AN EVALUATION OF A RANGE OF COMPUTER MODELS SIMULATING THE TRANSPORT OF SOLUTES AND WATER IN THE ROOT ZONE OR IRRIGATED SOILS

by

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VOLUME I

of a report to the Water Research Commission on the project

"AN EVALUATION OF THE ABILITIES OF SEVERAL ROOT ZONE SOLUTE AND WATER TRANSPORT MODELS TO ADEQUATELY PREDICT THE QUANTITY AND QUALITY OF WATER LEAVING THE ROOT ZONE"

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EXECUTIVE SUMMARY

1 INTRODUCTION

Much research in the fields of soil physics and soil chemistry has, since the early 1960's, been directed toward developing scientific aids to deal with subjects such as the impact of irrigation on the environment, water reuse projects, and estimations of the travel time of water and chemicals trough the root zone of soils. One such aid has been the development of unsaturated zone leaching models for predicting movement and, in some cases, the degradation of agricultural chemicals. Scientific reports describing various aspects of this research, i.e. theory and development, validation, application, etc., are abundant in the literature. The result is that, at least within the research community, modelling has become an accepted way of predicting and estimating the outcome of agricultural activities. However, there are serious difficulties which are hampering the selection of suitable models and which are preventing the use of these potentially powerful tools in everyday practical applications. Some of these problems include problems of scale, spatial variability, cost-benefit ratios and multidimensional flow directions.

Solute transport models have been used in a number of case studies in South Africa e.g. Van Rooyen (1977), Van Rooyen & Moolman (1980), Moolman and Beukes (1980) and Hall and Du Plessis (1984). These applications unveiled a number of questions and uncertainties regarding the use of solute transport models. An example of these uncertainties is how the results of different rootzone hydrosalinity models compare with respect to their potential applications under conditions such as:

i) varying the scale of application, e.g. catchment vs. farm scale;
ii) different conditions of spatial variability;
iii) different levels of input data availability;
iv) different irrigation management strategies, e.g. complete wetting vs. partial wetting of the soil surface (flood vs. drip irrigation).

2 OBJECTIVES

In order to try and resolve some of these issues a research project with the following aims was formulated and conducted by the Department of Soil and Agricultural Water Science, University of Stellenbosch:

i) To determine, with the aid of the most appropriate water and solute transport model, the minimum amount of input data necessary to adequately predict the quantity and quality of water leaving the root zone for various scales of application and modes of surface wetting.

ii) To investigate the sensitivity of various hydrosalinity models to a change in input variables, with special emphasis on the effect of spatial variability of soil properties on the accuracy of model predictions of the quantity and quality of the deep percolate.

iii) To illustrate how solute transport models can be used to change surface water management strategies in order to decrease the salt load of the deep percolate.

iv) To compile a comprehensive literature review of solute transport models. (This objective is not listed in the original research contract, but, on request of the steering committee, was included as a separate aim of the project.)

Several solute and water transport models for the root zone of agricultural lands are available. These models differ in their level of sophistication and input demands. Ideally all of these models should be included in a study of this kind. However, because of time and financial constraints, this is not a feasible approach. Therefore, the models included in this study were selected using the following guidelines:

i) A model should be able to simulate both the flow of water and solutes, with associated inorganic chemical processes, through the root zone. Models simulating the chemistry of pesticides and nitrogen were excluded.

ii) At least one example of a mechanistic model and one functional model should be evaluated.

iii) One of the models should describe the chemistry of all the major cations and anions.

iv) Duplication should be avoided, i.e. if two models differ only with respect to minor detail, one only will be studied.

Several models were found that met two or more of these criteria. Recognizing the criteria stated above, as well as constraints imposed by time and manpower, this study was limited to the following three models: BURNS (Burns, 1974), LEACHM (Wagenet and Hutson, 1989), and TETRans (Corwin and Waggoner, 1990).

In order to address adequately these research goals, observed field information from irrigated areas are required as reference data against which model predictions can be evaluated. Such reference data sets must include, on both a spatial and temporal scale:

i) salt composition and distribution within and below the root zone;

ii) soil water content and distribution within and below the root zone;

iii) drainage water (deep percolate) quantity, and chemical composition;

iv) irrigation, precipitation and evapotranspiration information;

v) all the necessary physical and chemical soil properties (including spatial statistics), required as input by solute transport models.

A survey of literature revealed that no local (South African) or international data set can meet all these requirements for periods exceeding two years. Consequently, during 1986 and 1987 two irrigated vineyards in the Breede River Valley were instrumented as "*field laboratories*" in which the parameters listed above were monitored at varying time scales up to June 1990.

The results of this research project are presented in two volumes. Volume I focuses on the main thrust of this research, i.e. to evaluate different solute transport models. Volume II deals with the data acquisition and surveys that were conducted as part of the field study.

In Volume I the three models used in this study are described in detail. Each of the research objectives were addressed separately and the results are presented as different chapters of Volume I. It includes a literature survey of models, the results of a sensitivity study of two different models, and the results of the application of some of the models mentioned above on both a micro- and mesoscale. The microscale study was conducted using the information of a drip irrigated vineyard located in the Breede River Valley of South Africa, while the mesoscale study was based on the results of an irrigation project conducted in the San Joaquin Valley of California.

Volume II of this report deals with the data acquisition programme and the various surveys and field studies that were conducted between 1986 and 1990 in the Breede River Valley of South Africa. Examples of the data and the format in which it can be made available to other interested people, are included in this volume. It also contains the interpretation of some the results which are presented in different chapters as independent scientific papers.

3 SUMMARY OF RESULTS AND CONCLUSIONS.

3.1 Evaluation of transport models of the unsaturated zone.

3.1.1 Literature Survey Of Transport Models.

The highlights of the review on transport models of the unsaturated zone can be summarized as follows:

a) No model can be identified as representing the ultimate state of the art. Neither has any one model, or even modelling approach, received wide scale acceptance. Furthermore, the reported success rate of model application studies, especially when used by non-modellers (i.e. researchers, managers, farmers, etc. etc.) can at best be described as being moderate to fair. According to Wagenet (1988), at present, only approximate prediction of water movement and chemical distributions can be made.

b) Based on the results and suggestions found in literature, it seems logical and scientifically sound to conclude that the more mechanistic models are superior to the more simple non-mechanistic, capacity type models. However, this alleged superiority might be negated when models are used to predict responses in large irrigated areas bordering on the order of basin scale. When models are applied to large areas, other factors might be of greater importance than, for example, the hydrologic variability of field soils.

c) None of the models reviewed can effectively describe the movement of chemicals under conditions of macropore flow.

d) Time and effort to meet the data demands of a specific model will play a role in model selection, especially for macroscale applications. On a macroscale, variables such as rainfall, irrigation and evapotranspiration amounts might be of far greater importance than detailed and accurate information of soil properties such as cation exchange capacity and cation selectivity coefficients.

e) The choice of the appropriate model to use will depend on three factors:
   i) the specific application;
   ii) the required accuracy of prediction;
   iii) how much information is available and how much time and effort can be spent in obtaining the required information, and
   iv) the knowledge of the user of the model.

3.1.2 Sensitivity analysis of two different transport models.

The objective of this study was to evaluate the effect of a number of model parameters on the predicted quantity and quality of soil water leaving the root zone of irrigated agricultural lands. The study was conducted using deterministic mechanistic, and deterministic capacity type of water and salt transport simulation models. A sensitivity analysis was performed which involved six input parameters required by the mechanistic LEACHM model. The parameters that were studied are: airentry potential, slope of the soil water characteristic (i.e. Campbell's *a* and *b* coefficients), saturated hydraulic conductivity, cation exchange capacity, Ca/Na selectivity coefficient, and the difference between the evapotranspiration and irrigation quantities. The latter parameter and field capacity were evaluated with the simpler Burns model. With both models a hypothetical soil profile and irrigation frequency were used. The results indicate that:

a) The net flux of water moving through the soil, simplified by the ratio of evapotranspiration and irrigation, i.e. the ET/I ratio, is by far the most important factor in determining the quantity of water and salt that will be leached out of the root zone. Both of the two models that were used, showed that even a relatively small change in the ET/I ratio, e.g. from 1,00 to 0,90, will significantly effect the flux of water and solutes through the soil. In practice this indicate that accurate estimates of the irrigation and evapotranspiration should receive more attention than other physical and chemical properties such as water retention, hydraulic conductivity and CEC when scaling up from the micro- to the macroscale.

b) Unbalanced combinations of hydrological parameters have a profound effect on model predictions of mechanistic models. In this regard the air entry potential was of particular importance. A high potential (i.e. small negative) in combination with medium to low saturated hydraulic conductivities had a critical effect on the estimate of the unsaturated conductivity. In extreme cases, such low values for the unsaturated hydraulic conductivities can be obtained that no movement of water and salt will be possible. It is quite possible that the unsuspecting model user could come to the spurious conclusion that soils in which macro pores predominate, i.e. soils with large airentry potentials, will have a low salt output irrespective of the ET/I ratio. This obviously is an inconsistent result.

c) The ranking of the rest of the parameters that were evaluated, was complicated by the large impact that one unbalanced combination of hydrological parameters had on the results. The ranking is also strongly influenced by the magnitude of the flux of water moving through the soil profile. By using the predicted results obtained with a certain combination of input parameters as the norm, the effect on the predicted salt load and water flux of the six variables that were evaluated could be evaluated. A moderate decrease in the ET/I ratio from 1,0 to 0,9 which, in this study corresponded to an in crease in the water flux from 49 to 182 mm m^{-1}, yielded the following rank (in order of decreasing effect):

ET/I > > Ksat > $a \geq b$ > CEC = k-Ca/Na

By using a similar procedure as above, but changing the ET/I ratio from 1,0 to 0,5 (which increased the water flux from 49 to 910 mm a^{-1}), a different rank order is obtained:

ET/I > > > CEC > b > k-Ca/Na = a > Ksat

This big increase in the water flux reduced the effect of Ksat to such an extent that it moved from the second to the last position in the rank order. In contrast, the salt supplying capacity of the soil, which in this study was quantified by using different CEC values, became more important and moved up several positions in the rank order.

In view of this result, it seems as if the relative importance of the cation exchange capacity and the hydraulic conductivity as properties that will influence the salt load in the deep percolate of irrigated lands, will depend on the magnitude of the water flux. At small fluxes, i.e. where AET ≈ irrigation, the rate of water movement through the soil is more important than the salt supply capacity of the soil. At greater fluxes, i.e. irrigation > > AET, the rate of water movement becomes less important while the capacity of the soils to supply salt, increases in importance.

d) With the capacity type model of Burns, the field capacity of the fictitious soil did influence the leachable quantity of water and salt, but it's effect was secondary to that of the ET/I ratio.

e) Several model parameters were not investigated, with the result that the effect of the chemical, but more specifically the hydrological parameters, remain somewhat inconclusive. The effect of the boundary conditions at the bottom of the soil profile might influence the relative importance of the a, b and Ksat parameters.

3.1.3 Microscale application of the mechanistic transport model LEACHM.

The objective of this part of the research project was to evaluate how accurately a mechanistic research model can simulate transport processes under microscale field conditions (< 1 ha). Only one model, namely LEACHM (Wagenet & Hutson, 1989), was used for this study. The data that were used to evaluate the predicted soil water and soluble salt contents over time, are based on field measurements made during a period of two and half years in a 0,5 ha drip irrigated vineyard in the Breede River Valley of South Africa. In addition to the primary objective, this application of LEACHM was also meant to serve as a test of the application of a one-dimensional model to a case where the irrigation is applied at a point source and the water and salts subsequently redistributed in three dimensions. LEACHM was used to simulate the chemistry and transport of soil water and salt that occurred during the period 1 May 1987 to 30 June 1989. Soil properties of four different locations in the vineyard were used as input for the model, and at each location the 2,5 m^2 area served by one emitter was divided into four sectors with each sector being simulated separately.

The results of this study gave a rather pessimistic picture on the ability of LEACHM to simulate accurately the chemical processes in drip irrigated row cropped fields. Some of the results are also conflicting and can be summarized as follows:

a) In terms of the predicted soil water contents and fluxes, the numerical statistics and visual comparisons give different impressions of the adequacy of LEACHM as a method to calculate accurately the fate of applied water in this drip irrigated vineyard. Based on statistical norms, neither the coefficients of determination (R^2), nor the d-index of Wilmot (1981) justify any confidence in the model at all. The maximum R^2 value and d-index that were obtained are 0,306 and 0,774 respectively. However, judging the adequacy of prediction in terms of visual comparisons only, give a slightly better view of the predictive ability of LEACHM. Except for marked underpredictions in the soil water content of the shallower soil layers during the summer of 1987/88, the predicted water contents as well as the temporal trends did not deviate too much from the measured values and trends.

b) The visual comparison between the predicted and observed drainage rates is promising, especially in view of the fact that the predicted daily drainage volumes and rates of a known area (0,5 ha) were compared with the observed values from an unknown area.

c) The poor prediction of soil water contents and fluxes should be judged against the complexity of the three dimensional flow patterns in the drip irrigated field to which a one-dimensional model was applied. Based on the results of the sensitivity study, it was concluded that in cases where a certain surface area of the soil only is wetted, even a small error in the conversion of volume of applied water to depth units is likely to result in substantial differences in the measured and predicted water contents and fluxes. Because the real wetted area is unknown and difficult to determine, using different areas when converting from volume to depth units of irrigation water can have a profound effect on the outcome of the modelling study. Consequently, in this particular application of LEACHM, the statistically poor match between predictions and observations might be related to either model inadequacies, or input errors and it is rather difficult to distinguish between these two.

d) Serious numerical problems were encountered with the chemistry version of LEACHM, i.e. LEACHC, and did little to install confidence in the model. It was found that the code of LEACHM is such that under circumstances, the square root of a negative number, or division of a value by zero, is attempted. However, it was virtually impossible to predict when and under which conditions this situation will occur. In this study all of these cases were associated with the chemistry of the calcium ion. It is speculated that the numerical instability is related to the large amount of non-saline, low salt water that was applied to a saline soil with a rather low cation exchange capacity in the presence of small quantities of gypsum and free lime. This set of conditions can possibly lead to a situation where, according to the algorithms used in, and rationale behind LEACHM, calcium concentrations become very small.

e) The information and experience gained with this microscale study indicate that the application of one-dimensional transport models to drip irrigated, widely spaced, row-cropped fields, by nature of the model construction will lead to poor results.

3.1.4 Evaluation of three transport models on a mesoscale.

The objective of this part of the research project was to apply one mechanistic research model, and two functional management models to field data and to assess their accuracy of prediction at a mesoscale (1 - 10 ha). The models used were LEACHM (Wagenet and Hutson, 1989), BURNS (Burns, 1974), and TETrans (Corwin and Waggoner, 1990). Because no local (South African) data on a meso scale could be found, use was made of the results of two treatments of a 61 ha irrigation experiment conducted in the San Joaquin Valley of California. The two treatments that were used are a 5,7 ha furrow irrigated, and a 2,4 ha drip irrigated plot. The main results and conclusions of this study are as follows:

a) Based on the quantitative statistics, it seems as if the predictive capability of the leaching model LEACHM when applied on a mesoscale, is rather poor. For example, predicted soil water contents, when evaluated on a temporal scale, could not adequately match the observed data. Furthermore very low R^2 values and d-indexes were obtained when the predicted and observed results were compared on a temporal scale. However, inspection of the observed soil water contents gave strong indications that the inadequate prediction by LEACHM might be related to measurement errors and inadequacies. This is supported when considering the few samples that were taken and the large spatial variability among them. One example of this is the case of the 5,7 ha furrow irrigated plot where the maximum number of samples taken at any one of the four sampling dates between 1983 and 1986, was never more than three. Previous studies on sampling strategies in saline soils, have proved that a large number of spatially distributed samples is required in order to detect trends and calculate means. Notwithstanding the inadequacies of the measured data that were available, the predicted results indicate that the chemistry of calcium and magnesium are not satisfactorily dealt with by LEACHM.

b) In contrast to the rather poor numerical statistics obtained with LEACHM, graphical comparison between the observed and predicted results at the end of the simulation period, i.e. the final ion concentrations, lead to a different conclusion, namely a good predictive capability. In this study, LEACHM predicted that the soluble salt content of soils that are irrigated with saline drainage water, will increase appreciably. Not only was this confirmed with measured data, but the predicted salt concentrations and distributions with depth closely matched the observed results. A similar result was obtained even when good quality water was used with furrow irrigation as an application method.

c) The two functional type models, i.e. Burns and TETrans, predicted chloride concentrations that bear no resemblance with the measured data, both in terms of numerical statistics and graphical comparisons. The accordance between the LEACHM predictions and observed data were substantially better than the Burns and TETrans predictions. The superior predictive ability of the LEACHM model over the Burns and TETrans models is supported by the root mean square error and d-index values.

d) The application of LEACHM, which is a one-dimensional flow model, to the 2,4 ha drip irrigated field, resulted in a fair to good prediction of the actual chemical composition of the soil as observed at the end of the irrigation experiment. This is contrary to what was found with the micro-scale study conducted in the drip irrigated vineyard in the Breede River Valley of South Africa. In the latter case the LEACHM-predicted salt concentrations did not accord with the observed data at all. It is concluded that this apparent anomaly can be explained by the differences in emitter spacing. In the mesoscale study the emitter spacing was 1 m x 1 m, as opposed to the 1 m x 2,5 m in the case of the microscale study. It is reasonable to assume that in the former case, the more densely spaced emitters will result in a flow pattern that is essentially one-dimensional, in contrast to the three dimensional flow pattern that is expected to predominate when the emitter spacing is less dense.

e) It was also found that the results of the drip simulation are more accurate than the furrow plot simulation. It was inferred that this is probably due to the fact that controlling and measuring the amount of water applied with drip irrigation is easier and more accurate than with furrow irrigation. Therefore, in the case of the drip irrigated plot, the amount of applied irrigation water supplied as input, was a more accurate account of the actual field infiltrated water than was the case with the furrow applied water.

3.1.5 Simulating the effect of different leaching strategies on the salt load of the deep percolate of irrigated lands

The aim of this study was to illustrate how solute transport models can be used to change surface water management strategies in order to decrease the salt load of the deep percolate. The effect of six different salinity control measures as affected by using various leaching strategies, simulated for three consecutive years, on the salt and water flux of a hypothetical irrigated soil were investigated. For each year and leaching strategy (with the exception of one scenario), the same rainfall and actual evapotranspiration (AET) data were used throughout. The soil properties, irrigation water composition and irrigation management strategies that were used as the basis for the different leaching strategies, are all common to the Breede River (South Western Cape, South Africa).

As was the case in Chapter 4 where LEACHM was used to simulate the water and salt distribution in a drip irrigated vineyard, numerical instabilities were also encountered in this study. A weekly irrigation frequency was the only salinity control measure that could be simulated for a full three year period. However, based on the results of the first summer and winter cycle, the following conclusions can be made regarding the effect of different leaching strategies that can be used to minimise the salt load of the deep percolate of irrigated lands:

a) For a particular leaching fraction, the total flux of water at the bottom of the root zone at the end of a summer and winter cycle will be nearly the same, irrespective of whether: i) a daily or weekly irrigation frequency is used during summer, and ii) the leaching water is applied with every irrigation during summer, or as a single application during winter.

b) Although only to a degree, the total salt load of the deep percolate will increase in the order: no leaching during summer, with a single leaching in winter < leaching during summer on a daily frequency < leaching during summer on a weekly frequency.

c) The temporal distribution of the salt load and water flux suggests that controlled leaching of salts during winter is more beneficial for the control of the salt concentration of receiving rivers.

d) For the irrigation water that was used (EC $\approx$ 100 mS m^{-1}), an irrigation practice where no leaching is employed during the summer period, will result in a considerable accumulation of salts in the bottom half of the root zone during the irrigation season. If a winter leaching is applied, a significant portion of these salts will be leached and the predictions suggest that the salt content within the root zone at the onset of the second irrigation season, will be less than the initial values.

e) The fact that LEACHM predicted similar water and salt fluxes for a daily and a weekly irrigation frequency should be treated with caution. This result, in all likelihood stems from the fact that LEACHM can handle D'Arcian type flow only and not macropore flow. In practice, low irrigation frequencies involving large amounts of irrigation water at greater applications rates than smaller quantities at higher frequencies but lower application rates, will yield larger water fluxes and salt loads.

f) In spite of the general shortcoming of the presently used water and salt transport models not being able to simulate non-D'Arcian type of water flow (e.g. macropore flow), they still are useful tools that can be used to evaluate and design different salinity control strategies. Computer investigations such as the one reported on in this study, are far cheaper to conduct than expensive field trials. The results of simulation studies can then be used to select, test and verify certain salinity control strategies under field conditions. Unfortunately, the particular model that was used in this study, LEACHM, under certain unknown and unpredictable circumstances, turned out to be numerically unstable.

3.2 Data acquisition and evaluation of changes in the temporal and spatial soil conditions in irrigated fields in the Breede River Valley

In Volume II of the report, a number of aspects associated with spatial and temporal variability of soil properties that impact on the validation of water and salt transport models, were investigated. This was done by investigating some aspects of the data that were acquired during the course of a three year field study which led to the establishment of a considerable data base on soil chemical and hydrological properties. The most important research findings will be highlighted here.

3.2.1 The effect of spatial variability on the estimation of the soluble salt content in a drip irrigated saline loam soil.

The distribution and total mass of soluble salt in a drip irrigated vineyard was investigated. Eighty four positions in a 0,475 ha area were sampled at five depths each, resulting in a total sample number of 420.

a) The salt content increased exponentially with distance from the emitter. At equal distances from the emitter, significantly higher values were observed outside, compared to within the vineyard row. Outside the row the salt content decreased significantly with depth, but within the row the salt content was constant down to 1 m. Depth, distance from emitter and position relative to the emitter could account for 52% of the observed variation in salt content.

b) The total salt mass within the study area to a depth of 1 m, was estimated to be ca. 22,5 ton ha^{-1}. Calculation of the required sample size, combining the central limit theorem with the statistics of the present study, showed that at certain spatial positions relative to an emitter, the type II error of erroneously accepting the null hypothesis and the first estimate of the salt content could be as high as 41%. The initial sampling scheme could be improved by taking account of the observed spatial variation.

3.2.2 Using the probability density function of soil water content to locate representative soil water monitoring sites in a drip irrigated vineyard.

This study investigated whether the probability density function of spatially measured soil water content at the first stage of a field study can be used to identify statistically important field locations. The soil water content at 14 sites was monitored at 15 different times over a period of 18 months in a drip irrigated vineyard.

a) It was found that certain sampling locations conserve the property to represent the mean and extreme values of the field water content over time. The presence of transpiring vines and irrigation applications increased the variability of the measured values without any big influence on the ranking position of the various monitoring sites as they initially appear on the probability density curve. The locations that were identified as being representative of the field mean water content during summer, also represented the mean during winter when irrigation and transpiration were absent.

b) The positions representing the field mean and extreme water contents of the topsoil differ significantly in space from the corresponding subsoil positions.

c) It was concluded that, because of the temporal stability of the ranking position of the measuring sites, the probability density curve of one sampling only can be used to identify representative sites (e.g. the median), that can be used for soil water monitoring and irrigation scheduling. However, cognizance should be taken of the confounding effects that are likely to occur with depth.

3.2.3 The design and use of a tipping flow gauge for the measurement of subsurface- and surface drainage water.

During the course of the study it became clear that there are few instruments available that can accurately measure flow rates in subsurface drains. A tipping bucket flow gauge was therefore designed for direct measurement of flow rates in subsurface drains of agricultural lands. The free-board problem in a manhole was overcome by using two reservoirs and pump system. The flow gauge was connected to a standard data logger with low power consumption. The flow gauge can also be easily adapted for measuring surface runoff. Results obtained with the flow gauge in irrigated vineyards in the Breede River Valley show a positive correlation between irrigation applications and flow rates in subsurface drains.

3.2.4 Water balance studies in a drip irrigated vineyard in the Breede River Valley: A comparison of different methods.

The evapotranspiration, irrigation, soil water content and drainage flow rates of three irrigation seasons were used to estimate the water balance of a 0,475 ha drip irrigated vineyard. The five different methods employed to calculate the leaching fraction, gave widely varying results.

a) From the field capacity of the soil, class A-pan estimated evapotranspiration data and measured irrigation quantities, it was inferred that with the exception of 1987/88, the amount of water that will percolate through the root zone of the drip irrigated vines, will be insignificant.

b) However, quantitative measurement of the soil water content and the applied irrigation amounts during two individual events, suggest significant losses of water out of the root zone, probably due to macropore- and preferential flow. The drainage hydrograph and chloride distribution in the soil volume in the immediate vicinity of the emitters, provide further evidence of significant losses due to macropore- and preferential flow.

c) It is inferred that a water balance based on irrigation and evapotranspiration amounts alone, might lead to spurious conclusions regarding the harmful, e.g. salinization, effects of irrigated agriculture on the water resources of an environment.

d) Most water and salt transport models cannot simulate macropore- and preferential flow. In view of the results of this study, it is possible that water and salt balances calculated using these models which rely heavily on evapotranspiration and irrigation inputs, might be far removed from actual field conditions.

3.3 Extent to which the contract objectives have been reached.

Although all of the objectives have been addressed in this study, not all of them have been met with equal success. Some of the original questions regarding the use of transport models in irrigated environments have been left unanswered. This study improved our knowledge about the strengths and weaknesses of soil and water transport models, as well as the role that they can play in the applied and predictive hydrology. This statement is based on the following aspects:

a) There are strong indications that the minimum input requirements in transport modelling involve those variables controlling the water and salt fluxes through the soil, i.e. irrigation, precipitation and evapotranspiration amounts, as well as the salt content of the soil and irrigation water.

b) Models designed to simulate one dimensional flow processes, should be expected to yield poor results when applied to irrigated field where the soil surface is only partially wetted, e.g. drip- and micro irrigated fields.

c) Validating models with field studies and on a scale larger than small experimental plots (i.e. >25 m^2), requires large data sets gathered using a sampling protocol that are designed to minimize the effect of statistical uncertainties, both in time and space.

d) This was one of the few studies of its kind that compared and evaluated different models at varying scales and under different environmental conditions.

4 RECOMMENDATIONS

a) In order to increase and improve data that can be used to validate water and salt transport models of the unsaturated zone, the monitoring of soil conditions in selected irrigated fields should continue.

b) A study involving the comparison of two sophisticated mechanistic models should be conducted. This should include LEACHM and another model also capable of simulating the chemistry of all the major cations and anions found in agricultural soils. However, the study will only have merit if another such a sophisticated model can be found.

c) Develop a two- and three dimensional model that can simulate the transport of water and chemical processes in drip irrigated fields.

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CHAPTER 1
INTRODUCTION

1.1 GENERAL

Modern irrigated agriculture is under pressure to maximize crop yields to provide food for an expanding population. Another form of pressure, and one which is steadily mounting, is public concern over residues of agricultural chemicals in groundwater and the concentration of toxic elements in plant tissue. Similarly, use of reclaimed municipal wastewater is a high priority for cities in arid areas with restricted water supply, but the use of such reclaimed water is constrained by severe discharge regulations which may render the reuse of wastewater unfeasible. Furthermore, in many countries environmental impact studies are now required before new irrigation schemes, water reuse projects, etc. etc. can be approved. In most cases the urgency of a particular project means that *in situ* field experiments cannot be used to conduct the environmental impact studies, mainly because of the long time required for salt and other agricultural chemicals to travel through the soil.

In order to overcome this conflict, much research in the fields of soil physics and soil chemistry has, since the early 1960's, been directed towards developing scientific aids to deal with this complex issue. One such aid has been the development of unsaturated zone leaching models for predicting movement and, in some cases, the degradation of agricultural chemicals. Scientific reports describing various aspects of this research, i.e. theory and development, validation, application, etc., are abundant in the literature. The result is that, at least within the research community, modelling has become an accepted way of predicting and estimating the outcome of agricultural activities.

These leaching models, which are also referred to as salt and water transport, or hydrosalinity models, are potentially powerful tools for use in a wide range of water resources-related applications. Examples of possible applications are:

i) the prediction of the quantity and quality of irrigation return flows (when appropriately linked with the rainfall-runoff and groundwater components of hydrological models);

ii) the design of minimum leaching irrigation management systems for water conservation, combating detrimental salinity effects on crops and simultaneously limiting salt loading on groundwater and river systems;

iii) optimizing methods of reclaiming degraded irrigated soils using appropriate ameliorants such as gypsum and sulfuric acid;

iv) predicting leaching of nitrogen and other nutrients from the root zone, with attendant problems of pollution of river systems;

v) assessing the possible reuse of agricultural drainage waters and other industrial effluents for the irrigation of salt tolerant crops.

1.2 PROBLEMS ASSOCIATED WITH THE APPLICATION OF MODELS

Proper management of salt in soil-water systems depends upon an understanding of the physico-chemical processes occurring during solute transport. The physical and chemical processes which take place in the so-called root zone is despite the complex nature thereof, fairly well understood. The appropriate knowledge and understanding are reflected in the wide range of simulation models which describe the dynamics of water and salt transport in the root zone. However, there are serious difficulties which are hampering the selection of suitable models and which are preventing the use of these potentially powerful tools in everyday practical applications. Some of these problems are:

i) **Problems of scale.** There are a number of hydrosalinity models available ranging from high resolution, highly mechanistic, to low resolution simpler models. The selection of an appropriate model for a particular application such as the prediction of irrigation return flow, where other components of the system are modelled at a fairly extensive scale, thus becomes problematical.

ii) **Spatial variability.** Little is known about the impact of spatial variability of soil properties on model output, as well as the choice of a model for specific applications. It is furthermore uncertain when using a deterministic approach, how to best cope with the uncertainties introduced by spatial variability.

iii) **Cost-benefit ratios.** The more sophisticated models are very labour intensive in terms of obtaining the necessary input data. However, for a specific application, it is uncertain whether it is cost-beneficial (as a consequence of more accurate information) to choose a model high up in the hierarchy of sophistication rather than one lower down. Obviously, data requirements are also factors that should be considered under i) and ii) above.

iv) **Multidimensional flow directions.** Most root zone hydrosalinity models simulate water flow in the vertical direction only. As such they may be of limited use on sloping and drip irrigated soils, where lateral movement of water and salt also occur.

1.3 THE NEED FOR LOCAL RESEARCH ON SOLUTE TRANSPORT MODELS

Solute transport models have been used in a number of case studies in South Africa. Van Rooyen (1977) applied the steady state chemistry model of Oster and

Rhoades (1975) to the Oudtshoorn irrigation scheme and predicted the effect of drainage water on downstream irrigation water quality. This application was a theoretical exercise with no attempt at verification with real data.

Van Rooyen & Moolman (1980) used the model of Shaffer et al. (1977) to predict the effect of the water table depth and irrigation frequency during the season on the salinization of soils. This was an encouraging application of the irrigation return flow model and reasonably reliable results were obtained, in that a critical water table depth of 2 m was defined as the minimum to avoid salt build-up in the soil profile to rooting depth. Moolman and Beukes (1980) tested the water and salt distribution component of the Shaffer et al. (1977) model by using 4 years of field data obtained at the Oudtshoorn experiment station of the then Department of Agriculture. Certain assumptions had to be made regarding internal drainage properties of the soils and the root distribution of crops as a function of depth. Considering the scarcity of input data and the assumptions that were made, the accordance between model predictions and measured data were reasonable. In another study Moolman, Van Rooyen and Weber (1983) used a solute transport model to describe the effect of irrigation return flow on the mean monthly base-flow salinity of the Poesjesnel river, a tributary of the Breede River. The model predicted results that could be reconciled with observations over a six month period from July to December 1979. However, model predictions and observations did not coincide closely during the period January to June.

On a basin scale, Hall and Du Plessis (1984) used the FLOSAL systems model to test various planning options available to the Department of Water Affairs for salinity control in the irrigated areas of the Great Fish River- and Lower Sundays River valleys. The latter two rivers form part of the larger Orange River Project, which include *inter alia* an interbasin water transfer system. Although FLOSAL originated as a basin scale hydrological model, and not a root zone model, it does include subroutines that simulate the irrigation return flow in response to water and salt inputs to irrigated land (Hall and Du Plessis, 1981). One of these subroutines, THOMAS, was used to predict the long-term chemical composition of drainage water reaching the Great Fish River. On the basis of their modelling effort, Hall and Du Plessis (1984) concluded that as more water from the Orange River is exported in to the Great Fish - Sundays River basins to meet the growing irrigation demands, the salinity levels of the supply water will fall. However, equilibrium conditions in the irrigation cycle will only be reached several years after any major change in irrigation water and salt inputs. For the Great Fish River, they predicted a time of about nine years for the total dissolved solid content (TDS). For individual ions the time to reach equilibrium were much longer.

These local (South African) applications unveiled a number of questions and uncertainties regarding the use of solute transport models. An example of these uncertainties is how the results of different rootzone hydrosalinity models compare with respect to their potential applications under conditions such as:

i) varying the scale of application, e.g. catchment vs. farm scale;

ii) different conditions of spatial variability;

iii) different levels of input data availability;

iv) different irrigation management strategies, e.g. complete wetting vs. partial wetting of the soil surface (flood vs. drip irrigation).

1.4 AIMS

Against this background, a research project with the following aims were formulated:

i) To determine, with the aid of the most appropriate water and solute transport model, the minimum amount of input data necessary to adequately predict the quantity and quality of water leaving the root zone for various scales of application and modes of surface wetting.

ii) To investigate the sensitivity of various hydrosalinity models to a change in input variables, with special emphasis on the effect of spatial variability of soil properties on the accuracy of model predictions of quantity and quality of the deep percolate.

iii) To illustrate how solute transport models can be used to change surface water management strategies in order to decrease the salt load of the deep percolate.

At the first meeting of this project, the steering committee requested that a comprehensive literature review of solute transport models be included in the research project. The literature review thus became the fourth aim of the research project.

1.5 BASIS OF MODEL SELECTION, EVALUATION AND COMPARISON

In order to address adequately these research goals, observed field information from irrigated areas are required as reference data against which model predictions can be evaluated. Such reference data sets must include, on a temporal basis:

i) salt composition and distribution within and below the root zone;

ii) soil water content and distribution within and below the root zone;
iii) drainage water (deep percolate) quantity, and chemical composition;
iv) irrigation, precipitation and evapotranspiration information;
v) all the necessary physical and chemical soil properties (including spatial statistics), required as input by solute transport models.

A survey of literature revealed that no local (South African) or international data set can meet all these requirements for periods exceeding two years. Consequently, during 1986 and 1987 two irrigated vineyards in the Breede River Valley were instrumented as "field laboratories" in which the parameters listed above were monitored. The results of this research project are described in two volumes. Volume I focuses on the main thrust of this research, i.e. to evaluate different solute transport models, while Volume II focuses on the field study.

As will be shown in the review of water and solute transport models, chapter 2 of this report, several solute and water transport models for the root zone of agricultural lands are available. These models differ in their level of sophistication and input demands. Ideally all of these models should be included in a study of this kind. However, it should be obvious that this is not a practical approach. Therefore, the models included in this study were selected using the following guidelines:
i) A model should be able to simulate both the flow of water and solutes, with associated inorganic chemical processes, through the root zone. Models simulating the chemistry of pesticides and nitrogen were excluded.
ii) At least one example of a mechanistic model and one functional model should be evaluated.
iii) One of the models should include the chemistry of all the major cations and anions.
iv) Duplication should be avoided, i.e. if two models differ only with respect to minor detail, one only will be studied.

Several models were found that met two or more of these criteria. Examples of these models are BURNS, (Burns, 1974), the USBR model of Shaffer et al (1977), HLDBACK (Addiscott, 1977), SWASAL (Kabat and Bolt, 1989), HYDRUS (Kool and Van Genuchten, 1989), LEACHM (Wagenet and Hutson, 1989), and TETrans (Corwin and Waggoner, 1990). Recognising the criteria stated above, as well as constraints imposed by time and manpower, this study was limited to the following three models: BURNS (Burns, 1974), LEACHM (Wagenet and Hutson, 1989), and TETRans (Corwin and Waggoner, 1990). These models are discussed in more detail in the literature review, presented as chapter 2 of Volume I.

The sensitivity analysis (aim ii), which used fictitious data, is presented as chapter 3. The data collected between December 1986 and July 1989 on one of the field laboratories, as well as other internationally available information were used to address aims (i) and (iii) above. The results are presented as chapters 4 and 5. Chapter 4 deals with data obtained from a field scale irrigation trial in the San Joaquin Valley in California. Some of the salt contents of the soils and irrigation water used in that study are very high with electrical conductivities of the saturated soil extract (EC_e) and irrigation water (EC_{iw}) being as high as 919 mS m^{-1} and 913 mS m^{-1} respectively. Chapter 5 is a micro-scale study of the water and salt movement in a drip irrigated vineyard in the Breede River Valley of South Africa. In this particular case a saline soil (EC_e = 197 to 1596 mS m^{-1}) is irrigated with non-saline water (ECiw ≈ 35 mS m^{-1}).

An illustration, using hypothetical but realistic data, of how water and salt transport models can be used to change surface water management strategies in order to decrease the salt load coming from irrigated lands, is presented as chapter 6. The general summary of this study of hydrosalinity models is presented as chapter 7. This is followed by a section containing all the references to the literature cited in Volume I of this repor I of this report.

In Volume II all the activities (e.g. instrumentation, data collection, etc. etc.) and results pertaining to the field study are dealt with. Also included in Volume II is a chapter which deals with the interpretation of some the results.

CHAPTER 2
A REVIEW OF WATER AND SOLUTE TRANSPORT MODELS SIMULATING LEACHING PROCESSES IN THE UNSATURATED ZONE

2.1 INTRODUCTION

Several reviews on leaching models have been published, e.g. Jury (1982), Addiscott and Wagenet (1985), Wagenet *et al* (1988), Jones *et al* (1988), and Feddes (1988). These reviews deal primarily with the theoretical and, in some cases, with the philosophy of modelling and represent a concentrated pool of knowledge upon which any researcher, manager and regulator of water resources can draw. However, few of these reviews cover the practical aspects of modelling such as concepts of validation, or present results of actual field scale applications. Consequently, in the present review of leaching models an attempt will be made to cover some of these aspects.

This review starts with a few theoretical considerations appropriate to modelling. Different approaches to classify or categorize models are then presented, followed by a review of validation techniques. Seven existing leaching models and some of their applications are presented, followed by a brief discussion and conclusions.

2.2 THEORETICAL CONSIDERATIONS

2.2.1 Defining a leaching model

According to Webster's dictionary the word "**model**" can have several meanings. One description of a model is "a miniature, three-dimensional representation of something existing in nature", but in this review the definition that will be used refers to the *mathematical representation of a natural process* such as root growth, nitrogen uptake, or rate at which water infiltrates the soil. More particularly, a leaching model is defined as a mathematical description of the fate and transport of water and chemicals in the soil. A distinction should be made between those leaching models describing transport processes in the unsaturated (vadose) zone, and those dealing with the water saturated zone of the earth's crust. Leaching models are also referred to as solute transport models (e.g. Jury, 1982), or solution flow models (e.g. Bresler *et al*, 1979).

Leaching models attempt to simulate natural processes active in the soil-plant-atmosphere system. In its simplest form a leaching model may be nothing more than a guide for interpreting measurements, while in the most complex form it may seek to describe the space and time dependence of all phases of every chemical species in the soil-water system (Jury, 1982).

Historically leaching models have evolved from two general approaches: those models that are empirical, and those that begin from some consideration of mass balance (Wagenet *et al*, 1988). During the last three decades different types of leaching models have evolved. The various categories into which models can be classified will be discussed in section 2 of this review, but irrespective of the type or class of leaching model, two principal aspects must be dealt with, namely the water regime, and the chemistry and transport of solutes in the partially saturated soil.

2.2.2 Water Regime

Concerning the water regime in soil, two processes are of importance, i.e. the transport and consumptive use of the soil water. Water transport in soil can be simulated in two ways: a) using the rigorous thermodynamic approach in which soil water moves according to differences in potential energy, or b) using a capacity approach in which the ability of the soil to retain water has a certain upper limit. Crop water uptake is usually simulated by employing a simple sink term that accounts for evapotranspiration, although some models are able to distinguish between the processes of evaporation and transpiration. Few leaching models attempt to simulate the actual physiological process of crop water uptake.

2.2.2.1 Thermodynamic approach

Soil water, like other bodies in nature, can contain energy in different quantities and forms, but water transport is concerned primarily with potential energy differences which are due to position or internal condition (Hillel, 1982). The relationship between water content and potential energy was first described by Buckingham (1907) and later in greater detail by Gardner (1920). The basic equation describing water flow in soil is generally known as the Richards equation (Richards, 1931) and combines D'Arcy's equation for saturated flow with the equation of continuity:

$$\delta\Theta/\delta t = \delta/\delta x[K(\Theta)\delta H/\delta x] \qquad \ldots.[2.1]$$

where

H = total hydraulic potential (L), which is the sum of matric (h) and gravitational (g) potentials;

$K(\Theta)$ = water content-dependent hydraulic conductivity (L T^{-1});

t = time;

x = distance (L).

Estimation of $h(x,t)$ automatically yields $\Theta(x,t)$, provided the soil water characteristic curve [$\Theta(h)$] is known. Knowledge of $\Theta(x,t)$ allows the soil water flux q (L T^{-1}) to be calculated. Because water movement is the result of energy differences in space, movement is not restricted to any particular dimension, e.g. vertically down only.

Use of equation 2.1 to calculate flux, or flow of soil water, depends on an accurate knowledge of both the $K(\Theta)$ relationship and the gradients $(\delta H/\delta x)$ that exist under field conditions. In vertically anisotropic soils, this knowledge must be available for each different soil layer which restricts the general application of equation 2.1 to field conditions. It is furthermore restricted by the fact that $K(\Theta)$ can be variable by orders of magnitude over the space of a single, seemingly homogeneous field (Nielsen *et al*, 1973). Similarly, gradients are spatially variable at any one time. As a consequence, calculated field-scale estimates of $\Theta(x,t)$ and $q(x,t)$ are in most cases, quite tenuous. (A more complete discussion of spatial variability and leaching models, is included in section 2.4.2 of this review).

When evapotranspiration is to be simulated, a sink term S is usually added to equation 2.1, where S represents both surface evaporation and transpiration losses. Arriving at a representative value for S and partitioning it into transpiration (crop water uptake) and evaporation can be accomplished in several different ways of varying complexity. The performance of four such root-water-uptake models were compared by Alaerts *et al* (1985). The four models tested were those of Nimah and Hanks (1973), Radcliffe *et al* (1980), Feddes *et al* (1978), and Hoogland *et al* (1981). Detailed descriptions of these four approaches are given by Alaerts *et al* (1985) and will not be repeated here. What is of importance however, is that all four methods attempt to relate crop water uptake to soil water energy differences within the root zone.

The Nimah and Hanks approach is the most complex, and therefore most data demanding, of the four methods. Water uptake is related to an electrical analogue. Resistance to flow in the soil-root system has to be compensated for by the potential drop between the bulk soil and the root xylem. The plant water potential that finally develops is balanced by the atmospheric demand and the soil water availability. Because water uptake is energy driven, knowledge of the $K(h)$ relationship (see equation 2.1) is required. Measurement of the various potentials and the $K(h)$ relationship *in situ* is time consuming and difficult. They are furthermore subject to both temporal and spatial differences.

Of the four methods tested, the sink term proposed by Radcliffe *et al* (1980) is the simplest to compute since root-water uptake is controlled in such a way that the expenditure of energy is a minimum. At each time step water uptake has to be computed. Water is withdrawn by the roots from only one compartment - namely the one with the lowest energy level, meaning specifically from the wettest soil layer.

Alaerts *et al* (1985) concludes that, even though a similar amount of water extraction can be simulated by the four sink terms if the input parameters are properly adapted (or calibrated), the simulated evolution of the extraction rate through time and the depth pattern of the root-water extraction depend strongly on the selected root term. Of particular importance to leaching models is the conclusion that the water-extraction-depth pattern will be of special importance if nutrient uptake and distribution is to be simulated. The simulated nutrient uptake (which indirectly will influence the solute leaching pattern) will depend greatly on the moisture extraction pattern. Alaerts *et al* (1985) furthermore warns that care should be taken when using a sink term for conditions for which it has not been designed and tested. The simple least-energy model of Radcliffe *et al* (1980), for example, performed similarly to the complex Nimah-Hanks model for unsaturated lower boundary conditions, but failed to simulate a realistic extraction pattern when a water table is present. Similarly, Hoogland's extraction term could not simulate daily fluctuating potential transpiration conditions.

Of importance to data collection for modelling studies, is the recommendation by Alaerts *et al* (1985) that a sensitivity analysis of the selected sink term can indicate the level of precision with which the input data and parameters should be controlled. This may save a sizable amount of superfluous experimental field work. Of equal importance is the conclusion that too little seems to be known about plant transpiration and water extraction patterns to result in a general extraction term, simple and economical in use, satisfying in concept and results. This is in accordance with an earlier statement of Molz (1981) who said that "*evidently there is a need for both engineering and agricultural hydrologists to further develop their quantitative understanding of water movement in plant and soil-plant systems*".

The conclusions of Molz (1981) and Alaerts *et al* (1985) are of consequence to leaching models as well. Intuition suggests that the two most important factors that will control the distribution and movement of soil water and chemicals, are the differences in the in- and output water and chemical fluxes. The net flux of solutes and water in turn are strongly influenced by crop water uptake and therefore it can be hypothesized that improved understanding of the process of crop water uptake will also lead to improved predictions of solute transport and distribution.

