T = T (G/G)  : ',WMT
      PRINT *,'12/ Mean prof. bulk density at time T = 1      : ',BD
      PRINT *,'13/ Annual water application                   : ',I
      PRINT *,'14/ Cl conc. of water (gm Cl/100 gm soil)      : ',C
      PRINT *,'15/ Time period of trial (years)         : ',T
      PRINT *,' '
      PRINT *,' Check: are the above entered data correct (Y/N)?'
      READ (5,'(A1)',END=200,ERR=200) OPT
```

```
      CALL u_cls
C
      IF (OPT.EQ.'Y'.OR.OPT.EQ.'y') GOTO 300
C
C
210   PRINT *,' '
      PRINT *,' '
      PRINT *,' '
      PRINT *,' 1/ Site identifier                         : ',SITE
      PRINT *,' 2/ Chemistry units                          : ',UNITS
      PRINT *,' 3/ Rooting depth (mm)                        : ',Z
      PRINT *,' 4/ Mean profile Cl at time zero              : ',CL0
      PRINT *,' 5/ Mean profile percent ADM at time 0        : ',ADM0
      PRINT *,' 6/ Mean profile Cl at time T                 : ',CLT
      PRINT *,' 7/ Mean profile percent ADM at time T         : ',ADMT
      PRINT *,' 8/ Cl conc at time T and depth Z            : ',CLZ
      PRINT *,' 9/ ADM at time T and depth Z                 : ',ADMZ
      PRINT *,'10/ Mean prof. field capacity at T = 0 (G/G)  : ',WM0
      PRINT *,'11/ Mean prof. field capacity at T = T (G/G)  : ',WMT
      PRINT *,'12/ Mean prof. bulk density at time T = 1      : ',BD
      PRINT *,'13/ Annual water application                  : ',I
      PRINT *,'14/ Cl conc. of water (gm Cl/100 gm soil)      : ',C
      PRINT *,'15/ Time period of trial (years)         : ',T
      PRINT *,' '
      PRINT *,' Enter the incorrect line number'
      READ (5,*,END=150,ERR=160) LINNO
      CALL u_cls
      GOTO (40,50,60,70,80,90,100,110,120,130,140,150,160,170,180) LINNO
C
C... WRITE INPUT DATA TO FILE
C    ==========================
C
300   CONTINUE
      WRITE (7,620) SITE
      WRITE (7,630) UNITS
      WRITE (7,640) Z
      WRITE (7,650) CL0
      WRITE (7,660) ADM0
      WRITE (7,670) CLT
      WRITE (7,680) ADMT
      WRITE (7,690) CLZ
      WRITE (7,700) ADMZ
      WRITE (7,710) WM0
      WRITE (7,720) WMT
      WRITE (7,730) BD
      WRITE (7,740) I
      WRITE (7,750) C
      WRITE (7,760) T
```

```
C
      IF (UNITS.EQ.1) CX = 1.71 * 10000
      IF (UNITS.EQ.2) CX = 2.82 * 0.01
      IF (UNITS.EQ.3) CX = 2.82 * 100
      IF (UNITS.EQ.4) CX = 2.82 * 10
C

      P = CLZ / CLT
      THE = WMT * BD
      IF (I.EQ.0.0) I=1
      C1 = I * C / P
      C2 = (T * P) / (Z * THE)
      C3 = P / (Z * THE)
C
C...  Conversion of Cl 1:5 to Wfc.
C     ================================
C

      CLZ = CLZ * (1 + ADMZ / 100)
      CLT = CLT * (1 + ADMT / 100)
      CL0 = CL0 * (1 + ADM0 / 100)
      S0 = CL0 * CX / WM0
      ST = CLT * CX / WMT
C
C ... SOLUTION FOR L
C      ===============
C
C        First approximation of solution for L.
C
C        F(L) is solved with successively greater values of L
C        until F(L) is < 0 . This value is then used as a first
C        approximation for the Newton - Raphson iteration.
C
      L = -305
310   L = L + 10
C
      FL = S0 - ST + ((C1 / L) - S0) * (1 - EXP(-C2 * L))
      IF (FL.GT.0) GOTO 310
      IF (L.LT.0) L = L - 10
C
C...  Newton - Raphson solution for leaching flux.
C
C         The initial guess is successively improved
C        by the term H = -F(L) / F'(L).
C
      PRINT*, 'First guess L is  ', L,' Continuing -'
320   FL = S0 - ST + (C1 / L - S0) * (1 - EXP(-C2 * L))
      DL = EXP(-C2 * L) * (C1 / L * (C2 / L - 1 / L) - C2 * S0)
```

```
     +        - C1 / (L * L)
      H = -FL / DL
      L = L + H
      IF (ABS(H).GT. 0.001) GOTO 320
      PRINT*,'Leaching flux = ', L
      WRITE (7,770) L
      SF = C1 / L
      CLF = SF * WMT / CX
C
C ..... SIMULATION AND OUTPUT
C       ======================
C
330  PRINT*,' '
      PRINT*,' DO YOU WISH TO SIMULATE TO EQUILIBRIUM (Y/N)?'
      PRINT*,' '
      READ (5,'(A1)',END=330) OPT2
      CALL u_cls

C
C
      WRITE (6,800)
      WRITE (6,810)
      WRITE (7,800)
      WRITE (7,810)
C
      DO 340 T = 0,200
C        T = J
         ST = S0 + (C1 / L - S0) * (1 - EXP(-C3 * T * L))
         CLT = ST * WMT / CX
         WRITE (6,820)      T, ST, CLT
         WRITE (7,820) T,ST,CLT
         IF (ABS(ST-SF).LT.0.001) GOTO 350
         IF (OPT2.EQ.'N'.OR.OPT2.EQ.'n') GOTO 350
340  CONTINUE
C
C
350  CONTINUE
      PRINT*,' '
      PRINT*,' '
      PRINT*,' Do you wish to model another site (Y/N)?'
      PRINT*,' '
      READ (5,'(A1)',END=350) OPT3
      IF (OPT3.EQ.'N'.OR.OPT3.EQ.'n') GOTO 370
C
 360 PRINT*,' '
      PRINT*,'Do you wish to change standard input (Y/N)?'
      READ (5,'(A1)',END=360) OPT4
C    IF (OPT4.EQ.'Y'.OR.OPT4.EQ.'y') GOTO 200
```