2.2.2.2 Capacity approach

An alternative approach to simulate and calculate the flow of water in soil is to consider a simple water balance. Here an upper limit to the amount of water that an individual soil layer can hold, is assigned. Added water moves into a designated soil layer until this limit (e.g. field capacity, saturation or any other value) is reached, with the excess water then moving into the next layer. The attractiveness of this method is that knowledge of the $K(\Theta)$ relationship and hydraulic gradients are not required. It also simplifies the numerical algorithms necessary to calculate soil water flow. Because movement of water is capacity driven, usually downward flow only is considered. In some cases an algorithm that mimics capillary rise can be added, e.g. Burns (1974).

Evapotranspiration in capacity type calculations is also much simpler to simulate because knowledge of the soil water potential regime within the root xylem and soil is not required. A simple sink term, representing water loss due to evapotranspiration for any given time period, is most often used, e.g. Burns (1974), and Addiscott (1977).

2.2.3 Chemicals

A number of mechanisms must be considered when predicting solute leaching. An inorganic salt in the soil or irrigation water can undergo any one or more of the following changes while moving through the soil:

dissolution, precipitation, adsorption, desorption, cation exchange, ion pair formation, plant uptake, volatilization (in the case of NH_3).

(The fate of agricultural chemicals, such as pesticides, which are mostly organic compounds, is not considered in this review).

Theoretical descriptions of the chemical reactions mentioned above can be found elsewhere, e.g. Bolt (1979), Lindsay (1979), and Bresler *et al* (1982) and will not be covered here. For the sake of completeness it should be noted that when modelling solute or nutrient transport in a soil which is at steady state with the infiltrating water (i.e. the mass of salt within the soil body remains constant with time), dissolution and precipitation only have to be considered. Consequently, leaching models which assume steady state conditions, are not only easier to construct but are also less data demanding. However, Jury (1982) is of the opinion that for soils with many meters of exchange surfaces above the groundwater table, steady state would never be reached.

Transient conditions where the soil either gain or lose salt with time, are the more general field condition that has to be modelled.

In leaching models, transient conditions are mathematically more complex to represent and solve and also more data demanding. For example, if cation exchange in a quaternary Ca, Mg, Na and K system is to be simulated, the cation exchange capacity and six selectivity coefficients are required as input. The determination of these parameters is time consuming and fraught with analytical errors and is consequently not routinely done.

Of equal importance are the description and mathematical representation of salt transport. Several approaches can be used to describe solute leaching, but according to Wagenet *et al* (1988), the one most often used is miscible displacement theory. This theory states that the flux of solute is the result of the combined effects of diffusion and convection. That is:

$$J_S = J_D + J_C \qquad \ldots[2.2]$$

where

J = the mass of solute transported through a cross-sectional area in unit time,

S = total solute,

D = solute transported by diffusion,

C = solute transported by convection.

A theoretical description and the derivation and extension of equation 2.2 is presented by Wagenet (1983). Certain key aspects only will dealt with here.

Miscible displacement theory assumes that a solute being transported through soil is subject to two types of mixing processes within the pores. One is chemical in nature, resulting from diffusion of solute in response to concentration gradients existing in soil solution. Fick's first law of diffusion is used to mathematically describe the diffusion process:

$$J_D = -D_p(dC/dx) \qquad \ldots[2.3]$$

where:

D_p = is the effective diffusion coefficient of the chemical in the soil,

C = solute concentration,

x = distance.

The other process leading to the mixing of solutes within the soil is physical in nature and results from variations in water flow velocity within each pore and between pores. This process is referred to as mechanical dispersion and can also be described by using an adapted version of Fick's law:

$$J_C = -\Theta D_m(v)[dC/dx] + v\Theta C \qquad ...[2.4]$$

where:

D_m = the mechanical dispersion coefficient

v = average interstitial flow velocity, and

J_C, Θ, C and x as defined before.

Combining equations 3 and 4 into 2 yield the convective dispersion equation of solute transport:

$$J_S = -\Theta D(v,\Theta)dC/dx + qC \qquad ...[2.5]$$

In this equation D_m and D_p are combined into D which is then referred to as the apparent diffusion coefficient, and q represent the volumetric water flux.

The use of equation 2.5 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. Studies by Biggar and Nielsen (1976) report a 420% coefficient of variation of a population of field determined D values. The population of 359 samples furthermore exhibited a skewed frequency distribution. The practical implication of this is that for the 150 ha field that was studied by Biggar and Nielsen (1976), 35 samples are required to estimate the mean within an order of magnitude, while 200 samples are needed to make the estimate within 50% of its true mean value! It should be clear that considering the apparent diffusion coefficient alone, the choice of the input value can have a profound effect on the predicted solute distribution.

2.3 CLASSIFICATION OF LEACHING MODELS

2.3.1 Traditional approaches

Mathematical models of leaching processes in the soil can be classified from the viewpoint of the modeler or the user (Wagenet *et al*, 1988). From the modeler's perspective mathematical models are represented, following the classification described by Clarke (1973), as:

$$q_t = f(p_{t-1}, p_{t-2},..;q_{t-1}, q_{t-2},..;a_1,a_2,..) + E_t \qquad ...[2.6]$$

where:

q_t = output variables,

p_t = input variables

a_n = system variables,

E_t = residual error, and

f = functional form of the model.

The functional form of the relationship can be either conceptual or empirical. The input and output variables, as well as the system parameters and the residual error, can be either stochastic or deterministic. Clarke (1973) categorized mathematical models into four major groups: stochastic-conceptual, stochastic-empirical, deterministic-conceptual, and deterministic-empirical. A model is regarded as stochastic if any of the variables in its mathematical expression are described by a probability distribution. A model is termed deterministic if all the variables are free from random variations. Models are called conceptual if their functional form is derived from consideration of physical processes, and empirical if its not.

Table 2.1 contains a number of leaching models categorized by Loague *et al* (1988) using Clarke's classification scheme.

Table 2.1 Examples of leaching models classified by the Clarke (1973) scheme (according to Loague *et al*, 1988)

stochastic-conceptual,	Dagan and Bresler (1979)
stochastic-empirical,	Jury (1982)
deterministic-conceptual	Wagenet and Hutson (1989)
deterministic-empirical	Carsel *et al* (1984).

In their review of modelling approaches Addiscott and Wagenet (1985) distinguished between deterministic-, stochastic-, mechanistic-, functional-, rate-, capacity-, analytical -, and numerical models. They also made a distinction between research and management models. The definition of **deterministic** and **stochastic** models are the same as that of Clarke (1973). **Mechanistic** models are defined to incorporate the most fundamental mechanisms of the process, as presently understood. An example of such a fundamental mechanism is the Richards equation which is derived from Darcy's Law for water flow. The term **functional** is used for models that incorporate simplified treatments of solute and water flow and make no claim to fundamentality but do thereby require less input data and computer expertise for their use (Addiscott and Wagenet, 1985).

Rate models are those that first define the instantaneous rate of change of water content in terms of the product of a hydraulic gradient and a rate parameter, the hydraulic conductivity, and then defines the rate of change of solute concentration in terms of two other rate processes, convection and diffusion. A capacity model, on the other hand, defines changes (rather than rates of change) in amounts of solute and water content. Such models usually do not use rate parameters but capacity factors, e.g. the volumetric water content at field capacity. Rate models are driven by time, while capacity models are usually driven by the amounts of rainfall, evaporation, or irrigation. According to Addiscott and Wagenet (1985) the distinction between rate and capacity models corresponds approximately to the distinction between mechanistic and functional models.

Analytical or numerical techniques can be used to solve the equations of deterministic-mechanistic models. For example, the convection-dispersion equation (eqn 2.5) can be solved analytically or numerically. However, the practical use of analytical techniques are greatly constrained by the boundary conditions required for the analytical solution (Addiscott and Wagenet, 1985). Numerical methods are most often used to solve equations 2.1 and 2.5, and then usually with finite differencing techniques. A detailed description of such a differencing technique can be found in Wagenet and Hutson (1989).

In deterministic models the model parameters are considered to be single valued. However, given the spatial and temporal variability of soils, crops and climate, each parameter is in fact represented by a population with a unique frequency distribution (Rao *et al*, 1989). The single valued assumption means that deterministic models operates such that the occurrence of a given set of events leads to a uniquely-definable outcome (Addiscott & Wagenet, 1985). Traditionally deterministic models have been constructed and validated based on column studies, mostly observed under controlled laboratory conditions. Consequently, the extrapolation from laboratory to field conditions have not always been met with a great deal of success.

Stochastic models are more suitable to conditions of spatial variability inasmuch as these models presuppose that soil properties vary spatially, so that solute and water movement also vary. Stochastic models therefore presuppose that the outcome will be uncertain and are structured to account for this uncertainty. However, these models are mainly used for research, not least because of the shortage of suitable field data against which to validate them (Addiscott & Wagenet, 1985).

A listing of some leaching models classified by Addiscott and Wagenet (1985) is given in Table 2.2.

2.3.2 Current Approaches

A more recent approach to classify models is that of Wagenet (1988). He is of the opinion that modelling as a science has evolved to the point where models should now be distinguished according to the purpose for which they were developed. His approach transcends the more classic framework for categorizing models used by purists which often focuses upon the mathematical technique used for solution, or the degree of determinism. The advent of microcomputers has put leaching models within reach of the society at large. Wagenet (1988) thus feels that the use to which a model will be put should be the norm for grouping and he identifies three such groups: researchers, action agencies, and a general class of extension/farm users. It is fitting to end this section with the following remark of P.J. Riordan: "*All models require the talents of a skilled model user. If you make the model [code] 'idiot-proof', you invite idiots to use it!*"[1]

Table 2.2 A classification of leaching models (adapted from Addiscott and Wagenet (1985))

I. **Deterministic models**

- A. Mechanistic
  1. Analytical (Nielsen & Biggar, 1962; Van Genuchten & Wierenga, 1976)
  2. Numerical (Childs & Hanks, 1977; Shaffer *et al*, 1977; Robbins *et al* 1980; Wagenet & Hutson, 1989)
- B. Functional (usually based on capacity parameters)
  1. Partially analytical (De Smedt & Wierenga, 1978; Rose *et al*, 1982).
  2. Layer and other simple approaches (Bresler, 1967; Tanji *et al*, 1972; Burns, 1974; Addiscott, 1977)

II. **Stochastic models.**

- A. Mechanistic (Dagan & Bresler, 1979; Amoozegar-Fard *et al*, 1982).
- B. Non-mechanistic (transfer function) (Jury 1982; Jury *et al.*, 1982)

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[1] Comment on a guest editorial by F.D. Arnold, 1989. "Who are these manuals for? The model documentation needs of practitioners". Ground Water 27:778-783.

2.4 VALIDATION OF MODELS

2.4.1 Concepts of Validation

Recently a certain amount of controversy has been associated with the terms *model validation* and *model verification*. One school of thought prefers the term *validate* while the other prefers to use *verify*. Those that give preference to the term *verify* justify their choice by saying that to validate a model, means "*to check the logic of the arguments used in the model*" while verify means "*to check that the scientific assumptions of the model are correct*". In this report, however, these two terms will be used interchangeably and will refer to the process whereby model predictions are compared to measured data. The terminology of researchers and modelers that was used in the original papers will also not be changed, i.e. if McLaughlin (1988) used the term *validate* in his study, then it will be used as such in this review.

The primary aim of validation studies are to prove that model predictions are realistic representations of field scale processes. However, it should also be remembered, as stated by Klemes (1986), "*for a good mathematical model it is not enough to work well. It must work well for the right reasons!*".

The validation of a model involves comparison of the model simulations against measured data. Thus, the model input parameters must be known, and experimental data to compare with the model outputs must be available. One problem with validation studies is that the term *validation* means different things to different people, largely because it is rarely defined with any precision (McLaughlin, 1988).

According to McLaughlin (1988) the general concept of model validation has both technical and policy origins. From a technical or scientific point of view, a model can be considered validated when it is a proper description of the physical processes. From a regulatory point of view it is considered validated when the model yields adequate predictions. In the latter case, the implicit goal seems to be to reduce the risk that a model will lead to inappropriate decisions.

When models are validated, care should be taken not to give subjective norms preference over objective statistical measures. According to McLaughlin (1988), traditional statistical methods are, however, not particularly useful in groundwater or leaching modelling studies. Several reasons are offered for this. First, there are rarely enough measurements in ground- and soil water applications to provide a statistically rigorous test of a model's explanatory capabilities. Second, the conditions prevailing when measurements were collected may not reflect those which the model is designed to simulate. Finally, most classical statistical tests are based on assumptions which are not necessarily met in complex subsurface environments. These tests typically assume that the model's structure is perfect and are based solely on an analysis of the effects of measurement error. In reality this might not be the case.

Validation should encompass the entire modelling process, e.g. sampling, input estimation, and prediction, and not just the simulation model alone (McLaughlin, 1988). Jones and Rao (1988) stress the importance of proper design of validation studies. Improper design may, for example, result in a validation exercise testing the ability of a modeler to select proper input parameters rather than the validity of the model.

Adequate description of processes is an integral part of model validation. Schweich *et al* (1988) questions whether an accurate description of chemical interactions is always necessary in a transport models. The answer depends on the problem posed and available experimental data concerning flow pattern and chemical interactions. If a pollutant is weakly sorbed and water flow is continuously varying, an accurate flow model is necessary and an overall distribution coefficient of the chemical may be sufficient. If safety rules concerning toxicity levels must be stated, flow description on the other hand may be secondary and a reliable chemical model is necessary.

A distinction should furthermore be made between calibration and validation. Loague *et al* (1988) points out that prediction models should first be calibrated and then validated and that the two processes should be independent. For solute transport models, field measured concentration profiles or summary variables can be used to calibrate a model at a given time by adjusting parameters until an acceptable simulation is achieved. Once this fit is obtained another simulation is performed for a later time and compared with a second set of measured data. If the second simulation is also acceptable, the model is considered validated. Model parameters are not adjusted, based on field data, during validation. If the parameters are adjusted for simulations subsequent to calibration, then the effort is not a validation but a recalibration. Loague *et al* (1988) furthermore suggest that the level of model performance be the same for the calibration and validation periods. However, Glass *et al* (1988) showed that goodness of fit during the calibration stage is no guarantee of success during the validation stage if the model does not describe the physical processes with sufficient precision.

In their overview of pertinent literature, Loague *et al* (1988) found that although there is a vast amount of information available on mathematical models, relatively little has been written about evaluation procedures that can/should be used. They distinguish between statistical criteria and graphical displays as techniques to evaluate model performance and feel that a model is a good representation of reality only if it can be used to predict, within a calibrated and validated range, certain observable phenomenon with acceptable accuracy and precision.

Loague *et al* (1988) give suggestions on procedures to be followed in validation studies. A suggested first step is to compare summary statistics (mean, standard deviation) for observed and predicted data. A second evaluation is to use a test statistics (e.g. Kolmogorov-Smirnov) to compare measured data against simulated results. A model's performance is judged acceptable if it is not possible to reject the hypothesis of no difference between observed and predicted values. As is the case with any statistical test, two types of errors are possible using a given confidence level. Type I error is a risk to the model builder and corresponds to rejecting a true hypothesis. Type II error is a risk to the model user and corresponds to accepting a false hypothesis. Analysis of residual errors can also be used to evaluate model performance by characterizing for example, systematic under- or over-prediction. Measures that are available to do this include a) maximum error, b) root mean square error, c) coefficient of determination, d) modelling efficiency, and e) coefficient of residual mass.

The results from any one statistical criteria or graphical display may not be sufficient to pronounce a model's validation even if established levels of confidence are available (Loague *et al*, 1988). Taken independently, each validation method can be limited by stringent assumptions, i.e. independence, equality of variance, and normality. If one or more assumption is violated then sole reliance on the method is suspect. A model should only be considered validated if a set of performance tests are met. In this context Loague *et al* (1988) propose the use of a so-called index of validity. The index of validity is composed of three sub-indices which test: a) stability, b) predictive ability, and c) sensitivity to major assumptions. Each sub-index is calculated as:

$$\frac{\sum_{j=1}^{m} (\%\ \textit{of favorable results}) \times (1/\textit{number of assumptions} + 1)}{\sum_{j=1}^{m} (1/\textit{number of assumptions violated} + 1)} \quad \ldots[2.7]$$

where m is the number of different statistical criteria and/or graphical display results included in each assessment. The sub-indices provide heuristic information for identifying model weaknesses. The index of validity is equal to the average value, when each is found acceptable, of the sub-indices. However, it seems as if a certain amount of subjectivity might be involved in calculating the "percentage of favorable results".

Wilmot (1981) warns against the use of correlation statistics (r) and coefficient of determination (r^2) as statistical measures during the validation process. He used a hypothetical data set to show that a high r (and r^2) value does not necessarily indicate good accordance between predicted and observed results. Wilmot (1981) defines an index of agreement, d, which he suggests is a better measure to use in validating model predictions. The index of agreement is defined as:

$$d = 1 - \frac{\sum_{i=1}^{N}(P_i - O_i)^2}{\sum_{i=1}^{N}[\,|P'_i| + |O'_i|\,]^2} \qquad \ldots[2.8]$$

where:

P_i = i'th predicted value;
O_i = i'th observed value;
$P'_i = P_i - O^-$
$O'_i = O_i - O^-$
O^- = arithmetic mean of the observed values.

The index of agreement is not a measure of correlation or association in the formal sense but rather a measure of the degree to which a model's prediction are error free. The index d varies between 0.0 and 1.0 where a computed value of 1.0 indicates perfect agreement between the observed and predicted observations, and 0.0 connotes one of a variety of complete disagreements. The index specifies the degree to which the observed deviations about the arithmetic mean O^- correspond, both in magnitude and sign, to the predicted deviations about O^-.

2.4.2 Spatial variability

Water and salt transport parameters have been shown to vary by orders of magnitude in space e.g. Nielsen *et al.* (1973), Jury *et al* (1987). In deterministic models one set of parameters are used as input and the procedure in the past has generally been to use the properties of a so-called "representative" soil profile as input, e.g. Van Rooyen & Moolman (1980), and Moolman *et al* (1983). The fact that the frequency distribution of rate parameters such as hydraulic conductivity, pore water velocity and the apparent diffusion coefficient are skew, makes the selection of representative values difficult.

Salt transport depends upon pore water velocity and therefore, the spatial distribution of soluble salt is expected to be highly variable also. Numerous studies have proved this to be the case, e.g. Wagenet & Jurinak (1978), Moolman (1985), Miyamoto & Cruz (1986), and Moolman (1989). The choice of a representative value for these highly variable parameters thus becomes difficult and prone to subjective decisions. Biggar and Nielsen (1976) showed that substantial errors can be made in estimating solute flux passing below the root zone of field soils by multiplying average values of water flux with average values of the soil solution concentration. In this case mean pore water velocities obtained from 20 field plots ranged across 2 orders of magnitude and varied between 0,1 and 11 m day^{-1}.

Part of this large variability of soil hydraulic properties is associated with cracks and channels in soils leading to macropore flow (Beven, 1981). Cameron *et al.* (1979) found that different rates of nitrate and chloride movement in a summer fallowed clay loam were significantly affected by non-uniformity in water storage and transport characteristics, non-uniformity in precipitation catchment of water due to soil surface micro-relief which redistributes water to depressed micro-locations prior to infiltration, and non-uniformity in distribution of applied N fertilizer. Rao & Wagenet (1986) noted that the total variability in field measurements of pesticide residue concentrations consists of two parts: intrinsic and extrinsic variability. The first may be a random component and is attributed to the variability introduced by inherent variability in soil properties. Extrinsic variability is introduced as a result of non-random patterns caused by management practices such as row cropping, drip irrigation, and banded applications of fertilizer or pesticides. An example of extrinsic variability and the effect of that on estimating the field mean salt content is given by Moolman (1989). Appropriate soil sample protocol to account for such extrinsic variability are not always used in field studies. As stressed by McLaughlin (1988) and Jones *et al* (1988) proper sampling design is an integral part of any model validation study.

Dudley *et al.* (1981) have suggested that the spatial variability in soil hydraulic properties is higher when leaching fractions are high or when water uptake by plants is low. A similar trend with regard to the spatial variability of solute leaching therefore cannot be ruled out. It is thus possible that the spatial variability of solute concentrations will be more pronounced on low efficiency furrow irrigated fields, than on high efficiency micro irrigated fields.

Wagenet (1988) is of the opinion that instead of attempting to accurately predict solute flux at a specific field location and which is greatly influenced by spatial variability, a more reachable goal would be to predict mean values for solute flux and concentration over the entire field. Deterministic models can be run using several different sets of input parameters and the outcome then averaged to predict mean water and solute fluxes for an irrigated field.

2.5 EXAMPLES AND FIELD APPLICATION OF SPECIFIC MODELS

2.5.1 Introduction

In the previous sections the theory, classification and validation of leaching models have been discussed. Most leaching models have been developed and tested under well controlled laboratory and, in a few cases, field conditions. Although the advent of micro-computers has put models within reach of a much wider audience than was previously the case, application of leaching models by users other than the original modeler still remain the exception rather than the rule. In the review of literature on leaching models, it became evident that non-mechanistic models, in view of their relative simplicity, have been more widely used and independently validated (by users other than the original model builder) than the more complex and data demanding models. A survey of literature in refereed scientific journals moreover reveal that the theoretical aspects and validation studies of models are more frequently published than are the results of field scale application studies. The same is true for cases where models were (successfully) used to solve a particular managerial or ecological problem.

In the following sections attention will be given to examples of specific leaching models that have been applied to field conditions. The list of models covered is not meant to be exhaustive and range from simple functional approaches to more complex, mechanistic and data demanding approaches. No conclusions should be drawn from the order in which the models are presented.

Factors considered in the selection of models were: a) the model should preferably have been used in more than one field- or plot scale study, and also by users other than the original modelers, b) the models should be able to deal with diffuse, non-point agricultural sources (opposed to point sources, such as waste dumps or factory spills), c) the models should simulate both water and solute flow, and d) preference was given to models simulating the fate of inorganic chemicals, i.e. pesticide models were not reviewed as thoroughly as "salinity" models. Models dealing with the flow and crop uptake of water only, e.g. De Jong and Cameron (1979), Belmans *et al*, (1983), and Torres and Hanks (1989), were excluded.

The discussion of each model will follow the same sequence, i.e. i) theory, ii) input requirements, and iii) application.

2.5.2 Description of specific models

2.5.2.1 Burns model

i) Theory

Burns (1974) proposed a capacity type leaching model for non-reacting (conservative) salts, including nitrate, based on the concept that soil segments (or "plates") in a fallow soil have a maximum storage capacity for water (field capacity, FC) and a minimum water content which is reached during drying, namely the evaporation limit. When water and/or nitrate is added to the uppermost segment, convection and dispersion are simulated by assuming that the added water remains in the uppermost layer long enough for equilibration of water and salt to occur. The newly generated water content of the uppermost layer is then compared with the corresponding FC value. If the water content is greater than FC, water and salts are transferred down to the next segment using the equation:

$$W_p = (R\text{-}E) + M - F , \qquad \ldots[2.9]$$

where W_p is the amount of water containing an equilibrium salt concentration that is lost, $(R\text{-}E)$ represents the net water applied (rainfall minus evaporation), M is the antecedent water content and F is the field capacity. This procedure continues down the profile until a layer is encountered which is either the bottom layer or in which the incoming water does not cause the water content to exceed field capacity. If $(R\text{-}E) < 0$, evaporation takes place and a routine which describes capillary movement of water and salt to the surface is employed. Redistribution of solutes within the profile (either upwards or downwards) are assumed to result solely from mass flow and convection; all diffusive movement is ignored.

ii) Input requirements

- Gravimetric water content initially in the profile, at field capacity, and evaporation limit for each soil segment of specified depth.
- Bulk density of each soil segment.
- Initial salt content ($kg.ha^{-1}$) of each soil segment.
- Daily actual evapotranspiration and precipitation.
- Amount of soluble salt in the irrigation water added to the soil. (This is an addition to the model made by Moolman, (1988)).

iii) Application

Burns(1974) applied this model for the period May to October 1970 to a fallow sandy loam soil and predicted the chloride, nitrate and water content distribution. Good agreement between the predictions of the model and the observed field results were obtained. Burns (1974) report that in most cases the predicted chloride values fell within two or three standard deviations of the mean field concentrations. The predicted Cl^- and NO_3^- concentrations for two dates, 13 July and 20 October 1970, redrawn from Burns (1974), are presented in Figures 2.1 and 2.2. A statistical analysis of the results from all sampling periods by Burns (1974) is summarized in Table 2.3.

Table 2.3 Statistical analysis of predicted vs. observed field values of chloride, nitrate and water deficit amounts (Burns, 1974)

Property	n[(a)]	Regression eqn.[(b)]	R^2 (%)
Chloride	84	F=0,917M+1,14	90,2
Nitrate	84	F=0,781M-1,17	84,4
Water deficit	84	F=0,580M+0,03	68,3

[a)] n= number of observations
[b)] F=field data, M=model data.

Cameron and Wild (1982) applied the Burns model to field observed data where a chloride tracer was introduced at the surface of a soil prior to the onset of irrigation and winter rainfall. After a total of 40 and 80 mm rainfall, the model under-estimated solute movement considerably, even when the input was modified to 5 mm water (precipitation) increments. A summary of the regression equations for measured against predicted chloride recovery percentages for each of four different sampling dates are given in Table 2.4.

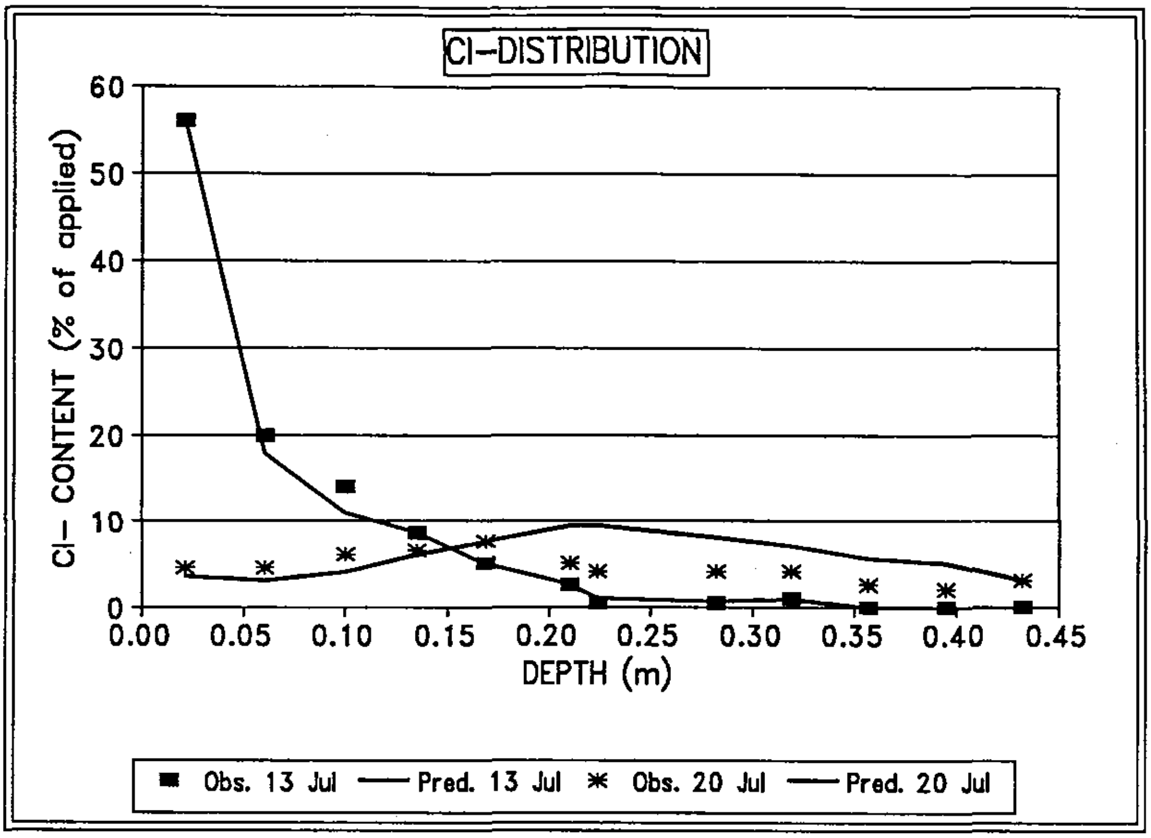


Figure 2.1 Chloride distribution profiles predicted with the Burns model for 13 July and 20 October 1970 (Redrawn from Burns, 1974)

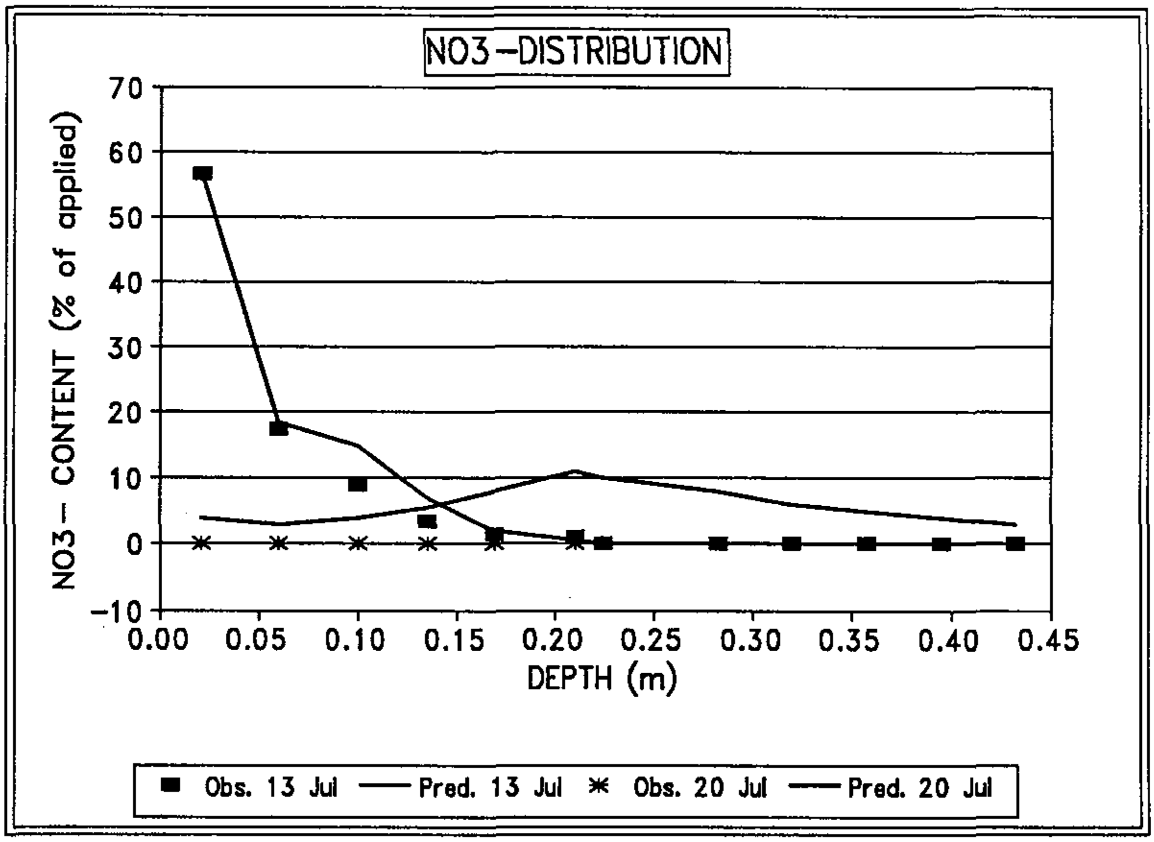


Figure 2.2 Nitrate distribution profiles predicted with the Burns models for two dates; 13 July and 20 October 1970 (Redrawn from Burns, 1974)

Table 2.4 Regression of field measured (F) chloride recovery on model predictions (M) for four different sampling dates (Cameron and Wild, 1982)

Sampling	Q[(a)]	Regression [(b)]	R^2 (%)
B	40	F=0,30M+1,98	19,0
C	80	F=0,38M+3,37	13,5
D	80	F=0,49M+1,76	31,6
E	180	F=0,57M-0,53	65,0

[a)] Q= mm of water added as rain (D,E) and irrigation (B,C)
[b)] F=field data, M=model data.

It is clear that the agreement between measured and predicted chloride contents were far less favorable than reported by Burns (1974). Cameron and Wild (1982) attributed this mainly to the fact that soil conditions regarding structure and texture differed markedly between the two studies. On the other hand, Khanif *et al.* (1984) and Haumann and Du Preez (1989) found good agreement between observed and predicted water content and nitrate concentration values when using the Burns model.

2.5.2.2 Addiscott model

i) Theory

A refinement of the functional approach of Burns (1974) is the multicompartment model of Addiscott (1977) for leaching of conservative salts in coarsely structured soils, in which retention of soil water and salt residing inside dead end and micro pores inside soil aggregates is simulated. Each layer is at field capacity (winter leaching) and the equilibrium soil solution is divided between mobile and a retained phases. The mobile phase corresponds to water held between -5 and -200 kPa and the immobile, retained phase below -200 kPa. Below -1500 kPa, diffusion is considered negligible and anion exclusion highly probable and this water is therefore omitted from the retained phase. The model functions in a similar way to the Burns model. Incoming water (precipitation and irrigation) causes piston flow in the mobile phase during which solute may move just from one layer to the next or, if a large amount of water is applied, through several layers. When piston flow ceases, solute movement between the phases occurs to equalize the concentrations in the soil water between the phases.

The model of Addiscott includes a fast leaching routine to distribute large water inputs down the profile to simulate fissure flow. The main uncertainty in the use of this model is in the allocation of values to mobile and retained water.

ii) **Input requirements**

- Water content of the mobile and immobile phases, in mm per soil segment.
- Water content at field capacity.
- Daily rain and open surface water evaporation.
- Solute content of rain or irrigation in mg per soil segment.
- Rainfall limit above which rain "overflows" into non-equilibrium channels.
- Maximum daily evaporation when the soil surface is dry.
- Retention, or "holdback" coefficients for the top- and subsoil.

iii) **Application**

This model was used successfully to simulate changes in concentrations of applied nitrate in the top 26 cm of a clay loam in the field (Addiscott, 1977). It was also used by Addiscott *et al* (1978) to predict the concentrations of chloride in water draining from the 20- and 40-inch drain gauges at Rothamsted after chloride application to the surface.

Cameron and Wild (1982) evaluated this model by predicting the chloride and nitrate movement through a soil on Upper Chalk under irrigation and winter rainfall. The output was compared with measured values after two irrigation events and two rainfall events (B,C,D & E in Table 2.5). The regression equations of field on model data for chloride distribution accounted for less than 10% of the total variance. The predicted distributions for the rainfall periods during winter was much improved. Cameron and Wild (1982) attributed this poor relationship to the fact that the first irrigation applied 40 mm of water to the soil. This required the use of the fast leaching routine, causing the water to be distributed down the profile before mixing with the resident solution. This was most significant in the surface layer where the chloride concentration was diluted but with very little solute movement to the lower layers taking place (Figure 2.3). When the water inputs were limited to 5 mm increments, an appreciable improvement was obtained.

Cameron and Wild postulated that another reason for the failure of the model could have the differences in the pore size distributions of the soil at Rothamstead (where the performance of the model was satisfactory) and the Upper Chalk soil. The model was developed and validated on the former soil.

In a different kind of application, Whitmore *et al.* (1987) used a more comprehensive version of Addiscott's (1977) model to successfully predict soil mineral N for the purpose of estimating fertilizer requirements for sugar beet.

Table 2.5. Regression equations for field measured recovery (F) on model predicted (M) chloride concentrations (adapted from Cameron and Wild, 1982)

Sampling	Q[(a)]	Regression [(b)]	R^2 (%)
B	40	F=0,01M+3,57	0,0
C	80	F=0,53M+6,13	7,3
D	80	F=0,44M+2,15	11,3
E	180	F=1,56M-2,63	77,7
5 mm increments			
B	40	F=0,91M+1,05	86,6
C	80	F=0,98M-0,65	83,1

a) Q= mm of water added as rain (D,E) and irrigation (B,C)
b) F=field data, M=model data.

2.5.2.3 TETrans

i) Theory

TETrans (acronym for Trace Element Transport) was developed by Corwin & Waggoner (1990) on the premise of mass balance and on a consideration of bypass flow. As such it can be considered to be a offshoot of the Burns and Addiscot models. TETrans is a capacity model which defines changes in amounts of solute and water content rather than rates of change. It is driven by the amounts of rainfall, irrigation or evapotranspiration (ET) and only considers time indirectly by using time from one irrigation or precipitation event to another. From a knowledge of water inputs and losses, and of soil-solute chemical interactions, TETRans predicts the average movement of reactive and nonreactive solutes in the unsaturated zone of the soil. Transport through the soil profile is modeled as a series of events or processes for a finite collection of discrete depth intervals.

The assumptions made in TETrans are similar to that of the Burns model with the exception that the former does not consider upward movement of water and salts. The major advantage of TETrans over the Burns approach is that it attempts to simulate by-pass flow and chemical exchange and adsorption reactions. The model is specifically designed for real-world applications where little transport information is known by, or is available to the user. It is a user-friendly, menu driven model and is available in both an IBM-PC and Macintosh II computer version.

ii) Input requirements

- The number, time, amounts and solute concentration of the irrigation/precipitation events.
- Evapotranspiration amounts
- The number and thickness of the soil depth increments.

- The pH of the soil solution and the adsorption coefficients for each depth increment.
- The field capacity and minimum soil water content of each soil increment.
- Bulk density.
- Initial soil water content, soil solute concentration and pH for each soil depth.
- Number of crops, planting, maturing and harvesting days, and maximum crop root penetration.

iii) Application

Because TETrans was only recently (August 1990) released by the authors (Corwin & Waggoner, 1990) very little is known about the actual field application of the model. Only one application of the model to a soil lysimeter column have been reported (Corwin *et al*, 1990). In this study, excellent agreement between measured and predicted boron concentrations are reported.

2.5.2.4 Rose model

i) Theory

Rose *et al* (1982) derived an approximate analytical equation that can be used to compute solute profiles with dispersion in soils but their method deals only with solutes that undergo no sorption or transformation. Precipitation, dissolution and cation exchange cannot be accommodated. The theory of the Rose model is described by Rose *et al* (1982). Abbreviated versions of this theory are also given by Cameron and Wild (1982), and Addiscott and Wagenet (1985).

This model first computes the position of the solute peak ignoring the effects of dispersion and diffusion and then impose on this peak the computed effects of dispersion and diffusion. The depth of the solute peak, i.e. depth of maximum solute concentration, is given by:

$$\alpha = Q/\Theta_{fc} \qquad \ldots[2.10]$$

where:

α = depth (from surface) of solute peak,

Q = amount of infiltration, $= V_f\, t$

V_f = rate of infiltration,

t = effective time of infiltration,

Θ_{fc} = average profile water content at field capacity.

(Equation 2.10 can be derived by removing the dispersion term from equation 2.5).

The effect of dispersion around the peak is calculated from approximate analytic steady state solutions to the convection dispersion equation (eqn. 2.5):

$$C = \frac{C_0}{2}\left| erfc \frac{z-\alpha}{2(D_0 t + m\alpha)^{0.5}} - erfc \frac{z-\beta}{2(D_0 t + m\beta)^{0.5}} \right| \qquad ...[2.11]$$

where:

C = solute concentration;
C_0 = initial solute concentration;
z = distance from soil surface;
β = (α - F) where F is the thickness of the initial solute pulse;
D_0 = molecular diffusion coefficient for the particular solute;
m = dispersivity, defined as $\epsilon = D_0 + mU$;
ϵ = hydrodynamic dispersion coefficient;
U = average pore water velocity;
erfc = complementary error function.

Equation 2.11 allows concentrations to be calculated for values of t and z.

ii) Input requirements

- Amount and rate of infiltration.
- Time of infiltration.
- Average profile soil water content at field capacity.
- Width of the solute pulse introduced at the soil surface.
- Molecular diffusion coefficient of the solute.
- Dispersivity.
- Initial solute concentration.
- Actual daily evapotranspiration rate.

iii) Application

Rose *et al* (1982) used their model to predict the time of arrival of the peak concentration of N in the drainage water of four undisturbed column lysimeters with a silt loam topsoil. Good agreement was found between their predictions and the observed data previously reported by Chichester and Smith (1978). The model was less successful in predicting solute movement in a lysimeter back-filled with a loamy sand. The less successful part of the simulation was attributed to preferential water movement and the effects of diffusion between mobile and less mobile water in the lower part of the soil profile.

Cameron and Wild (1982) also applied the Rose model to the same data on which the Burns and Addiscott models were evaluated (see sections 2.5.2.1 and 2.5.2.2). They found that the Rose model simulated the movement of the chloride tracer with considerable success. The regression equations of measured on predicted chloride concentration had coefficients of determination that ranged between 70% and 96% when a diffusion coefficient of 0,1 cm^2 day^{-1} and a dispersivity value of 3 were used. Increasing the dispersivity value generally led to a decrease in the coefficient of determination (R^2) while increasing the diffusion coefficient from 0,1 to 1,0 cm^2 day^{-1} had little effect on the predicted results.

2.5.2.5 Shaffer (USBR) model

i) Theory

The Shaffer model (Shaffer *et al*, 1977) is the result of 15 years of research and development, funded mostly by the U.S.B.R., into efforts to accurately predict irrigation return flow qualities and quantities on irrigation schemes in the western parts of the U.S.A. Theoretical aspects of the model have been published by Dutt *et al* (1972), Skogerboe *et al* (1976), Shaffer *et al* (1977), and Moolman and Beukes (1980). The model simulates chemical and physical processes associated with agricultural lands drained by subsurface tile drainage systems. The simulation starts with field applications of water, salt and nutrients (nitrogen) and ends with predictions of flow and water quality from the drains. According to the classification scheme of Addiscott and Wagenet (1985) the Shaffer model is both mechanistic and deterministic and solves both the Richards flow, and convection dispersion equations numerically.

The overall model consists of several submodels and is schematically represented in Figure 2.3. Only a brief, qualitative description of each submodel, according to Shaffer *et al* (1977) will be dealt with here.

The unsaturated flow submodel describes the infiltration, redistribution, drainage, and soil water extraction by plants. Layered soils can also be accommodated. Flow is described using the Richards flow equation in its diffusivity form.

$$\delta\Theta/\delta t = \delta/\delta x[D\delta\Theta/\delta x - K] - S \qquad \ldots.[2.12]$$

where D is the hydraulic diffusivity, S is a sink term accounting for evapotranspiration, and the other symbols defined as before (see equation 2.1). The unsaturated hydraulic conductivity is calculated according to the method of Campbell

(1974). Actual semimonthly values of evapotranspiration can be used in the sink term and the water loss is distributed through the soil profile by assuming a specific root distribution for the crop under consideration.

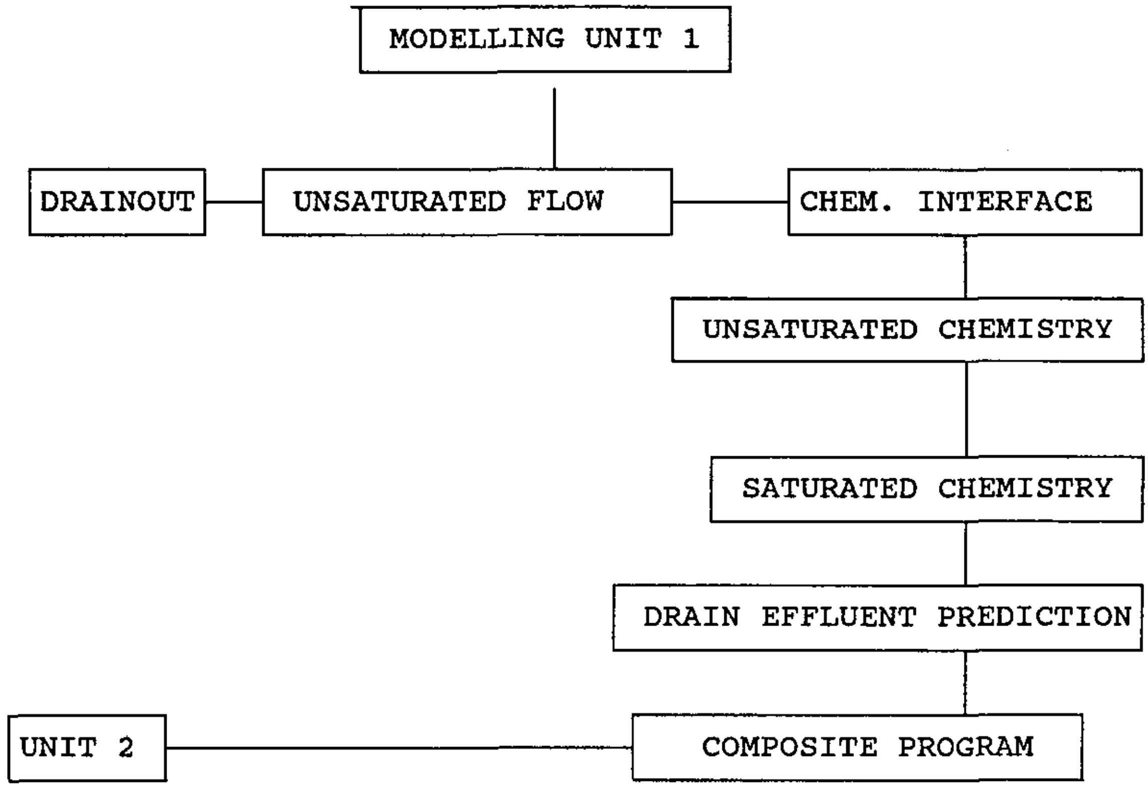


Figure 2.3 Schematic representation of the return flow salinity model of Shaffer *et al* (1977)

Simulating flow in the profile is accomplished by dividing the soil into small nodes and by solving equation 10 at successive time steps with a finite difference approximation technique. At each time step the computer program calculates the moisture flux between adjacent nodes. A limitation of the model is that the bottom boundary of the soil should be at a fixed location with a fixed water content. Fluctuating water conditions can therefore not be accommodated as the bottom boundary. In order to accommodate soils where the water content at the bottom boundary do fluctuate, the unsaturated flow program was changed in an empirical and qualitative way (Moolman, 1982). Although the method violates the conservation of mass, test runs showed that the error introduced to the water balance is negligible.

The chemistry of the unsaturated zone is described by simulating the following processes for each of the user specified number of soil segments: a) various forms of nitrogen reactions (which can be bypassed by the user), b) inorganic chemistry including ion exchange, solution-precipitation of slightly soluble salts, the formation of undissociated ion pairs, and the bicarbonate buffer system, and c) movement and redistribution of the soluble constituents of the unsaturated zone.

One-dimensional salt transport is described by equation 2.5 (convection dispersion). Following the recommendation of Bresler *et al* (1979) and which was later experimentally proved as correct by Amoozegar-Fard *et al* (1982), Shaffer *et al* (1977) assumes that dispersion due to diffusion is negligible compared to convective dispersion. This yields an abbreviated form of equation 2.5:

$$\delta C/\delta t = -v\delta C/\delta x \qquad \ldots[2.13]$$

where v is the flux or Darcy velocity. By means of an interfacing program the nodal concept of the unsaturated flow submodel is changed to the segment concept of the unsaturated chemistry submodel.

The drainout program (Fig 2.3) is designed to predict the response of a subsurface drainage system of parallel, equally spaced tile drains to percolation inputs. The quantity of water crossing the water table during any given day, as computed by the unsaturated flow program, is used to calculate the position of the water table and drain discharge as a function of time. Discharge values, computed on a daily basis, are accumulated to yield monthly or yearly values (Shaffer *et al*, 1977).

The saturated flow program predicts the average or steady-state responses of a subsurface drainage system to deep percolation inputs. The total amount of deep percolation computed by the unsaturated flow program is converted to an annual rate for input to the saturated flow submodel. Implementing the geometry of the drainage system, as used by the drainout program, a steady-state potential theory solution is employed to define stream paths or lines to a circular drain.

The saturated chemistry program (Fig. 2.3) deals with the chemical processes taking place in the saturated zone, as water flows from the water table to a drain. It accepts as input the quantity and quality of the leachate predicted by the unsaturated chemistry program. Water is assumed to move by piston displacement through successive soil segments until it reaches the drain. After each displacement, the solution phase is equilibrated with the solid and exchangeable phases.

The drain effluent prediction program mixes the water from each drainage tube in the saturated zone. Mean travel times, monthly drain discharges, and water qualities generated in the previous programs are used to calculate transient qualities for the soluble constituents of the drain (Shaffer 1976).

ii) Input requirements

The Shaffer model is very data demanding, more so because it simulates processes both in the unsaturated as well as in the saturated zone. However, this review deals with transport models of the unsaturated zone and therefore, the input requirements for the unsaturated flow and unsaturated chemistry programs only (Fig 2.3) will be listed. A full description of the input requirements can be found in the users manual of this model (Shaffer *et al*, 1977):

The input required for each soil node or segment is:

- Saturated hydraulic conductivity.
- Minimum water content below which the diffusivity and conductivity are assumed negligible and set to zero (usually taken as the permanent wilting point).
- Water content at saturation.
- Initial water content.
- Slope of the soil moisture characteristic curve.
- Air entry potential.
- Initial soil analysis including:

  soluble salt content (Ca^{2+}, Mg^{2+}, Na^{+}, HCO_3^{-}, CO_3^{2-}, Cl^{-}, SO_4^{2-})
  cation exchange capacity and selectivity coefficients
  gypsum content
  presence of lime (yes/no)
  bulk density
  saturation percentage of a watersaturated soil paste.

Additional input requirements are:

- Semimonthly actual evapotranspiration data.
- Root distribution information.
- Water application information, including chemical composition of irrigation water.
- Fertilizer application dates and amounts.

ii) Applications

The model was verified by Shaffer *et al* (1977) using information of a 2200 acre area in southwestern Colorado which has been irrigated for 75 years. Soil samples from an adjacent unirrigated area were used to estimate the initial soil conditions and the model was then run simulating the 75 year irrigation period. The predicted chemical composition after 75 years of irrigation was then compared to the measured data obtained at two field sites within the 2200 acre area. The results are summarized in Table 2.6.

Table 2.6 Predicted and observed soil conditions after 75 years of irrigation (adapted from Shaffer *et al*, 1977)

Site	M2		M3		
Variable	Obs	Pred	Obs	Pred	Units
Ca	25	28	23	27	me dm^{-3}
Na	50	27	61	49	me dm^{-3}
Mg	29	43	59	60	me dm^{-3}
HCO_3	2	3	2	2	me dm^{-3}
CO_3	0	0	0	0	me dm^{-3}
Cl	3	4	10	7	me dm^{-3}
SO_4	97	89	131	123	me dm^{-3}
Sums	206	184	286	268	me dm^{-3}
TDS	6885	6298	9342	8668	mg dm^{-3}
Percent error	8,5		7,2		

With the possible exception of Na, the predicted ion concentrations were in good accordance with the observed values. The predicted total salt content was within 10% of the observed data. Considering some of the assumptions made concerning the climate (evapotranspiration) and irrigation quantities, the good accordance between predicted and measured data was taken to be a valid verification of the predictive capabilities of the model.

Moolman and Beukes (1980) tested the Shaffer model under field conditions using four years of data of an irrigation experiment with alfalfa in the Southern Cape Province of South Africa. Two irrigation treatments were simulated, being irrigation applications of respectively 180 mm every six weeks, and 45 mm every three weeks. The two treatments were referred to as the low (LIF) and high (HIF) irrigation frequency plots and each plot was irrigated with water with an electrical conductivity (EC) of 2.32 $dS.m^{-1}$ and SAR of 9.01. The plots were underlain by a water table which was assumed to be static at a depth of 3360 mm. Due to a lack of data the physical properties of the soil below 1200 mm were empirically chosen using the textural composition (which was available) as a guideline. At the onset of the irrigation experiment, the soil was analyzed to a depth of 1200 mm only. Consequently, no information on the initial chemical composition of the soil deeper than 1200 mm was available. To overcome this problem the authors extended the properties of the 900-1200 mm layer to the water table at 3360 mm depth. At the end of the four year irrigation experiment, the soil was analyzed to a depth of 1920 mm.

Due to a lack of measured data, the predicted water contents of the soil layers deeper than 880 mm could not be verified. In general good agreement between measured and predicted data was found (Moolman and Beukes, 1980). Soil water content profiles of the HIF plot (Fig 2.4) suggest that the Shaffer model is able to yield acceptable results under field conditions. The relative error in the absolute water content of individual soil layers appeared to be unacceptably large, but when the authors compared the differences to the actual water holding capacities of the different soil layers, the relative error was found to be within acceptable limits. For the HIF plot the mean percentage error in the predicted water content per profile (0-880 mm) was 6.1% and for the LIF plot 16.1%.

The predicted and measured depth weighted mean soluble salt concentrations for the HIF plot, after four years of irrigation, are summarized in Table 2.7. On a depth-weighted basis for the soil layers shallower than 1200 mm, the predicted soluble salt concentration compared favorably with the measured data, with the percentage error of TDS being about 10%. However, if the salt content of the soil layers between 1200 mm and 1920 is also taken into account, the percentage error increases to about 40% for both of the irrigation treatments. Moolman and Beukes (1980) attributed this discrepancy to three possible causes: a) salt releasing by the weathering of primary minerals in the semi-arid soil, b) the assumption that the chemical composition of the 1200-3360 mm layer is similar to that of the 900-1200 mm layer, and c) capillary rise of saline water from the water table into the 1200-1920 mm zone.

The Shaffer model has also been used in macro scale field studies, e.g. McLinn and Gelhar (1979), and Moolman *et al* (1983). The former authors applied certain components of the model to ten years of information of 43800 ha of irrigated soil in the Mesilla Valley, New Mexico. The Shaffer model was combined with a conjunctive use model to predict the total salt content of the Rio Grande river, which receives the irrigation return flow from the irrigated area. The authors concluded that the model was able to simulate the seasonal variation in water quality quite well.

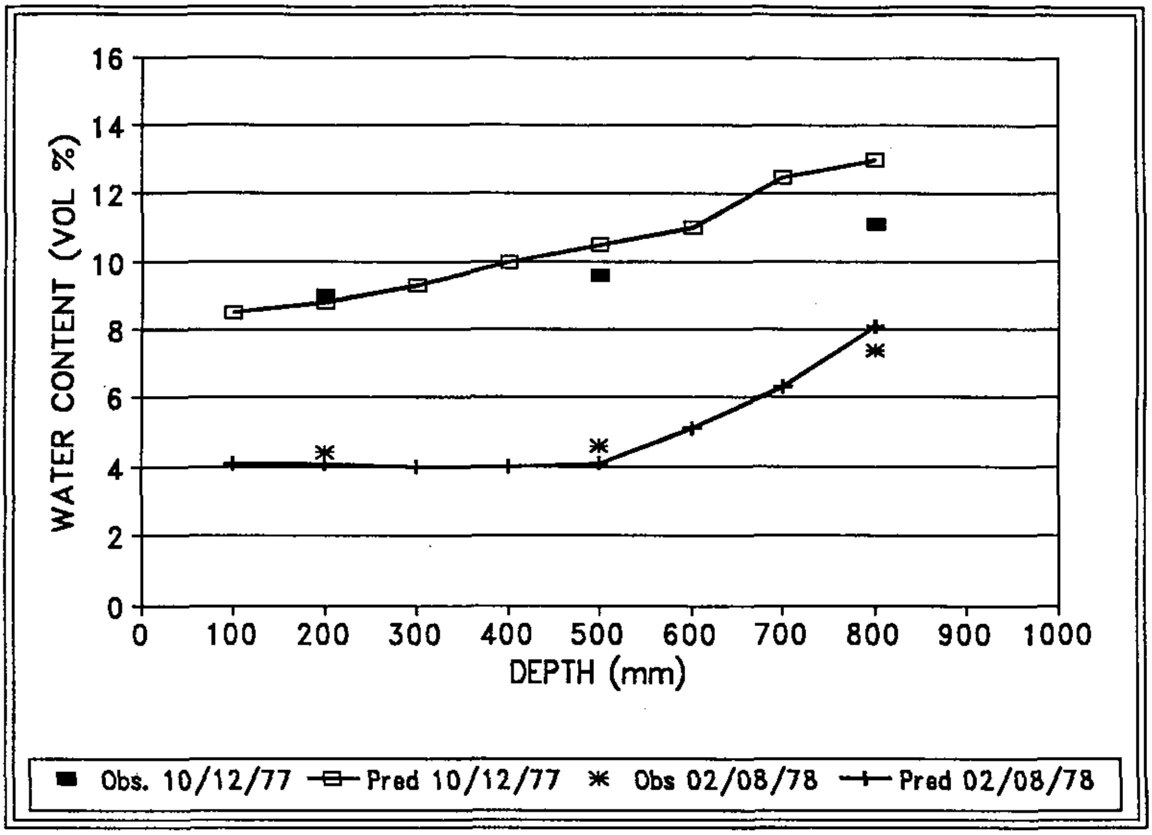


Figure 2.4 Observed and predicted soil water content of the HIF plot (Redrawn from Moolman and Beukes, 1980)

Table 2.7 Predicted and measured depth weighted mean soluble salt concentration for the HIF plot after four years of irrigation (adapted from Moolman and Beukes, 1980)

Depth (mm)	1200		1920		
Ion	Meas	Pred	Meas	Pred	Units
Ca	9,56	12,37	11,55	12,42	me dm^{-3}
Mg	11,20	3,93	15,60	3,37	me dm^{-3}
Na	23,80	21,13	29,06	16,58	me dm^{-3}
HCO_3	1,08	3,96	0,90	3,10	me dm^{-3}
Cl	33,67	26,99	44,20	23,37	me dm^{-3}
SO_4	10,17	7,00	11,33	6,40	me dm^{-3}
Sum	89,48	75,38	112,70	65,24	me dm^{-3}
TDS	2623	2316	3256	1996	mg dm^{-3}
Error		11,7		38,7	%

Moolman *et al* (1983) used the model to predict irrigation return flow volumes of 770 ha of irrigated vineyard as a possible explanation for the observed fluctuations in the mean monthly baseflow TDS content of a tributary of the Breede River in South Africa. It was found that the practice of vineyard irrigation which involved a large amount of water being applied as a pre-bud-burst irrigation in late August or early September, followed by more or less fixed amounts of water being applied at set frequencies during the rest of the irrigation season, resulted in deep percolation losses and accompanying salt loads which are much bigger during the last six months (July-December) of a calender year than during the first six months (January-June). On a half yearly time basis, the computer predictions were in fair accordance with the observed TDS content of the receiving river, which for three consecutive years (1978-1980) were substantially higher for the period July to December than from January to June (Fig 2.5). However, on a monthly time basis, it was found that the fair comparison between predicted (in the irrigation return flow) and observed (in the river) mean monthly TDS contents for the months July to December does not apply to the period January to July. During 1979 the root mean square error for the months January to June (637 mg dm^{-3}) was more than double that of the period July to December (308 mg dm^{-3}). The authors hypothesized that this lack of agreement might be related to the fact that the Shaffer model lacks the ability to route unsaturated flow to a receiving river.

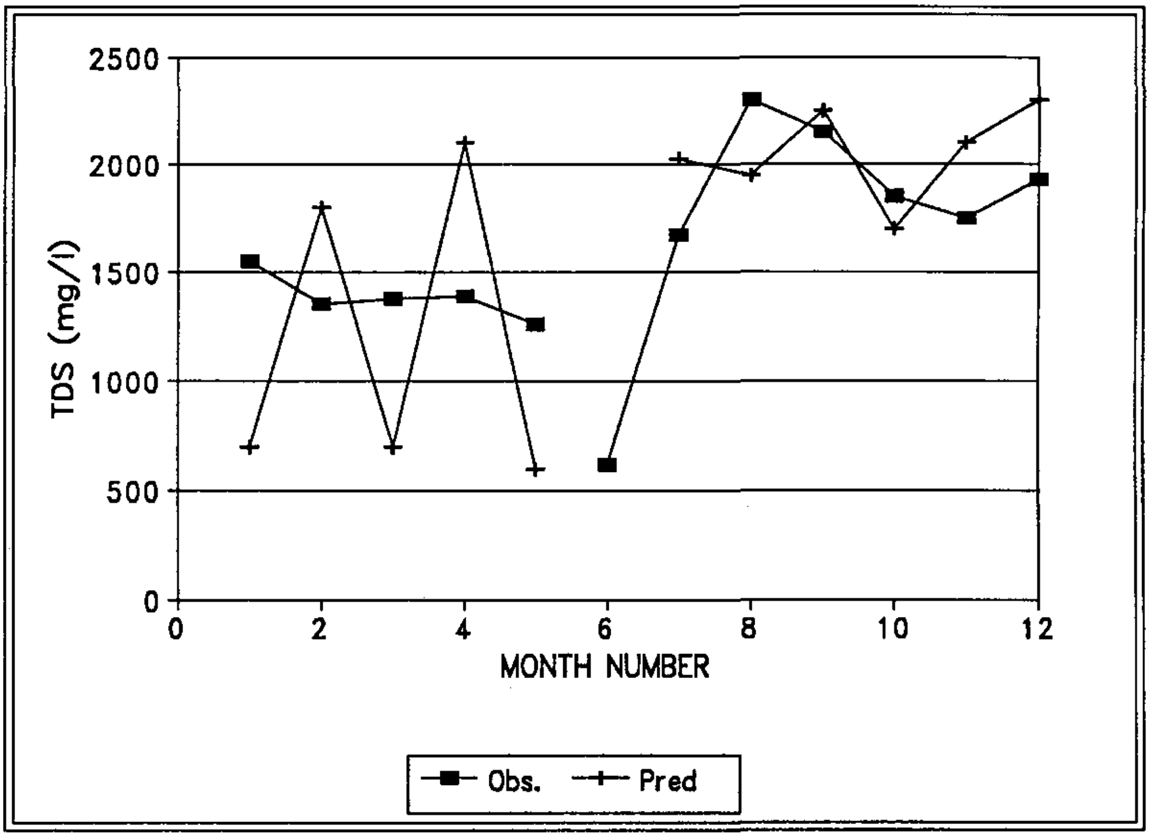


Figure 2.5 Mean monthly predicted and observed TDS content of the Poesjesnel River during 1979 as predicted with the Shaffer model (Redrawn from Moolman *et al* (1983)

2.5.2.6 Jury model

i) Theory

Jury (1982) states that "*the many causes of spatial variability of water and solute transport, renders measurement of the hydraulic and retention parameters of a field soil all but impossible*". As a consequence he abandoned the deterministic approach to modelling chemical transport in favor of a stochastic approach by using a transfer function model.

The concept of a transfer function is to predict the movement of non-reacting solutes, such as the chloride ion, through a field of spatially variable hydraulic properties. This approach measures the distribution of solute travel times from the soil surface to some reference depth. A distribution function of the form:

$$P_L(I) = \int_0^i f_L(I)dI \qquad \textit{...[2.14]}$$

is constructed in which $f_L(I)$ represents the probability density function summarizing the probability (P_L) that a solute added at the soil surface will arrive at depth L as the quantity of water applied at the surface increases from I to $(I + dI)$. The model considers the soil to be composed of twisted capillaries of different lengths within which water moves by piston flow. An estimate of the probability density function $f_L(I)$ can be obtained using soil solution samples located at depth L at various field locations. Jury (1982) assumes that the transfer function is log-normally distributed.

Addiscott and Wagenet (1985) are of the opinion that the most important characteristic of this model is that it attempts to simulate spatially variable field processes with only minimum of input data.

ii) Input requirements

The only input requirements of this model are:

- Amount of water infiltrated at the surface.
- Concentration, measured at a number of locations in a field at depth z, of a pulse of tracer (e.g. chloride) introduced at the surface at time zero.
- Evapotranspiration information.

iii) Application

Only one field application of this model could be found, i.e. Jury *et al* (1982) and Jury and Sposito (1985), both reports describing essentially the same experiment. The transfer function model was tested on a 0,64 ha field instrumented with a set of solution samplers at various depths. A tracer of NaBr solution was applied at the surface and the vertical movement of the Br^- pulse was monitored as a function of the amount of infiltrated water. The 30 cm depth (L=30 cm) was used to calibrate the transfer function. This was achieved by determining at which infiltrated water content (I) the maximum concentration of Br_- was detected at the 30 cm depth. The population of I values was used to obtain the required probability density function f_L which appear in equation 2.14. This function was then used to predict the breakthrough curves for Br^- at the deeper depths, as well as the movement of the solute pulse down to depths exceeding 360 cm.

In general the agreement between observed and predicted solute concentrations was good, although the model tended to overpredict the amount of spreading at the greater depths. The good agreement was found to also hold for the predicted and measured fractions of the sample population (n=14) which had moved past the 330 cm depth by the time 70 cm water had infiltrated.

It is not yet known whether this transfer function approach will be satisfactory in soils which are anisotropic with depth, or whether it will give accurate estimates of flux as well as concentration (Addiscott and Wagenet, 1985). Furthermore, it is unclear how this model, and other stochastic approaches, will be used in management to predict the amount and quality of the deep percolate crossing the bottom boundary (e.g. how much water and salt will enter a water table). The transport volume required to move the non-sorping solute by convection must also be measured experimentally by observing the movement of a pulse of solute for any given field situation. It cannot be predicted *a priori* from independent measurements of the soil (Jury *et al*, 1988). Obtaining the probability density function, which is the essential part of this model, is thus a time consuming and labor intensive process.

2.5.2.7 Wagenet-Hutson (LEACHM) model

i) Theory

a) General Overview

LEACHM is a general acronym (Leaching Estimation And CHemistry Model) that refers to four versions of a simulation model which describes the water regime and the chemistry and transport of solutes in unsaturated or partially saturated soils (Wagenet and Hutson, 1989). These models utilize similar numerical solution schemes to simulate water and chemical movement. They differ in that one model (LEACHN) is organized to describe nitrogen transport and transformation, a second model (LEACHP) is intended for simulation of pesticide displacement and degradation, a third model (LEACHC) is formulated to describe transient movement of inorganic ions (Ca^{2+}, Mg^{2+}, Na^{+}, K^{+}, SO_4^{2-}, Cl^{-}, CO_3^{2-}, HCO_3^{-}) and a fourth (LEACHW) describes the water regime only. In the rest of this discussion attention will be devoted to the inorganic chemistry version of LEACHM only, i.e. LEACHC.

Estimates of plant growth and absorption of water and solutes by plant roots are included together with a flexible means of describing precipitation and surface evaporation of water. The numerical differencing procedures used in LEACHC were developed from several earlier models (Bresler, 1973; Nimah and Hanks, 1973; Tillotson *et al.*, 1980). The chemical equilibrium and cation exchange subroutines were developed from those of Robbins *et al.* (1980a,b). The water flow subroutine is based upon that developed by Hutson (1983). Improvements to these models include applicability to a wider range of field conditions, flexibility of simulating layered or non homogeneous profiles, improved mass balancing and orderly and self explanatory input and output tables.

The model is organized on a modular basis. A main program initializes variables, calls subroutines and performs mass balancing. Subroutines deal with data input and output, time step calculation, evapotranspiration, water flow, solute movement, sources, sinks (degradation, volatilization) and chemistry, leaf and root growth, temperature, and solute absorption by plants. Segregation of each of these processes into subroutines called by the main program enables any subroutine to be replaced by an improved or different formulation if desired. The main features of some of the more important subroutines will be dealt with in the next section.

b *Subroutine structure*

LEACHM uses a numerical solution to the Richard's equation (eqn 2.1) as a means of predicting water contents, fluxes and potentials. In order to solve this equation the soil hydrological characteristics (K-Θ-h relationships), boundary conditions, and source and sink (rainfall, irrigation, evaporation and transpiration) terms need to be defined or calculated. Subroutines involved in the water regime simulation are:

- RETPRED: retentivity and conductivity parameters from particle size distribution can be estimated using regression relationships such as those of Rawls and Brakensiek (1982).
- RETFUN: contains the various K-Θ-h relationships and functions, using the methods of Campbell (1974) and Hutson and Cass (1987). According to the Campbell approach, the relationship between matric potential (h) and soil water content can be formulated as

$$h = a(\Theta/\Theta_s)^{-b} \qquad ...[2.15]$$

where a is the airentry potential, b is the slope of the soil water characteristic curve, and Θs volumetric water content at saturation (or total porosity). By applying a capillary model to [2.1] Campbell (1974) derived a conductivity equation,

$$K(\Theta) = K_s(\Theta/\Theta_s)^{2b+2+p} \qquad ...[2.16]$$

where $K(\Theta)$ is the hydraulic conductivity (mm d^{-1}) at a water content Θ, Ks is the hydraulic conductivity at saturation (Θs), and p is a pore interaction parameter, currently set to 1 in RETFUN.

- WATDAT: calculates and prints the relationships between hydraulic conductivity, water content and matric potential, which are required to drive the flow of water during execution of the model.
- GROWTH: empirical simulation of plant cover and root growth.
- POTET: calculates daily potential evapotranspiration from pan evaporation data. It is assumed that evapotranspiration starts at 0.3 day (07h12) and ends at 0.8 day (19h12) and that during this period potential evapotranspiration flux density (mm d^{-1}) varies sinusoidally.
- ETRANS: calculates potential evapotranspiration for the time step.
- WUPTAK: transpiration sink term for each soil segment using the method of Nimah and Hanks (1973).
- WATFLO: numerical solution of the Richard's equation (eq. 1) using a finite difference technique. WATFLO calculates water flux density, water content and matric potential changes during the time increment using the Richards equation. To reduce the dependent variables in equation 2.1 to pressure potential only, Θ is eliminated by defining the differential water capacity $C(\Theta)$, as

$$C(\Theta) = \delta\Theta/\delta h \qquad ...[2.17]$$

where h is the soil water pressure head. Equation 1 is then defined as

$$\delta h/\delta t . C(\Theta) = \delta/\delta z[K(\Theta) . \delta H/\delta z] \qquad ...[2.18]$$

This equation is used as a basis to simulate the flux of water between the specified depth increments in the soil by the finite differencing techniques given by Wagenet and Hutson (1989).

Subroutines involved in the chemical and solute regime are:

- CHEM: brings the solution salts into chemical equilibrium with lime, gypsum and PCO_2, and adjusts exchange equilibria.
- XCHANG: in this subroutine the free cations in solution and exchangeable cations are brought into equilibrium, satisfying the Gapon selectivity coefficients. Exchange reactions of Ca^{2+}, Mg^{2+}, Na^+ and K^+ are considered.
- SOLC: transports the major inorganic cations and anions (Ca^{2+}, Mg^{2+}, Na^+, K^+, Cl^-, SO_4^{2-}, HCO_3^-, CO_3^{2-}, OH^-, H^+) using equation 2.5.

Subroutine TSTEP calculates the time as the minimum of a) a specified maximum (usually 0.05 day), or b) the time remaining to the end of a 0.1 day interval, and c) the time for a specified maximum water flux to occur.

ii) Input requirements

Simulations begin at 00h00 on the first day, for which a set of initial conditions are required. The soil need not be homogeneous in the vertical direction. Plants can be present or absent. If present, crop cover and root expansion can be simulated, or a static, established root system and crop cover can be defined. The four versions of LEACHM all require the following inputs, which are read from data files constructed appropriately for each version. Input required for the LEACHC version are:

- Soil properties and initial conditions for each soil segment:
  - water content or water potential
  - hydrological constants for calculating retentivity and hydraulic conductivity or particle size distribution, i.e. saturated hydraulic conductivity and the a and b parameters of the Campbell equation.
  - appropriate chemical contents and soil chemical properties for each version, i.e. the chemical composition of both the solution and exchange phases of the soil, and the exchange characteristics.
- Soil surface boundary conditions of:
  - irrigation and rainfall chemical composition, amounts and rate of application.

- pan evaporation (weekly totals).

- Crop details (if it is assumed that no crops are present, a control variable allows bypass of the plant related subroutines):
  - time of planting.
  - root and crop maturity and harvest dates.
  - root and cover growth parameters.
  - a pan factor for adjusting pan evaporation to potential crop evapotranspiration.
  - lower soil and plant water potentials for water extraction by plants.
- Other constants used in determining bottom boundary conditions, time steps, diffusion coefficients and output details. The bottom boundary conditions that can be accommodated are a) a fixed water table, b) a fluctuating water table, c) a free-draining profile, d) zero flux, or e) lysimeter tank.

iii) Application

No field studies where LEACHC was applied could be found in literature (excluding the earlier versions of the model, i.e. Robbins *et al,* (1980 a,b) and Tillotson and Wagenet (1982)). Three studies (Wagenet and Hutson, 1986; Wagenet *et al,* 1989; Fuller, 1989) with the pesticide and nitrogen versions of LEACHM, (LEACHP and LEACHN) will be used to demonstrate the field application and validation of the modelling approach of this model, with greater emphasis on the predicted water balance and hydrologic characteristics.

In the first of these studies, Wagenet and Hutson (1986) used LEACHP to predict the fate of aldicarb in the unsaturated zone of a 18 by 36 m plot of sandy Palmyra soil. Good agreement between measured and simulated aldicarb residues and water content was reported. The simulated mass balance error for water was 0,1 mm and 3,7 mm after 7 and 124 days respectively.

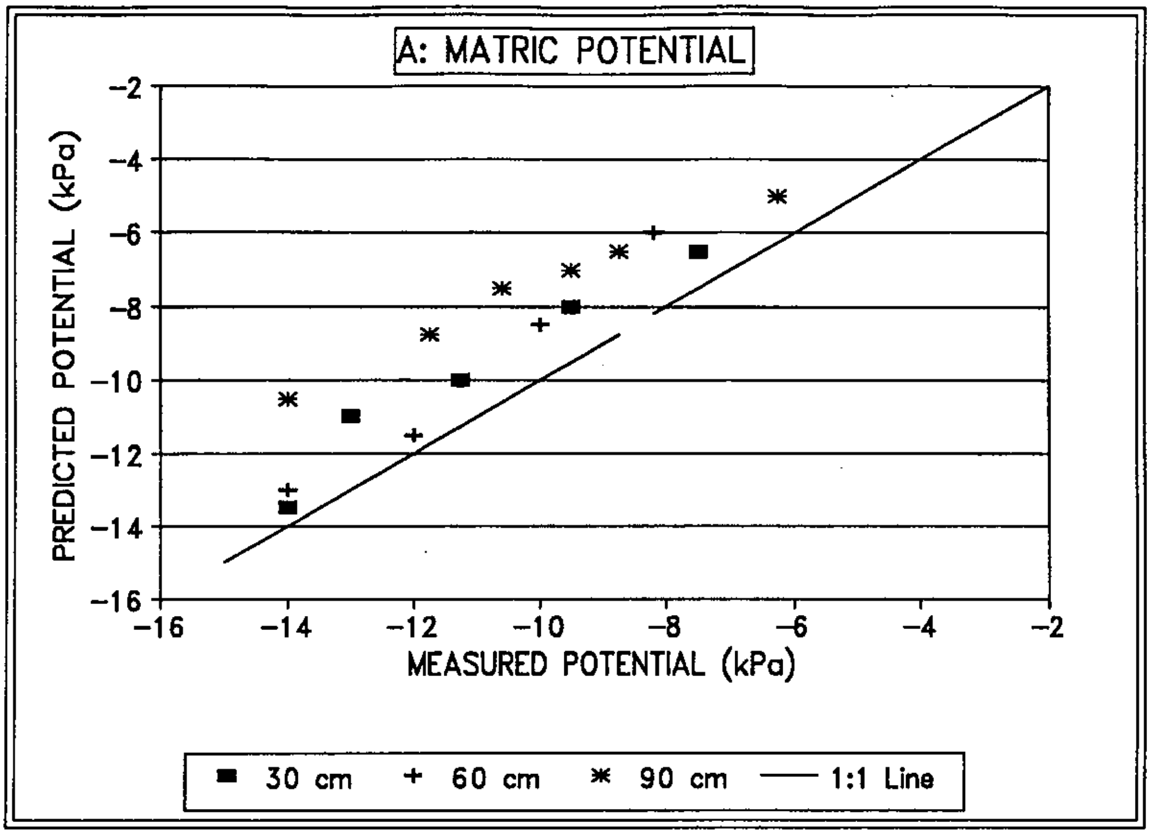
In the second of these studies Wagenet *et al* (1989) LEACHP was used to interpret a field experiment that measured DBCP distribution during leaching through the unsaturated soil of a 6,1 m by 6,1 m plot of a Panoche clay loam. The redistribution of a 150 mm pulse of water (without DBCP), in the absence of evapotranspiration, was simulated for a forty day period. After forty days another 150 mm pulse (with DBCP) was added and the fate of the water and pesticide simulated. There was good agreement between simulated and measured values of matric potential (h) and soil water flux for the first 40 d redistribution period (Fig

2.6). Plotted points for h represent tensiometer measurements taken 2, 4, 6, 8, 12, and 20 days after water application, and for q represent fluxes calculated from measured h and Θ at 4, 6, 8, 12, and 20 days. The authors conclude that the good agreement between measured and predicted h and q illustrate that LEACHM can accurately estimate water flow under the given experimental conditions. However, it should be mentioned that the agreement between predicted and observed DBCP concentrations was less favorable.

Fuller (1989) used LEACHN to simulate the field-observed redistribution of an ammonium nitrate (AN) pulse, introduced at different stages during irrigation on a sandy orchard soil. The predicted movement of NH_4^+ and NO_3^- was compared to the observed distribution obtained 48 hours after an AN solution was introduced during the first and fourth quarters of a 23 or 58 mm irrigation, referred to as pulse stages 1 and 4 respectively. The two irrigation applications correspond to 20 and 50% depletion of profile available water.

The flux of water through the profile was generally underestimated, especially in the case of the 58 mm irrigation where no water was predicted to percolate deeper than 600 mm (Table 2.8). The relatively low observed water contents in the upper layers after irrigation are in all probability due to degree of lateral movement during redistribution, a process not considered by LEACHM. Fuller (1989) speculate that the overprediction in the water content of the surface layer might also be due to an underestimate of the simulated evaporative loss of soil water (which was in excess of 8 mm d^{-1}). When the AN pulse was introduced during the first quarter of the 58 mm irrigation, the model also underestimated the movement of the NH_4^+ (Fig. 2.7a). In contrast, where the AN pulse was applied with the last quarter of irrigation water, excellent agreement was found between observed and predicted NH_4 distributions (Fig. 2.7b). This latter result is probably an artefact of the small surface flux of water following the introduction of the AN pulse. Too little water was added to affect any real redistribution of the solute.

Wilmott's index of agreement (eqn 8) for the predicted depth distributions of NH_4^+ and NO_3^- are listed in Table 2.9. The index indicate that as the flux of water through the soil increased (i.e. pulse stage 1 vs 4) the index of agreement decreased. No explanation for this behavior could be offered other than spurious input values used for the hydrologic characteristics of the soil.



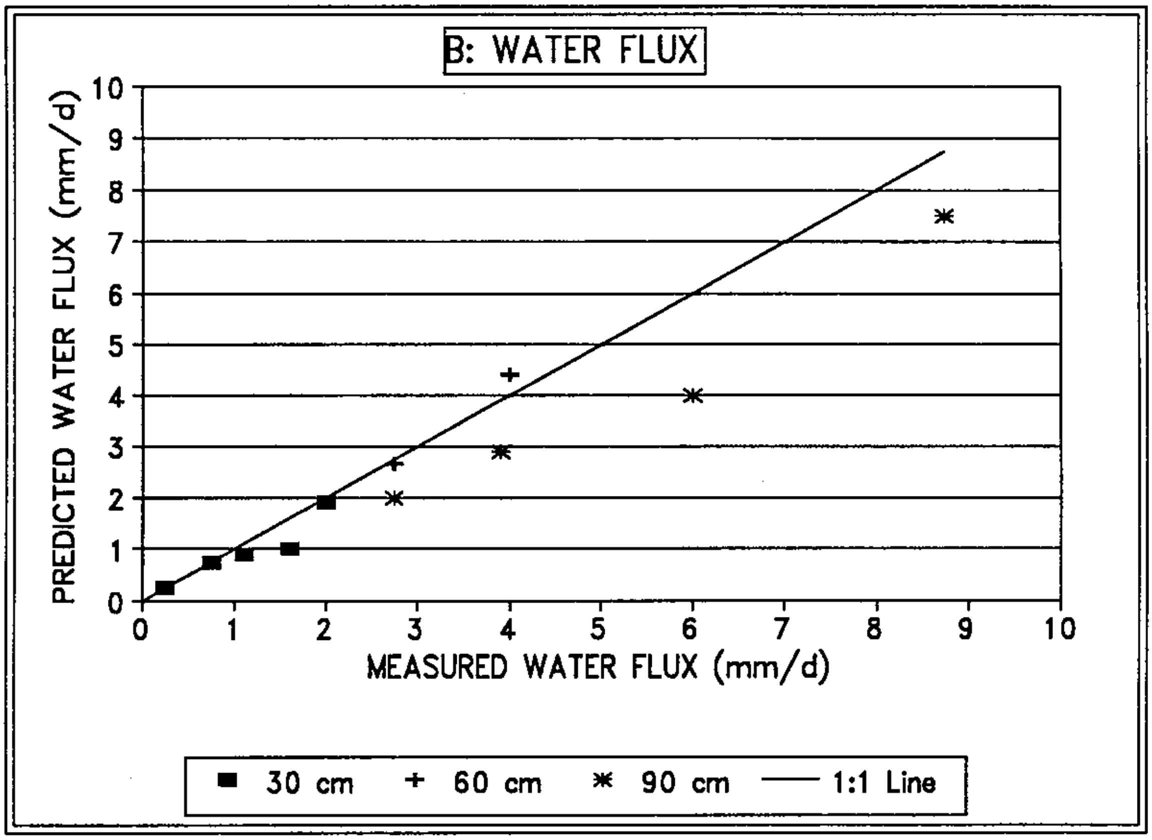


Figure 2.6 Comparison of field-measured and LEACHM-predicted matric potential (A) and water fluxes (B) at selected times after application of water. (Redrawn from Wagenet *et al* 1989)

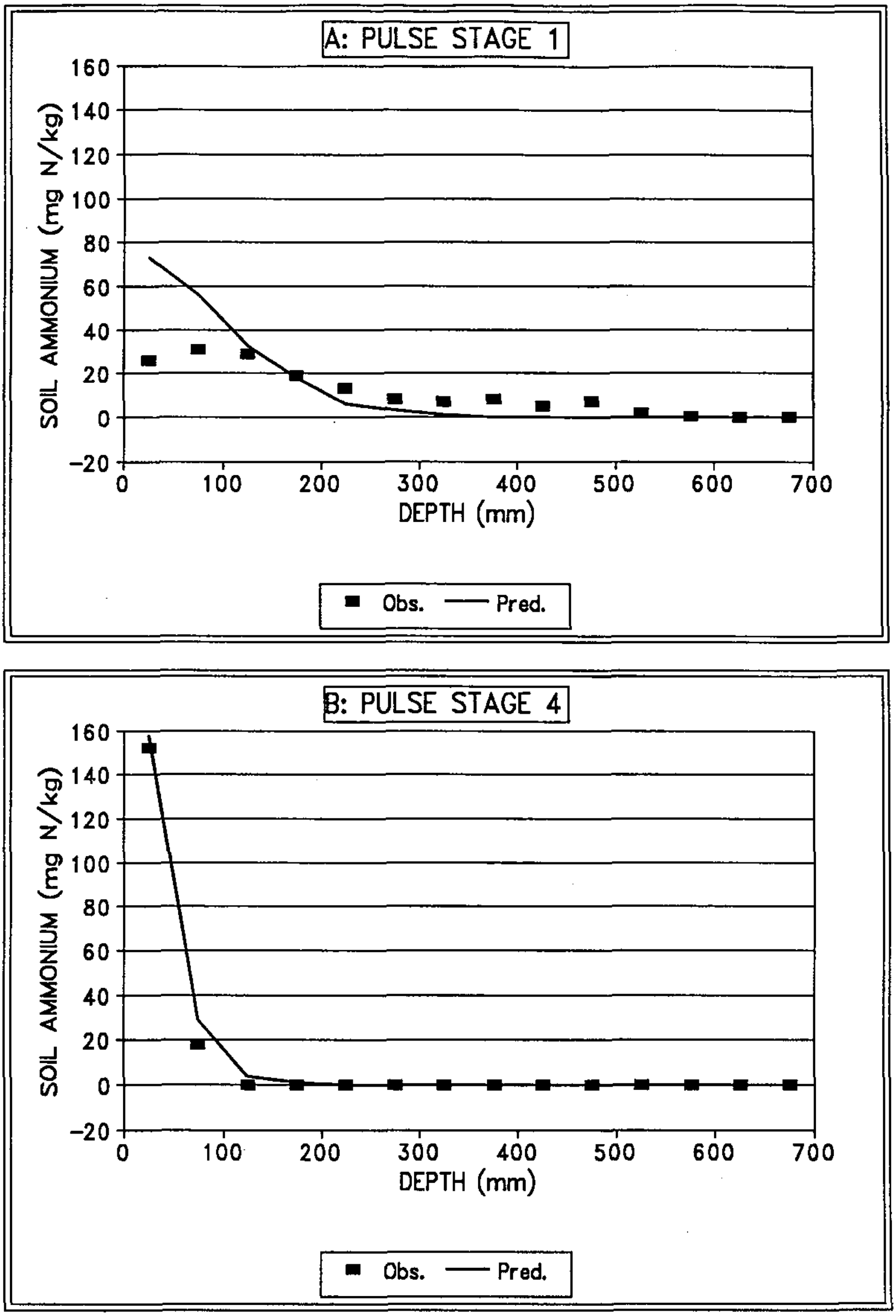


Figure 2.7 Observed and predicted distribution of applied ammonium after 58 mm of irrigation at A: pulse stage 1, and B: pulse stage 4 (Redrawn from Fuller, 1989)

Table 2.8 Measured and predicted water contents 24 hours after a 58 mm irrigation (Fuller, 1989)

Depth (mm)	Soil water content ($m^3\ m^{-3}$) Antecedent	24 hours Measured	Predicted
150	0,044	0,064	0,143
300	0,085	0,113	0,177
450	0,102	0,130	0,175
600	0,118	0,140	0,119
750	0,124	0,132	0,125

Table 2.9 Wilmott's indices of agreement for observed and predicted depth distributions of NH_4^+ and NO_3^- for two irrigation quantities and two pulse stages (Fuller, 1989)

Pulse stage	23 mm irrigation		58 mm irrigation	
	NH_4^+	NO_3^-	NH_4^+	NO_3^-
1	0,65	0,74	0,79	0,36
4	1,00	0,98	1,00	0,93

2.7 DISCUSSION AND CONCLUSIONS

Since 1960 there has been a proliferation in the number of models that can be used to predict water and salt movement in soils. However, in the majority of cases the published reports on the theory and validation of these models have been by the original modeler. Very few examples exist where a model has been tested and validated by non-modellers.

Based on the published results no model can be identified as representing the ultimate state of the art. Neither has any one model, or even modelling approach, received wide scale acceptance. Furthermore, the reported success rate of model application studies, especially when used by non-modellers (i.e. researchers, managers, farmers, etc. etc.) can at best be described as being moderate to fair. Wagenet (1988) therefore quite rightly poses the question: "*What is the result of the substantial efforts directed to modelling of soil hydrology, if in fact we have yet to produce a comprehensive tool useful in directly addressing and resolving field-scale problems?*".

The answer of Wagenet (1988) to this prudent question is equally enlightening: "*The answer without doubt is more agreeable to the scientist than to the manager or regulator, as it lies within the region of the scientific method where the answers lurk,* *but are not well identified, and where the light shines most clearly not on the answers, but on the next questions."* Wagenet (1988) proceeds by stating: "*Despite the lack of resolution of many modelling issues, the efforts to date had a very useful effect on that subset of modelers who not only build models but use them as tools in designing experiments and interpreting field data. For these individuals one very important benefit has been gained from use of a modelling approach. That is, their intuition has been enhanced, tuned, and honed to a finer edge than existed before the modeling/experimental exercise was undertaken*".

Despite this philosophical view and answer to the question posed, the researcher and manager interested in using models, are still faced with the problem which model to use for his particular application. Published results do not really help in formulating an answer to this question, partly because few scientific reports are available that compares different models, or approaches, to each other (using similar data sets). In a plot scale study Moolman (1988) found that the simple Burns model gave unrealistic and inferior predictions compared to the more mechanistic Shaffer model. Cameron and Wild (1982) reported similar results in their comparison of the Burns, Addiscott and Rose models with the latter, more mechanistic approach of Rose being superior to the other two models. In their theoretical comparison of different pesticide leaching models, Jones *et al* (1988) speculate that little difference in predicted solute movement would be expected between models using a simplified water balance (i.e. no movement until field capacity is exceeded, then instantaneous movement). They are furthermore of the opinion that models that calculate the rate of water movement according to the Richards equation is likely to predict slower solute movement than predicted by models using the simplified water balance. However, indications are that in coarse textured soils where the rate of water movement is relatively fast, such differences will not be significant.

Based on these results and suggestions, it seems logical and scientifically sound to conclude that the more mechanistic models are superior to the more simple non-mechanistic, capacity type models. However, this alleged superiority might be negated when models are used to predict responses in large irrigated areas bordering on the order of basin scale. All comparisons between models reported in this review were conducted on rather small plots, where the influence of spatial variability of rate parameters on the outcome of the study is expected to be less than would be the case in larger areas. Also, none of the models reviewed can effectively describe the movement of chemicals under conditions of macropore flow. When models are applied to larger areas, other factors might be of greater importance than the hydraulic variability of field soils. In fact, one such study (Hutson *et al.* 1988) demonstrated that under the transient upward and downward fluxes of water and chemical in a real California soil, it was not the variability in soil hydraulic properties that determined the distribution of the applied chemical, it was rather the sorption processes and net water fluxes, which were primarily a function of surface boundary conditions. This result obviously will vary by soil type and leaching fraction, but it demonstrates that the (to date) rather single minded focus upon hydraulic variability in modeling of soil leaching in fact may be misplaced concern. Addiscott and Wagenet (1985) have stated that the capacity type inputs required for the simple water balance type models are less spatially variable than rate parameters used in mechanistic models. Furthermore, because these models can cope with non-uniform initial distributions of solute in the profile together with a large number of pulses of added solute, they might be useful for management purposes.

Time and effort to meet the data demands of a specific model also play a role in model selection, especially for macroscale applications. On a macroscale, variables such as rainfall, irrigation and evapotranspiration amounts might be of far greater importance than detailed and accurate information of soil properties such as cation exchange capacity and cation selectivity coefficients. Jones *et al* (1988) quotes a study in which the predicted solute movement has been substantially altered in several simulations with the same pesticide model depending on whether the potential evaporation was estimated using average temperature data or pan evaporation data. Furthermore, if irrigation return flow volumes and salt loads are to be predicted, an inaccurate estimate of actual irrigated surface area might have a far greater effect on predicted results, than for example an inaccurate estimate of the "average, representative" hydraulic conductivity of the soil.

In conclusion, the choice of the appropriate model to use will depend on four factors:

a) the specific application;
b) the required accuracy of prediction;
c) how much information is available and how much time and effort can be spent in obtaining the required information, and
d) the knowledge of the user of the model.