```
      CALL u_cls
      GOTO 10
  370 CONTINUE
C
      PRINT*,' PROGRAM TERMINATED'
      CLOSE (7)
C
C... WRITE FORMAT STATEMENTS
C    ========================
C
600   FORMAT ('MODEL SODICS INPUT DATA')
620   FORMAT (' FOR SITE  : ',A20)
630   FORMAT (' CHEMISTRY DATA INPUT UNITS               : ',I6)
640   FORMAT (' ROOTING DEPTH (mm)                       : ',I6)
650   FORMAT (' MEAN PROFILE Cl AT TIME ZERO             : ',F6.4)
660   FORMAT (' MEAN PROFILE PERCENT ADM AT TIME 0       : ',F6.2)
670   FORMAT (' MEAN PROFILE CL AT TIME T                : ',F6.4)
680   FORMAT (' MEAN PROFILE PERCENT ADM AT TIME T       : ',F6.2)
690   FORMAT (' Cl CONC AT TIME T AND DEPTH Z            : ',F6.4)
700   FORMAT (' ADM AT TIME T AND DEPTH Z                : ',F6.2)
710   FORMAT (' MEAN PROF. FIELD CAPACITY AT T = 0 (G/G) : ',F4.2)
720   FORMAT (' MEAN PROF. FIELD CAPACITY AT T = T (G/G) : ',F4.2)
730   FORMAT (' MEAN PROF. BULK DENSITY AT TIME T = 1    : ',F4.2)
740   FORMAT (' ANNUAL WATER APPLICATION                 : ',I6)
750   FORMAT (' Cl CONC. OF WATER (gm Cl/100 gm SOIL)    : ',F6.2)
760   FORMAT (' TIME PERIOD OF TRIAL (YEARS)             : ',I6)
770   FORMAT (' MEAN LEACHING FLUX FOR TRIAL PERIOD      : ',F6.2)
C
800   FORMAT (' Time        S(T)        Cl(T)')
810   FORMAT ('(years)    (meq/l)     (gCl/100g)')
820   FORMAT (I5,7X,F9.4,5X,F9.4)
830   FORMAT (I1,I4,F6.3,F6.2,F6.3,F6.2,F6.3,F6.2,F6.2,F6.2,F6.2,
     +         I6,F6.1,I6)
C
C
      END
C*****************************************************************
C*****************************************************************
C
C
      SUBROUTINE ERR_LST (Err_stat)
C
      INTEGER * 4 Err_stat
C
      IF (Err_stat.EQ.6413) THEN
         WRITE (*,'(A\)') ' File already connected to different unit - '
C
         ELSE IF (Err_stat.EQ.6414) THEN
```

```
         WRITE (*,'(A\)') ' Access not allowed - '
C
      ELSE IF (Err_stat.EQ.6415) THEN
         WRITE (*,'(A\)') ' File already exists - '
C
      ELSE IF (Err_stat.EQ.6416) THEN
         WRITE (*,'(A\)') ' File not found - '
C
      ELSE IF (Err_stat.EQ.6417) THEN
         WRITE (*,'(A\)') ' Too many open files - '
      END IF
C
      WRITE (*,'(A\,I5)') ' Error number :\a'C, Err_stat
      WRITE (*,'(A1)')
      WRITE (*,'(A1)')
      Err_stat = 0
      RETURN
      END
```

APPENDIX B

```
C...   PROGRAM PEAKM
C
C... Fortran version of program developed BY PETER THORBURN
C    of the Soil Conservation Research Branch of the
C    Queenslans Department of Primary Industries
C
C... A Program to calculate the movement of a solute concentration
C    peak through the soil during a series of infiltration and
C    evapotranspiration events, based on the model of Rose et. al., 1982
C
C
C... VARIABLE LIST
C    =============
C
C    N         = number of time events
C    T         = time events
C    I(T)      = depth of infiltrating rain or irrigation water
C    E(T)      = depth of evapotranspiration
C    R(T)      = depth of roots
C    P(T)      = depth of penetration of solute concentration peak
C    DP(T)     = difference in P with each event
C    J         = constant (proportion of E which is assumed to occur
C                  before I)
C    G         = constant (either R or P)
C    THETA(T)  = volumetric water content
C    DM        = difference in soil moisture content with each event
C    THEFC     = field capacity
C    CF        = crop factor for adjusting evaporation
C
C
C... VARIABLE DECLARATION
C    ====================
C
     INTEGER  T,N,CC
C
     REAL  I(0:100),E(0:100),R(0:100),P(0:100),F(100),
    +      DP(0:100),THETA(0:100),THEFC,J,CF,AE(100),LEACH(100)
C
C
     DATA OPT/'Y'/,CC/66/
C
     CHARACTER*25 File_In, File_Out, PeakD_In
C
C... OPEN DATA FILES
C
     OPEN (5)
     OPEN (6)
C
```

```
C
10   PRINT *,' '
     PRINT *,' '
     PRINT *,'Please enter name of input data file'
     PRINT *,' '
     READ (5,'(A1)'), END = 10 ) File_In
     CALL u_cls
     OPEN (7,FILE = 'File_In ',FORM = 'FORMATTED', STATUS = 'OLD',
                    IOSTAT = Err_stat, ERR = 20)
     GOTO 30
C
20   CALL ERR_LST (Err_stat)