It might be fitting to end this review with the following perception of Wagenet (1988): "*At present, only approximate prediction of water movement and chemical distributions can be made. The reliability of these predictions, whether made by simplified or more mechanistic and data intensive approaches, however remains obscure.*"

CHAPTER 3
THE SENSITIVITY OF TWO HYDROSALINITY MODELS TO A CHANGE IN THE INPUT VALUES OF SOIL PROPERTIES, IRRIGATION AMOUNTS AND ESTIMATES OF EVAPOTRANSPIRATION

3.1 THE OBJECTIVE OF A SENSITIVITY ANALYSIS

3.1.1 Introduction

In deterministic modeling, the input variables are single valued and supposedly free from random variations. For a certain combination of initial input values, these models will therefore always lead to a uniquely-definable result. In practice, however, it has been found that water and salt transport parameters vary substantially in space and that no single value can represent the real nature of a field. Because of this variability, reliable estimates of the mean often requires large numbers of field measurements. The problem of spatial variability is compounded by the time involved to make these field measurements, as well as by the number of different measurement techniques that are available. For example, seven different techniques to measure saturated hydraulic conductivity in the field are discussed in "Methods of Soil Analysis" (Amoozegar & Warrick, 1982). These methods furthermore do not necessarily yield the same results. This also applies to analytical laboratory techniques used for example, to determine the chemical status of soils. A good example is determining the cation exchange capacity of a soil, where the result depends on the pH and nature of the ionic exchanger that was used.

Consequently, the final outcome of any modelling study involving deterministic approaches, relies heavily on the selection of appropriate input values. The number of variables involved, and selections to be made, increases with the degree of mechanism and number of processes that are simulated. In order to direct the selection of values assigned to input variables, a sensitivity analysis can be performed. This technique can also be used to select those variables that have the biggest impact on model predictions.

Theoretically a sensitivity analysis should include all the variables that are required as input by the particular model. One parameter (or variable) at a time are then evaluated over a range of values, while all other variables are held constant. It is obvious that such an analysis will become increasingly more complicated and time consuming as the number of input variables increase.

A distinction should be made between a "*sensitivity analysis of a model* " and a "*sensitivity analysis of a system using simulation models*". In the former the prime concern is the accuracy of the algorithms within the model code itself. In contrast, the latter kind of analysis investigates (along theoretical lines) how a system (e.g. soil) will respond to changes in for example, irrigation frequency, chemical composition of the irrigation water, or gypsum additions to a sodic soil. Response analyses of soil systems assumes that the simulation model used to conduct the study, is a fair representation of all the processes involved. In the present study it was intended to use elements of both of these two approaches, i.e. the sensitivity analysis of a model, but with reference to a particular soil-plant-atmosphere system.

3.1.2 Defining the goals.

The primary aim of the study was:

a) to use two different water and salt transport models to determine which variables play the most important role in determining the **quantity and quality of water leaving the root zone** of irrigated agricultural lands.

The secondary goal was:

b) to evaluate the effect of a range of changes in input values on the stability of, and results produced by, a mechanistic type deterministic transport model.

The selection of the different input values and the definition of the hypothetical soil system were based on field observations in an irrigated vineyard in the Breede River Valley made during the period 1986 to 1989. However, the range of values evaluated are such that the results can be extrapolated to other irrigated soil systems as well.

3.2 METHODS

3.2.1 General approach

The methodology that was decided upon was to use the deterministic models LEACHM (Wagenet and Hutson, 1989), and BURNS (Burns, 1974) to simulate the water and salt transport in a hypothetical irrigated soil, for an irrigation period of one year, and using different initial conditions, and each initial condition with a set of different input values. The two starting conditions were:

a) starting with a uniform saline soil (EC_e = 904 mS m^{-1}) under irrigation with non-saline water (EC_w = 30 mS m^{-1}, TDS = 192 mg dm^{-3})*, and

b) starting with a non-saline soil (EC_e = 100 mS m^{-1}) but irrigated with saline water (ECw = 125 mS m^{-1}, TDS = 824 mg dm^{-3}) with a 25% uncertainty associated with the actual total salt content.

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*ECe = electrical conductivity of a saturated soil paste extract; ECw = electrical conductivity of irrigation water; TDS = total dissolved solids.

The theoretical description and input requirements of the two simulation models were discussed in detail in Chapter 3 of this report and are not repeated here.

3.2.2 Selection of which variables to evaluate

The procedure that was followed in deciding which variables should be included in the sensitivity study, was based on the input requirements of LEACHM. These variables, where appropriate, were then also used in the BURNS study. In LEACHM there are approximately 22 different soil, plant and meteorological variables to which values must be assigned. If the physical nature and chemical composition of the soil differs with depth, this number increases significantly. It should be obvious that a sensitivity analysis involving each of one these variables over range of for example four different values, is a formidable task in terms of computer processing time, data storage and interpretation of the results. Consequently, it was decided to divide the input variables empirically into three groups based on the amount of information available, and uncertainty normally associated with each one of them.

The three categories were:

a) Variables to which values can be assigned based on certain boundary conditions, system limitations, and prior knowledge of the particular system. These included the quantity and quality of irrigation water, soil depth, texture, estimates of the bulk density (or total porosity) and rooting pattern;

b) Variables that are either difficult to measure (and therefore include a certain amount of analytical uncertainty and variability), are subjected to spatial variability, or where a field determination often yield markedly different results compared to the laboratory determined equivalents. Variables that were included in this group are the field scale hydrological properties of soils, (i.e. water retention, hydraulic conductivity, etc.), and the chemical composition of the exchange complex and cation exchange selectivity coefficients. Also included in this group was the net flux of water through a field soil, which normally is a function of the difference between evapotranspiration, and rain and irrigation water infiltrating the soil surface. Uncertainties associated with the measurement of evapotranspiration and actual infiltrated and stored soil water can be expressed as the ET/I ratio where ET is the evapotranspiration, and I the quantity of infiltrated water;

c) Variables that will have a small effect on the quantity and quality of water leaving the root zone. This included variables such as chemical diffusion and dispersivity values, the effect of root flow resistance to crop water uptake, and temporal changes in the surface and bottom boundary conditions of soils.

With these three categories in mind, the effect of the following variables on the quantity and quality of water leaving the root zone of soils were investigated.

i) The *a* and *b* coefficients of the Campbell equation (i.e. the airentry potential and slope of the soil water characteristic curve);

ii) Saturated hydraulic conductivity (Ksat);

iii) Cation exchange capacity (CEC);

iv) Cation exchange selectivity coefficients, with specific reference to the Ca-Na exchange process (k-Ca/Na);

v) ET/I ratio, which was used as an index of the potential flux of water through the root zone.

3.2.4 Defining the limits of each variable

The environmental and soil conditions observed in a 0,5 ha drip irrigated vineyard in the Breede River Valley were used to define the bounds within which each of the above variables were evaluated. In this vineyard, which was used as the "field laboratory" (see Chapter 2, and Volume II of this report), soil water content, matric potential, chemical composition of the soil and irrigation water, quantity of irrigation and class A-pan evaporation are monitored on a continuous basis. The soil is underlain by a tile drain at 2 m depth and the flow rate within the drains as well as the water table have been observed to fluctuate seasonally, reaching a peak during spring to mid summer.

3.2.4.1 Campbell *a* and *b* coefficients

Several methods are available to calculate the airentry potential and slope of the soil water characteristic (also referred to as a soil water retention curve). In the sensitivity study, three of these methods were used to obtain values for the *a* and *b* coefficients. Firstly, linear least squares fitting routines were applied to soil water retention data from undisturbed soil cores. Secondly, the same fitting procedures were applied to *in situ* tensiometer and neutron moderation data. Thirdly, estimates of the retention properties were made using as a guideline the soil texture (fine sandy loam) and regression equations relating texture to water retention, (e.g. Rawls and Brakensiek, 1982). The following range of *a* and *b* values were obtained:

a (kPa):	-0,04	to	2,5
b (dimensionless):	2,25	to	32,15

The extremely high b value of 32,15 was rejected on the basis that it is an outlier. Campbell (1985) shows that a is expected to decrease (become more negative) as the mean pore size diameter becomes smaller, and b to increase as the standard deviation of pore size increases. He furthermore shows that in typical soils airentry values will generally range between -9,0 and -0,6 kPa, while the b coefficient can range between 2 and 24. Inspection of equation [3.15] reveals that when $b=0$, all of the soil water is held at a single potential, and when it approaches infinity, no change in water content occurs when h (matric potential) changes.

In view of this, and considering the soil texture, it was decided to define eight a and b combinations and assign the following values and to the two coefficients:

a(kPa)	b 5	7	10
-0,2	X	X	X
-1,0	X		X
-3,0	X	X	X

3.2.4.2 Saturated hydraulic conductivity (Ksat)

Field determined saturated hydraulic conductivity exhibits a large amount of variation. Nielsen and Warrick (1980) categorizes it as a "high variation" variable and cite three field studies where a coefficient of variation of 86 to 190% has been found. In the present study, an attempt was made to determine *in situ* hydraulic conductivities using the instantaneous profile method described by Hillel (1982). The values obtained ranged between 15 and 550 mm d^{-1}, while laboratory methods (using undisturbed soil cores) returned conductivities in excess of 1000 mm d^{-1}. It is unlikely that soils with saturated hydraulic conductivities of less than 50 mm d^{-1} are representative of irrigated soils. Therefore it was decided to restrict this investigation to conductivities bounded by 50 and 1000 mm d^{-1}. Three conductivities were defined namely 50, 100 and 1000 mm d^{-1}.

3.2.4.3 Cation exchange capacity

Soils of the South Western Cape are known to have low cation exchange capacities (CEC). The loamy soil of the field laboratory is no exception, and according to the NH_4-acetate extraction method, the CEC vary between 34,9 and 131,4 mmol(+) kg^{-1} with a coefficient of variation of 19,4 %. This variation is much less than for example, the hydraulic conductivity values. However, the cation exchange subroutine used in LEACHM assumes that CEC remains constant for a given soil, independent of pH, ion type and concentration (Wagenet and Hutson, 1989). In reality, it is known that CEC is affected by all three of these soil conditions, but it is uncertain to what extent changes in the CEC will influence the predicted chemical composition of the deep percolate. Based on these uncertainties, but also recognizing intuitively that its effect will be limited, only two CEC values were evaluated, namely 30 and 100 mmol(+) kg^{-1}.

3.2.4.4 Selectivity coefficients

In a Ca-Mg-Na-K exchange system, six combinations of selectivity coefficients are possible, each involving two cations. Because of the known adverse effect of sodium on soil physical properties (Richards, 1952), it was decided in the present study to concentrate on the Gapon Ca-Na selectivity coefficient only. In this report this selectivity coefficient will be referred to k-Ca/Na. The six different selectivity coefficients must be consistent, and changing the Ca/Na coefficient will also have an effect on the other selectivity coefficients.

The method of Robbins and Carter (1983) were used to determine the cation exchange selectivity coefficients of 160 soil samples. (For more detail, see volume II of this report). The results exhibited considerable variation, which in most cases could be ascribed to analytical problems caused by the presence of phosphogypsum and potassium fertilizers in the soil.

The 160 k-Ca/Na coefficients had a mean and standard deviation of 3,93 and 4,68 respectively. Against this background, it was decided to select two sets of coefficients which approximately reflect the mean and two times the mean of the analytical data i.e. Ca/Na = 4,0 and Ca/Na = 9,3. These two values fall within the range of coefficients found in international literature, e.g. Robbins *et al* (1980a), and Robbins and Carter (1983). The two sets of selectivity coefficients that were used, are listed in Table 3.1.

Table 3.1 Cation exchange selectivity coefficients used in the sensitivity study

	Low Ca/Na	High Ca/Na
Ca/Na	4,00	9,30
Mg/Ca	1,00	0,50
Ca/K	0,10	0,19
Mg/K	0,10	0,10
Mg/Na	4,00	4,65
K/Na	40,00	46,50

3.2.4.5 Ratio of evapotranspiration to infiltrated water (ET/I ratio)

The net flux of water trough a soil is influenced by a number of factors, three important ones being the difference between evapotranspiration and rainfall or irrigation, the total amount of water applied, and reduced infiltration (caused by clay swelling and/or surface crusting). Version 2 of LEACHM (Wagenet and Hutson, 1989) cannot simulate the latter condition and this study thus concentrated on the difference between evapotranspiration and applied irrigation water only. Different ET/I ratios can be simulated in several ways, e.g. keeping evapotranspiration constant and varying the amount of applied irrigation water, or keeping the applied irrigation water constant and varying the evapotranspiration amounts. Although similar ratios will be obtained, the results in terms of profile salt distribution and chemical composition might not be the same, reason being that evapotranspirational losses occur over the entire depth of the root zone (because of root water uptake), while applied irrigation water can infiltrate through the soil surface only (disregarding subsurface drip irrigation systems). In this study preference was given to the latter method.

As used in this study, ET/I is equivalent to the LEACHM input variable "crop factor" and was used as a method to vary the actual evapotranspiration and therefore, water flux. For example, by keeping the amount and rate of irrigation applications constant, (e.g. 35 mm week^{-1} = 1820 mm year^{-1}) and by varying the variable "crop factor", different ET/I ratios and therefore fluxes can be simulated. An ET/I value of 0,5, for example, means that the applied water exceeds the total evapotranspiration by 50%, and *vice versa* for ET/I = 1,5. It also means that in theory, the leaching factor will range from -1,0 (capillary rise) to 1,0 (deep percolation). In the sensitivity study the following six ET/I ratios were studied: 0,50 0,75 0,9 1,00 1,25 and 1,50.

3.2.5 Combinations of input values evaluated

Different combinations of physical and chemical parameters were made but unrealistic and atypical combinations were intentionally avoided. For example, a Campbell *b* value of 5 which is accepted to be more representative of a sandy soil, was not combined with the high CEC value of 100 mmol(+) kg^{-1}. Similarly, a hydraulic conductivity of 50 mm d^{-1} was not tested with the combination of *a* (airentry) = -0,02 kPa and *b* = 5.

An example of how the different hydrological, chemical and ET/I values were combined is given in Figure 3.1. From Figure 3.1 it can be seen that the combination of the Campbell coefficients *a* =-0,2 kPa and *b* = 5, was evaluated under eight different sets of conditions. In total 65 combinations of *a*, *b*, Ksat, CEC, k-Ca/Na and ET/I ratios were evaluated and are listed in Table 3.2.

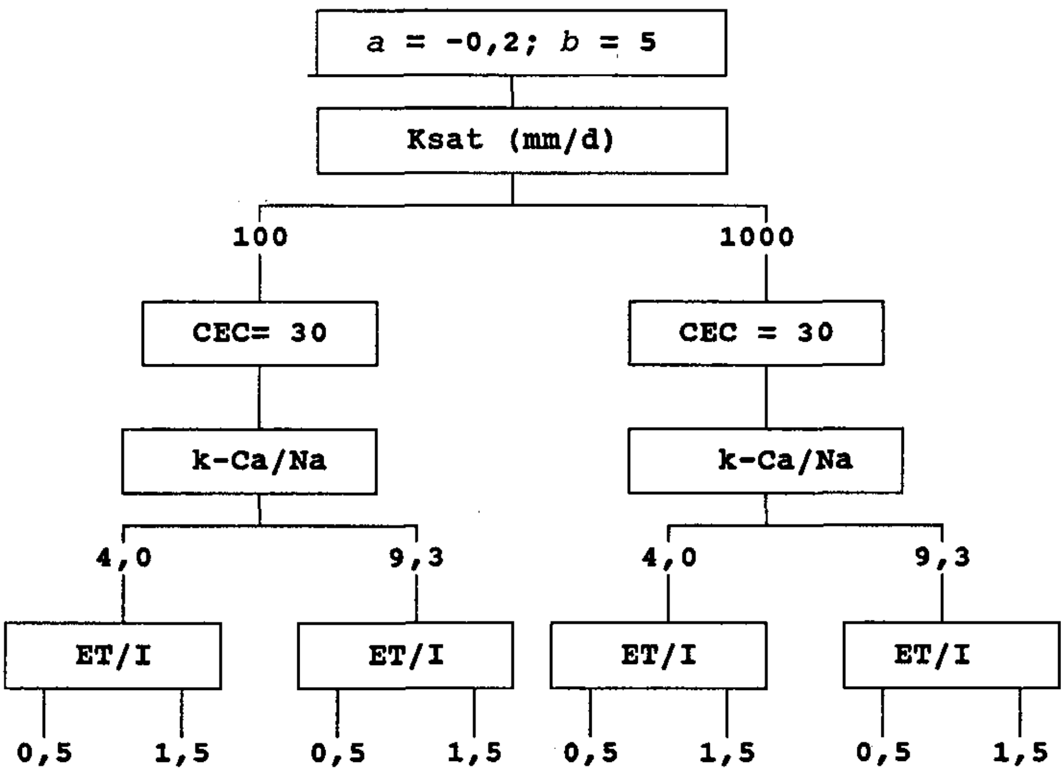


Figure 3.1 An example of how the Campbell coefficients *a*=-0,2 kPa and *b*=5 were combined with the other input variables used in the sensitivity study

For identification purposes, the hydrological soil properties that were evaluated were classified into 12 groups depending on the particular combination of values. For the ease of discussion and data presentation, these groups were referred to as P1 to P11. The combinations are listed in Table 3.3.

Table 3.2 Combination of the different LEACHM input variables that were used in the sensitivity study

a			b			HC			CEC		kCa/Na		ET/I					
0,2	1,0	3,0	5	7	10	50	100	1000	30	100	4,0	9,3	0,50	0,75	0,90	1,00	1,25	1,50
x			x					x	x		x		x					
x			x					x	x		x							x
x			x					x	x			x	x					
x			x					x	x			x						x
x			x				x		x		x		x					
x			x				x		x		x							x
x			x				x		x			x	x					
x			x				x		x			x						x
		x	x					x	x		x		x					
		x	x					x	x		x					x		
		x	x					x	x		x							x
		x	x					x	x			x	x					
		x	x					x	x			x				x		
		x	x					x	x			x						x
		x	x					x		x	x		x					
		x	x					x		x	x					x		
		x	x					x		x	x							x
		x	x					x		x		x	x					
		x	x					x		x		x				x		
		x	x					x		x		x						x

contd.

Table 3.2 (contd.)

a			b			HC			CEC		kCa/Na		ET/I					
0,2	1,0	3,0	5	7	10	50	100	1000	30	100	4,0	9,3	0,50	0,75	0,90	1,00	1,25	1,50
		x	x				x		x		x		x					
		x	x				x		x		x					x		
		x	x				x		x		x							x
		x	x				x			x	x				x			
		x			x		x			x	x					x		
	x		x				x			x	x					x		
		x			x		x			x	x				x			
	x		x				x			x	x				x			
		x	x					x	x		x				x			
		x	x				x			x		x			x			
		x	x				x		x			x	x					
		x	x				x		x			x				x		
		x	x				x		x			x						x
		x	x				x			x	x		x					
		x	x				x			x	x					x		
		x	x				x			x	x							x
		x	x				x			x		x	x					
	x	x				x			x		x		x					
		x	x				x			x		x				x		
		x	x				x			x		x					x	

contd.

Table 3.2 (contd.)

a			b			HC			CEC		kCa/Na		ET/I					
0,2	1,0	3,0	5	7	10	50	100	1000	30	100	4,0	9,3	0,50	0,75	0,90	1,00	1,25	1,50
		x	x				x			x		x						x
x					x		x			x	x		x					
x					x		x			x	x					x		
x					x		x			x	x							x
x					x		x			x		x	x					
x					x		x			x		x				x		
x					x		x			x		x						x
x					x	x				x	x		x					
x					x	x				x	x					x		
x					x	x				x	x							x
x					x	x				x		x	x					
x					x	x				x		x				x		
x					x	x				x		x						x
		x			x		x			x	x		x					
		x			x		x			x	x							x
		x			x		x			x		x	x					
		x			x		x			x		x						x
		x			x	x				x	x		x					
		x			x	x				x	x							x

-----contd.

Table 3.2 (contd.)

a			b			HC			CEC		kCa/Na		ET/I					
0,2	1,0	3,0	5	7	10	50	100	1000	30	100	4,0	9,3	0,50	0,75	0,90	1,00	1,25	1,50
		X			X	X				X		X	X					
		X			X	X				X		X						X
X				X			X			X	X					X		
		X		X			X			X	X					X		
	X				X		X			X	X		X					
	X				X		X			X	X					X		
21	4	40	39	2	24	10	38	17	21	44	36	29	21	1		17	1	20
Total 65			Total 65			Total 56			Total 65		Total 65		Total 65					

Table 3.3 Combinations of the different airentry, slope and hydraulic conductivity values

Group	Airentry *a* (kPa)	Slope *b*	Hydraulic conductivity Ksat (mm d^{-1})
P1	-0,2	5	1000
P2	-0,2	5	100
P3	-3,0	5	1000
P4	-3,0	5	100
P5	-0,2	10	100
P6	-0,2	10	50
P7	-3,0	10	100
P8	-3,0	10	50
P9	-1,0	10	100
P10	-0,2	7	100
P11	-3,0	7	100
P12	-1,0	5	100

3.2.6 Description of the hypothetical soil

3.2.6.1 General definition of the soil profile

For the ease of interpretation it was decided to define the soil profile as being uniform with depth with respect to the physical (hydrological) and chemical properties. It was furthermore decided to use the subsurface properties observed in the drip irrigated vineyard (*the field laboratory, see section 3.2.4*) to define the bottom boundary condition. The field laboratory is underlain by a water table which, over the three year period during which it was monitored, never subsided to below the tile drain depth at 2 m depth. Field measurements also indicate a slow rise in the water table when the irrigation season commences in September of each year. With these observations in mind, the hypothetical soil profile was defined as having the following characteristics:

a) Two meter deep profile with equally spaced 100 mm depth nodes, and a water table as the bottom boundary at the 2 m depth;

b) Uniform bulk density of 1325 kg m^{-3} (porosity=0,50);

c) Uniform textural and other hydrological characteristics, i.e. the same water retention and hydraulic conductivity properties were used for each of the depth nodes. The only exception was the 1900 - 2000 mm depth node where a hydraulic conductivity of 1 mm d^{-1} was defined (see below);

d) Uniform soluble salt content with depth. Two initial conditions were used: namely a saline, and a non-saline starting condition.

3.2.6.2 Hydrological properties

As can be deduced from Table 3.2, twelve different combinations of water retention and hydraulic conductivity values were used and had to be merged with the hypothetical profile defined above. In order to ensure that the results of the different combinations are comparable in all respects, the initial soil water content and matric potential had to be in equilibrium with the defined water table and low conductivity node at the bottom of the profile. If this was not the case, the predicted results could have been influenced more by non-equilibrium starting conditions, than by the defined input values of the variables under investigation.

The equilibrium condition was achieved by using the waterflow model of LEACHM to calculate the so-called field capacity for each combination of *a*, *b* and *Ksat* values. For each combination of hydrological properties (Table 3.3) the hypothetical profile was allowed to drain for a period of two months, starting with a water saturated profile. The shape of the soil water retention curves (h-Θ curves), and the hydraulic conductivity - matric potential curves (K-h curves) for some of the different *a-b-Ksat* combinations, are given in Figures 3.2 and 3.3.

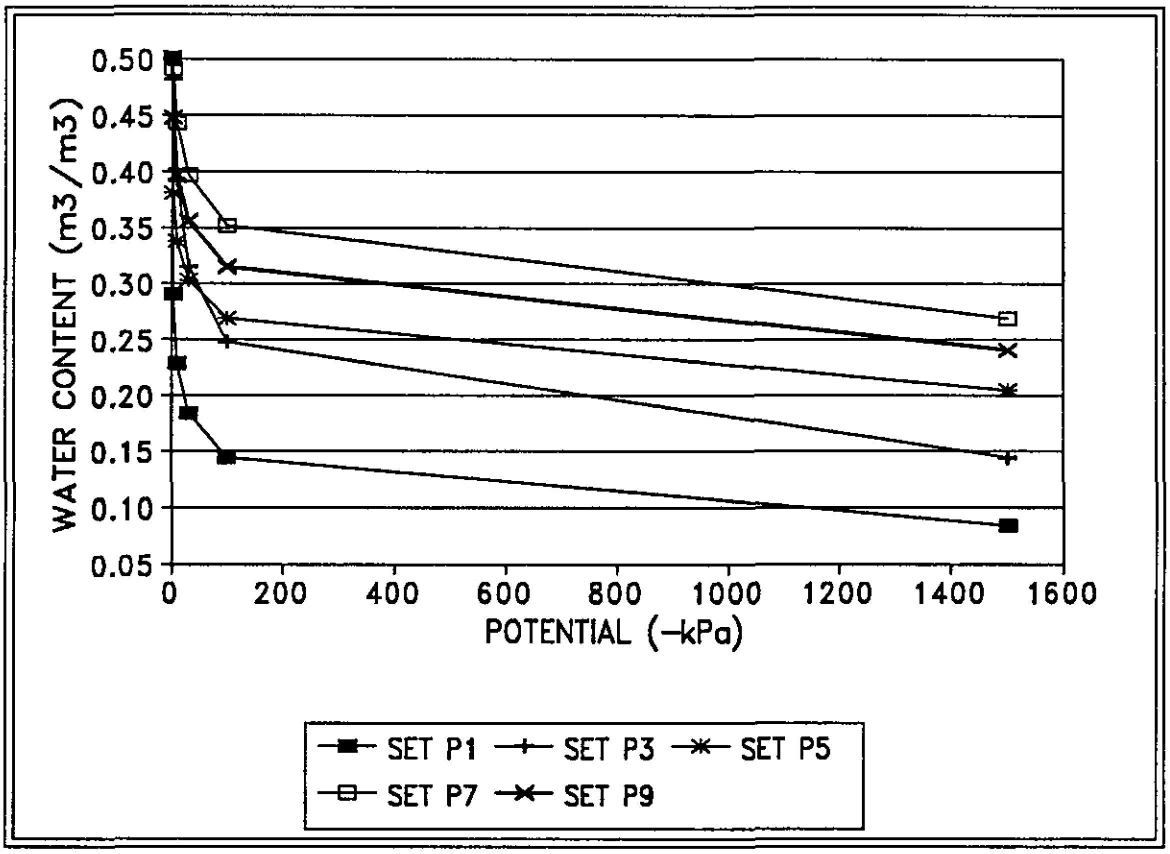


Figure 3.2 Shape of the soil water retention curve as determined by the Campbell *a* and *b* coefficients

An example of the soil water content after two months of drainage in the absence of evapotranspiration, for four of the hydrological combinations are given in Figure 3.4(a-d). Distinct differences in water content, and especially the matric potential values, were predicted. It is also clear that where an airentry value of -0,2 kPa was used, two months were not sufficient to reach equilibrium.

3.2.6.3 Soil chemistry

As mentioned above, it was decided to use the same soluble salt content for each of the 65 different combinations of input variables. The ionic composition for the initial saline condition was derived from the mean concentration of the soil solutions of four monitoring positions in the field laboratory, namely the 450 mm depth layer of site A3 (see Volume II of this report). The mean composition of these particular samples is given in Table 3.4.

Table 3.4 Initial soluble salt composition used for all input combinations evaluated in the sensitivity study

	Concentration at water content of:	
	40% mass (paste)	35% vol (field)
EC (mS m^{-1})	904	ca 1130
pH	7,74	Variable
Ca (mmol dm^{-3})	9,04	13,69
Mg (mmol dm^{-3})	10,32	15,62
Na (mmol dm^{-3})	57,30	86,77
K (mmol dm^{-3})	0,35	0,53
HCO_3 (mmol dm^{-3})	2,58	3,91
Cl (mmol dm^{-3})	50,10	75,87
SO_4 (mmol dm^{-3})	21,84	33,07
Lime (kg kg^{-1})	0,001	0,001
Gypsum (kg kg^{-1})	0,007	0,007
B.D. (kg m^{-3})	1,325	1,325

B.D.=bulk density; mass=gravimetric %; vol=volumetric %.

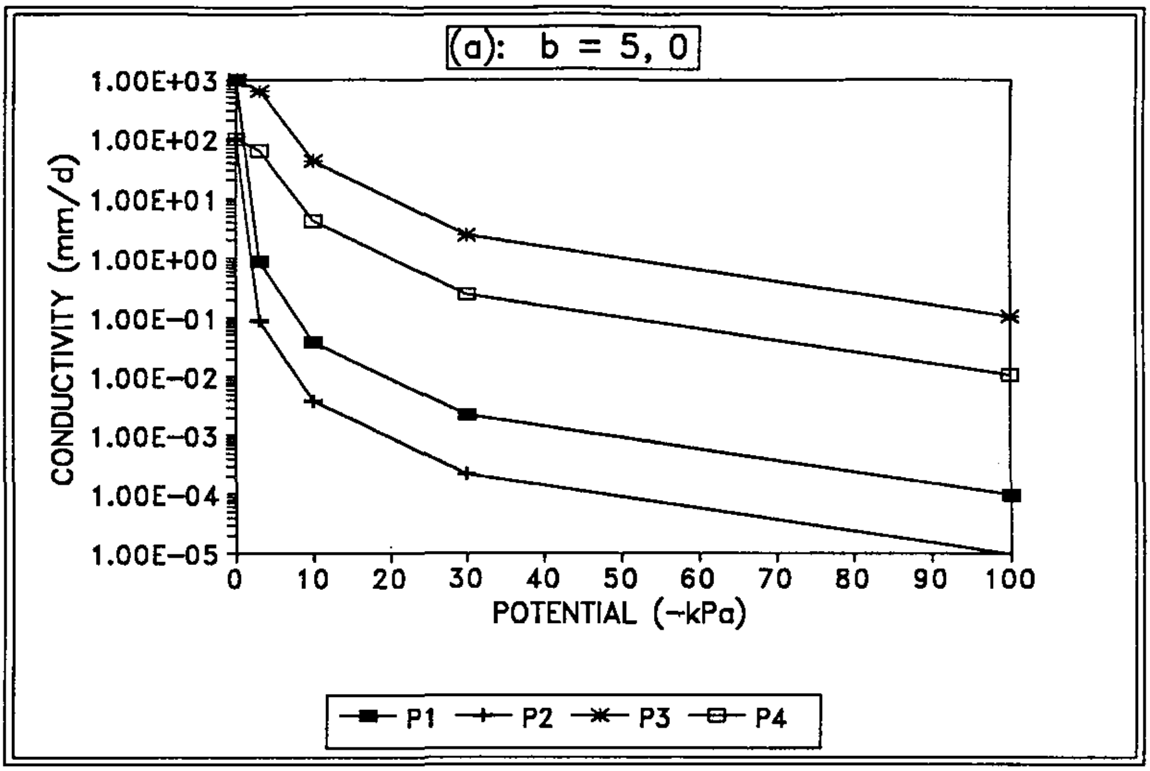
Four combinations of CEC and k-Ca/Na values were evaluated. These combinations were:

CEC = 30 mmol(+) kg^{-1}; k-Ca/Na = 4,0 (set 1)

CEC = 30 mmol(+) kg^{-1}; k-Ca/Na = 9,3 (set 2)

CEC = 100 mmol(+) kg^{-1}; k-Ca/Na = 4,0 (set 3)

CEC = 100 mmol(+) kg^{-1}; k-Ca/Na = 9,3 (set 4)



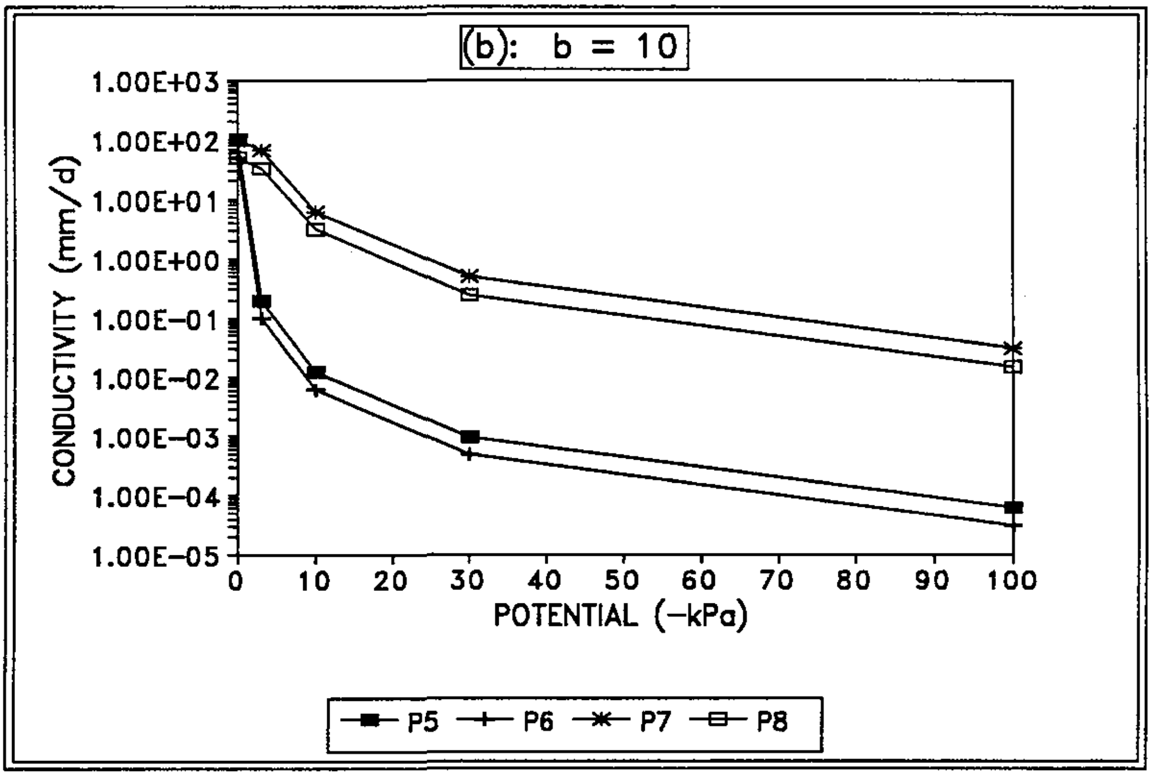
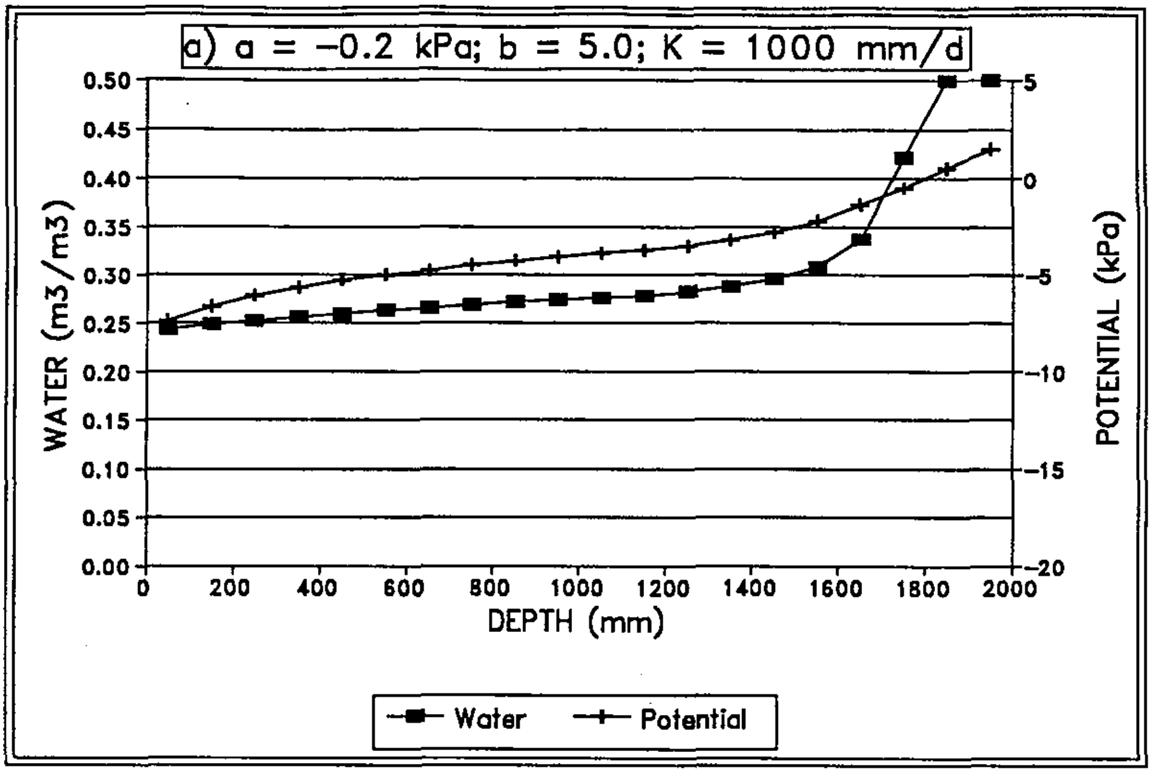


Figure 3.3 Calculated hydraulic conductivity as a function of matric potential and the Campbell *a* and *b* coefficients: a) *b* = 5; b) *b* = 10



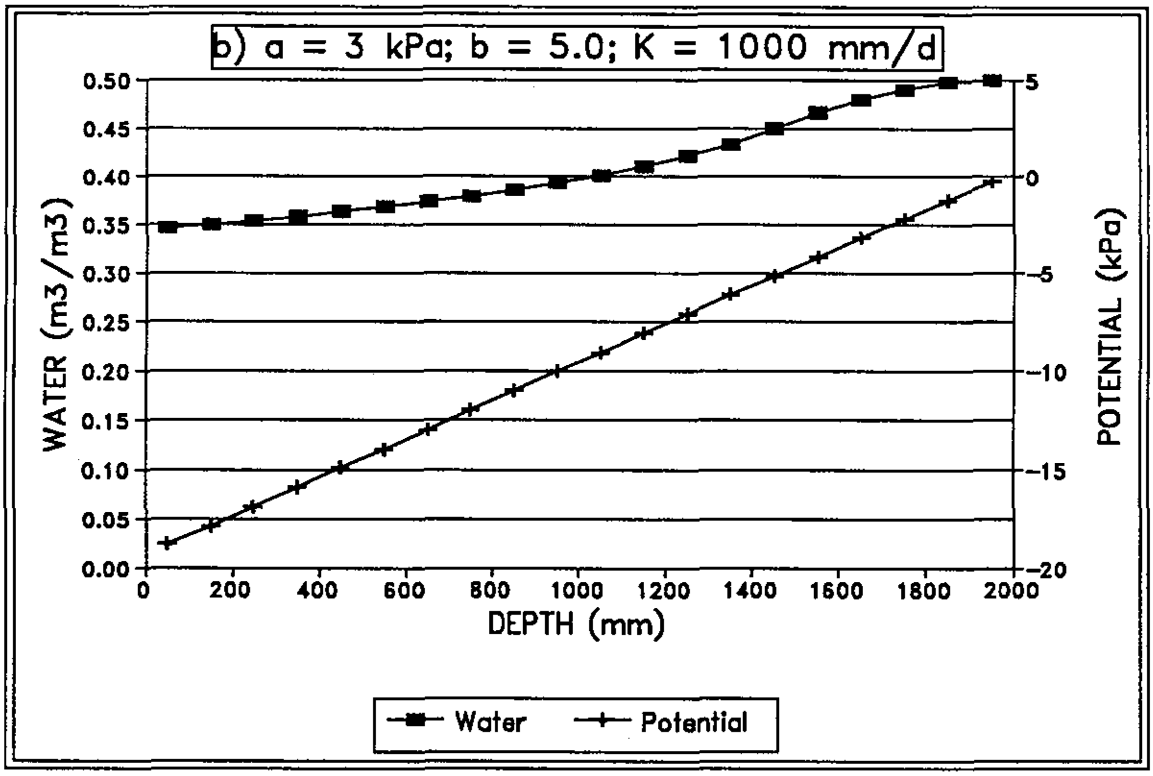
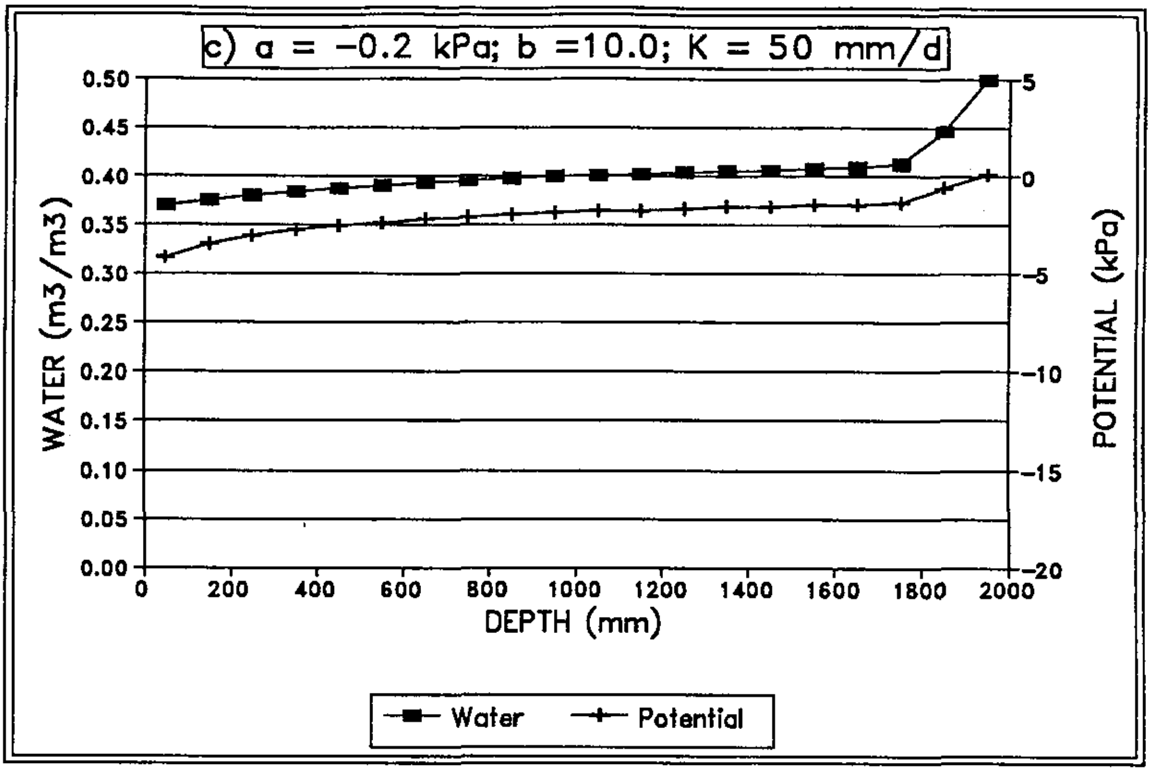


Figure 3.4 Predicted soil water content and matric potential after two months of continuous drainage as determined by the Campbell *a* and *b* coefficients and saturated hydraulic conductivity:
a) a=-0,2 kPa; b= 5,0; Ksat=1000 mm d^{-1}
b) a=-3,0 kPa; b= 5,0; Ksat=1000 mm d^{-1}



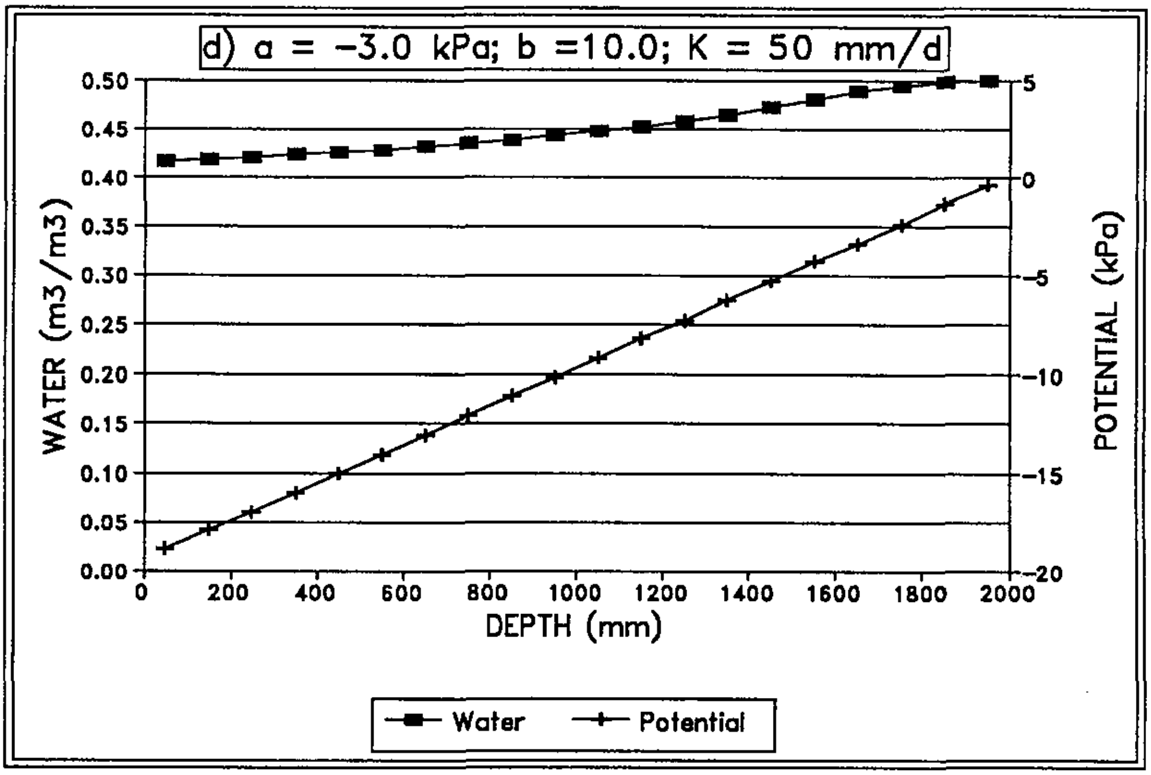


Fig 3.4
c) *a*=-0,2 kPa; *b*=10,0; Ksat=50 mm d^{-1}
d) *a*=-3,0 kPa; *b*=10,0; Ksat=50 mm d^{-1}

Analogous to the water content, the initial soil chemistry had to resemble a soil in chemical equilibrium. This meant that for each of the above CEC and selectivity coefficient combinations, a different exchangeable cation composition in equilibrium with the defined soluble salt content (Table 3.4), had to be calculated. This was done by using the stand-alone chemical equilibrium model, CHEMEQ, which is part of the LEACHM family of programs. The resulting equilibrium exchangeable cation concentrations for the four CEC-kCa/Na combinations are given in Table 3.5.

Table 3.5 Equilibrium exchangeable cation composition as a function of CEC and k-Ca/Na selectivity coefficient

Set	ExCa	ExMg	ExNa	ExK	CEC	k-Ca/Na
1	2,14	13,47	3,54	0,85	30	4,0
2	17,49	9,70	2,19	0,61	30	9,3
3	40,47	44,90	11,80	2,83	100	4,0
4	58,31	32,34	7,31	2,04	100	9,3

The non-saline starting condition that was used, was based on the chemical properties (soluble and exchangeable) of a particular depth node at the end of the one year simulation period during which the hypothetical saline soil was irrigated with non-saline water. The detailed description of the non-saline soil will be dealt with as part of the results in section 3.3.2.

3.2.6.4 Irrigation water and evapotranspiration

For the sake of simplicity and because the prime concern was to evaluate the effect of the different input values of the variables under study on the salt transport and chemical reactions (rather than to reflect real field conditions), an annual potential class A-pan evaporation of 1820 mm, divided into 52 weekly values of 35 mm each, was defined. Similarly, the irrigation application and frequency were specified as being 35 mm per week, also totaling to 1820 mm. As stated in a previous section the different ET/I ratios were attained by using different crop factors (or crop coefficients). A summary of the actual evapotranspiration (AET) and the theoretical water flux at the bottom of the root zone that resulted from the six different ET/I ratios that were used, is given in Table 3.6.

Table 3.6 Actual evapotranspiration (AET) and theoretical water flux as a function of the different crop factors (ET/I ratios) for 1820 mm of potential evaporation (PET) and 1820 mm applied irrigation water

PET mm a^{-1}	ET/I*	AET mm a^{-1}	Irrigation mm a^{-1}	Flux mm a^{-1}
1820	0,50	910	1820	910
1820	0,75	1365	1820	455
1820	0,90	1638	1820	182
1820	1,00	1820	1820	0
1820	1,25	2275	1820	-455
1820	1,50	2730	1820	-910

* ET/I = value assigned to the variable "crop factor" in LEACHM.

The chemical composition of the irrigation water that was used in the study reflect the prevailing conditions in the upper reaches of the Breede River Valley in the sense that it is non-saline (TDS = 192 mg dm^{-3}). The actual ionic composition was taken from the data base containing the irrigation water quality used in the drip irrigated field plot. For the second scenario, where the starting condition was that of a non-saline soil, the total salt content of the water used in the simulation study was empirically raised to 824 mg dm^{-3}. Also used in the second study, is a water that has 25% less dissolved salt than the 824 mg dm^{-3} water. This chemical composition represent a hypothetical case where a 25% analytical error was made in the chemical analysis of the irrigation water. The composition of the two types of water are listed in Table 3.7.

Table 3.7 Chemical composition of the irrigation water used in the sensitivity study

	Salt content of Irrigation water		
	Low TDS	**High TDS**	**High - 25%**
Ca (mmol dm^{-3})	0,503	1,800	1,35
Mg (mmol dm^{-3})	0,313	2,500	1,88
Na (mmol dm^{-3})	1,370	4,700	3,53
K (mmol dm^{-3})	0,740	0,140	0,11
Cl (mmol dm^{-3})	1,770	7,000	5,25
SO_4 (mmol dm^{-3})	0,463	2,420	1,82
HCO_3 (mmol dm^{-3})	0,379	1,600	1,20
TDS (mg dm^{-3})	192	824	618

3.2.6.5 Input variables of LEACHM not included in the sensitivity study

As mentioned previously, not all of the input variables of LEACHC were included in the sensitivity analysis. For these variables a fixed (constant) value was used in each of the modelling runs. The variables and values are:

Largest time interval	day	0,05
Max.theta change/time step		0,01
No. of time steps/chemeq		10,00
Wilting point (soil)	kPa	-1500,0
Min.root water pot'l	kPa	-3000,0
Max.root water pot'l	kPa	0,0
Root flow resistance term		1,05
Molecular diffusion	D0	120,0
coefficient (mm^2 d^{-1})	DIFA	0,001
(Bresler's eq)	DIFB	100,0
Dispersivity	mm	40,0
PCO2 for whole profile	bar	0,003
Root fraction	(0-300 mm)	0,25
Root fraction	(300-400 mm)	0,12
Root fraction	(400-500 mm)	0,07
Root fraction	(500-600 mm)	0,06
Planting date	Julian day	1
Emergence date	Julian day	1
Root maturity date	Julian day	120
Plant maturity date	Julian day	120
Harvest date	Julian day	365
Relative crop cover		0,80
Irrigation water application rate mm d^{-1}		144,0
Fertilizer applications (mol m^{-2})		
Ca= 2,90	SO_4= 2,90	
Date of application	Julian day	2,00

3.2.7 Starting conditions for the BURNS model

With the Burns model, the input requirements are considerably less than with the LEACHM model. It also clear from the structure of the model that only two factors will determine how much water and salt will be leached, namely the field capacity of the soil, and the difference between the evapotranspiration and irrigation (or rainfall) quantities. The model was furthermore designed to reflect free draining conditions and the transport of conservative salts only. Consequently, the sensitivity analysis only had to involve the field capacity and the ET/I ratio. Because of the big difference between the LEACHM and Burns models, the design of two sensitivity studies could not be exactly the same. Nevertheless, an attempt was made to keep the two studies comparable by using the same underlying principles. Some of the equilibrium soil water properties calculated with LEACHM were also used as starting conditions for the Burns model.

With the Burns model a **free draining**, two meter deep soil with 100 mm segments (or nodes) was defined as the hypothetical soil profile under study. Each segment had the same soluble salt content, but the actual chemical composition of the soil solution was not specified (although it can be interpreted as being similar to chloride). Unlike the salt content, a different field capacity for each 100 mm soil segment was used. The field capacity used in the Burns model were calculated with LEACHM using the P12 group of hydrological variables (Table 3.3). The field capacity and evaporation limits (in volumetric units), salt content (kg ha^{-1} per layer) and bulk density are listed in Table 3.8.

In the sensitivity study the field capacity (FC) was changed ten percent above and below the values listed in Table 3.8, while the ET/I ratios were changed by ten- and twenty percent above and below the 1:1 ratio. Twelve different sets of FC and ET/I combinations were used and are listed in Table 3.9.

The same amount of irrigation water was used for all of the combinations and were applied at a frequency of 35 mm per week, giving an annual total of 1820 mm. The total salt content of the irrigation water was 100 mg dm^{-3}. No precipitation and/or adsorption of the dissolved salt were considered, i.e. the salt was assumed to be conservative. An irrigation application of 35 mm amounted to a salt application of 35 kg ha^{-1}.

3.2.8 Interpretation of the Results

The objective of this study was to see to what extent the quantity and quality of the soil water that percolates out of the root zone is influenced by changes in the input values of certain variables. The bottom boundary of the root zone was defined as the 1 m depth and the net daily flux of water and salt across this depth were recorded. The amount of salt was converted to a load and expressed in units of mass per hectare. The chemical composition of the deep percolate was also recorded to see to what extent the CEC and k-Ca/Na selectivity coefficient influence chemical processes in the root zone. The initial and final chemical composition of the soil solution within the root zone, i.e. 0 - 1 m, were also recorded. The most convenient method of interpreting and comparing the results was found to be visual techniques (graphs) in combination with tabulated information.

Table 3.8 Starting soil water and soluble salt conditions used in the Burns sensitivity study

Depth (mm)	BD (kg m^{-3})	FC (m^3 m^{-3})	EL (m^3 m^{-3})	Salt (kg ha^{-1})
100	1325	0,304	0,116	10000
200	1325	0,308	0,116	10000
300	1325	0,312	0,116	10000
400	1325	0,316	0,116	10000
500	1325	0,319	0,116	10000
600	1325	0,322	0,116	10000
700	1325	0,325	0,116	10000
800	1325	0,327	0,116	10000
900	1325	0,329	0,116	10000
1000	1325	0,332	0,116	10000
1100	1325	0,334	0,116	10000
1200	1325	0,336	0,116	10000
1300	1325	0,337	0,116	10000
1400	1325	0,339	0,116	10000
1500	1325	0,341	0,116	10000
1600	1325	0,342	0,116	10000
1700	1325	0,344	0,116	10000
1800	1325	0,345	0,116	10000
1900	1325	0,346	0,116	10000
2000	1325	0,346	0,116	10000

BD=bulk density; FC=field capacity; EL=evaporation limit;
Salt=salt content (Cl)

Table 3.9 Field capacity and ET/I combinations used in the Burns study

ET/I	FC (1)	Irrigation water quantity (mm)	quality (Cl; mg dm^{-3})
1,0	1,0	1820	100
1,0	1,1	1820	100
1,0	0,9	1820	100
1,1	1,0	1820	100
1,1	1,1	1820	100
1,1	0,9	1820	100
0,9	1,0	1820	100
0,9	1,1	1820	100
0,9	0,9	1820	100
0,8	1,0	1820	100
0,8	1,1	1820	100
0,8	0,9	1820	100

1) Given as a fraction of the values listed in Table 3.8

3.3 RESULTS

3.3.1 LEACHM; Saline soil irrigated with non-saline water

3.3.1.1 General

Computational instabilities in the code of LEACHC aborted the processing of the data in all the cases where the combination CEC=30 mmol(+) kg^{-1} and k-Ca/Na=9,3 were used. (In August 1990, the authors of LEACHM were notified of this problem). Because of this instability, the original 65 combinations of input values (Table 3.2,) were reduced to 56. The processing time on a Toshiba T3200SX desktop computer was approximately 2,25 hours per simulated year. The total processing time for the 56 simulation runs was 135 hours, i.e. 5,6 days.

The calculated annual water flux, salt load, cumulative infiltration and surface evaporation are summarised in Table 3.10.

Table 3.10 Summary of the effect of the input values used in the sensitivity study on the predicted annual total salt load, water flux, cumulative infiltration and surface evaporation

a kPa	b	Ksat mm d^{-1}	CEC mmol(+) kg^{-1}	Ca/Na	ET/I	Load t ha^{-1}	Flux mm	Inf mm	E mm
-0,2	5	1000	30	4,0	0,50	45,500	921,0	1820	174
-0,2	5	1000	30	4,0	1,50	-0,437	5,3	1820	278
-0,2	5	100	30	4,0	0,50	29,200	355,0	1260	175
-0,2	5	100	30	4,0	1,50	1,380	13,1	1740	276
-3,0	5	1000	30	4,0	0,50	52,800	955,0	1820	183
-3,0	5	1000	30	4,0	1,00	15,100	136,0	1820	347
-3,0	5	1000	30	4,0	1,50	-56,500	-682,0	1820	510
-3,0	5	1000	100	4,0	0,50	59,900	955,0	1820	183
-3,0	5	1000	100	4,0	1,00	16,200	136,0	1820	347
-3,0	5	1000	100	4,0	1,50	-57,400	-682,0	1820	510
-3,0	5	1000	100	9,3	0,50	58,000	955,0	1820	183
-3,0	5	1000	100	9,3	1,00	15,900	136,0	1820	347
-3,0	5	1000	100	9,3	1,50	-57,300	-682,0	1820	510
-3,0	5	100	30	4,0	0,50	51,800	891,0	1820	187
-3,0	5	100	100	9,3	0,50	56,900	891,0	1820	187
-3,0	5	100	100	4,0	0,50	58,800	891,0	1820	187
-3,0	5	100	100	4,0	0,75	40,500	473,0	1820	273
-3,0	5	100	100	9,3	1,00	6,080	49,1	1820	358
-3,0	5	100	100	4,0	1,00	6,140	49,1	1820	358
-3,0	5	100	30	4,0	1,00	6,220	49,1	1820	358
-3,0	5	100	100	4,0	1,25	-35,000	-374,0	1820	442
-3,0	5	100	100	4,0	1,50	-66,900	-715,0	1820	512
-3,0	5	100	100	9,3	1,50	-66,700	-715,0	1820	512
-3,0	5	100	30	4,0	1,50	-66,000	-715,0	1820	512

.....contd.

Table 3.10 Contd.

a kPa	b	Ksat mm d^{-1}	CEC mmol(+) kg^{-1}	Ca/Na	ET/I	Load t ha^{-1}	Flux mm	Inf mm	E mm
-0,2	10	100	100	4,0	0,50	18,700	191,0	1390	174
-0,2	10	100	100	4,0	1,00	0,604	6,1	1600	292
-0,2	10	100	100	4,0	1,50	0,173	4,8	1710	260
-0,2	10	100	100	9,3	0,50	18,600	191,0	1390	174
-0,2	10	100	100	9,3	1,00	0,604	6,1	1600	292
-0,2	10	100	100	9,3	1,50	0,174	4,8	1710	260
-0,2	10	50	100	4,0	0,50	1,470	11,3	814	165
-0,2	10	50	100	4,0	1,00	0,580	6,7	1110	165
-0,2	10	50	100	4,0	1,50	0,500	6,1	1130	166
-0,2	10	50	100	9,3	0,50	1,460	11,3	814	165
-0,2	10	50	100	9,3	1,00	0,580	6,7	1110	165
-0,2	10	50	100	9,3	1,50	0,502	6,1	1130	166
-3,0	10	100	100	4,0	0,50	62,700	918,0	1820	184
-3,0	10	100	100	4,0	1,50	-74,700	-797,0	1820	521
-3,0	10	100	100	9,3	0,50	60,900	918,0	1820	184
-3,0	10	100	100	9,3	1,50	-74,500	-797,0	1820	521
-3,0	10	50	100	4,0	0,50	58,600	812,0	1710	184
-3,0	10	50	100	4,0	1,50	-60,800	-653,0	1820	495
-3,0	10	50	100	9,3	0,50	57,000	812,0	1710	184
-3,0	10	50	100	9,3	1,50	-60,600	-653,0	1820	495
-1,0	10	100	100	4,0	0,50	60,600	916,0	1820	173
-1,0	10	100	100	4,0	1,00	11,000	107,0	1820	335
-0,2	7	100	100	4,0	1,00	1,230	10,9	1600	303
-3,0	7	100	100	4,0	1,00	7,180	51,4	1820	359
-1,0	5	100	100	4,0	0,90	23,500	259,0	1820	304
-3,0	7	100	100	4,0	1,00	7,18	51,4	1820	359
-1,0	5	100	100	4,0	1,00	9,90	100,0	1820	334

Ca/Na=Ca-Na exchange selectivity coefficient; CEC=cation exchange capacity in mmol(+) kg^{-1}; Inf=infiltration; E=surface evaporation.

3.3.1.2 Total water flux

The total amount of water crossing the 1 m boundary depth, was (as expected) linearly related to the ET/I ratio (Figure 3.5). Both positive (downward) and negative (upward = capillary rise) are indicated in Figure 3.5. The amount of water leaving the root zone decreased as the ET/I ratio increased, i.e. as evapotranspiration increased. A similar result could have been obtained by decreasing the amount of applied irrigation water but this was not investigated. With an ET/I > 1, the net movement of water across the 1 m depth becomes negative, which is indicative of capillary movement of water from the water table into the root zone.

Combinations P5 and P6, i.e. a high airentry potential (small negative number e.g. -0,2 kPa) combined with a slope of 10, suppressed the flow of water both upward and downward. These combinations are indicated by asterisks on Figure 3.5. The most extreme case was the combination of a = -0,2 kPa, b = 10 and Ksat = 50 mm d^{-1}, which yielded less than 12 mm of water flux across the 1 m depth, irrespective of the ET/I ratio. Investigation of the two Campbell equations that are used in LEACHM to calculate water retentivity and conductivity, i.e. eqns [2.15] and [2.16], showed that these particular combinations of *a* and *b* with Ksat values of 50 and 100 mm d^{-1}, will lead to extremely low unsaturated hydraulic conductivities. From Figure 3.3(b) it can be deduced that at a matric potential of -10 kPa (with an associated water content of about 0,34 m^3 m^{-3}), the hydraulic conductivity will be approximately 0,01 mm d^{-1}. The calculated conductivities at the same potential, but with other *a* and *b* combinations are between 3 and 8 mm d^{-1}. Because of these low conductivities, and despite large hydraulic potential gradients, very little water will flow in the soil. This particular combination of *a* and *b* also decreased infiltration and surface evaporation, and increased runoff losses (Table 3.10). It is uncertain, but unlikely, whether a real soil will react similarly in the field. In the present study, this particular result was consequently regarded as being an artefact of computational methods. However, it does illustrate the effect of unbalanced input values on model predictions.

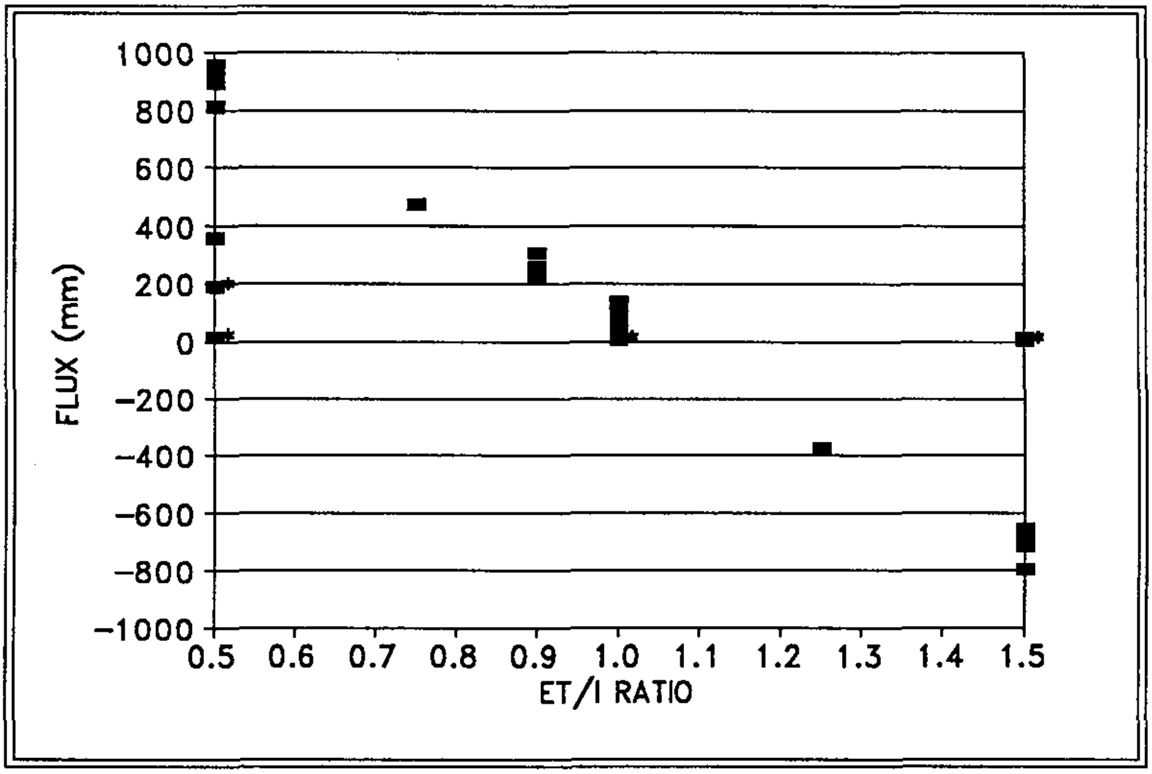


Figure 3.5 Relationship between the ET/I ratio and total annual soil water flux at the 1 m depth. Negative values indicate upward flow. The points marked with asterisks indicate the hydrological combination *a*=-0,2 kPa and *b*=10

The sensitivity of the Campbell equation (and, consequently the calculated water flux) to airentry values, was investigated in more detail with hydrological combination P9 (Table 3.3). This combination differed from the P2 group in that the *a* value was decreased from -0,2 to -1,0 kPa. At an ET/I ratio of 0,5, this relatively small change in the airentry value increased the annual flux from 191 mm to 916 mm (Table 3.9). Theoretically, the flux of water could also have been increased by increasing the saturated hydraulic conductivity to 1000 mm d^{-1}, but the combination of a=-0,2 kPa, b=10 and Ksat=1000 mm d^{-1} was not used in this study.

3.3.1.3 Total salt load

i) Effect of ET/I

The influence of the difference between irrigation applications and evapotranspiration losses on the salt load, quantified by the ET/I ratio in this study, is illustrated in Figure 3.6. The results show that, irrespective of the values of the other physical and chemical properties that were evaluated, the ET/I ratio alone can be used to divide the predicted salt loads into distinct groups. With an ET/I ratio of 0,5, a **salt loss** that ranged between approximately 50 and 60 t ha^{-1} are predicted. An ET/I ratio of 1,5 led to **salt accumulations** within the root zone that ranged between 40 and 75 t ha^{-1}. When the evapotranspiration equals the amount of infiltrated water, i.e. ET/I = 1,0 , salt losses of approximately 0 to 15 t ha^{-1} are predicted (Figure 3.6).

Within an ET/I group, the differences were considerably less than across the groups. A noticeable exception again is the P5 and P6 combination of hydrological variables where the airentry value of -0,2 kPa was used. The restricted flow of water into and out of the root zone would also have prevented any convective salt movement. This is indicated by the 13 salt load values given in Figure 3.6 that all are located on or about the zero line.

Within a specific combination of hydrological variables, the great impact of the ET/I ratio on salt gains and losses becomes even more evident. In Figure 3.7, the ET/I - salt load relationship for the P4 combination of *a, b* and *Ksat* is given. Also indicated on the bargraph are the two CEC values that were used, but the effect of the latter variable, was completely overshadowed by the ET/I ratio. It can therefore be deduced that of all the variables that were used in this study, barring the P5 and P6 combination, the ET/I ratio had the greatest single effect on the amount of salt that were either leached out of, or accumulated in the root zone.

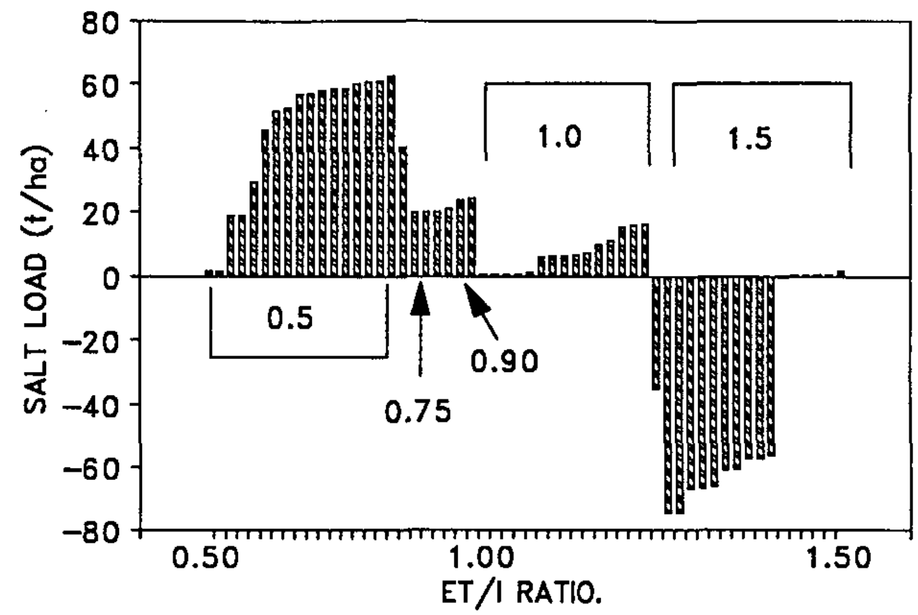


Figure 3.6 The relationship between the ET/I ratio and the predicted annual salt load, expressed as t ha^{-1}, irrespective of all other input values. Those points falling on the zero line, represent the hydrological combination of a=-0,2 kPa and b=10

ii) Effect of the variables *a*, *b*, Ksat, CEC and k-Ca/Na

Within an ET/I group, e.g. ET/I = 0,5 , differences of up to 30 t ha^{-1} in the annual salt load were found. (This does not include the P5 and P6 combinations, which will not be discussed any further). These differences for the most part could be attributed to the two Campbell coefficients and are illustrated in Figures 3.8 (a-c). Although no clear trend is discernible, it does seem as if solute movement, and hence the salt load, increases with a decrease in the airentry potential. For example, compare the two combinations b=5 a=-0,2 , and b=5, a=-3,0 kPa, both with a hydraulic conductivity of 100 mm d^{-1} and ET/I ratio of 0,5; by decreasing the airentry value from -0,2 to -3,0 the salt load increased from 29,1 t ha^{-1} to 51,8 t ha^{-1}. Similar results were obtained with the other *a*-*b* combinations.

An increase in the saturated hydraulic conductivity also seems to increase the movement of water and solutes across the 1 m depth. Combinations P1 and P2 differed only with respect to their hydraulic conductivity values, with the former being 1000 mm d^{-1} and the latter 100 mm d^{-1}. Increasing the Ksat value from 100 to 1000 mm d^{-1}, increased the salt load from approximately 30 to 45 t ha^{-1} at an ET/I ratio of 0,5 (Figure 3.8a). Although it might be argued that such a large increase in the Ksat value is rather drastic (one order of magnitude), similar variations are observed in natural soils, e.g. Biggar and Nielsen, 1976.

Within an ET/I ratio, the higher of two CEC values increased the salt load by up to 7 t ha^{-1} compared to the lower value. The Ca-Na selectivity coefficient also had a small effect on the salt load with the 9,3 coefficient increasing the salt load by 2 t ha^{-1} over that of the 4,0 coefficient.

3.3.1.4 Chemical composition of the deep percolate

The effect of the CEC, k-Ca/Na values, and the cumulative flux on the salt load within the P4 hydrological combination (a=-3,0 kPa; b=5; Ksat=10 mm d^{-1}), are expressed in Figure 3.9. As is to be expected, the load increases with flux, but the differences caused by the different values of the exchange properties were less than 10 t ha^{-1} at the end of the simulation period. Despite this small effect, it seems as if this difference might increase with an increase in the cumulative flux. Initially the three CEC-k-Ca/Na combinations yielded the same salt load, but when the net flux of water had accumulated to approximately 350 mm, an increasing deviation in predicted salt loads started to develop. The lower CEC and k-Ca/Na values resulted in the lowest salt load.

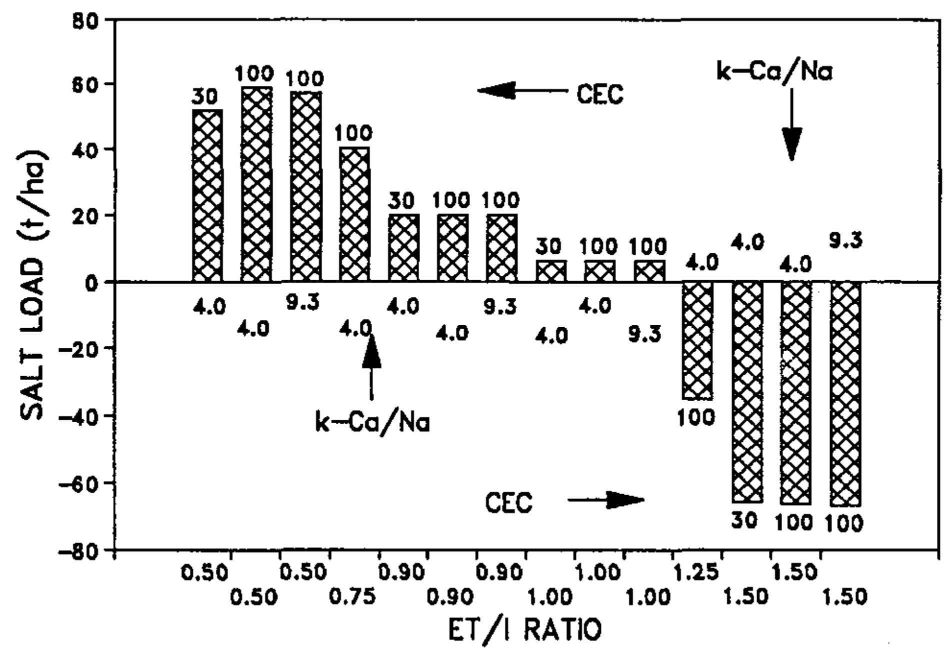


Figure 3.7 Effect of the ET/I ratio on the predicted annual salt load (t ha^{-1}) for the hydrological combination a=-3,0 kPa, b=5, and Ksat=100 mm d^{-1} (The numbers above each bar indicate the particular CEC and k-Ca/Na values)

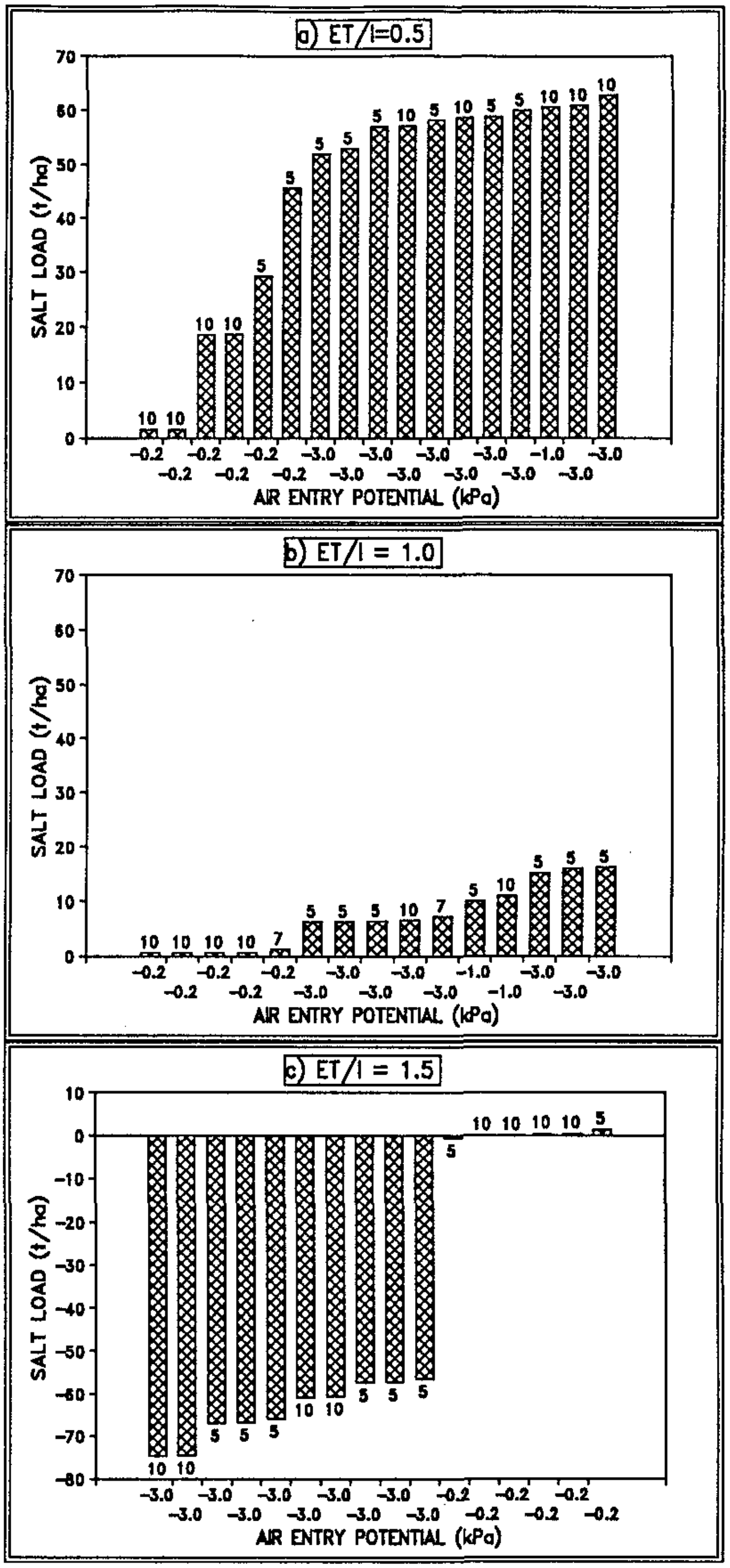


Figure 3.8 Relationship between the Campbell *a* (X-axis) and *b* (number above each bar) values, and the predicted annual salt load within an ET/I ratio group (irrespective of the effect of Ksat, CEC and k-Ca/Na)
a)ET/I = 0,5; b)ET/I=1,0; c)ET/I=1,5

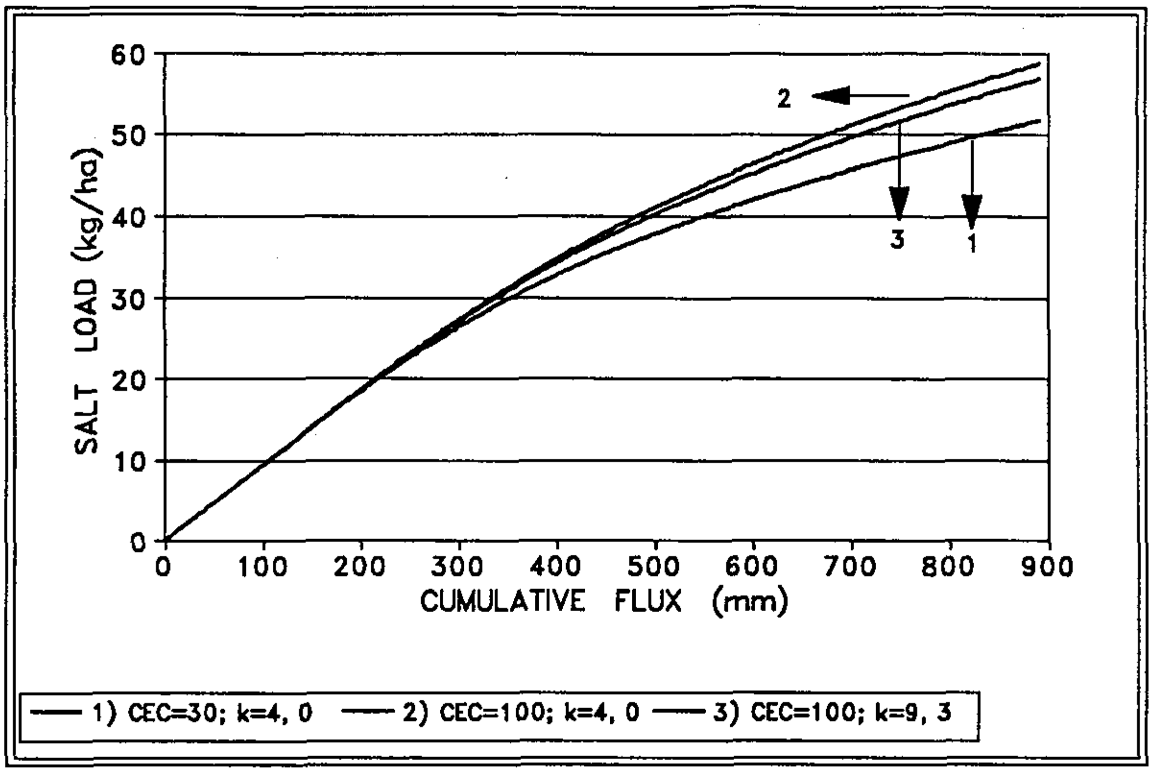


Figure 3.9 Relationship between the cumulative flux and cumulative salt load for three different CEC and k-Ca/Na combinations within the hydrological combination a=-3,0 kPa, b=5 and Ksat=100 mm d^{-1}, and for an ET/I ratio of 0,5

Although the two chemical properties, i.e. CEC and the k-Ca/Na coefficient seemingly will have a minor effect on the annual salt load, it does influence the chemical composition of the deep percolate. Considering the fact that the hypothetical soil is irrigated with low salt water, it is reasonable to expect that the concentrations of all the major soluble cations and anions in the deep percolate will decrease as the soil becomes progressively more leached, i.e. with an increase in the cumulative flux. This is illustrated in Figure 3.10 which shows that, with the exception of Ca, the concentrations of all the other major ions decreased with an increase in flux. Sodium and chloride exhibited the greatest decrease. The initial concentrations were in excess of 2000 mg dm^{-3}, while the final concentrations were less than 200 mg dm^{-3}.

In view of the different Ca/Na selectivity coefficients that were used, the temporal changes in Ca, Na and SO_4 warrant further discussion. These changes are illustrated in Figures 3.11 (a-c). After an initial decrease, the Ca concentration is predicted to increase with cumulative flux. This is probably caused by the dissolution of gypsum once the exchange complex had become equilibrated with the less saline soil solution. Inspection of results not presented here also show that for both of the two CEC values (30 and 100 mmol kg^{-1}), the exchangeable calcium concentration increased from the initial values. This might explain the initial decrease in the dissolved calcium content of the deep percolate, i.e. calcium in solution is removed from the soil solution through the Ca-Na, Ca-Mg and Ca-K exchange reactions. The extent of the initial Ca decrease was less for the CEC = 30 than for the CEC = 100 value. Compared to the higher CEC value, a CEC of 30 mmol(+) kg^{-1} also produced higher final Ca concentrations, the difference being approximately 40 to 60 mg dm^{-3} at the end of the simulation run. This difference is attributed to the fact that the capacity of the CEC=100 soil to adsorb and remove calcium from the soil solution, exceeds that of the CEC=30 soil. This greater capacity effectively lowers the calcium concentration of the soil solution and ultimately the deep percolate.

The Na concentration of the deep percolate is predicted to first increase slightly, and then to decrease with increasing flux. The CEC=100 value gave higher concentrations than the CEC=30 value. The initial increase coincides with the decrease of calcium and these two observations are in support of the explanation concerning the Ca-Na exchange reaction mentioned in the previous paragraph. After going through a stage where the differences in the concentrations caused by the different CEC and k-Ca/Na values are as much as 500 mg dm^{-3}, the final concentrations all converge on a value of approximately 250 mg dm^{-3}. The biggest difference in the individual ion concentrations are exhibited by the SO_4 content of the deep percolate. At a cumulative flux of 400 mm the difference between the highest and lowest SO_4 concentration is 900 mg dm^{-3}, with the CEC=30 k-Ca/Na=4 combination having a concentration of 2600 mg dm^{-3}, while that of the CEC=100 k-Ca/Na=4 combination is 3500 mg dm^{-3}. A possible explanation is that the higher the CEC is, the more calcium will be adsorbed (until a new chemical equilibrium has been reached), and therefore the more gypsum will dissolve. An increase in the dissolution of gypsum will increase the concentration of sulfate in the soil solution and deep percolate. Similar model predictions were made by Jury *et al* (1978). As the exchange complex of the two CEC soils approaches calcium saturation, this difference should decrease. Inspection of Figure 3.11c shows that this is the case. The information of Figure 3.11a-c also show that the simulated period of one year is not long enough for a new chemical equilibrium to be reached.

3.3.1.5 Changes in the chemical composition of the soil solution in the root zone

The changes in the chemical composition of the soil solution at field water contents are depicted in Figures 3.12 (a,b) and 3.13 (a,b) for the P4 hydrological group. For the sake of brevity only the results of the CEC=30 mmol(+) kg^{-1} k-

Ca/Na=4 chemical combination are given. Similar trends were observed with the other combinations of these two variables.

In Figure 3.12 the depth distributions of the Ca, Na, SO_4 and Cl concentrations at the ET/I=0,5 ratio are given. With the exception of Ca, the concentration of all the ions decreased markedly. The opposite is predicted if the evapotranspiration exceed the irrigation quantity by a ratio of 1,5 (Figure 3.13). The solubility product of gypsum determines how much Ca and SO_4 can be in solution before precipitation sets in. Therefore, the limited solubility of gypsum ($CaSO_4$) prevented the Ca and SO_4 concentrations to increases as much as the Na and Cl concentrations did. The latter two ions increased dramatically at the depth of maximum water penetration, i.e. at approximately 500 mm depth.

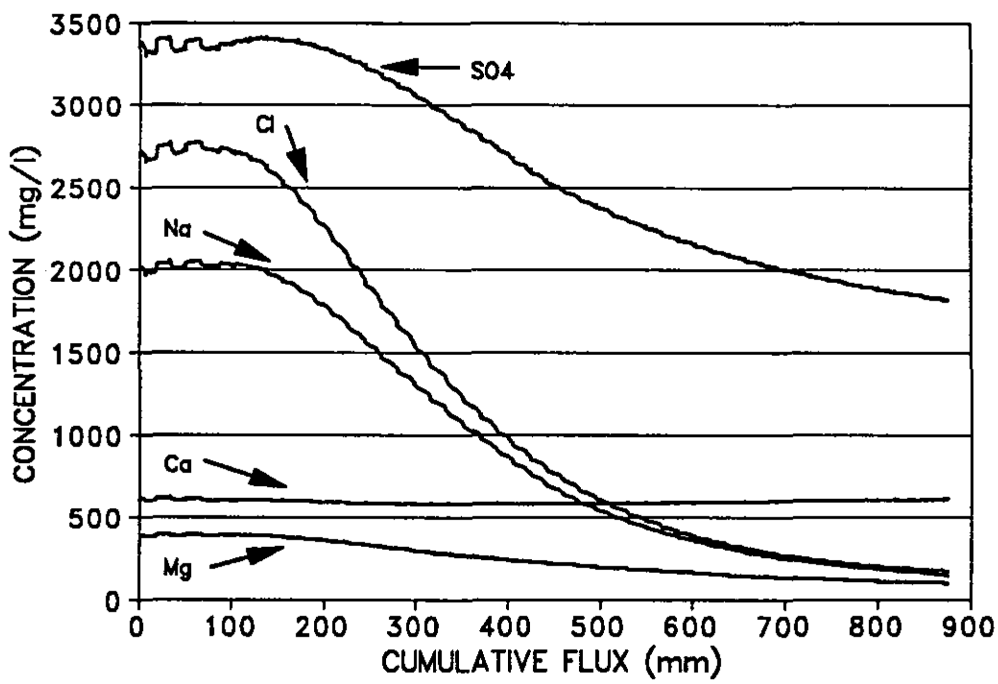


Figure 3.10 Effect of the cumulative soil water flux across the 1 m depth on the concentration of the major cations and anions in the deep percolate: input combination *a*=-3,0 kPa, *b*=5,0 and Ksat=100 mm d^{-1}, ET/I=0,5, CEC=30 mmol(+) kg^{-1} and k-Ca/Na=4,0

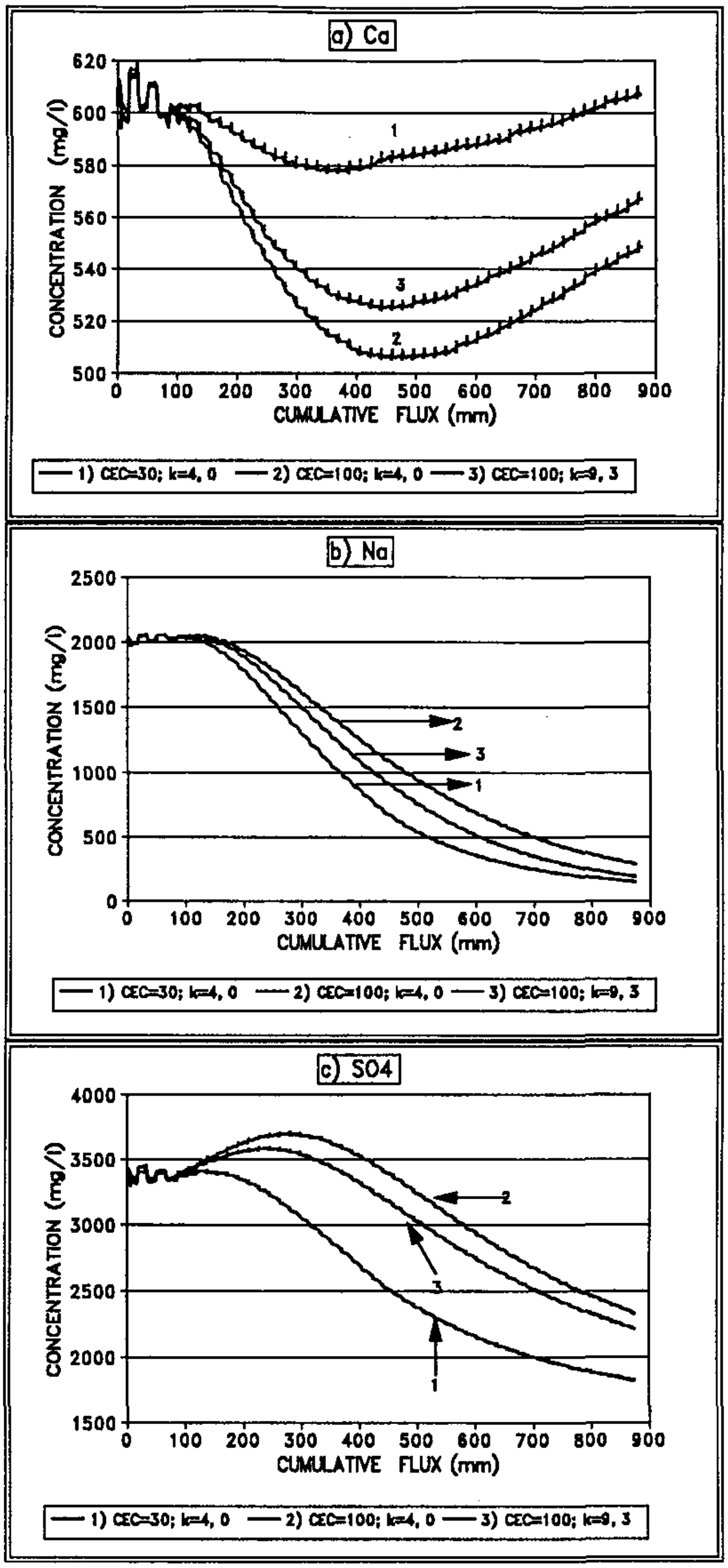
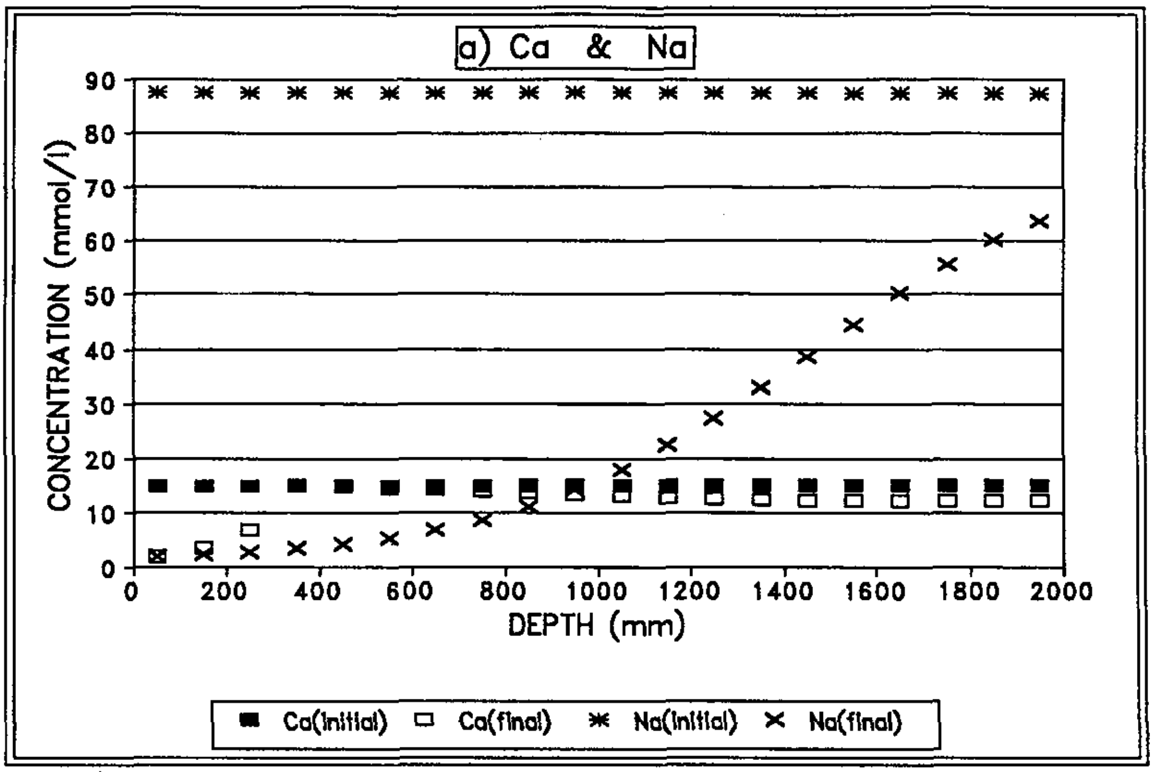


Figure 3.11 Salt concentrations in the deep percolate as function of cumulative flux, CEC and k-Ca/Na for the hydrological combination a=-3,0 kPa, b=5 and Ksat=100 mm d^{-1}, and ET/I=0,5:
a) Calcium; b) Sodium; c)Sulfate.