30   PRINT *,' '
     PRINT *,' '
     PRINT *,'PLEASE ENTER NAME FOR OUTPUT DATA FILE'
     PRINT *,' '
     READ (5,'(A1)'), END = 20 ) File_Out
     CALL u_cls
     OPEN (8,FILE = 'File_Out', FORM = 'FORMATTED', STATUS = 'NEW')
                    IOSTAT = Err_stat, ERR = 40
     GOTO 50
C
40   CALL ERR_LST (Err_stat)
     GOTO 30
C
50   PRINT *,' '
     PRINT *,' '
     PRINT *,'PLEASE ENTER NAME FOR PEAKD INPUT DATA FILE'
     PRINT *,' '
     READ (5,'(A1)'), END = 20) PeakD_In
     CALL u_cls
     OPEN (9,FILE = ' ',FORM = 'FORMATTED', STATUS = 'NEW'
                    IOSTAT = Err_stat, ERR = 60
     GOTO 70
C
60   CALL ERR_LST (Err_stat)
     GOTO 50
C
70   CONTINUE
C
C... READ INPUT DATA
C    ================
C
     READ (7,700) N,THEFC,CF,J
     WRITE (9,900) N,THEFC,CF,J
     WRITE (8,901)
     WRITE (8,900) N,THEFC,CF,J
```

```
      PRINT*,'NUMBER OF ITERATIONS        : ',N
      PRINT*,'FIELD CAPACITY              : ',THEFC
      PRINT*,'CROP FACTOR                 : ',CF
      PRINT*,'PROPORTION OF EVAP BEFORE I : ',J
      WRITE (6,820)
      WRITE (8,820)
C
      DO 10 T =1,N
          READ  (7,710) I(T),E(T),R(T),F(T)
          AE(T)=E(T)*CF
           WRITE (6,830) I(T),E(T),AE(T),R(T),F(T)
           WRITE (8,830) I(T),E(T),AE(T),R(T),F(T)
   10 CONTINUE
      P(0) = 0
      THETA(0) = THEFC
      J=0
      WRITE (6,800)
      WRITE (8,800)
C
C... CALCULATIONS
C    ============
C
C
C... For each time step (month), values of G, DELTA THETA, and
C    the DELTA P and P are calculated. Then, THETA is updated.
C
      DO 100 T=1,N
         IF (P(T-1).LT.R(T)) THEN
             G = P(T-1)
         ELSE
             G=R(T)
         ENDIF
         DM = G*(THEFC-THETA(T-1)+J*AE(T)/R(T))
         DP(T) = (I(T)-DM)/THEFC
         IF (DP(T).LT.0) DP(T) = 0
         P(T) = P(T-1) + DP(T)
         THETA(T) = THETA(T-1) + (I(T)-AE(T))/R(T)
         IF (THETA(T).GT.THEFC) THEN
              LEACH(T) = THETA(T) - THEFC
              THETA(T) = THEFC
         ENDIF
          WRITE (6,810)     T, P(T), DP(T), THETA(T),LEACH(T),I(T),AE(T)
          WRITE (8,810)     T, P(T), DP(T), THETA(T),LEACH(T),I(T),AE(T)
         WRITE (9,910)  P(T),F(T)
100       CONTINUE
C
C... READ AND WRITE FORMAT STATEMENTS
C    ================================
```

```
C
 800 FORMAT (/,’TIME’,5X,’P’,9X,’DP’,6X,’THETA’,5X,’LEACH’,
    + 5X,’IRRIGAT’,4X,’EVAP’)
 810 FORMAT(I3,6F10.3,F6.2)
 820 FORMAT (/,’IRRIGAT   EVAP   ACT EVAP   ROOT DEP   F(T)’)
 830 FORMAT (4F8.2,F8.4)
 900 FORMAT (I3,F5.2,F4.2,F5.2)
 901 FORMAT (/,’  N     THETA    CF  J’)
 910 FORMAT (F10.3,F10.4)
C
C... READ FORMAT STATEMENTS
C
 700 FORMAT (I3,3F5.2,)
 710 FORMAT (F5.1,F9.1,F7.0,F9.2)
     STOP
     END
C***************************************************************
C***************************************************************
C
     SUBROUTINE ERR_LST (Err_stat)
C
     INTEGER * 4 Err_stat
C
     IF (Err_stat.EQ.6413) THEN
        WRITE (*,’(A\)’) ’ File already connected to different unit - ’
C
         ELSE IF (Err_stat.EQ.6414) THEN
            WRITE (*,’(A\)’) ’ Access not allowed - ’
C
         ELSE IF (Err_stat.EQ.6415) THEN
            WRITE (*,’(A\)’) ’ File already exists - ’
C
         ELSE IF (Err_stat.EQ.6416) THEN
            WRITE (*,’(A\)’) ’ File not found - ’
C
         ELSE IF (Err_stat.EQ.6417) THEN
            WRITE (*,’(A\)’) ’ Too many open files - ’
     END IF
C
     WRITE (*,’(A\,I5)’) ’ Error number :\a’C, Err_stat
     WRITE (*,’(A1)’)
     WRITE (*,’(A1)’)
     Err_stat = 0
     RETURN
     END
```

APPENDIX C

```
C... Program PEAKD
$DEBUG
C
C... Program to calculate the dispersion of solute around a
C    concentration peak moving through the soil, based on
C    the model of Rose et. al. (1982). Solute peak
C    position is calculated in the program PEAKM.
C
C... VARIABLE LIST
C    =============
C
C    N              = number of time events
C    T       = time increment
C    I0       = initial depth of infiltrating rain or irrigation water
C    F       = proportion of solute taken up by crop
C    THEFC   = field capacity
C    ZMM      = depth from soil surface in mm
C    ZMAX     = maximum calculation depth
C    P(T)     = depth of penetration of solute conc. peak - leading edge
C    Q(T)      = depth of penetration of solute conc. peak - trailing edge
C    D0       = molecular diffusion coeff.
C    D              = field dispersion coeff.
C    C0       = irrigation water solute concentration
C    S(Z,T,) = soil solute conc. at depth Z & time T
C    V(I)     = ERFC numerical integration constants
C    A & B    = 'leading' & 'trailing' parts of the dispersion equation solution
C
C
C... DECLARATION OF VARIABLE
C    ========================
C
      INTEGER*2 N,I0,T,CC,Z,ZINT,ZMAX,ZMM,NDEPTHS,DEPTH,Err_stat
C
      REAL*4  F(100),THEFC,D0,D,C0,P(200),Q(200),S(200,100),
     +        A,B,TS(0:200)
C
      CHARACTER* 1 OPT
      CHARACTER* 25 File_In, File_Out.
C
      OPEN (5)
      OPEN (6)
C
      DATA OPT/'Y'/,CC/66/
C
      CALL u_cls
C
1     PRINT *,' '
      PRINT *,' '
```