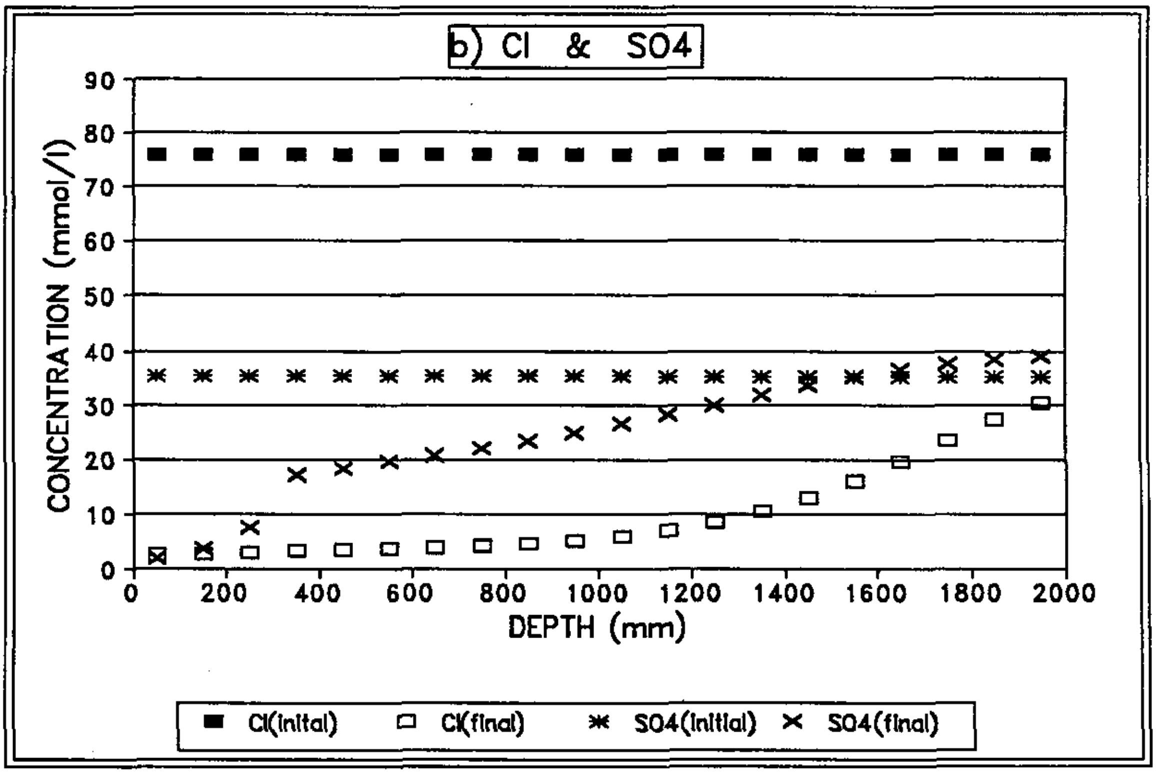


Figure 3.12 Initial and final soluble salt concentrations within the hypothetical soil profile at field water content as influenced by the ET/I ratio = 0,5 (input combination a=-3 kPa, b=5, Ksat=100 mm d^{-1}, CEC=100 mmol(+) kg^{-1}): a) Calcium and Sodium; b) Chloride and Sulfate

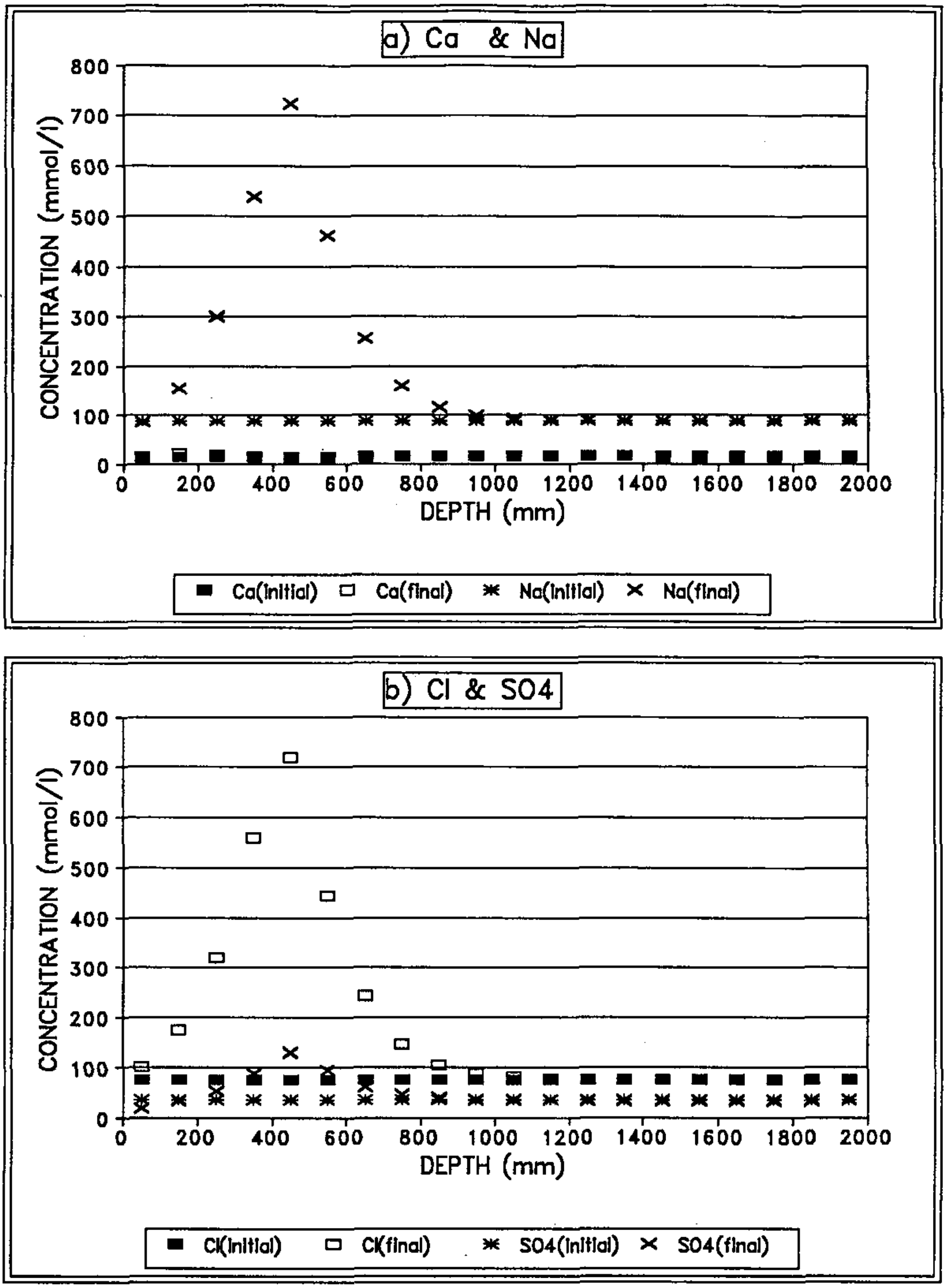


Figure 3.13 Initial and final soluble salt concentrations within the hypothetical soil profile at field water content as influenced by the ET/I ratio = 1,5 (input combination a=-3 kPa, b=5, Ksat=100 mm d^{-1}, CEC=100 mmol(+) kg^{-1}): a) Calcium and Sodium; b) Chloride and Sulfate

3.3.2 LEACHM: Non-saline soil irrigated with saline water

3.3.2.1 Objectives

In the first part of the sensitivity study with the LEACHM model, it was established that the ET/I ratio, more specifically the water flux quantity, is the most important factor that will determine the quantity of water and salt leaving the root zone. Secondary factors, mostly chemical of nature, influenced the chemical composition, and thus the quality of the water leaving the root zone. There is no evidence to show that the results would have been different if the starting conditions were the opposite, i.e. a hypothetical non-saline soil irrigated with saline water. The dominant factor controlling the amount of the applied water that will percolate through the root zone, would also have been the ET/I ratio. In can be argued that the absolute amount of soluble salt, and consequently the salt load, initially would have been less than that draining out of a saline soil. However, if a non-saline soil is irrigated with saline water, the salt load will at some stage start to increase with cumulative flux. The purpose of this part of the sensitivity study was to determine the temporal pattern of such an increase in the salt load and to evaluate the influence of the CEC and Ca/Na selectivity coefficient on the chemical composition of the deep percolate. Another goal was to evaluate how a 25% change in the total salt content of the irrigation water will effect the predicted salt load in comparison with a similar change in the ET/I ratio.

In order to achieve this goal, two ET/I ratios, namely 0,50 and 0,75 were used but with one combination of hydrological variables only. The combination of a, b and *Ksat* values that was decided upon, was the P4 combination, i.e. a = -3,0 kPa, b = 5, and *Ksat* = 100 m d^{-1} (Table 3.3). In terms of the defined objective, the initial chemical composition had to reflect a non-saline soil in chemical equilibrium. Furthermore, the combinations of chemical properties used in this second part of the sensitivity study had to be comparable for those used in the first. The combinations of input values that were used are listed in Table 3.11.

Table 3.11 Combinations of values used in the LEACHM sensitivity study where the starting conditions was a non-saline soil

Combination	a (kPa)	b	Ksat (mm d^{-1})	CEC (mmol(+) kg^{-1})	k-Ca/Na	ET/I
1	-3	5	100	30	4,0	0,75
2	-3	5	100	100	4,0	0,75
3	-3	5	100	100	9,3	0,75
4	-3	5	100	100	9,3	0,50

The hypothetical soil used in the second part of the study was the same as that used in the first part, i.e. physically and chemically uniform with depth. The only difference was in the chemical composition where non-saline initial conditions were defined. The chemical compositions used were selected from the predicted data at the end of the one year "saline" simulation period with the same chemical parameter combinations as those listed in Table 3.11. At that stage the ET/I=0,5 ratio yielded non-saline, chemical equilibrium conditions throughout the root zone. To keep the initial conditions of the three chemical combinations comparable with respect to the soluble salt content, the electrical conductivity of all three was empirically chosen to be approximately 100 mS m^{-1}. The soluble and exchangeable ionic compositions of three depths that matched this criteria are listed in Table 3.12. These concentrations defined the starting conditions for the one year simulation period that was used. The two irrigation waters that were used to irrigate the non-saline soil are listed in Table 3.7. The water with a TDS content of 618 mg dm^{-3} has 25% less dissolved solids than the 824 mg dm^{-3} water, and as mentioned earlier, represent a hypothetical case where a 25% analytical error was made in determining the chemical composition of the irrigation water. The amounts and rates of water applied were exactly similar to that of the first study.

Table 3.12 Initial chemical composition of the hypothetical non-saline soil used in the sensitivity study

	Combination	1	2	3
Cl	mmol dm^{-3}	3,70	3,30	3,30
SO_4	mmol dm^{-3}	16,80	17,10	16,80
HCO3	mmol dm^{-3}	2,00	1,40	1,40
Ca	mmol dm^{-3}	15,50	15,10	15,30
Mg	mmol dm^{-3}	2,20	2,80	2,30
Na	mmol dm^{-3}	3,80	3,40	2,90
K	mmol dm^{-3}	0,30	0,30	0,40
EC	mS m^{-1}	107	109	102
XCa	mmol(+) kg^{-1}	20,52	67,70	81,20
XMg	mmol(+) kg^{-1}	8,16	29,10	16,80
XNa	mmol(+) kg^{-1}	0,55	0,70	0,30
XK	mmol(+) kg^{-1}	0,77	2,60	1,70
CEC	mmol(+) kg^{-1}	30	100	100
pH		7,4	7,4	7,4

X=exchangeable cation; EC=electrical conductivity of the soil solution

3.3.2.2 Total salt load

The two CEC values that were used had an insignificant effect on the total salt load at the end of the one year simulation period. Decreasing the ET/I ratio from 0,75 to 0,50 led, as expected, to an increase of approximately 10 ton in the annual salt output (Figure 3.14). With an ET/I ratio of 0,75, the salt load increased curvilinearly with the water flux (Figure 3.15). The differences between the three CEC-k-Ca/Na combinations were marginal - less than 1 t ha^{-1} per year. The effect of a 25% analytical error in the chemical composition of the irrigation water is illustrated in Figure 3.16. Within an ET/I ratio the 25% reduction in the total salt content of the irrigation water reduced the annual salt load by approximately 1 ton ha^{-1}. This is substantially less than the 12 ton ha^{-1} which is predicted to occur when the ET/I ratio is changed from 0,50 to 0,75. However, it should be realised that this increase in the ET/I ratio, decreased the water flux from 910 mm a^{-1} to 455 mm a^{-1}.

3.3.2.3 Chemical composition of the deep percolate

The CEC and k-Ca/Na values did influence the chemical composition of the deep percolate, but only too a limited extent. The differences between the various combinations were accentuated most in the Ca and SO_4 concentrations. These changes and differences as a function of the cumulative flux, are shown in Figures 3.17 (a,b). The combination that yielded the highest SO_4 concentration (CEC=30, Ca/Na=4) were predicted to have the lowest Ca concentration. Similarly, the combination with the lowest SO_4 concentration (CEC=100, k-Ca/Na=4), had the highest Ca concentration in the deep percolate. However, the magnitude of the differences between lowest and highest values were quite different for the two ions. In the case of Ca this difference was less than 20 mg dm^{-3} at the end of the simulated one year irrigation period, but for the SO_4 ion it was five times as large, i.e. approximately 100 mg dm^{-3}. Whether these differences in a real world situation will be of practical significance, will depend on the actual case under study.

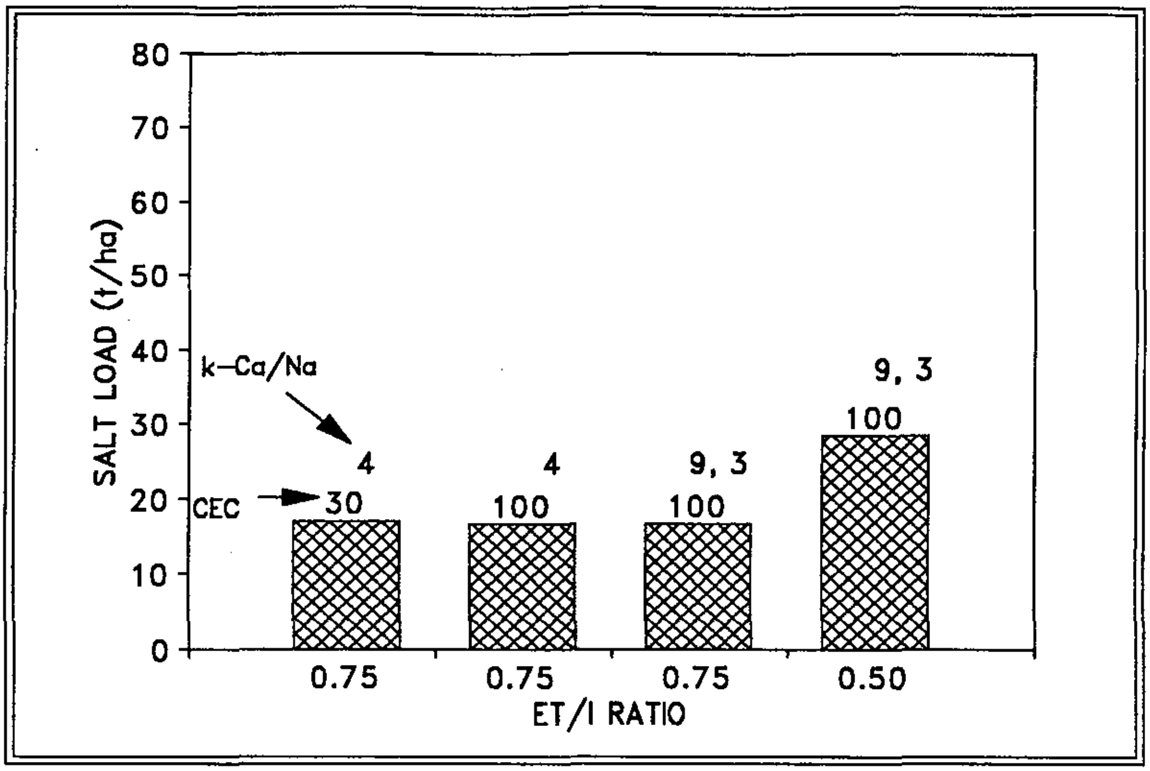


Figure 3.14 Effect of ET/I ratio, and CEC on the predicted salt load in the deep percolate of the initially non-saline soil (input combination a=-3,0 kPa, b=5 and Ksat=100 mm d^{-1})

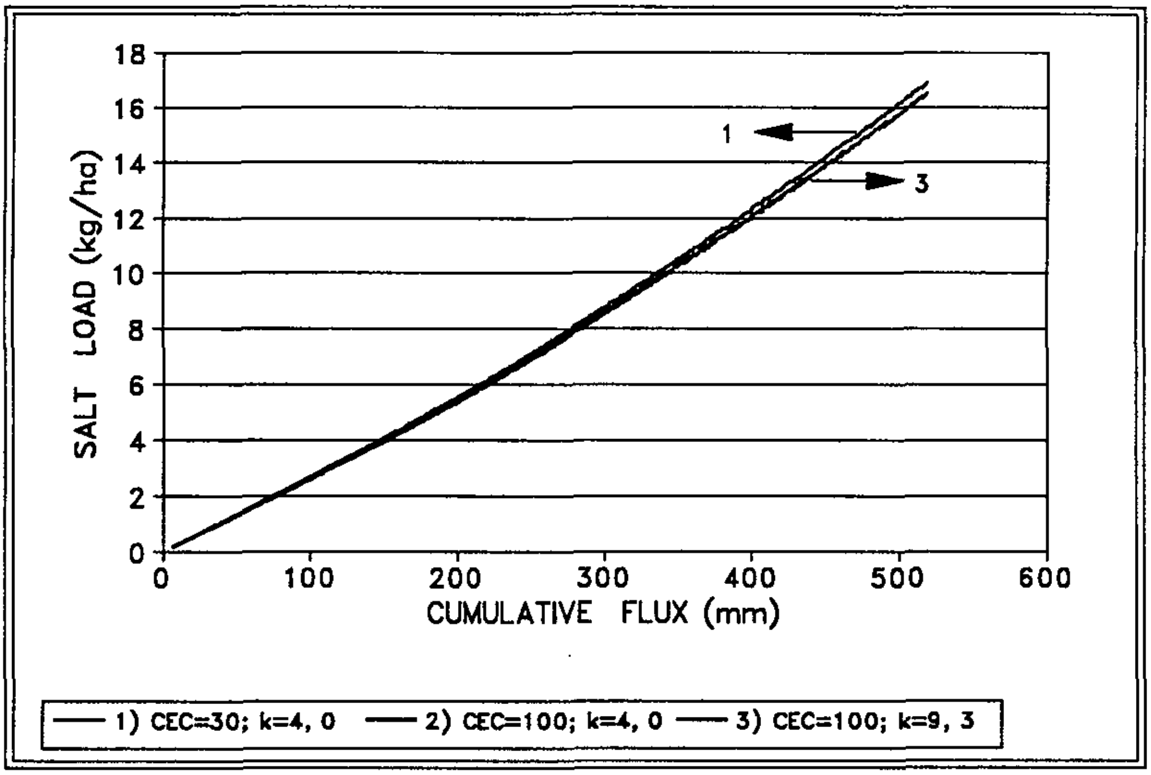


Figure 3.15 Relationship between cumulative flux and the salt load of the deep percolate of the initially non-saline soil, for three different CEC-k-Ca/Na combinations (the combination CEC=100, k-Ca/Na=9,3 is the bottom line, and combination CEC=30, k-Ca/Na=4,0 the top line)

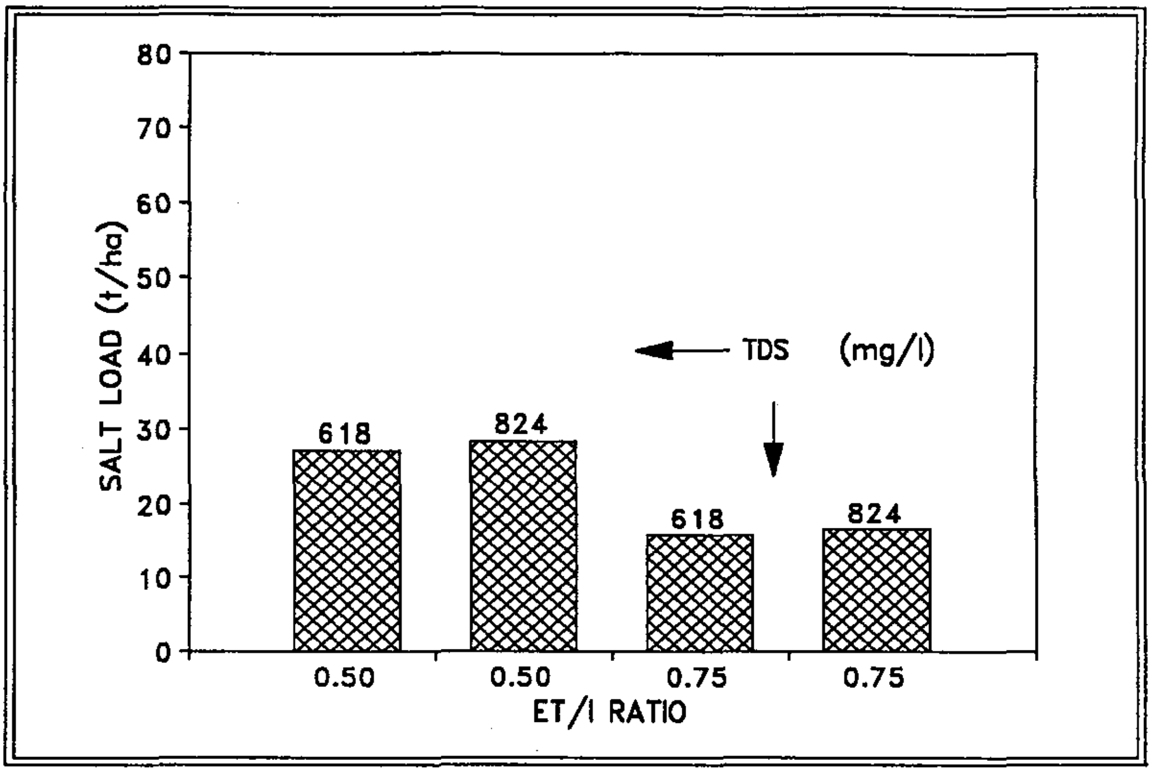


Figure 3.16 Effect of a 25% reduction in the irrigation water TDS content and ET/I ratio on the predicted annual salt load for the combination CEC = 100 and k-Ca/Na = 9,3

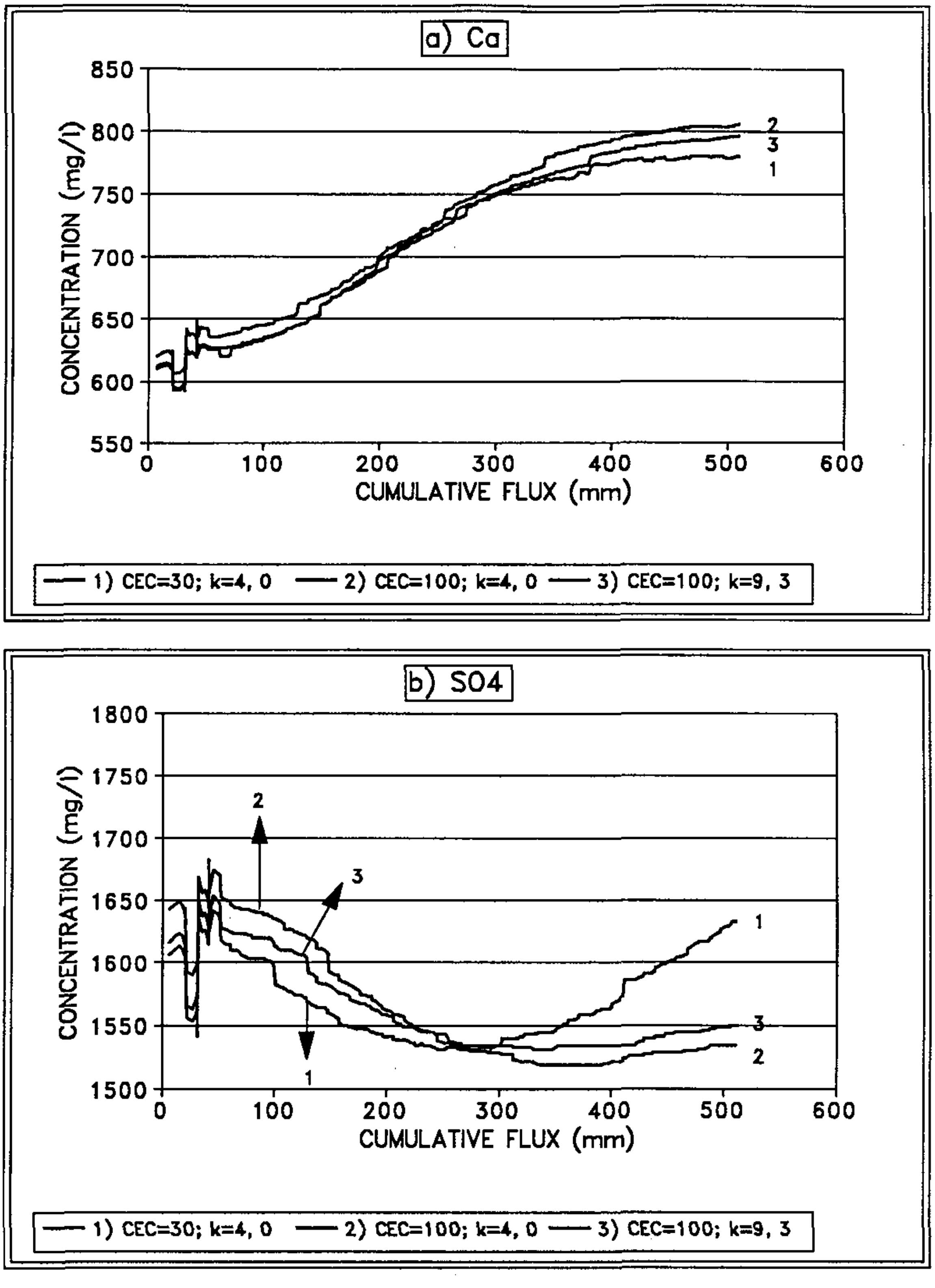


Figure 3.17 Influence of cumulative flux, CEC and k-Ca/Na on the calcium and sulfate concentrations of the deep percolate of the initially non-saline soil (input combination a=-3,0 kPa, b=5, Ksat=100 mm d^{-1}, and ET/I=0,5): a) Calcium; b) Sulfate

3.3.3 BURNS: Saline soil irrigated with non-saline water

As explained in section 3.2.2.2, the Burns model uses a capacity approach to simulate the transport of water and salt. In this sensitivity study, the initial soil water content was set at field capacity for all of the twelve combinations that were used. Consequently, where evapotranspiration was equal to, or exceeded the amount of applied irrigation water, no leaching occurred. Although no leaching was predicted, the salt content in the 2 m deep profile did increase by the amount of salt applied, which in this case is 1820 kg ha^{-1} per year (35 mm * 52 weeks * 100 mg dm^{-3}).

The only instance in which water and salt were leached out of the two meter deep profile, is when the ET/I ratio was less than 1. The total flux and salt (chloride) load for these ET/I ratios, are summarized in Table 3.13.

Table 3.13 Predicted annual soil water flux and salt load as a function of the ET/I ratio and field capacity (expressed as a fraction of the original values in Table 3.8)

ET/I	FC	Flux mm	Load t ha^{-1}
0,90	1,1	182	40,93
0,90	1,0	182	53,00
0,90	0,9	182	75,18
0,80	1,1	364	82,44
0,80	1,0	364	107,16
0,80	0,9	364	149,45

The same results are visually presented as Figure 3.18. As was observed with the LEACHM model, the effect of the ET/I ratio is dominant, especially within a specific field capacity value. For example, by decreasing the ET/I from 0,90 to 0,80, the salt load increases from 53,0 to 107,16 t ha^{-1}. A ten percent decrease in the water content at field capacity increased the salt load from 53,00 to 75,18 t ha^{-1}. In absolute terms this is a significant increase in the load, but it is substantially smaller than the increase in the load which resulted from a 10% change in the ET/I ratio.

For the defined set of circumstances, the ten percent decrease in the ET/I ratio (0,9 --> 0,8), increased the annual flux by 100%, i.e. from 182 to 364 mm. A simple water balance, using the annual figures (mm a^{-1}) employed in this study, elucidate this result:

Pan Evap	Crop Fact	AET	Irrig	Balance
1820	0,8	1456	1820	364
1820	0,9	1638	1820	182

These figures illustrate the profound effect that inaccurate estimates of AET, or inappropriate crop factors, will have on the predicted (calculated) salt load.

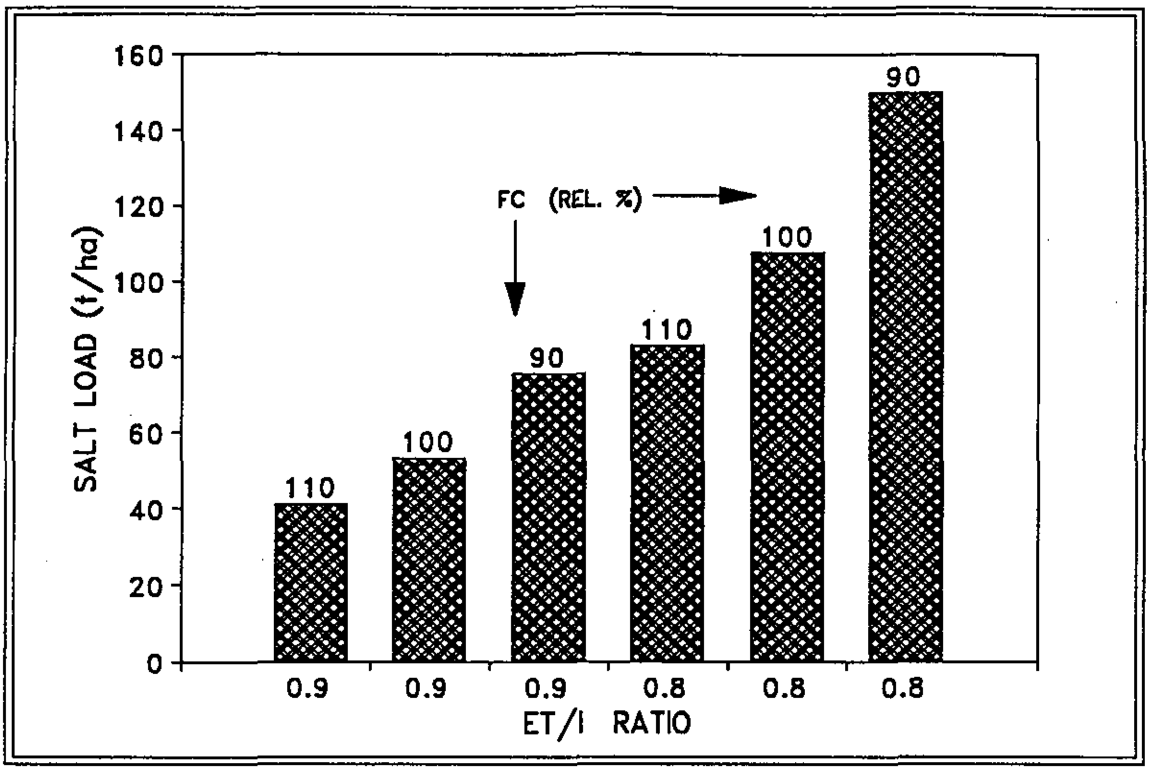


Figure 3.18 Effect of the ET/I ratio and field capacity on the annual salt load (chloride) predicted with the Burns model

3.4 DISCUSSION AND CONCLUSIONS

The objective of this study was to evaluate the effect of a number of input variables on the predicted quantity and quality of soil water leaving the root zone of irrigated agricultural lands. The study was conducted using two different deterministic water and salt transport models. The one model was deterministic mechanistic- and the other a deterministic capacity type of model. A sensitivity analysis was performed which involved six of the input variables required by the mechanistic LEACHM model. The variables that were studied are: airentry potential, slope of the soil water characteristic (i.e. Campbell's *a* and *b* coefficients), saturated hydraulic conductivity, cation exchange capacity, Ca/Na selectivity coefficient, and the difference between the evapotranspiration and irrigation quantities. The variables evapotranspiration, irrigation and field capacity were evaluated with the simpler Burns model. In both cases a hypothetical soil profile and irrigation frequency were used. The results indicate that the quantity of water moving through the soil (i.e. the water flux), is by far the most important factor that will determine the quantity of water and the amount of salt that will be leached out of the root zone. In this study different fluxes of water through the soil was affected by varying the actual evapotranspiration rate in the presence of a constant irrigation application rate. This resulted in different ratios of evapotranspiration and irrigation, i.e. ET/I ratios. Both of the two models that were used, showed that even a relatively small change in the ET/I ratio, e.g. from 1,00 to 0,90 will significantly effect the flux of water and solutes through the soil. For example, in the case of LEACHM, changing ET/I from 1,0 to 0,9 increased the calculated salt load from 6,1 ton ha a^{-1} to 20,1 ton ha a^{-1}. This indicate that accurate estimates of the irrigation and evapotranspiration quantities should receive more attention than other physical and chemical soil properties such as water retention, hydraulic conductivity and CEC when predicting the salt load coming from irrigated lands.

With the mechanistic model LEACHM, another important result was that unsound combinations of input values for the hydrological variables have a profound effect on model predictions. In this regard the air entry potential was of particular importance. A high potential (i.e. small negative) in combination with medium to low saturated hydraulic conductivities had a critical effect on the estimate of the unsaturated conductivity. In extreme cases, such low values for the unsaturated hydraulic conductivities can be obtained that no movement of water and salt will be possible. In this study a particular combination of hydrological variables yielded a water flux of less than 12 mm a^{-1} and a salt load of 11 t ha a^{-1}. This prediction was made despite the fact that the amount of irrigation water that was specified as input, exceeded evapotranspiration by as much as 910 mm a^{-1}. In such a case the unsuspecting model user might come to the conclusion that soils in which macro pores predominate, i.e. soils with large airentry potentials, will have a low salt output irrespective of the ET/I ratio. This obviously is an inconsistent result.

It is necessary to put this particular result in its proper perspective. In the Campbell approach to estimate hydraulic conductivities, the airentry potential is the term that quantifies the effect of pore size distribution on water movement. According to Poiseuille's law, the volume of water flow in a tube is proportional to the hydraulic gradient and the ***fourth power of the radius of the tube***. A large airentry potential is indicative of large soil pores which in turn, according to Poiseuille's law, should be associated with large hydraulic conductivities. Selecting a large air entry potential, without balancing it with a matching hydraulic conductivity can thus lead to water and salt production estimates that is entirely spurious.

Ranking the other variables of LEACHM in terms of their effect on the amount of salt that will be leached from the root zone, was done by calculating their effect on a "base line" salt load obtained with a certain combination of input values. The combination of values used for this purpose is the P4 group (Table 3.3), i.e. a = -3,0 kPa, b = 5,0, Ksat = 100,0 mm d^{-1} which was combined with CEC=100 mmol kg^{-1}, k-Ca/Na = 4,0 and ET/I = 1,0. LEACHM predicted that this set of input values will yield an annual salt load of 6,1 t ha^{-1}. The ET/I ratio was then changed from 1,0 to 0,9 and the new salt load calculated. By changing ET/I from 1,0 to 0,9, the water flux at 1 m increased from 49 to 182 mm a^{-1}. Subsequent to this change, each variable was changed individually while the other variables, except ET/I, were kept at their base line values. The effect of these changes was expressed as a percentage relative to the base line salt load. The results are listed in section I of Table 3.14. Based on the percentages listed in Table 3.14(I) the rank order is:

ET/I $>>$ Ksat $> a \geq b >$ CEC = k-Ca/Na

By using the same procedure as above, but changing the ET/I ratio from 1,0 to 0,5 (which increased the water flux from 49 to 910 mm a^{-1}), a different rank order is obtained (Table 3.14 II):

ET/I $>>>$ CEC $> b >$ k-Ca/Na $= a >$ Ksat

This big increase in the water flux reduced the effect of Ksat to such an extent that it moved from the second to the last position in the rank order. In contrast, the salt supplying capacity of the soil, which in this study was quantified by using different CEC values, became more important and moved up several positions in the rank order.

In view of the above, it seems as if the relative importance of the cation exchange capacity and the hydraulic conductivity as properties that will influence the salt load in the deep percolate of irrigated lands, will depend on the magnitude of the water flux. At small fluxes, i.e. where AET $\approx$ irrigation, the rate of water movement through the soil is more important than the salt supply capacity of the soil. At greater fluxes, i.e. irrigation $>>$ AET, the rate of water movement becomes less important while the capacity of the soils to supply salt, increases in importance. However, it should be realised that this conclusion is based on a flux which in the first case increased from 49 to 259 mm a^{-1}, and in the second case from 49 to approximately 900 mm a^{-1}. It is doubtful whether the error associated with the measurement and/or estimation of the actual evapotranspiration and irrigation quantities will ever be as large as 900 mm a^{-1}.

Table 3.14 Increase in the initial base line salt load due to a sequential change in input values (excluding the a = -0,2 kPa b = 10 combination)*

Variable	Base line value	New value	Range (%)	New Load (ton ha^{-1})	% Increase in load	% Due to variable
I: Change in ET/I: 1,0 to 0,9						
ET/I	1,0	0,9	10	20,1	330	330
b	5,0	10,0	200	21,1	346	+16
a	-3,0	-1,0	300	23,5	385	+55
Ksat	100,0	1000,0	1000	24,5	398	+68
CEC	100,0	30,0	333	19,6	321	-9
k-Ca/Na	4,0	9,3	233	20,0	328	-2
II: Change in ET/I: 1,0 to 0,5						
ET/I	1,0	0,5	200	58,8	858	858
b	5,0	10,0	200	62,7	921	63
a	-3,0	-1,0	300	60,6	887	29
Ksat	100,0	1000,0	1000	59,9	875	17
CEC	100,0	30,0	333	51,8	744	-114
k-Ca/Na	4,0	9,3	233	56,9	827	-29

* Each variable was changed individually while the other variables, except ET/I, were kept at their base line values

The hydrological variables a, b and Ksat will determine the so-called field capacity of the soil. With the Burns model, the input value used as the field capacity of the soil had a significant influence on the water and salt flux, but it's effect remained secondary to that of the ET/I ratio.

Several input variables of LEACHM were not investigated, neither was the quantity of applied irrigation water varied. Consequently, the effect of some of the chemical and even some of the hydrological input variables, remain somewhat inconclusive. It can be hypothesized that the effect of the boundary conditions at the bottom of the soil profile might influence the relative importance of the a, b and Ksat variables. Similarly, the variables controlling the dispersion and diffusion of the solutes might increase or decrease the effect of CEC and the selectivity coefficients. The study furthermore did not attempt to distinguish between the difference in salt loads stemming from saline as opposed to non-saline soils. Despite these shortcomings, it is very clear that the evapotranspiration and irrigation quantities play the dominant role in determining the quantity and quality of soil water percolating out of irrigated lands. The effect of all the other variables are nominal, although the actual chemical composition might to a limited extent be influenced by factors such as the cation exchange capacity and the exchange selectivity coefficients.

In summary, this sensitivity analysis has showed that studies which attempt to predict the salt and water fluxes coming from irrigated lands, should concentrate more on accurate estimates of the evapotranspiration and irrigation amounts, than elaborate methods to get accurate values for the chemical and hydrological soil properties.

CHAPTER 4
PREDICTING WATER AND SOLUTE MOVEMENT IN A DRIP IRRIGATED VINEYARD IN THE BREEDE RIVER VALLEY: A MICROSCALE SPATIAL STUDY WITH LEACHM

4.1 INTRODUCTION

The objective of this part of the study was to evaluate how accurate a mechanistic research model can simulate transport processes under microscale field conditions (< 1 ha). Only one model, namely LEACHM (Wagenet & Hutson, 1989), was used for this study. The data that were used to evaluate the predicted soil water and soluble salt contents over time, are based on field measurements made during a period of two and half years in a 0,5 ha drip irrigated vineyard in the Breede River Valley of South Africa. In addition to the primary objective, this application of LEACHM was also meant to serve as a test of the application of a one-dimensional model to a case where the irrigation is applied at a point source and the water and salts subsequently redistributed in three dimensions. LEACHM was used to simulate the chemistry and transport of soil water and salt that occurred during the period 1 May 1987 to 30 June 1989.

4.2 DESCRIPTION OF THE DRIP IRRIGATED FIELD AND INPUT DATA

4.2.1 Physical description of the field

As mentioned in Chapter 1 of this report, no reference data suitable for the evaluation of model predictions could be found in South-Africa. (The requirements for a set of data that can be used to evaluate/validate soil and water transport models, are listed on page 1.5). Consequently, in May 1987 an area representing 5000 m^2 of a drip irrigated vineyard in the Breede River Valley were equipped with 30 neutron access tubes and other necessary instruments such as tensiometers, soil water cup samplers, rain gauges and water meters. In addition, the chemical composition of the soil solution and exchange complex, were determined during May 1987, August 1988 and June 1989. The samples of May 1987 were also used to determine the textural composition of the soil at each site where a neutron access tube was installed. Between May 1987 and June 1989 the following soil properties were monitored on a continuous basis:

a) spatially distributed soil water content;
b) spatially distributed matric potential;
c) spatially distributed soluble salt content;
d) drainage rate (two-hourly) and chemical composition (daily) of the leachate in a tile drain located at two meter depth.

The emitter spacing in the vineyard is 1 m x 2,5 m. Details of the instrumentation, monitoring actions, *ad hoc* surveys and results are presented and discussed in detail in Volume II of this report. A schematic representation of the physical layout and instrumentation of the field only will be presented here (Figure 4.1).

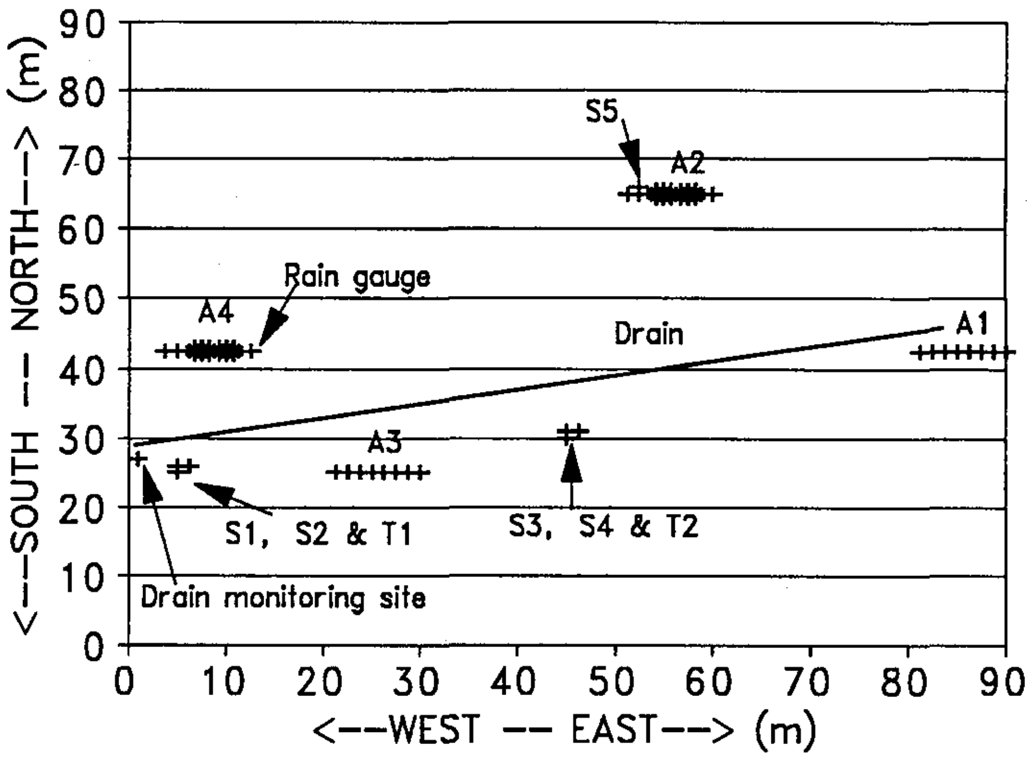


Figure 4.1 Map of the drip irrigated vineyard that was monitored from May 1987 to June 1989. Also indicated are the locations of the various monitoring points: S = soil water cup sampler, T = tensiometer, A=neutron access tube.

4.2.2 Input data

4.2.2.1 Irrigation water: Conversion from volume to depth of applied water

The amount of water that was applied per irrigation event was measured with a tipping bucket rain gauge placed at one of the emitters located close to site A4 (Figure 4.1). The volume and rate of water flow through the emitter were recorded every two hours using an onsite datalogger. The statistical uniformity of emitter flow in the 5000 m^2 vineyard was determined as 93%. This was done by measuring the flow at 25 randomly selected emitters, all in close proximity to the neutron access tubes where the soil water content was measured (Figure 4.1), and by using the following equation (Bralts and Edwards, 1987):

$$U_s = 100(1-S_q/q')$$

with U_s = statistical uniformity, S_q = standard deviation of emitter flow, and q' = mean emitter flow rate or volume. Based on the high coefficient of uniformity, the information gathered at the one emitter where the irrigation amounts were recorded, was assumed to be valid for all of the 2000 emitters in the 5000 m^2 vineyard.

In drip irrigation the wetted surface area can be substantially smaller than the cultivated area. As a consequence the volume of water that was measured per irrigation event cannot be divided by the cultivated surface area to obtain an equivalent depth. In the field under consideration, the surface area per emitter is 2,5 m^2. An irrigation application of, for example 50 m^3 ha^{-1}, which is equivalent to 12,5 liter per emitter, is, depending on the actual wetted area, equivalent to the following depths:

Area (m^2)	Depth (mm)
2,50	5,00
2,00	6,25
1,00	12,50
0,50	25,00
0,25	50,00

During the sensitivity study of LEACHM it was established that the depth of water percolating through the soil, relative to the loss due to evapotranspiration, is the most important factor determining the fate of water and chemicals in the root zone of crops. Therefore, at an early stage during this microscale study, it was recognized that the method used to convert the volume of water to equivalent depths per irrigation, will have a profound effect on the outcome of any modelling study. In order to minimise this effect, an attempt was made to distribute the volume of water from the point source (i.e. emitter) using an area- and leaching fraction-weighted procedure, but at all times adhering to the conservation of mass. The chloride distribution at various distances and depths from the emitter, established during December 1986 (Moolman, 1989), was used as an estimate of the field scale leaching fraction at different distances from the emitter. The 2,5 m^2 area surrounding each emitter was divided into four different subsectors, each with its own area and leaching fraction. A schematic diagram of these four sectors for one emitter, is given in Figure 4.2.

The inverse of each of the four areas and associated leaching fractions were then used to calculate a weight factor to convert the volume of irrigation water applied per event to an equivalent depth. An example of this conversion is summarised in Table 4.1. Because rainfall was assumed to be uniformly distributed in space, this weighted distribution procedure was used for irrigation water only, i.e. a rainfall event of, for example 10 mm, was assumed to fall evenly over the whole of the cultivated area.

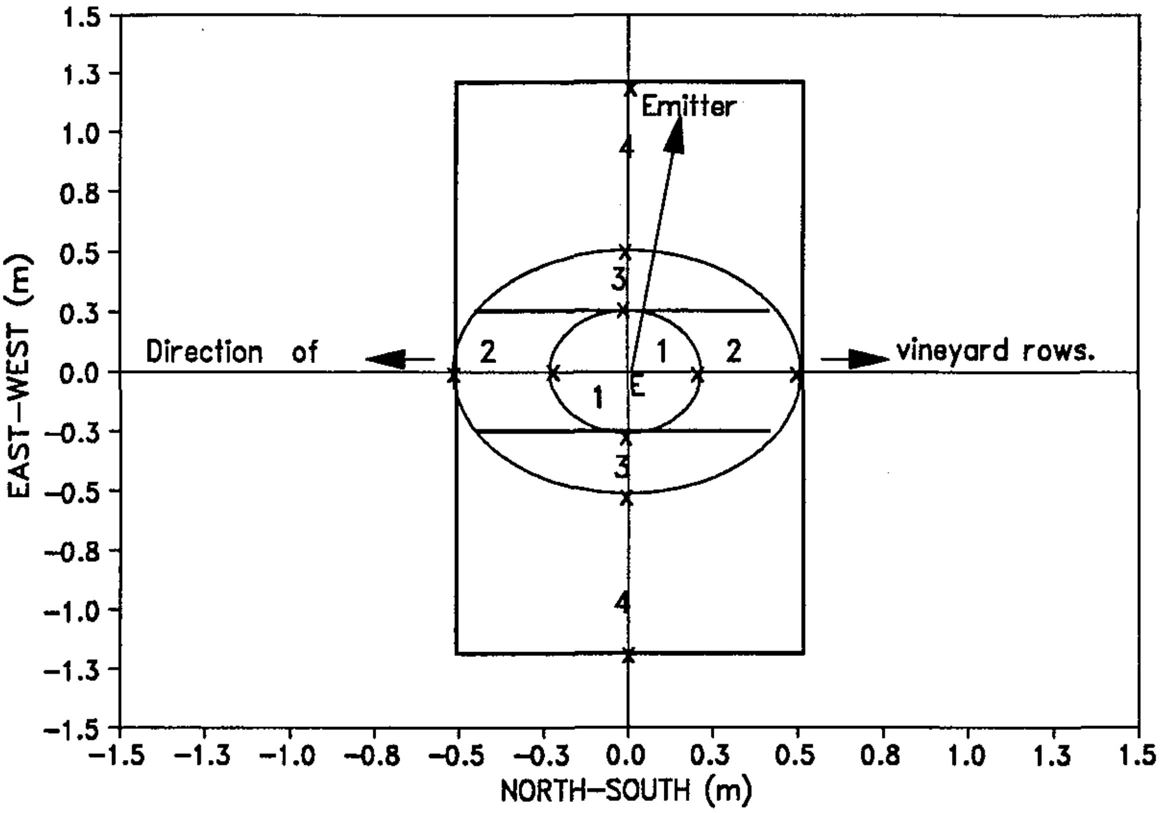


Figure 4.2 Schematic diagram of the division of the 2,5 m² area around each emitter into four sectors -- indicated as 1, 2, 3 and 4

Table 4.1 Conversion of irrigation volumes to equivalent depths at four different distances and directions from an emitter

	Sector 1	Sector 2	Sector 3	Sector 4	Total
Direction	0°	0°	90°	90°	
Distance (m)	0,0-0,25	0,25-0,5	0,25-0,5	0,5-1,0	
LF	0,267	0,253	0,155	0,085	
Area per emitter(m^2)	0,196	0,304	0,50	1,500	2,50
Area per ha (m^2)	784	1216	2000	6000	100
00					
LF*(1/Area)	1,361	0,833	0,310	0,057	2,561
Weight factor	0,531	0,325	0,121	0,022	1,000

Depending on the actual area and weight factor assigned to each sector of the 2,5 m^2 total area, different equivalent depths were obtained. According to this procedure, 53,1 % of an irrigation application will wet the surface area that are situated within 0,25 m from the emitter, while only 2,2 % of the water reaches those areas that fall outside the vineyard row and are situated between 0,5 m and 1,25 m away from an emitter. An example of the different depths that were obtained for the series of irrigation events between cumulative day numbers 104 and 144 (relative to 1 May 1987), are given in Table 4.2. Also indicated is the cumulative total of irrigation and rain water applied from May 1987 to June 1989 at each of the four sectors.

The model was used to simulate each of the "macro" areas indicated in Figure 4.1, i.e. A1, A2, A3 and A4, and each "macro" site was divided into four different sectors each of which was studied (i.e. simulated) separately. At each of the four macrosites, an additional simulation, representing the rectangular 0,5 m x 0,25 m-area surrounding the emitter, was made. This latter area is the sum of sectors 1 and 2 (Figure 4.2). Consequently, it was planned to do the simulation of the 5000 m^2 vineyard with twenty different runs of LEACHM. As will be shown in a following section, these twenty simulation runs were done with the waterflow version of LEACHM only, i.e. LEACHW, while less than twenty were used to simulate the chemical processes.

4.2.2.2 Irrigation water: Chemical composition

The vineyard under consideration is irrigated with water from the Robertson canal. Although the chemical data of the Roberston canal, as determined on a weekly basis by the Department of Water Affairs, were available, it was thought better to sample the irrigation water on site and to use that data as input for LEACHM. The chemical composition of the irrigation water was therefore determined at a number of times throughout the study period. On a few occasions the farmer flushed the irrigation lines with phosphoric acid which lowered the pH of the water to approximately 3. However, on an overall time scale the effect of the volume of low pH-water on the chemical processes in the soil was considered to be unimportant. Even if its effect cannot (and probably should not) be ignored, LEACHM cannot deal with chemical processes associated with low pH waters. The summary statistics of the chemical composition of 32 water samples are listed in Table 4.3. As can be deduced from the figures in the table and considering the effect of the phosphoric acid on the statistics of the chemical composition of the water (i.e. to increase the variance), the temporal variation in the chemical composition was insignificant. Consequently, a mean chemical composition, which did not include the low pH samples, was used throughout as input for LEACHM. The input concentrations in mmol dm^{-3} are also given in Table 4.3.

4.2.2.3 Meteorological data and crop coefficients

Pan evaporation measurements, recorded on site, were used as the index of potential evapotranspiration. The conversion to actual evapotranspiration (AET) was accomplished by using a set of crop factors supplied by V.O.R.I.* for use in the drip irrigated vineyards of the Breede River Valley. The crop factors are:
October 0,27; November 0,37; December and January 0,42; February 0,46; March 0,44; April to September 0,20.

Although these crop factors are applicable to drip irrigated surfaces, they in actual fact were adjusted by V.O.R.I. to represent full surface wetting. Consequently, the calculated full surface AET figures (i.e. AET = crop factor x pan evaporation), were adjusted to represent a weighted AET for each of the four sectors within the 2,5 m^2 around an emitter (Figure 4.2). The weights that were used are the same as those employed to convert the volume of irrigation water to depth units per sector (see section 4.2.2.1). It discretisizes AET according to the wetted surface area but conserves the mass balance of a full surface evapotranspiration. This weighing was applied to the evapotranspiration data of the active growing season only, i.e. September to March. An excerpt of the complete data set per wetted sector is listed in Table 4.4.

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* Viticultural and Oenological Research Institute, Stellenbosch

Table 4.2 Irrigation applications and rainfall amounts between day number 104 and 144 at the four empirically chosen sectors around an emitter (See also Table 2.1)

Day	Total per ha Irrig (m^3)	Rain (mm)	Depth of water (mm) applied to sectors: 1 (mm)	2 (mm)	3 (mm)	4 (mm)	Irrigation mass balance (m^3 ha^{-1})
104	0,0	14,0	14,00	14,00	14,00	14,00	0,0
114	0,0	2,5	2,50	2,50	2,50	2,50	0,0
115	0,0	4,5	4,50	4,50	4,50	4,50	0,0
123	0,0	7,5	7,50	7,50	7,50	7,50	0,0
124	0,0	5,0	5,00	5,00	5,00	5,00	0,0
126	0,0	9,0	9,00	9,00	9,00	9,00	0,0
127	29,5	0,0	20,02	7,91	1,79	0,11	29,5
128	25,8	0,0	17,48	6,90	1,56	0,10	25,8
129	4,4	0,0	2,99	1,18	0,27	0,02	4,4
130	13,9	0,0	9,40	3,71	0,84	0,05	13,9
131	72,8	0,0	49,36	19,49	4,41	0,27	72,8
132	1,6	0,0	1,05	0,42	0,09	0,01	1,6
135	0,0	3,0	3,00	3,00	3,00	3,00	0,0
137	0,0	10,0	10,00	10,00	10,00	10,00	0,0
138	74,3	2,0	50,33	19,87	4,49	0,27	74,3
142	0,0	1,0	1,00	1,00	1,00	1,00	0,0
144	67,6	2,0	45,85	18,10	4,09	0,25	67,6
Total 1987-1989			6862,9	2950,9	975,3	433,0	9539,1

Table 4.3 Summary statistics of the chemical composition of the water used to irrigate the vineyard

	Mean (n=32)	SD	Max	Min	LEACHM ($mmol\ dm^{-3}$)
pH	6,21	0,99	7,33	3,10	
Ca ($mg\ dm^{-3}$)	7,7	3,4	18,0	4,0	0,503
Mg ($mg\ dm^{-3}$)	7,6	2,7	14,9	4,1	0,313
K ($mg\ dm^{-3}$)	2,9	6,5	36,0	0,5	0,074
Na ($mg\ dm^{-3}$)	31,5	9,2	54,0	19,0	1,370
HCO_3 ($mg\ dm^{-3}$)	23,1	15,7	48,8	0,0	0,379
Cl ($mg\ dm^{-3}$)	62,9	16,8	103,8	34,6	1,771
SO_4 ($mg\ dm^{-3}$)	44,4	17,3	57,6	0,0	0,463
EC ($mS\ m^{-1}$)	34,5	21,3	122,6	19,9	
TDS ($mg\ dm^{-3}$)	224,6	52,9	291,7	70,9	

Table 4.4 An example of the area-weighted weekly, and total evapotranspiration data used in LEACHM

Sector*	----->	1	2	3	4	Per ha
Area (m^2)	----->	784	1216	2000	6000	10000
Weight	----->	0,531	0,325	0,121	0,022	1
	PET mm	AET mm	AET mm	AET mm	AET mm	AET mm
Week						
1	19,4	3,9	3,9	3,9	3,9	3,9
2	19,4	3,9	3,9	3,9	3,9	3,9
3	19,4	3,9	3,9	3,9	3,9	3,9
4	19,4	3,9	3,9	3,9	3,9	3,9
5	18,7	3,7	3,7	3,7	3,7	3,7
6	18,2	3,6	3,6	3,6	3,6	3,6
7	18,2	3,6	3,6	3,6	3,6	3,6
8	18,2	3,6	3,6	3,6	3,6	3,6
9	19,7	3,9	3,9	3,9	3,9	3,9
10	23,5	4,7	4,7	4,7	4,7	4,7
20	36,1	49,0	19,3	4,4	0,3	7,2
21	32,0	43,4	17,1	3,9	0,2	6,4
22	35,6	48,3	19,1	4,3	0,3	7,1
23	31,5	57,6	22,8	5,1	0,3	8,5
24	42,5	77,8	30,7	6,9	0,4	11,5
25	50,0	91,5	36,1	8,2	0,5	13,5
26	55,0	100,6	39,7	9,0	0,5	14,9
27	60,5	110,7	43,7	9,9	0,6	16,3
28	56,5	141,7	56,0	12,7	0,8	20,9
29	66,5	166,8	65,9	14,9	0,9	24,6
30	70,0	175,5	69,3	15,7	1,0	25,9
Totals (mm) 1 May 1987 - 30 June 1989						
	4382	8073	3348	962	308	1417

* See Figure 4.2 for identification of different sectors; Week 1-10 = winter, 20-30 = summer

4.2.2.4 Soil water retention properties and hydraulic conductivity

As was mentioned in earlier chapters, LEACHM uses the soil water retention (*h*-Θ) and hydraulic conductivity (*K*-Θ) relationships of Campbell (1974) to estimate the unsaturated hydraulic conductivity and matric potential as a function of water content. The sensitivity analysis of LEACHM (Chapter 3) indicated that the Campbell *a* and *b* coefficients (i.e. airentry potential and slope of the soil water characteristic curve) have a relatively small effect on the flux of water and salt through the soil. In the present study the airentry potentials were not measured. However, it was possible to obtain estimates of the airentry potential and the *b* coefficient using either the laboratory- or field measured soil water characteristic curves. It was also possible to use the method of Rawls & Brakensiek (1982) to infer the water characteristic from the available particle size data. If the shape of the soil water characteristic curve is known (from which the *b* coefficient is obtained), the method of Hutson and Cass (1987) can be used to estimate the value of the air entry potential. This method fits equation 2.1 to the water characteristic curve and determines the *a* and *b* values with a least squares technique. In the present study, the programme RETFIT (i.e. "retention fitting") was used to estimate *h* as a function of the particle size distribution using the Rawls and Brakensiek (1982) approach. Subsequent to this estimation, the *a* and *b* coefficients were calculated from the $h\text{-}\Theta/\Theta_s$ relationship.

The following values are typical of the different *a* and *b* values that were obtained by calculating the coefficients from:

i) the soil water characteristic curves determined in the laboratory using undisturbed soil cores;

ii) the soil water characteristic curves using tensiometer and neutron probe data determined *in situ*;

iii) particle size distribution data as described above.

Method	Sample	airentry *a* (kPa)	slope *b*
i	1	-1,00	7,33
ii	1	-0,04	10,94
iii	1	-2,20	5,93
i	2	-1,75	8,42
ii	2	-1,00 x 10^{-5}	23,30
iii	2	-1,70	5,97

It is clear that depending on the method that is used to calculate the *a* and *b* coefficients, vastly different values can be obtained. The coefficients calculated from the retention data of undisturbed soil cores and those calculated using *in situ* tensiometer and neutron probe data yielded coefficients that were highly suspect. In view of this, it was decided rather to infer the *a* and *b* values from the particle size distribution data.

LEACHM was run in the mode where it calculates the two coefficients from the particle size distribution data supplied as input. The clay and silt contents for the four different macrosites and depths and the calculated air entry potentials and slopes of the retention curves, are listed in Table 4.5.

Table 4.5 Campbell's *a* and *b* coefficients, saturated hydraulic conductivities, clay and silt percentages, bulk densities and organic matter contents for each depth layer of the different macrosites

Depth mm	*a* kPa	*b*	Ksat mm day^{-1}	Clay %	Silt %	Bulk Dens Mg m^{-3}	Org.Mat %
A1							
50	-2,20	5,93	110,0	20,0	42,5	1,527	0,71
250	-1,70	5,97	71,6	21,8	44,2	1,465	0,30
450	-2,50	6,20	70,8	21,8	44,2	1,624	0,10
550	-2,90	6,43	310,0	23,8	44,5	1,624	0,05
750	-2,20	6,32	310,0	23,8	44,5	1,554	0,00
1050	-2,70	6,42	105,0	23,5	44,1	1,626	0,00
1350	-2,20	6,08	500,0	21,0	44,6	1,626	0,00
1950	-2,10	6,00	500,0	20,3	44,4	1,626	0,00
A2							
50	-1,60	6,42	108,0	20,9	35,3	1,575	0,60
350	-2,50	6,71	50,9	20,0	35,6	1,787	0,20
450	-2,50	6,78	50,8	20,0	35,6	1,814	0,10
550	-1,60	7,38	45,0	21,1	29,6	1,814	0,05
750	-2,10	7,56	45,0	21,1	29,6	1,870	0,00
1050	-0,41	7,42	186,0	19,9	22,8	1,705	0,00
1350	-0,34	6,51	300,0	15,6	24,9	1,705	0,00
1650	-0,41	5,99	300,0	13,7	27,9	1,705	0,00
1950	-0,41	5,99	90,7	13,7	27,9	1,705	0,00

Table 4.5 (contd.)

Depth mm	*a* kPa	*b*	Ksat mm day^{-1}	Clay %	Silt %	Bulk Dens Mg m^{-3}	Org.Mat %
A3							
50	-2,00	5,96	203,0	19,2	39,6	1,529	0,92
250	-1,20	6,16	31,1	21,6	39,0	1,464	0,30
350	-1,20	6,15	34,9	21,6	39,0	1,464	0,20
450	-1,30	6,25	29,2	21,6	39,0	1,530	0,10
550	-0,93	6,45	210,0	21,6	35,0	1,530	0,05
750	-1,90	6,93	210,0	21,9	35,0	1,742	0,00
1050	-1,50	6,89	20,2	19,5	32,2	1,798	0,00
1350	-2,30	6,34	25,0	18,6	38,9	1,798	0,00
1650	-1,00	6,85	25,0	18,3	30,0	1,798	0,00
1950	-1,00	6,85	1,5	18,3	30,0	1,798	0,00
A4							
50	-1,20	5,53	102,0	16,4	38,7	1,441	0,85
250	-1,80	5,80	42,2	17,8	42,0	1,627	0,30
350	-1,70	5,79	44,6	17,8	42,0	1,627	0,20
450	-1,10	5,60	78,6	17,8	42,0	1,495	0,10
750	-1,20	5,68	550,0	18,2	42,4	1,532	0,00
1050	-1,30	5,99	93,9	20,4	41,6	1,529	0,00
1650	-1,80	6,39	201,0	24,1	42,8	1,529	0,00
1950	-1,80	6,39	1,5	24,1	42,8	1,529	0,00

The reference hydraulic conductivities (assumed to represent field scale saturated hydraulic conductivity) of the different depth layers were determined at eight different sites (two each per macrosite) within the 5000 m^2 area, using the instantaneous profile method (Hillel, 1980). An arithmetic mean value (per depth) for each macrosite was calculated and used as the reference hydraulic conductivity in LEACHM. These values for the various depths and locations are also listed in Table 4.5. The bulk density of each depth layer was determined *in situ* using the standard soil core method (Blake & Hartge, 1986).

4.2.2.5 Soluble salt content

During May 1987, the soil that was excavated while installing the 30 neutron access tubes (Figure 4.1), were analysed. The soluble salt content and chemical composition of a 40 % water saturated extract were determined using standard analytical techniques. The chloride and bicarbonate concentrations were determined from colorometric titrations while sulphate was determined using gravimetric techniques. The cations Ca, Mg, Na and K were determined with an atomic absorption spectrophotometer. Two arithmetic mean values for each macrosite were calculated. The one value represented the soluble salt composition of the soil volume within 0,5 m of an emitter (sectors 1, 2 and 3 of Figure 4.2), while the second value represented the conditions between two vineyards rows, i.e. at a distance approximately 1,25 m from the emitters (sector 4, Figure 4.2). The chemical composition of the water saturated extracts are listed in Table 4.6. It is clear that the soil between two vineyard rows are much more saline than the soil situated closer to the emitter. The chemical compositions of the saturated extracts given in Table 4.6 were adjusted to the field water contents that were used as input and the new chemical equilibria (at the lower water contents) calculated using the CHEMEQ utility program of LEACHM. The adjusted chemical concentrations are given in Table 4.7. It is these values that were finally used as input for LEACHM.

LEACHM also requires as input the lime and gypsum content of the soil. Only trace amounts of free lime were present in the soil at the onset of the simulation period (May 1987). Gypsum as a mineral (i.e. in its natural state) also do not occur freely in the soil. However, phospho-gypsum is regularly applied as an soil ameliorant to the soil of the Breede River Valley. Therefore, the gypsum content can fluctuate substantially between years. The gypsum and lime contents that were initially used as input are summarised in Table 4.8. With the exception of the different depths, the same lime and gypsum contents were used for all of the wetted sectors and macrosites.

Table 4.6 Mean soluble salt composition used as input for each macrosite and emitter sector (4 samples per mean): concentrations of a 40% saturated extract

Depth	EC	pH	Ca	Mg	Na	K	HCO_3	Cl	SO_4
m	mS m^{-1}		<--------	--------	mmol(+) dm^{-3}§	--------	--------	--------	-------->
A1 (sectors 1,2 & 3)									
0,15	347	7,56	20,61	8,21	12,71	1,83	4,18	8,34	30,85
0,45	493	7,65	16,48	13,47	21,07	0,21	1,80	14,94	34,49
0,75	476	7,48	7,96	10,98	32,02	0,07	1,20	18,00	31,83
1,05	478	7,45	11,34	11,72	31,86	0,05	0,95	15,66	38,36
1,35	462	7,39	8,77	10,77	31,92	0,03	0,73	16,20	34,57
1,50	448	7,65	8,69	10,41	30,30	0,04	1,20	15,00	33,24
A1 (sector 4)									
0,15	1596	7,72	48,71	43,44	68,11	0,66	1,25	104,01	55,67
0,45	1253	7,72	33,81	34,42	59,42	0,29	1,25	80,40	46,29
0,75	848	7,71	17,17	19,76	61,79	0,11	1,35	46,50	50,98
1,05	863	7,55	20,93	22,60	59,61	0,06	1,40	45,30	56,49
1,35	783	7,28	9,84	17,92	55,31	0,04	0,53	51,30	31,28
1,50	744	7,44	8,27	17,94	48,67	0,04	0,83	49,68	24,41
A2 (sectors 1,2 & 3)									
0,15	253	7,76	15,46	5,84	6,56	0,30	3,23	5,46	19,47
0,45	233	7,97	6,01	5,22	10,17	0,11	2,08	7,80	11,64
0,75	240	8,09	2,42	2,97	14,33	0,05	2,08	7,62	10,08
1,05	235	7,97	2,34	3,15	13,96	0,05	1,90	6,18	11,41
1,35	197	7,92	2,36	1,47	12,69	0,03	1,05	6,06	9,43
1,50	256	8,06	2,73	3,27	15,90	0,04	1,48	6,72	13,74
A2 (sector 4)									
0,15	730	7,90	18,18	14,75	43,86	0,47	1,75	27,60	47,89
0,45	639	7,97	9,19	10,76	43,89	0,17	1,65	34,62	27,74
0,75	531	8,01	4,86	7,39	39,79	0,08	1,75	31,98	18,38
1,05	509	7,96	4,45	7,03	36,46	0,06	1,65	28,68	17,67
1,35	476	7,83	4,80	6,84	31,81	0,05	1,08	26,52	15,90
1,50	423	7,98	4,47	6,25	29,57	0,04	1,23	24,36	14,74

§ mmol(+) dm^{-3} = meq dm^{-3}

Table 4.6 (contd.)

Depth	EC	pH	Ca	Mg	Na	K	HCO_3	Cl	SO_4
m	mS m^{-1}		<-----			mmol(+) dm^{-3}§			----->
A3 (sectors 1,2 & 3)									
0,15	320	7,65	19,28	6,76	7,17	0,64	4,63	5,46	23,75
0,45	487	7,57	16,46	16,61	20,13	0,23	3,65	18,48	31,30
0,75	487	7,58	11,44	12,59	24,29	0,22	2,58	18,48	27,48
1,05	503	7,35	6,60	10,37	31,33	0,20	3,08	25,50	19,92
1,35	618	6,95	9,08	16,62	40,31	0,14	1,30	27,44	37,42
1,50	653	7,34	10,63	17,25	39,59	0,18	3,75	33,84	30,06
A3 (sector 4)									
0,15	1515	7,70	45,16	39,16	112,18	0,70	2,65	99,30	95,24
0,45	903	7,74	18,08	20,64	57,30	0,35	2,58	50,10	43,68
0,75	840	7,38	12,91	21,07	55,50	0,24	2,18	46,20	41,35
1,05	699	6,87	8,73	17,34	45,52	0,15	0,95	35,10	35,68
1,35	570	6,58	7,02	13,70	37,09	0,14	0,47	28,80	28,67
1,50	727	7,01	12,18	17,32	43,44	0,28	1,77	34,00	37,46
A4 (sectors 1,2 & 3)									
0,15	521	7,50	39,88	10,08	9,04	0,65	4,80	8,52	46,32
0,45	414	7,81	17,43	12,76	11,02	0,27	2,73	8,40	30,36
0,75	488	7,92	10,68	13,23	24,94	0,26	2,50	13,08	33,52
1,05	554	7,77	9,40	9,43	35,15	0,16	2,50	21,42	30,22
1,35	547	7,33	6,56	8,98	35,81	0,10	1,88	24,78	24,80
1,50	661	6,17	8,73	12,86	40,00	0,13	1,10	31,60	29,02
A4 (sector 4)									
0,15	1309	7,86	39,05	25,55	82,91	0,49	2,23	68,40	77,38
0,45	924	7,84	17,56	16,80	55,08	0,39	2,80	54,90	32,14
0,75	688	7,95	10,28	10,92	42,78	0,35	2,78	36,84	24,71
1,05	769	7,72	13,45	12,60	48,11	0,18	2,35	42,30	29,69
1,35	669	7,32	8,90	8,85	42,56	0,10	1,23	35,10	24,09
1,50	573	7,10	8,40	6,01	31,04	0,12	2,60	21,60	21,38

§ mmol(+) dm^{-3} = meq dm^{-3}

Table 4.7 Mean soluble salt composition used as input for each macrosite and emitter sector (4 samples per mean): concentrations at field water content

Depth	Ca	Mg	Na	K	HCO_3	Cl	SO_4
m		<----------------------	--mmol dm^{-3}	----------------------	---------->		
A1 (sectors 1,2 & 3)							
0,15	35,75	14,24	44,11	6,37	14,49	28,94	53,52
0,45	28,60	23,37	73,09	0,73	6,25	51,84	59,84
0,75	13,81	19,04	111,12	0,26	4,16	62,46	55,23
1,05	19,68	20,33	110,54	0,18	3,30	54,34	66,55
1,35	15,22	18,68	110,77	0,11	2,52	56,21	59,97
1,50	15,07	18,06	105,12	0,15	4,16	52,05	57,66
A1 (sector 4)							
0,15	84,51	75,37	236,33	2,29	4,34	360,89	96,58
0,45	58,66	59,72	206,18	1,00	4,34	278,98	80,31
0,75	29,79	34,28	214,42	0,40	4,68	161,35	88,45
1,05	36,30	39,20	206,83	0,21	4,86	157,19	98,01
1,35	17,07	31,10	191,91	0,13	1,82	178,01	54,27
1,50	14,35	31,12	168,86	0,14	2,86	172,39	42,35
A2 (sectors 1,2 & 3)							
0,15	26,83	10,13	22,75	1,04	11,19	18,95	33,78
0,45	10,43	9,06	35,30	0,37	7,20	27,07	20,19
0,75	4,20	5,16	49,71	0,18	7,20	26,44	17,48
1,05	4,06	5,46	48,43	0,16	6,59	21,44	19,80
1,35	4,09	2,54	44,02	0,12	3,64	21,03	16,37
1,50	4,73	5,67	55,17	0,13	5,12	23,32	23,84
A2 (sector 4)							
0,15	31,53	25,58	152,18	1,62	6,07	95,77	83,10
0,45	15,94	18,66	152,30	0,60	5,73	120,13	48,13
0,75	8,43	12,81	138,06	0,27	6,07	110,97	31,89
1,05	7,71	12,20	126,50	0,22	5,73	99,52	30,65
1,35	8,33	11,86	110,36	0,18	3,73	92,02	27,58
1,50	7,76	10,84	102,59	0,15	4,25	84,53	25,58

Table 4.7 (contd.)

Depth m	Ca	Mg	Na	K	HCO_3	Cl	SO_4
		<-------------------	mmol dm^{-3}	------------------>			
A3 (sectors 1,2 & 3)							
0,15	33,44	11,72	24,86	2,22	16,05	18,95	41,21
0,45	28,56	28,82	69,85	0,80	12,67	64,12	54,31
0,75	12,88	22,39	107,95	0,68	6,85	82,86	44,73
1,05	11,45	17,99	108,70	0,68	10,67	88,48	34,56
1,35	15,76	28,84	139,86	0,50	4,51	95,22	64,92
1,50	18,43	29,92	137,37	0,64	13,01	117,42	52,15
A3 (sector 4)							
0,15	87,64	68,37	382,34	2,55	8,85	325,83	181,12
0,45	31,36	35,80	198,81	1,21	8,94	173,84	75,78
0,75	22,40	36,56	192,58	0,83	7,55	160,31	71,74
1,05	15,14	30,08	157,96	0,51	3,30	121,79	61,90
1,35	12,17	23,77	128,69	0,48	1,62	99,93	49,75
1,50	16,37	27,10	132,31	0,63	7,75	102,71	54,71
A4 (sectors 1,2 & 3)							
0,15	69,18	17,49	31,35	2,24	16,66	29,56	80,36
0,45	30,23	22,14	38,25	0,95	9,46	29,15	52,67
0,75	18,52	22,96	86,52	0,91	8,67	45,39	58,16
1,05	16,31	16,35	121,98	0,56	8,67	74,33	52,43
1,35	11,39	15,58	124,25	0,35	6,51	85,99	43,02
1,50	15,15	22,30	138,80	0,46	3,82	109,65	50,35
A4 (sector 4)							
0,15	67,75	44,33	287,70	1,71	7,72	237,34	134,25
0,45	30,47	29,15	191,12	1,36	9,72	190,50	55,75
0,75	17,83	18,94	148,45	1,21	9,63	127,83	42,87
1,05	23,34	21,86	166,94	0,63	8,15	146,78	51,51
1,35	15,44	15,35	147,67	0,36	4,25	121,79	41,79
1,50	14,57	10,44	107,71	0,43	9,02	74,95	37,09

Table 4.8 Lime and gypsum contents used as input to represent the conditions at the start of the simulation period

Depth m	Lime[a]	Lime[b]	Gypsum
	<--------------------	fraction	-------------------->
0,05	0,001	0,011	0,007
0,45	0,001	0,011	0,003
0,75	0,001	0,011	0,001
1,05	0,001	0,011	0,007
1,95	0,001	0,011	0,001

a=content initially used; b=adjusted content to prevent negative Ca concentrations (see later).

4.2.2.6 Exchangeable cation composition and selectivity coefficients

The exchangeable cation composition was determined using the same samples referred to in section 4.2.2.5 (soluble salt content) above. These samples were collected in May 1987, and were used to represent soil conditions at the start of the simulation period. The standard ammonium acetate method was used to obtain the extractable cations which was subsequently corrected for the soluble cations to yield the exchangeable composition. It should be mentioned that, because of the presence of phosphogypsum and traces of free lime in the soil, the exchangeable calcium content had to be determined by subtracting the sum of the sodium, magnesium and potassium concentrations from the cation exchange capacity (CEC). The latter was determined with the ammonium acetate and potassium sulfate procedure at pH 7. The mean values for the different exchangeable cations and associated CEC values are given in Table 4.9.

The six different pairs of cation selectivity coefficients for the quaternary exchange processes between Ca, Mg, Na and K were calculated using the soluble and exchangeable cation compositions referred to above, and by assuming that the respective concentrations reflect equilibrium conditions. The calculation was performed on all 180 samples (i.e. 30 sites and six depths each) using the CHEMEQ utility program. In the absence of any discernable microspatial or depth trends within each of the four macrosites (A1, A2 A3 and A4), the results were, for the sake of simplicity reduced to six mean values for each of the four macrosite positions. The mean and standard deviation of the six pairs of coefficients are listed in Table 4.10. A considerable variation around each mean was found. However, the results of the sensitivity study indicate that the effect of the selectivity coefficient on the calculated salt and water fluxes are minimal. Therefore, only the mean values were used.

Table 4.9 Mean cation exchange capacity and exchangeable cation composition of May 1987 per macrosite and emitter sector

Depth	CEC	Ca	Mg	Na	K
m	<---	---	mmol(+) kg^{-1}	---	--->
A1 (sectors 1,2 & 3)					
0,15	104,5	65,1	29,3	1,5	8,6
0,45	94,7	40,1	41,1	10,2	3,2
0,75	115,9	42,3	56,4	15,6	1,6
1,05	104,2	38,5	49,4	15,0	1,2
1,35	92,0	25,8	48,7	16,4	1,1
1,50	92,1	32,7	45,4	13,2	0,8
A1 (sector 4)					
0,15	96,9	41,9	42,4	8,2	4,3
0,45	100,7	31,6	50,1	16,1	2,9
0,75	113,3	38,8	53,7	18,8	2,0
1,05	97,2	27,3	51,9	16,9	1,1
1,35	92,9	23,6	49,7	18,9	0,6
1,50	84,7	18,5	47,2	18,3	0,7
A2 (sectors 1,2 & 3)					
0,15	89,2	50,2	32,6	2,5	3,9
0,45	92,5	38,8	46,7	4,8	2,2
0,75	86,7	27,4	45,9	12,2	1,2
1,05	71,3	20,7	39,3	10,3	1,1
1,35	70,0	18,4	38,1	12,7	0,8
1,50	59,0	15,5	32,3	10,5	0,7
A2 (sector 4)					
0,15	82,4	28,6	39,9	9,9	3,9
0,45	87,3	22,4	46,6	15,9	2,4
0,75	77,6	14,5	44,9	16,7	1,5
1,05	79,4	20,9	41,2	16,2	1,2
1,35	61,0	11,8	34,7	13,6	0,8
1,50	60,7	15,3	32,4	12,3	0,6

Table 4.9 (contd.)

Depth	CEC	Ca	Mg	Na	K
m	<---------------------	mmol(+) kg^{-1}			----------------------->
A3 (sectors 1,2 & 3)					
0,15	98,4	59,2	30,6	3,4	5,2
0,45	98,4	33,7	53,7	8,2	2,8
0,75	91,4	27,5	50,5	11,0	2,4
1,05	85,1	21,6	46,7	14,7	2,0
1,35	82,0	23,0	44,2	13,4	1,4
1,50	54,0	10,2	31,8	10,8	1,1
A3 (sector 4)					
0,15	91,8	32,7	42,2	13,6	3,3
0,45	93,4	15,1	55,1	19,6	3,5
0,75	97,0	16,0	58,1	20,3	2,5
1,05	87,3	24,7	45,3	16,0	1,4
1,35	60,2	14,3	34,3	10,6	1,0
1,50	62,8	12,0	36,1	12,6	2,0
A4 (sectors 1,2 & 3)					
0,15	85,1	50,8	27,9	2,9	3,5
0,45	85,2	26,2	51,3	4,8	2,9
0,75	84,6	13,2	58,6	10,0	2,8
1,05	96,8	23,2	55,0	16,5	2,1
1,35	98,0	27,4	52,1	17,1	1,4
1,50	88,0	43,9	36,5	6,4	1,2
A4 (sector 4)					
0,15	79,1	11,5	47,1	17,2	3,4
0,45	88,7	9,9	59,7	15,5	3,6
0,75	84,4	5,1	60,1	16,0	3,1
1,05	86,2	11,6	55,2	17,4	2,1
1,35	95,3	23,0	51,7	19,3	1,3
1,50	87,5	26,5	49,8	10,1	1,2

Table 4.10 Mean Gapon type cation selectivity coefficients for each of the four macrosites

Coefficient	A1		A2		A3		A4	
	Mean	SD	Mean	SD	Mean	SD	Mean	SD
Mg/Ca	1,46	0,87	1,89	0,95	3,02	5,95	5,81	6,72
Ca/Na	6,19	7,11	3,05	1,88	3,39	2,66	2,93	4,13
Ca/K	0,09	0,08	0,08	0,03	0,11	0,07	0,09	0,08
Mg/K	0,10	0,04	0,13	0,03	0,16	0,05	0,20	0,06
Mg/Na	6,55	5,63	4,71	1,78	4,83	1,75	5,84	1,62
K/Na	63,75	31,42	37,02	12,94	31,18	12,80	33,10	20,91

SD = standard deviation

4.2.2.7 Crop information

Because vines are perennial crops, only one crop with a fixed rooting pattern was simulated. The respective important phenological dates for the 1987/88 and 1988/89 growing seasons, as required by LEACHM, are listed in Table 4.11.

Table 4.11 Dates (as YYMMDD) for different phenological growth stages of vines and other crop information

	Year 87/88	Year 88/89
Planting	870901	880901
Emergence	870901	880901
Root maturity	871215	881215
Plant maturity	871130	881130
Harvest	870228	880228
Crop cover	0,7	0,7
Plant per m^2	0,4	0,4

4.2.3 Data available for model validation

The whole purpose of instrumenting and monitoring the soil water content and soil chemistry of the study area was to assemble a set of data that can be used to evaluate the results of any modelling study. The matric potential of the soil at one site (close to A4, Figure 4.1) was monitored every two hours using datalogging tensiometers. At another two sites tensiometric readings were obtained on a daily basis. Throughout the period May 1987 to June 1989 *ad hoc* surveys of the soil water content at 30 sites were also made using the neutron moderation technique. During November of 1988 and 1989 more detailed surveys of the soil water content were made at sites A2 and A4. This was an attempt to determine the water balance and leaching fraction at various distances from the emitter.

Five sets of soil water cup samplers were also installed. Each set consisted of samplers at the following five depths: 0,15 m, 0,30 m, 0,60 m, 0,90 m and 1,20 m. The purpose was to establish a data base of the soluble salt content of this vineyard on a continuous temporal scale by collecting *in situ* samples every two weeks. However, for a number of different reasons, mostly caused by leakages and dry soil conditions, very few samples could be collected. Therefore, the original idea of a complete record of the temporal and spatial changes in the chemistry of the soil solution, could not be realized. Nevertheless, it was possible to collect samples at thirty different occasions between May 1987 and June 1989. Unfortunately, it was seldom possible to gather information at each site and depth. The result is therefore, that, although some knowledge on the spatial and temporal changes in the soluble salt content are available, it might not be good enough for a complete and thorough validation of model predictions.

In August 1988 and June 1989 soil samples were collected in the near vicinity of the soil water monitoring sites (i.e. the neutron access tubes) at sites A1, A2, A3 and A4 (Figure 4.1). The samples of August 1988 were analysed for the soluble salt content only while those of June 1989 were analysed in full (i.e. soluble and exchangeable salts determined). These results, especially those of June 1989, provided another measure for the validation and evaluation of transport model predictions. However, as will be shown in the following sections, numerical instabilities caused LEACHC (which is the chemistry version of LEACHM), to consistently abort after approximately 300 days of irrigation had been simulated. The length of the modelling run could be increased beyond 300 days by altering some of the chemical input (see following sections), but even then it was possible to simulate the whole study period (May 1987 to June 1989) with four of the twenty runs only. Because they fell outside the time period for which predictions could be made, the observed data of August 1988 and June 1989 were of very little value to validate the predicted trends in chemical composition of the study area.

On the few occasions that it was possible to compare the predicted results with observed data, use was made of visual techniques (graphical interpretation), linear regression analysis and Wilmot's coefficient of agreement (see chapter 2, section 2.4.1).

4.3 RESULTS

4.3.1 General

From the first attempt in 1987 to apply the chemistry version of LEACHM, i.e. LEACHC, to the soil and water conditions found in the drip irrigated vineyard, numerical problems were encountered. These problems were restricted to LEACHC only because the waterflow version, LEACHW, could be used successfully throughout this study. It should also be mentioned that in a separate study, Fuller (1989) successfully used the nitrogen version of LEACHM, i.e. LEACHN, to simulate the movement of nitrogen in irrigated orchards. It therefore seems as if the numerical instabilities of LEACHM occurs within LEACHC only, and specifically in the CHEM- or XCHANGE subroutines. Furthermore, the abortion of the model were always triggered when the square root of a negative number, or division by zero were attempted. However, it was impossible to know beforehand when such a condition would crop up.

During the course of this study, several unsuccessful attempts were made to rectify the problem. The fact that the actual computer processing time up to the point where the program aborted, normally exceeded several hours (i.e. in excess of 200 to 300 days of simulation time) also hampered the debugging of the model. The authors of the model, Prof R.J. Wagenet and Dr J.H. Hutson of Cornell University, U.S.A. were notified of these and other problems during 1988. Although they were normally successful in rectifying a particular problem, it invariably happened that such a "debugged" version of LEACHC, just by using a slightly different set of input data, also aborted.

Version 2 of LEACHM, which was released during the second half of 1989, also did not solve all the numerical instabilities of LEACHC. In the course of time it became apparent that, whereas the first problems were associated with either a very high soil salinity and associated ionic activities, or with low TDS irrigation waters, the problems of version 2 invariably were linked to the chemistry of calcium. More than often the model predicted that calcium will decrease to the point where it becomes zero or negative. Again the authors (Wagenet and Hutson) debugged the model and the latest "corrected" version was received in November 1990. This is the version which was finally used in the study of microscale soil processes in the drip irrigated vineyard.