```
      PRINT *,'Please enter name for input data file'
      PRINT *,' '
      READ (5,'(A)') File_In
      CALL u_cls
      OPEN (7,FILE = 'File_In',FORM = 'FORMATTED', STATUS = 'OLD',
     +     IOSTAT = Err_stat,ERR = 2)
      GOTO 5
C
2     CALL ERR_LST (Err_stat)
      GOTO 1
C
5     PRINT *,' '
      PRINT *,' '
      PRINT *,'Please enter name for output data file'
      PRINT *,' '
      READ (5,'(A)') File_Out
      CALL u_cls
      OPEN (9,FILE = 'File_Out',FORM = 'FORMATTED', STATUS = 'NEW',
     +     IOSTAT = Err_stat, ERR = 6)
      GOTO 10
C
6           CALL ERR_LST (Err_stat)
            GOTO 5
C
C
   10 CONTINUE
      PRINT*,'Enter molecular diffusion coef D0 (mm**2/day)'
      READ (5,*,END=10) D0
      CALL u_cls
      IF (OPT.EQ.'N'.OR. OPT.EQ.'n') GOTO 60

   20 PRINT*,'Enter filed dispersion coefficient D (mm)'
      READ (5,*,END=10) D
      CALL u_cls
      IF (OPT.EQ.'N'.OR.OPT.EQ.'n') GOTO 60

   30 PRINT*,'Enter solute conc. of irrigation water C0 (meq/l)'
      READ (5,*,END=10) C0
      CALL u_cls
      IF (OPT.EQ.'N'.OR.OPT.EQ.'n') GOTO 60
C
   40 PRINT*,'Enter max. calculated depth (m)'
      READ (5,*,END=10) ZMAX
      CALL u_cls
      IF (OPT.EQ.'N'.OR.OPT.EQ.'n') GOTO 60
C
   45 PRINT*,'Enter depth increment (mm)'
      READ (5,*,END=10) ZINT
```

```
      CALL u_cls
      IF (OPT.EQ.'N'.OR.OPT.EQ.'n') GOTO 60
C
   50 PRINT*,'Enter initial depth of I0 (mm)'
      READ (5,*,END=10) I0
      CALL u_cls
      IF (OPT.EQ.'N'.OR.OPT.EQ.'n') GOTO 60
C
  60  CONTINUE
      PRINT*,' '
      PRINT*,'    PLEASE CHECK THE BELOW ENTERED DATA '
      PRINT*,' '
      PRINT*,' 1/ Molecular diffusion coef. D0 (mm^2/day)      :',D0
      PRINT*,'  '
      PRINT*,' 2/ Field dispersion coef. D (mm)                :',D
      PRINT*,'  '
      PRINT*,' 3/ Solute conc. of irrigation water C0 (meq/l)  :',C0
      PRINT*,'  '
      PRINT*,' 4/ Maximum calculated depth  (m)                :',ZMAX
      PRINT*,' '
      PRINT*,' 5/ Depth increment (mm)                         :',ZINT
      PRINT*,' '
      PRINT*,' 6/ Initial depth of I0 (mm)                     :',I0
      PRINT*,' '
      PRINT*,' IS THE ABOVE ENTERED DATA CORRECT (Y/N)?'
      READ (5,'(A1)',END=60) OPT
      CALL u_cls
      IF (OPT.EQ.'Y'.OR.OPT.EQ.'y') GOTO 100
C
   70 CONTINUE
      PRINT*,' '
      PRINT*,'    PLEASE CHECK THE BELOW ENTERED DATA '
      PRINT*,' '
      PRINT*,' 1/ Molecular diffusion coef. D0 (mm^2/day)      :',D0
      PRINT*,'  '
      PRINT*,' 2/ Field dispersion coef. D (mm)                :',D
      PRINT*,'  '
      PRINT*,' 3/ Solute conc. of irrigation water C0 (meq/l)  :',C0
      PRINT*,'  '
      PRINT*,' 4/ Maximum calculated depth  (m)                :',ZMAX
      PRINT*,' '
      PRINT*,' 5/ Depth increment (mm)                         :',ZINT
      PRINT*,' '
      PRINT*,' 6/ Initial depth of I0 (mm)                     :',I0
      PRINT*,' '
      PRINT*,' '
      PRINT*,' PLEASE ENTER THE LINE NO OF THE INCORRECT DATA'
      READ (5,*,END=70) LINNO
```

```
      CALL u_cls
      GOTO (10,20,30,40,45,50) LINNO
C
  100 CONTINUE
C
      READ (7,700) N,THEFC
      WRITE (6,700) N,THEFC
      DO 110 T=1,N
         READ (7,710) P(T),F(T)
         WRITE (6,710) P(T),F(T)
  110 CONTINUE
C
C... CALCULATIONS
C
C     For each time step (month), Q is calculated, then
C     the soil solute conc. at each depth (ZMM) is calculated.
C     Variables in the equation to calculate solute concs. are
C     calculated, with co-error function (ERFC) values being
C     calculated in a subroutine.
C
      WRITE (9,900) N,ZMAX
C
      P1 = I0/THEFC
      NDEPTHS=ZMAX/ZINT
      DO 130 T=1,N
         Q(T) = P(T) - P1
          DO 120 Z = 1,NDEPTHS
            ZMM = Z * ZINT
            IF (D0*T+D*Q(T).LE.0.0) THEN
               S(Z,T)=-9
               GOTO 119
            ENDIF
            A = (ZMM - P(T)) / (2*SQRT(D0*T + D*P(T)))
           B = (ZMM - Q(T)) / (2*SQRT(D0*T + D*Q(T)))
C
           CALL SUBERFC(A)
           CALL SUBERFC(B)
           S(Z,T) = (C0 / 2 * (A - B))*F(T)
  119   CONTINUE
  120   CONTINUE
  130 CONTINUE
C
C... DATA OUTPUT
C
C       WRITE (6,920) N,ZMAX
C       DO 150 T=1,N
C         DO 140 Z=1,NDEPTHS
C            DEPTH = Z*ZINT
```

```
C             WRITE (6,930) T,DEPTH,S(Z,T)
C             WRITE (9,930) T,DEPTH,S(Z,T)
C   140            CONTINUE
C   150 CONTINUE
C
C... SUM OF S(Z)'S FOR PERIOD T
C
C
      DO 170 Z=1,NDEPTHS
           TS(Z) = 0.0
           DO 160 T=1,N
              TS(Z)= TS(Z) + S(Z,T)
  160      CONTINUE
           DEPTH=Z*ZINT
           WRITE (6,940) Z,DEPTH,TS(Z)
           WRITE (9,950) Z,DEPTH,(S(Z,T), T=1,N),TS(Z)
  170 CONTINUE
C
            PRINT*,' PROGRAM  TERMINATED ON COMPLETION'
C
C
C... READ AND WRITE FORMAT STATEMENTS
  700 FORMAT (I3,F5.2)
  710 FORMAT (F10.3,F10.4)
  900 FORMAT (I3,I6)
  910 FORMAT (2I3,F5.2)
  920 FORMAT (I10,I10)
  930 FORMAT (I10,I10,F10.6)
  940 FORMAT (I6,I6,F16.9)
  950 FORMAT (I6,I6,20F10.6,F16.9)
C
      STOP
      END
C
C*********************************************************************
C*********************************************************************
C
      SUBROUTINE SUBERFC (ERFC)
C
C... This subroutine uses the method of Carslaw and Jaeger (1959)
C    to calculate ERF values
C
      INTEGER FLAG
C
      REAL  ERFC,ERF,V(0:5),V1,V2
C
C
      DATA V/0.3275911,0.254829592,-0.284496736,
```

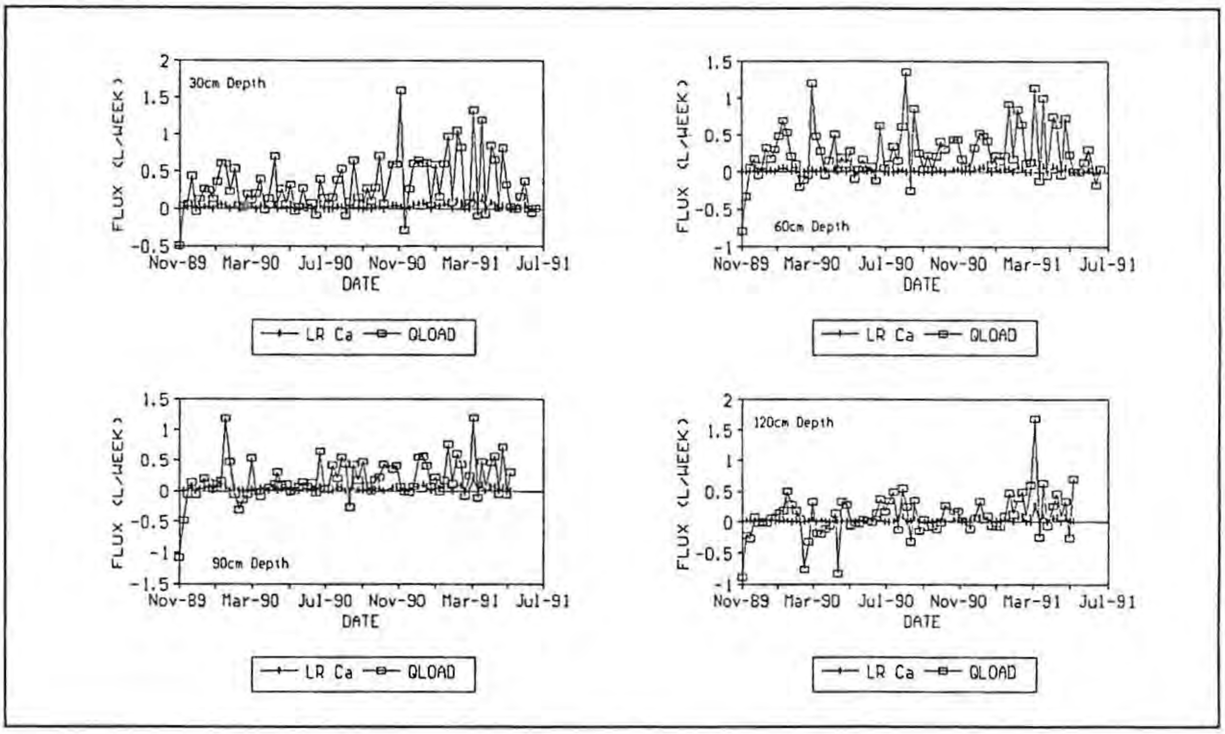
```
     +      1.421413741,-1.453152027,1.06140543/
C
C       DO 300 I=0,5
C       PRINT*,'V(I) : ',V(I)
C  300 CONTINUE

      IF (ERFC.LT.0.0) THEN
         FLAG=1
      ELSE
         FLAG=0
      ENDIF
C
      IF (FLAG.EQ.1) THEN
         ERF = ERFC * (-1)
      ELSE
          ERF=ERFC
      ENDIF
C
      V1 = 1 / (1 + V(0)*ERF)
      V2 = V(1)*V1 + V(2)*V1**2 + V(3)*V1**3 + V(4)*V1**4 + V(5)*V1**5
      ERF = 1 - (V2 * EXP ( -(ERF**2) ) )
      IF(FLAG.EQ.1) ERF = ERF * (-1)
      ERFC = 1 - ERF
      RETURN
      END
```

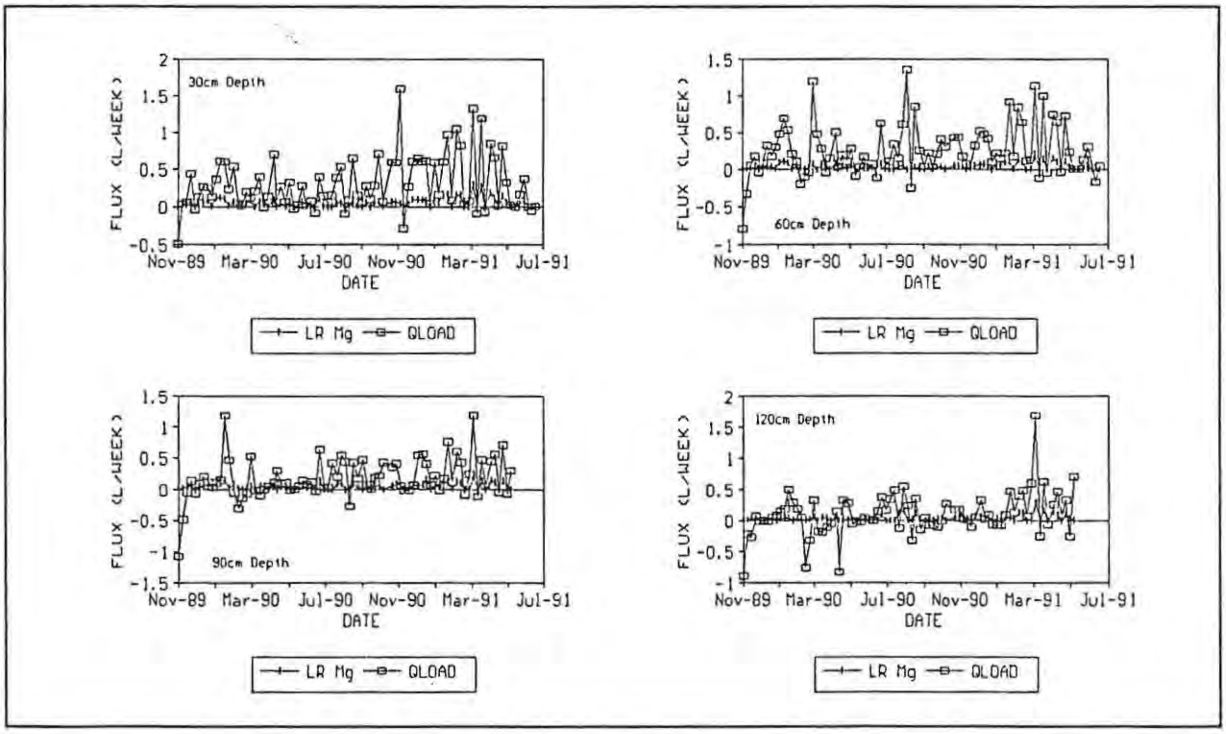
APPENDIX D

Weekly leaching fluxes predicted using the Leaching Requirement (LR) model for all cation concentrations (Calcium, Magnesium, Sodium, Potassium)

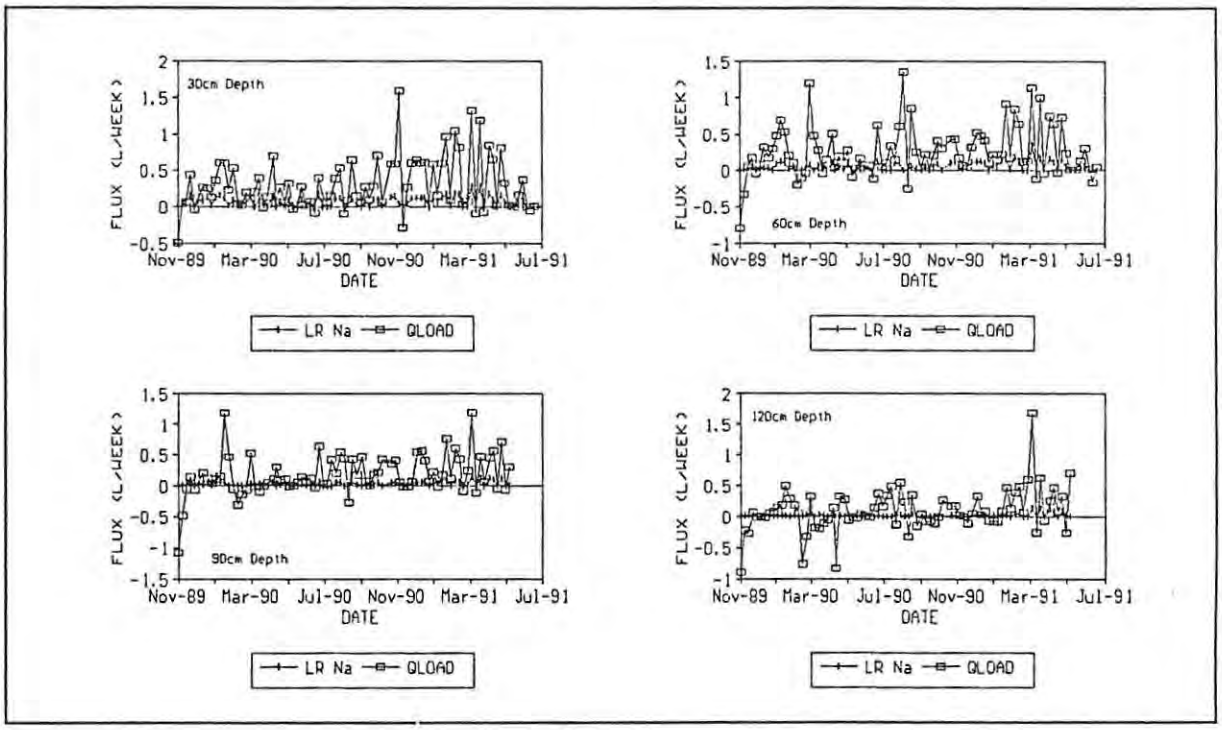
1. Calcium



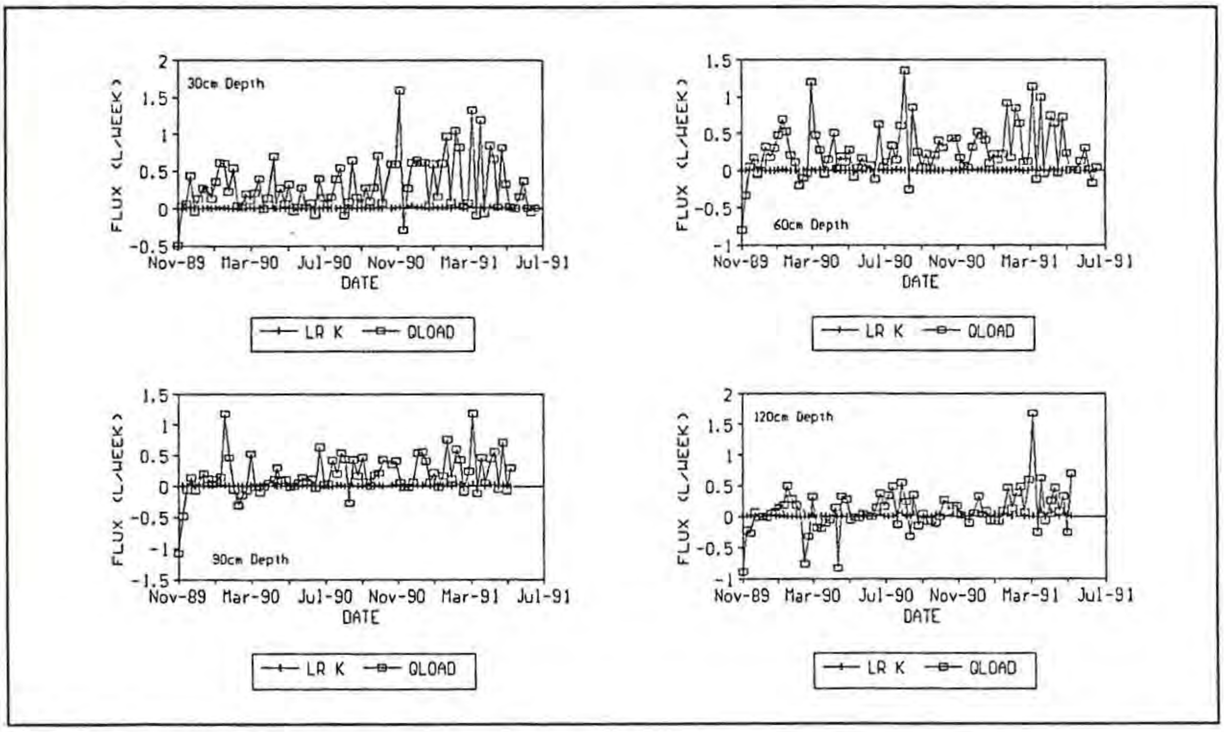
2. Magnesium



3. Sodium



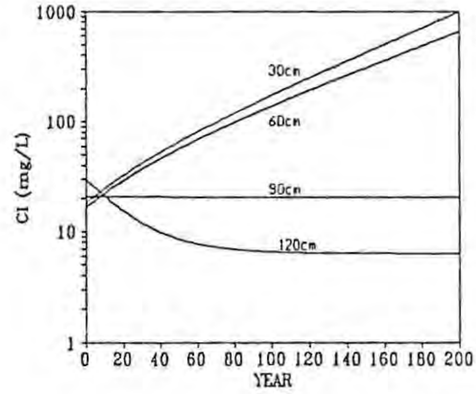
4. Potassium



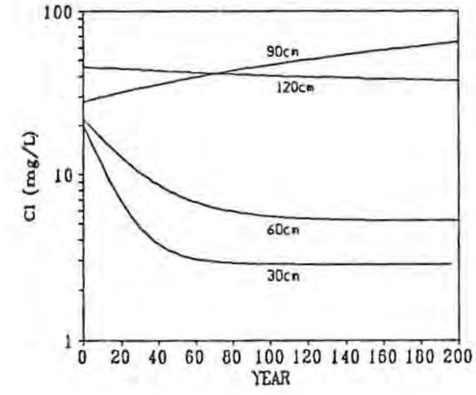
APPENDIX E

Soil Chloride profiles predicted for 200 years, or until steady state conditions are reached, using SODICS.

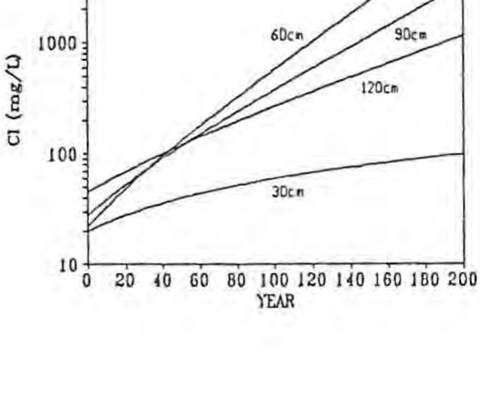
1. Bailes Orchard 13



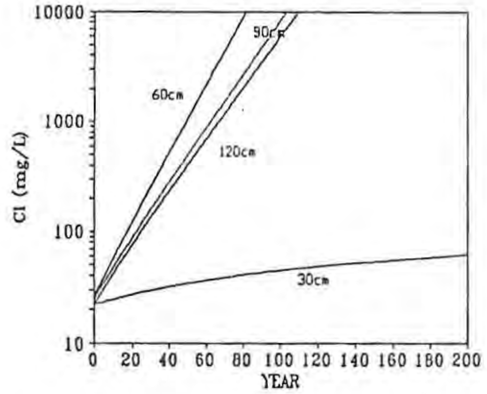
2. Beachey Orchard 45



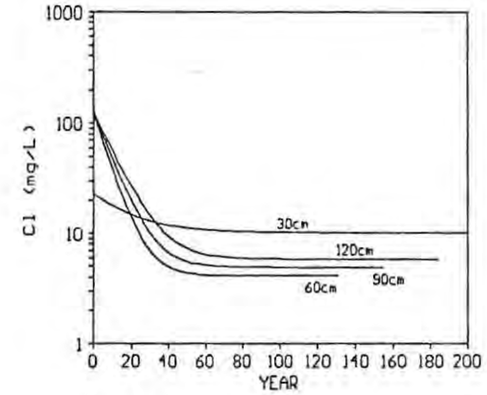
3. Blighty Farm Orchard 38



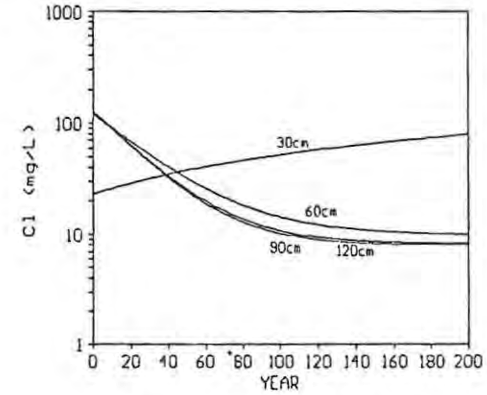
4. Daisy Dell Orchard



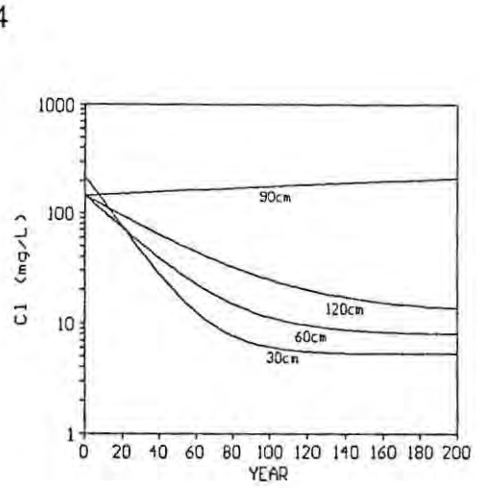
5. Goodhope Farm Orchard 02



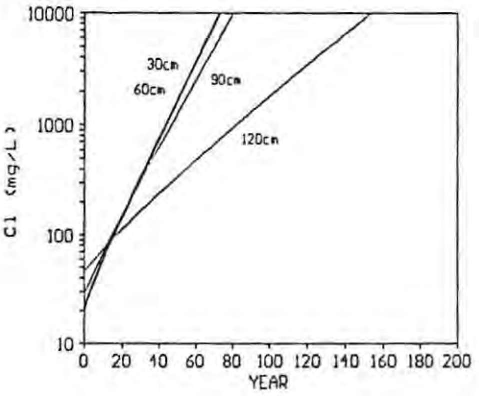
6. Goodhope Farm Orchard 24



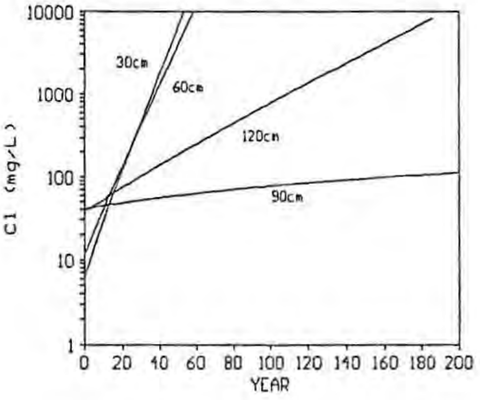
7. Hurter Farm Orchard A4



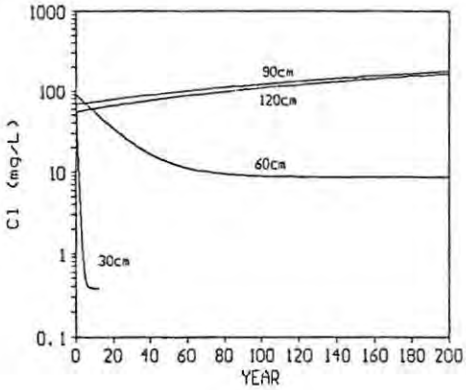
8. Lennie Farm Orchard 07



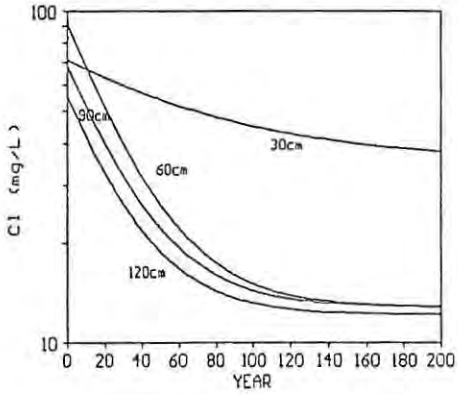
9. Sun Orange Farm Orchard A26



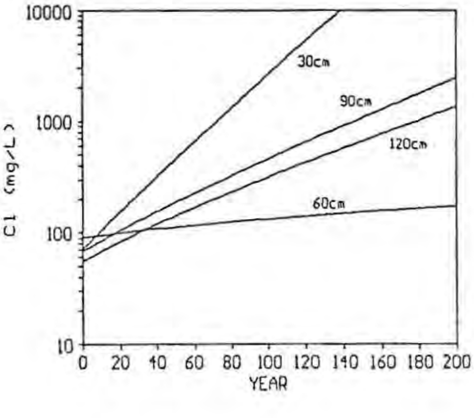
10. Sunland Farm Orchard E04



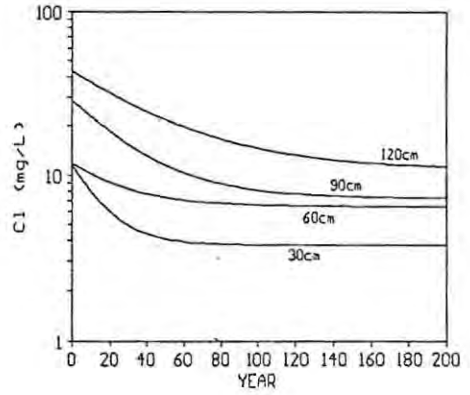
11. Sunland Farm Orchard E22



12. Sunland Farm Orchard E32



13. Willowtree Farm Orchard 05



14. Willowtree Farm Orchard 43