Even with the latest version of the model, LEACHC unexpectedly aborted at different simulation times and conditions. By trial and error it was established that increasing the lime content of the soil (expressed as a mass fraction), the number of days that could be simulated increased to a minimum of 300 (see also Table 4.8). For some of the macrosites and emitter sectors the whole period of 792 days between 1 May 1987 and 30 June 1989 could be studied. The maximum number of days that could be simulated for the different sectors (or wetted areas around an emitter) for each of the macrosites, are summarised in Table 4.12. From the contents of the table it should be clear that it was difficult to predict when and why LEACHC would abort. Finally after more than three years of unsuccessful attempts, it was decided that it was not worthwhile to continue with the trial and error process of debugging LEACHC. As a consequence, no attempt was made to simulate the chemical processes in sector 3 of the different macrosites. Some of the results, up to the point where the computer program aborted, will be discussed in section 4.3.2 of this chapter.

Table 4.12 Maximum number of days that could be simulated with the chemistry version of LEACHM for each wetted sector and macrosite

Site	Emitter sector (wetted zone)			
	1	2	4	5§
A1	792	792	329	792
A2	575	792	534	792
A3	516	508	308	486
A4	528	640		574

§ (sector 5 = 1+2 combined)

4.3.2 Soil water content

4.3.2.1 Linear regression statistics of the predicted and observed soil water content at selected sites and depths

The 1:1-relation between the predicted and measured soil water contents of three selected depths within the wetted zone 0,25 m from an emitter (i.e. sector 1) at site A2 are presented in Figure 4.3. It is clear that although the predicted data vaguely resembles the observed values, a fair amount of scatter was present, especially at the 0,30 m depth. The approximate maximum deviation from the observed water contents were respectively 0,06, 0,02 and 0,02 $m^3\ m^{-3}$ for the 0,30 m, 0,60 m and 0,90 m depths. When sectors 1 and 2 were combined and treated as a single wetted area with a radius of 0,5 m from an emitter (as opposed to when sectors 1 and 2 were simulated separately as two different zones), the scatter increased substantially (Figure 4.4). For example, the soil water content at the 0,60 m depth was predicted to range between approximately 0,22 and 0,30 $m^3\ m^{-3}$, while the actual observed water contents fluctuated between 0,25 and 0,275 $m^3\ m^{-3}$ only. Similar observations were made at the other sites.

A full set of coefficients of determination (R^2) and the accompanying d-indices of Wilmot (1981) were calculated for all the wetted sectors of macrosite A2 only. These statistics and the R^2 values of the other macrosites are listed in Table 4.13.

The rather low R^2 values give the impression of an inadequate and poor prediction of soil water transport and content. Although the d-indices are appreciably higher than the associated R^2 values (see Table 4.13, site A2), even they do not justify any form of confidence in the performance of LEACHW. However, it should be remembered that the reason for the poor results might not be the model itself but rather the fact that a one-dimensional model was applied to a three dimensional case. Also, the way in which the volume of water applied at a point source is converted to equivalent depths, can play a major role in the simulation of soil water movement, storage and uptake by plants. Furthermore, the visual comparison (Figure 4.3) to a certain extent gives a slightly different impression of the adequacy of model predictions than the coefficients of determination. As will be shown in the next section, this statement is supported by the comparison of predicted and observed soil water contents on a temporal scale.

Table 4.13 Summary of the relationship between predicted and observed soil water contents in terms of the coefficients of determination (linear regression) and d-indices (Wilmot, 1981) for the different macrosites and wetted sectors in the drip irrigated vineyard (n=21)

		Macrosite				
		A1	A2	A2	A3	A4
Sector	Depth (m)	R^2	R^2	d-Index	R^2	R^2
1	0,3	0,175	0,051	0,489	0,215	0,047
1	0,6	0,070	0,008	0,227	0,002	0,000
1	0,9	0,104	0,074	0,306	0,047	0,038
1	Total	0,178	0,031	0,363		0,006
2	0,3	0,209	0,091	0,521	0,040	0,048
2	0,6	0,252	0,048	0,774	0,017	0,017
2	0,9	0,296	0,063	0,321	0,009	0,033
2	Total	0,290	0,060	0,405		0,022
3	0,3	0,003	0,142	0,440	0,039	0,106
3	0,6	0,039	0,064	0,262	0,015	0,011
3	0,9	0,008	0,015	0,376	0,002	0,003
3	Total	0,001	0,143	0,530		0,067
4	0,3	0,030	0,222	0,439	0,000	0,015
4	0,6	0,131	0,306	0,726	0,120	0,002
4	0,9	0,166	0,006	0,493	0,010	0,001
4	Total	0,035	0,258	0,596		0,010
Avg(1+2+3)	0,3		0,124	0,443		
	0,6		0,047	0,282		
	0,9		0,015	0,356		
	Total		0,117	0,527		
1+2	0,3	0,199	0,083	0,510	0,185	0,054
1+2	0,6	0,236	0,043	0,270	0,019	0,059
1+2	0,9	0,297	0,076	0,358	0,030	0,031
1+2	Total	0,277	0,054	0,398		0,040

Avg (1+2+3)=area weighted average of predicted water contents within sectors 1,2 and 3 compared with measured data; 1+2=sectors 1 and 2 simulated together as one area; Total=total profile water content 0-1,05 m.

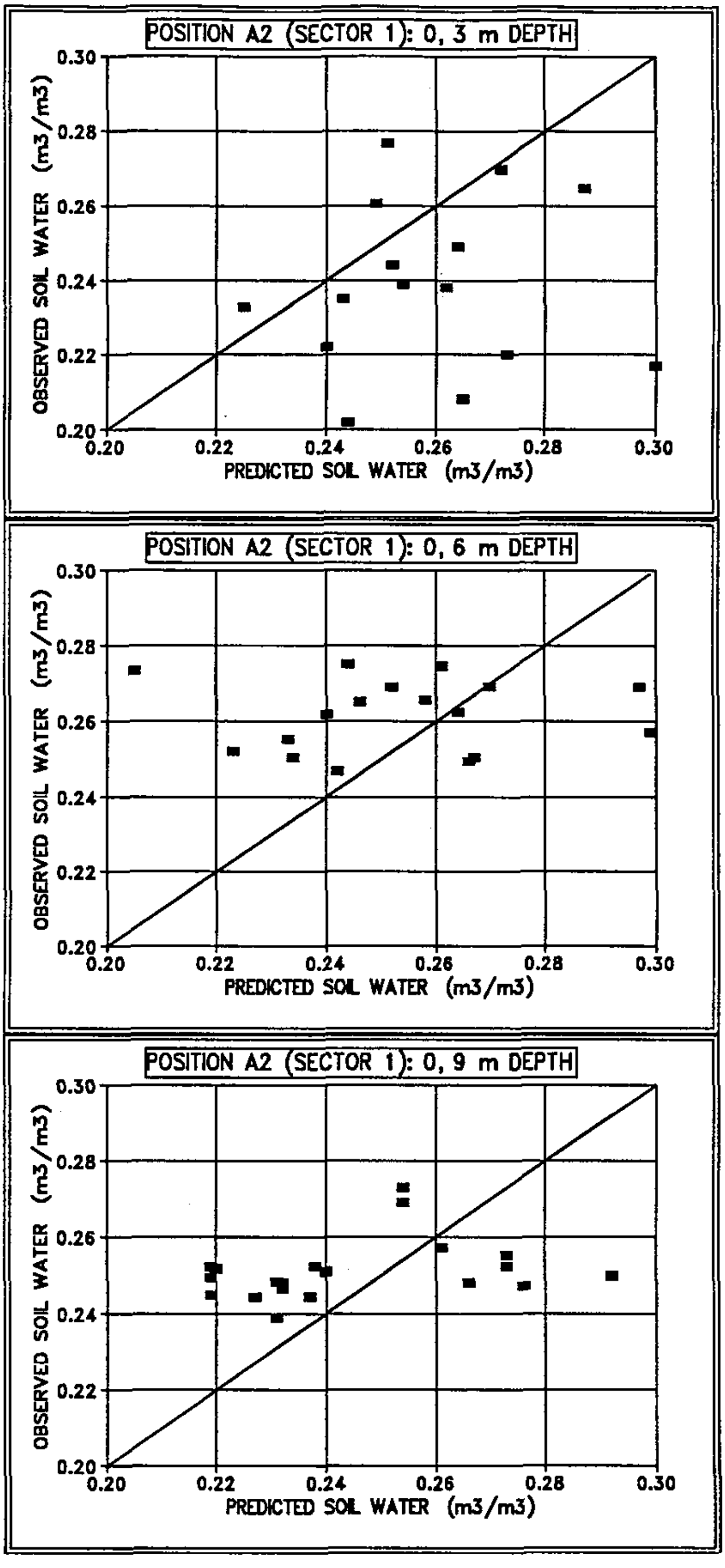


Figure 4.3 Comparison of predicted and observed soil water content at the 0,30, 0,60 and 0,90 m depths in sector 1 of site A2.

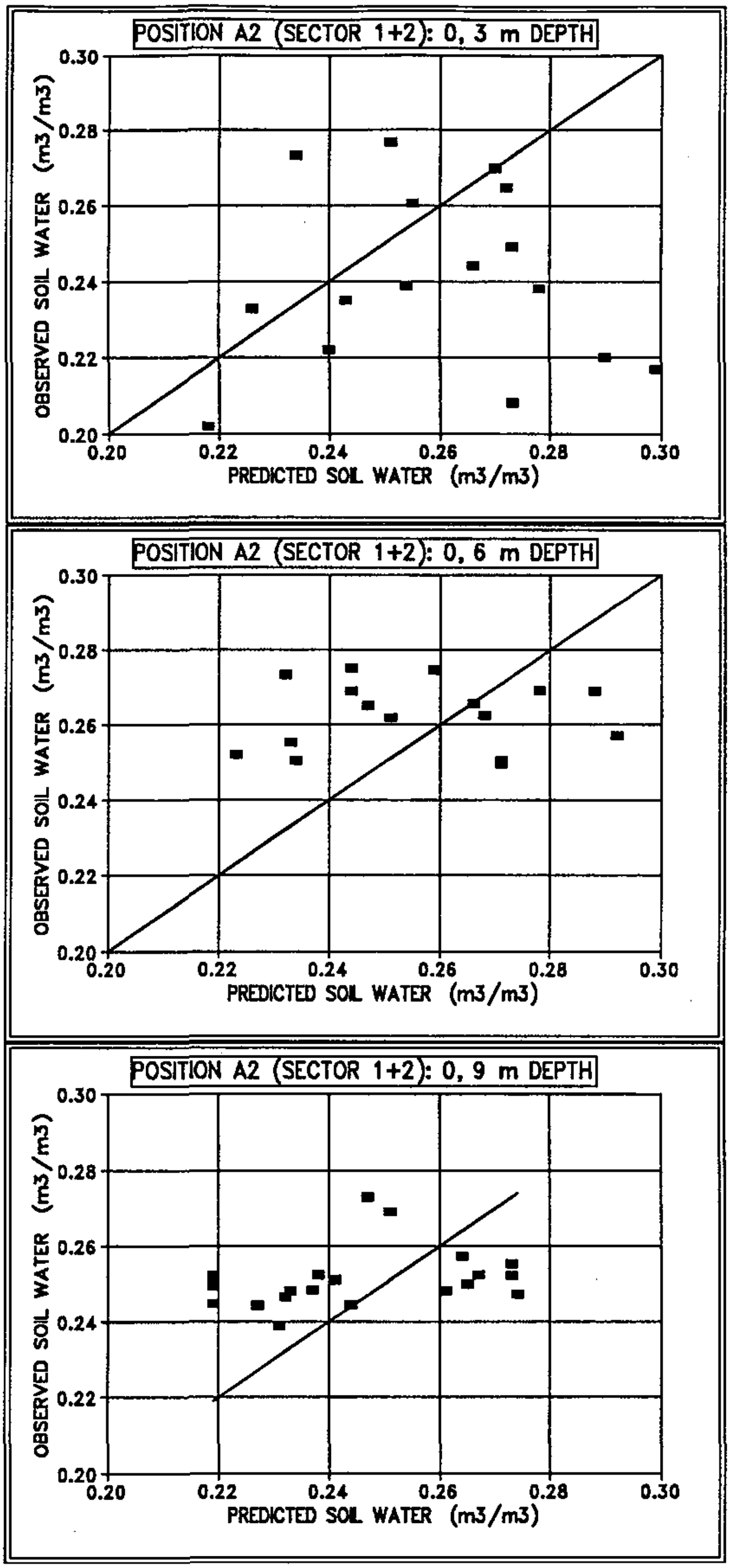


Figure 4.4 Comparison of predicted and observed soil water content at the 0,30, 0,60 and 0,90 m depths of the combined sectors 1 and 2 of site A2.

4.3.2.2 Temporal trends of predicted soil water content

The temporal relationship between predicted and observed soil water contents for the 0,30 m, 0,60 m and 0,90 m depths within wetted sectors 1,2 and 3 of macrosites A2 and A4 are presented in Figures 4.5 a and b respectively. At both sites the water contents at the 0,30 and 0,60 m depths were consistently underpredicted between day number 150 and 280. This period coincided with the summer (active growing) season of 1987/88. The progressive decrease in the predicted soil water content of the upper soil layers did not extend through to the 0,90 m depth. In the case of site A2 the predicted water content at the 0,9 m depth accorded quite well with the observed values throughout the study period (Fig. 4.5 a). At all the sectors of site A4 the water content at the 0,90 m depth was consistently overpredicted with a rather sharp increase occurring around day number 300 (Fig.4.5 b). This predicted increase was also observed at site A2, albeit less dramatic, and coincides with the so-called "post-harvest" irrigation applied to vineyards in the Breede River Valley between the end of February and March of each year. This irrigation is generally accepted to be associated with high leaching fractions. It is not certain why the post-harvest irrigation of the 1988/89 season (±day number 650) did not produce the same increase in the predicted water content. In fact, at the time of the 1988/89 post-harvest irrigation, the predicted water content at site A4 decreased while the observed values increased (Fig. 4.5 a & b). At site A2 the results were similar, but the difference between the predicted and observed water content was smaller.

The model can only react to the input it receives. It is therefore possible that some of the hydrological data supplied as input did not reflect the real field conditions. Because of similar textural compositions at the four macro sites, the *b*-coefficients inferred from the clay and silt percentages were also quite similar (Table 4.5). However, the measured soil water contents suggest that the hydrology of the four sites are quite different. For example, throughout the study period it was found that site A2 is drier than the other three sites. Yet, the estimated *a* and *b* coefficients of site A2 did not differ all that much from those of sites A1, A3 and A4. It is therefore possible that the consistent over- and under predictions of the soil water content are related to faulty *a* and *b* values. Although the sensitivity study indicated that the *a* and *b* coefficients should have a minor effect on the calculated water flux, this does not prove that the effect on the soil water content will be equally small. Another possible explanation for the discrepancies, is that the actual plant water uptake (evapotranspiration) is spatially variable as well as different to the values supplied as input. In chapter 3 it was found that LEACHM is particularly sensitive to irrigation and evapotranspiration inputs. As mentioned in section 4.2.2.3, although evapotranspiration was discretisized according to distance from an emitter, the same values were used as input at each of the four sites that were simulated. Because of time constraints and the difficulties encountered with the chemistry version of the model, these different possible causes for the inconsistencies between predicted and observed water contents were not investigated any further.

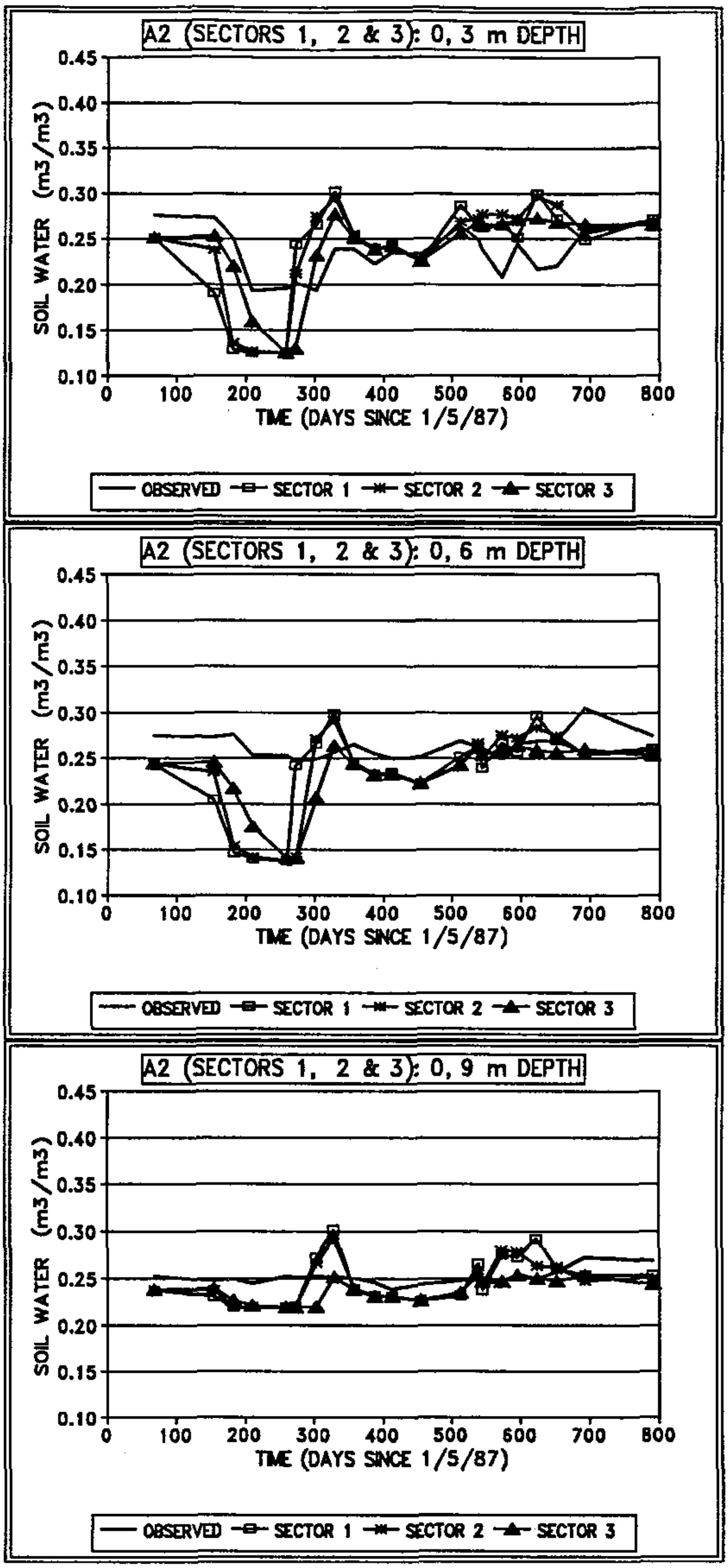
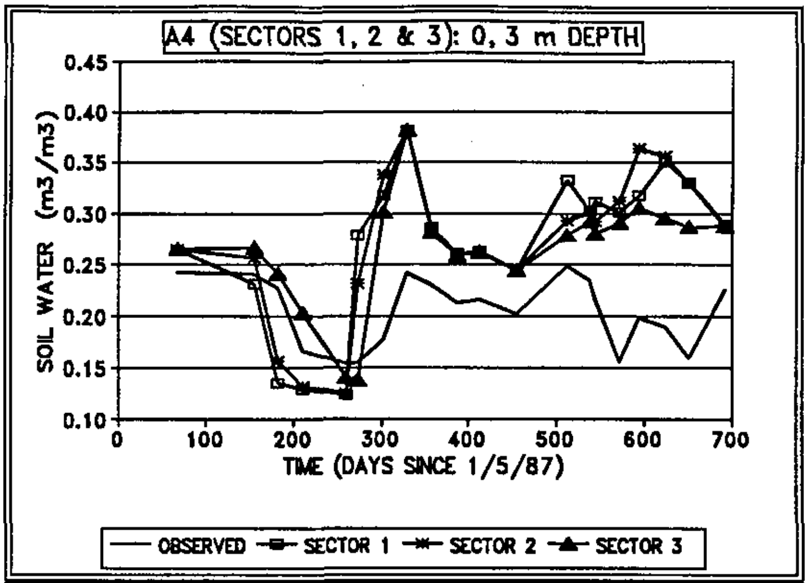
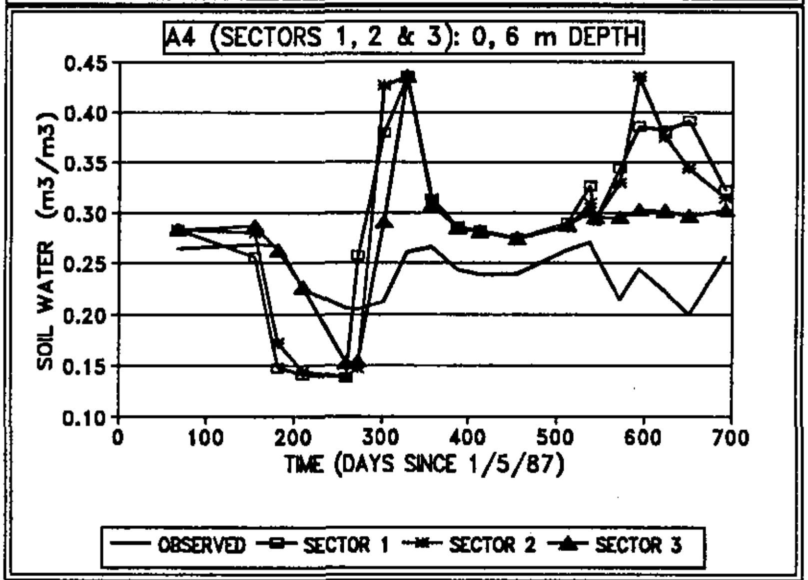


Figure 4.5 Temporal trend of the observed and predicted volumetric soil water content at the 0,3 m, 0,6 m and 0,9 m depths of sectors 1, 2 and 3: a: Site A2





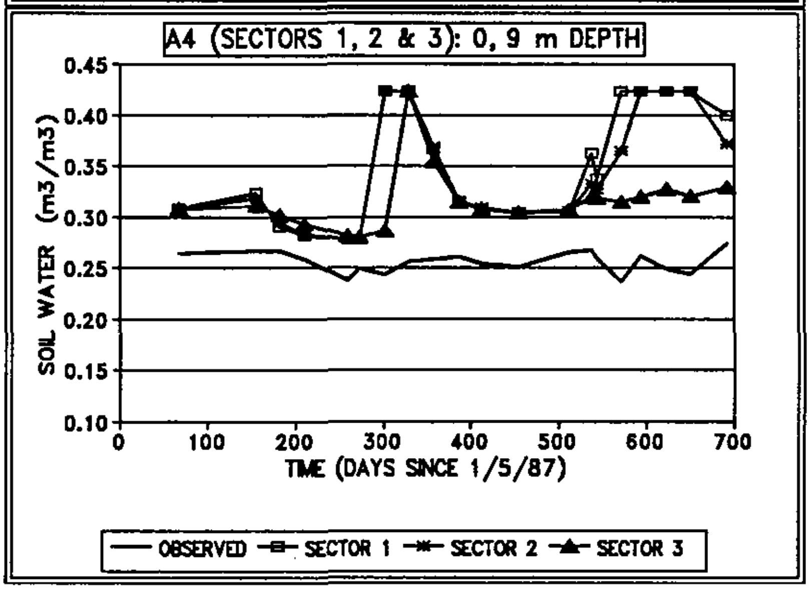


Figure 4.5 b: Site A4

4.3.3 Chemical composition of the soil

4.3.3.1 Temporal trends

The original intention was to use LEACHC to simulate water and salt transport processes for a period of 792 days commencing on 1/5/87 and ending on 30/6/89. As mentioned in section 4.3.1 this could be accomplished in four cases only. Consequently, a comparison between predicted and observed salt concentrations in the soil solution for the complete period of 792 days was possible for sectors 1 and 2 of site A1 and sector 2 of site A2 only, as well as when sectors 1 and 2 were combined and simulated as one wetted area (Table 4.12). In Figures 4.6 to 4.8 the temporal trend in predicted and observed EC (in mS m^{-1}) and chloride concentration (in mg dm^{-3}) at the 0,30, 0,60 and 0,90 m depths of site A2 are presented. It should be noted that both the predicted and observed values reflect concentrations at field water content. The observed data is that of soil solution sampler S5 in sector 2 of macrosite A2 (Figure 4.1). The predicted results represent the wetted area within 0,5 m from an emitter and comprise three different scenarios. In Figure 4.6 the EC and chloride content within sector 1 only (i.e. the area 0,25 m from the emitter) are given. The results given in Figure 4.7 are the area-weighted mean concentrations of sectors 1 and 2, which were simulated in two separate runs. Figure 4.8 also gives the results of the area covered by sectors 1 and 2, but this time simulated and treated as one wetted area (see Table 4.2 for the different equivalent depths of applied water). The following are amongst the more discernable inferences that can be made from these figures:

i) The EC (i.e. the measure of total soluble salt content) was overpredicted at all depths up to day 300, which in all likelihood is the result of the underprediction in the soil water content. Towards the end of the simulation period the comparison between predicted and observed EC was very good, but interestingly enough, very poor in the case of chloride.

ii) The period when the total salt content increases, coincides with the progressive decrease in soil water content (as could be expected).

iii) Distinct differences developed between the three different depths during the latter dry period, with the differences in total salt content being more pronounced than the chloride differences.

iv) The soil solution sampled at position S5 indicate a steady increase in the electrical conductivity as well as a drastic increase in the chloride concentration, especially from day 500 onwards. In a study in which they evaluated ceramic cups for determining soil solution chemistry, Debyle *et al* (1988) found that solute samples collected with 1-year-old and 6-year-old ceramic cups had significantly higher Mg, Na, NO_3 and K concentrations than samples from new ceramic cups. They attributed this to gradual plugging of the pores in the ceramic cup, as well a CEC that gradually developed in the cup matrix with time. This could also have happened with the solution sampler at site S5. Obviously, LEACHM cannot simulate this process.

v) Within sectors 1 and 2 the predicted EC decreases in the order sector 1 < sector 2 (not shown) < weighted average of sectors 1 and 2 < sectors 1 and 2 combined and treated as one area.

4.3.3.2 Comparison of predicted salt content with the measured data of 23 August 1988

The reason for LEACHM not being able to simulate the full 792 day period in all cases was related to calculations in the model that led to negative or zero calcium concentrations, which in turn resulted in run time errors. In view of this error in the model, it is not clear what the value of a comparison between the predicted and observed chemical compositions will be. Nevertheless, for the sake of completeness, such a comparison was made by using the measured electrical conductivities (of a saturated soil paste) of 32 soil samples collected at several distances and directions from the emitter on 23 August 1988. The measured and predicted EC's of sectors 1 and 2 of sites A2 and A4 are presented in Figures 4.9 (a,b) and 4.10 (a,b) respectively. The predicted conductivities were adjusted (diluted) from the field water contents predicted for 23/08/88, to a gravimetric water content of 40%, which is similar to the saturation percentages of the soil pastes. No correction was made for any chemical reaction (such as increased dissolution of minerals) at the higher water content.

With the exception of the 0,90 and 1,50 m depths, the predicted EC's fall within one standard deviation from the observed values in sector 1 of site A2 (Fig. 4.9a). From 1,20 m and deeper the predicted values deviates markedly from the observed EC's. In the case of sector 2 of site A2, the EC is predicted to increase with depth, while the observed EC's suggest a slight decrease (Fig 4.9b). Although both the observed and predicted salt contents are higher, similar observations were made at site A4 (Fig. 4.10 a & b).

It can be argued that the overprediction of the soluble salt content at the lower depths of sector 2, is indicative that the predicted flux of water that percolates through the soil at a distance 0,25-0,50 m from the emitters, is less than the actual flux. A smaller flux of water in turn implies less leaching and therefore higher salt contents.

Still, the temporal distribution of the predicted soil water content in sector 2 of site A2 (Figure 4.5) accords well with the observed values. At site A4 the water content was overpredicted. It is reasonable to assume that a consistent overprediction of water content will also be associated with an increased (and not decreased) flux of water through the root zone. The water contents of given in Figure 4.5 therefore do not support the deduction that an underpredicted water flux is the reason for the overpredicted salt content. The effect of an increase in the weight factor (which will increase the depth of water applied at sector 2), was not investigated.

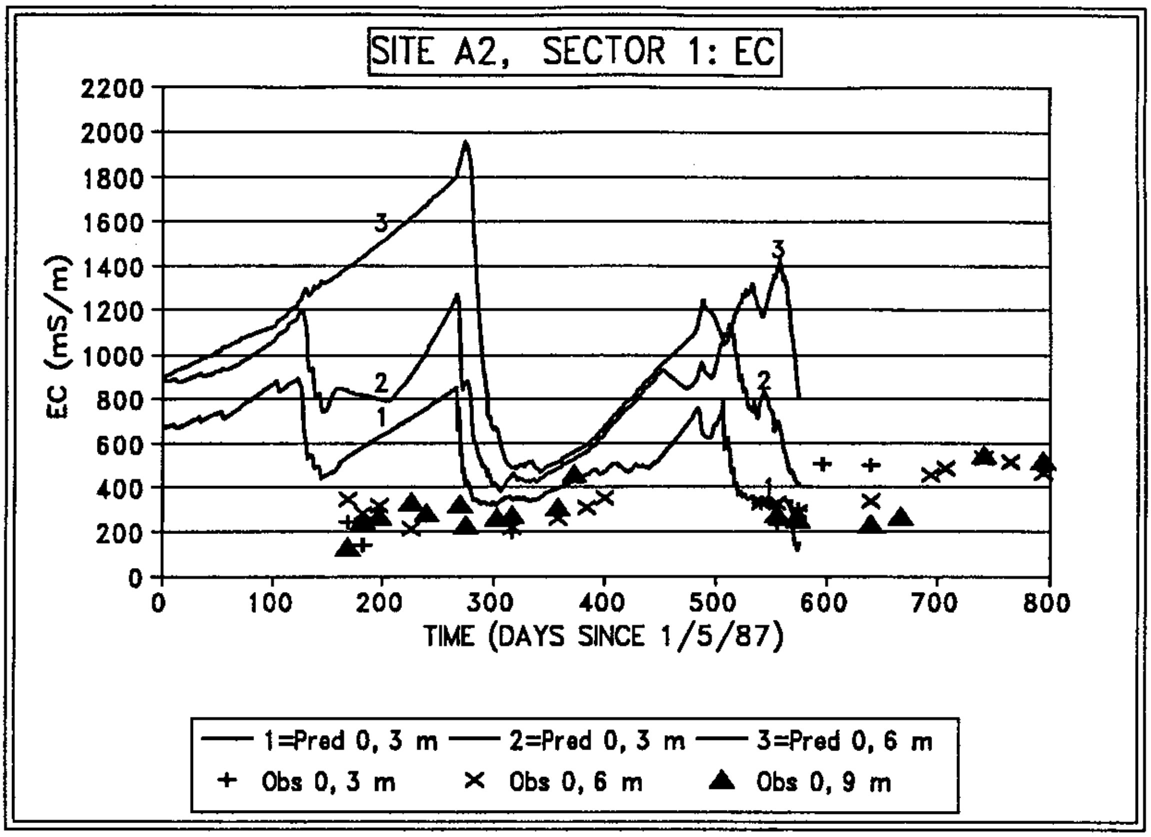
4.3.4 Field averaged water flux at 2 m depth

The field averaged flux of soil water flowing into the water table at 2 m depth, was calculated by first obtaining the wetted surface area-weighted mean flux of each of the four macrosites. This weighted mean was calculated as follows (see also Table 4.1):

[(Flux sector 1 * 0,196)+(Flux sector 2 * 0,304)+(Flux sector 3 * 0.50)+(Flux sector 4 * 1,50)]/2,5

The field averaged mean flux was obtained by calculating the arithmetic mean of the four weighted mean values for macrosites A1 to A4. This arithmetic mean was converted to a volume (m^3) by using the appropriate area of the vineyard (ca. 5000 m^2). This field averaged predicted daily water flux value was then compared with the daily drainage rate measured in the tile drain on the west side of the vineyard (Figure 4.1). The results are presented in Figure 4.11. It should be stressed that the observed drainage volumes do not necessarily constitute the deep percolate of the 5000 m^2 irrigated area only. Lateral movement of water from outside the irrigated area could also enter the drainage pipes. The predicted fluxes and travel times were also not lagged according to the different flow distances from the various macrosites to the drain. Despite the complexity of the flow regime in a drip irrigated soil the predicted temporal trend given in Figure 4.11 mimics the observed trend surprisingly well.

The negative flux values predicted from day 150 to 270 indicate upward flow of water from the water table into the root zone. This coincides with the period during which the water content was a) underpredicted and b) progressively decreasing (Fig 4.6 and 4.7). The predicted flux generally underestimate the measured drainage rates. This is particularly noticeable between day 500 and 700 (Figure 4.11). However, this does not necessarily mean that the predicted values and/or input data are totally erroneous. The underestimate might also be explained by lateral flow of water from outside the area into the drain underlying the vineyard.



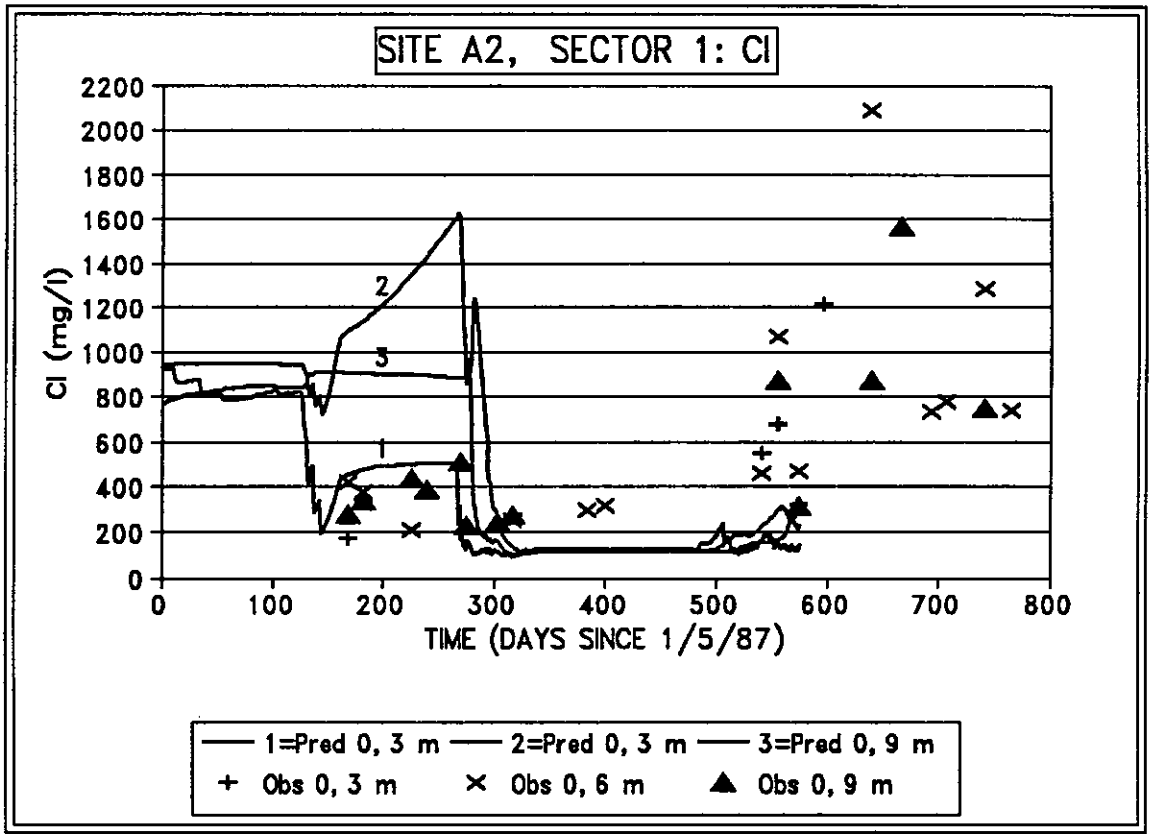
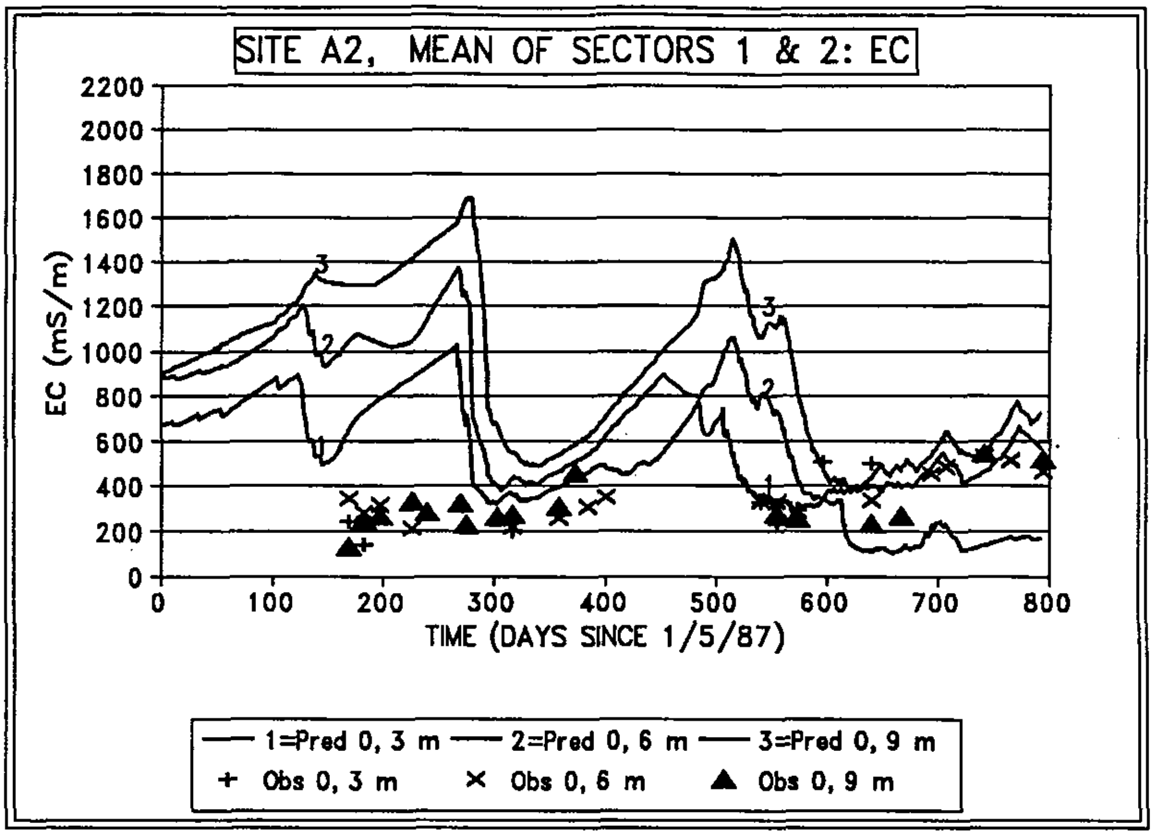


Figure 4.6 Temporal trend of the electrical conductivity and chloride content of the soil solution at field water content in sector 1 of site A2



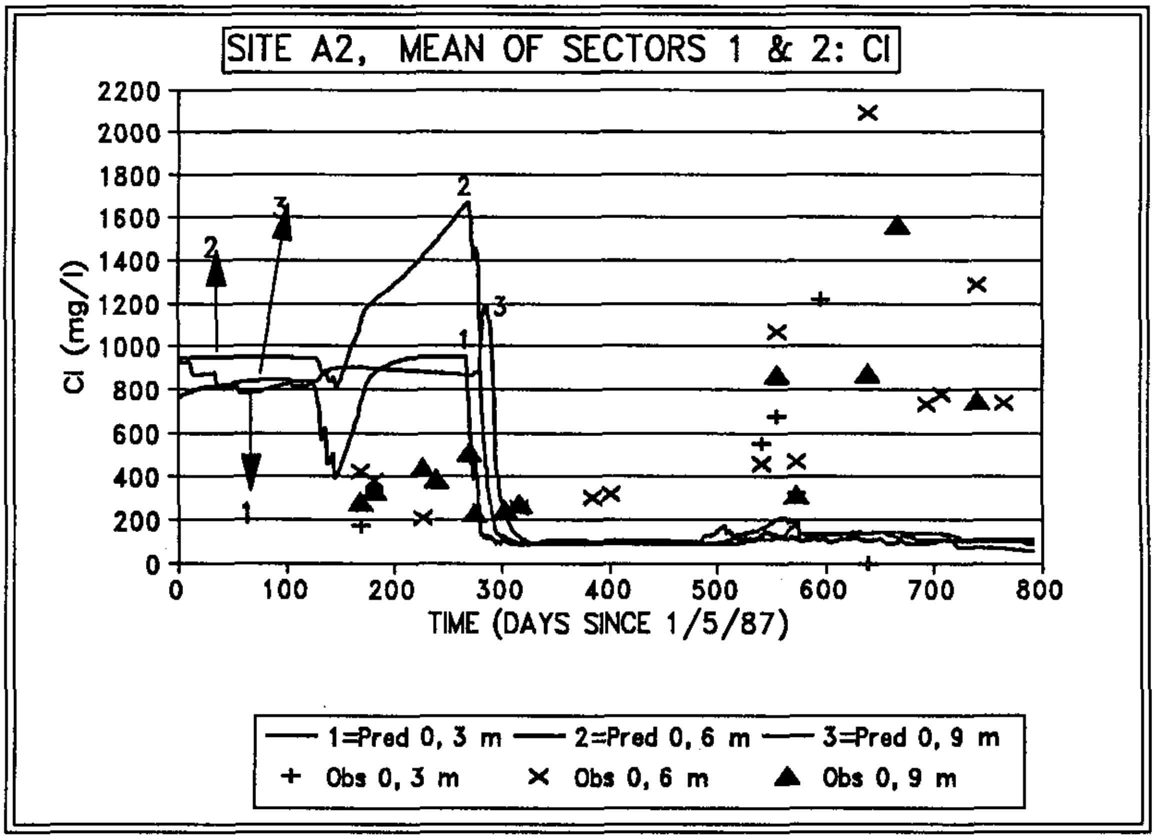
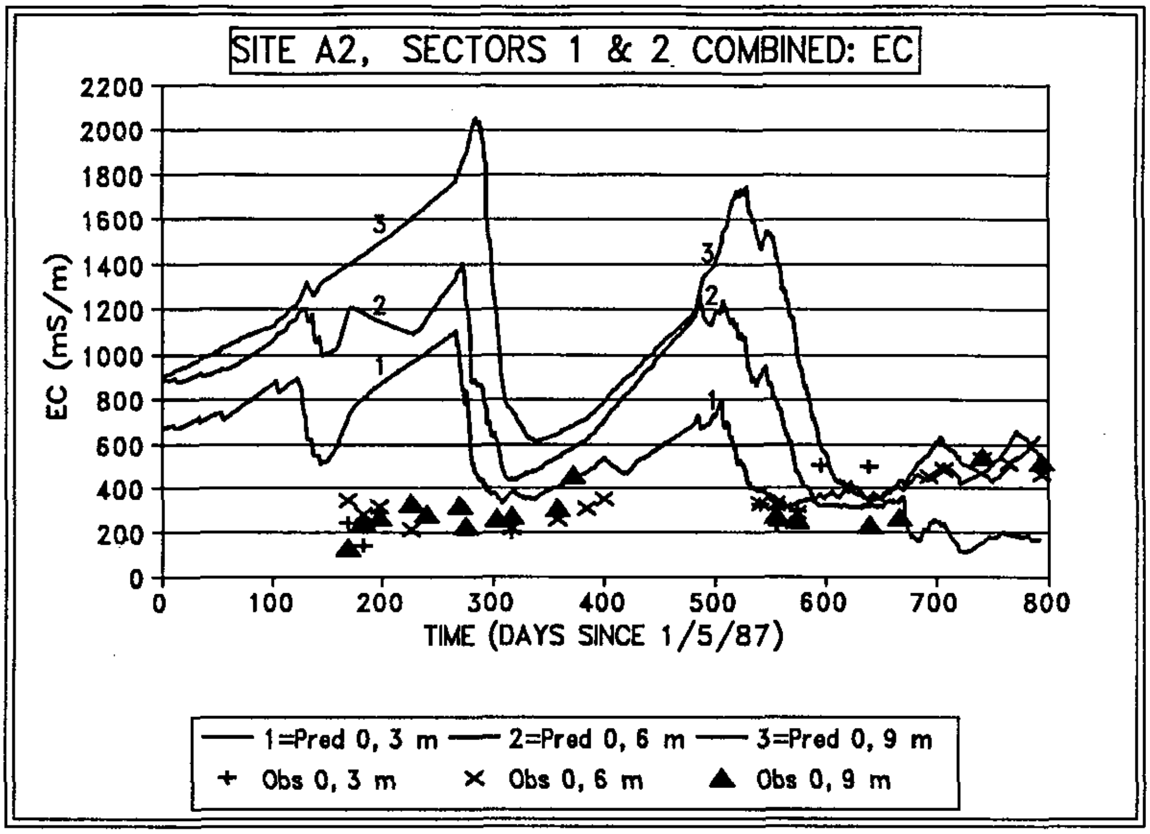


Figure 4.7 Temporal trend of the weighted mean electrical conductivity and chloride content of the soil solution in sectors 1 and 2 of site A2



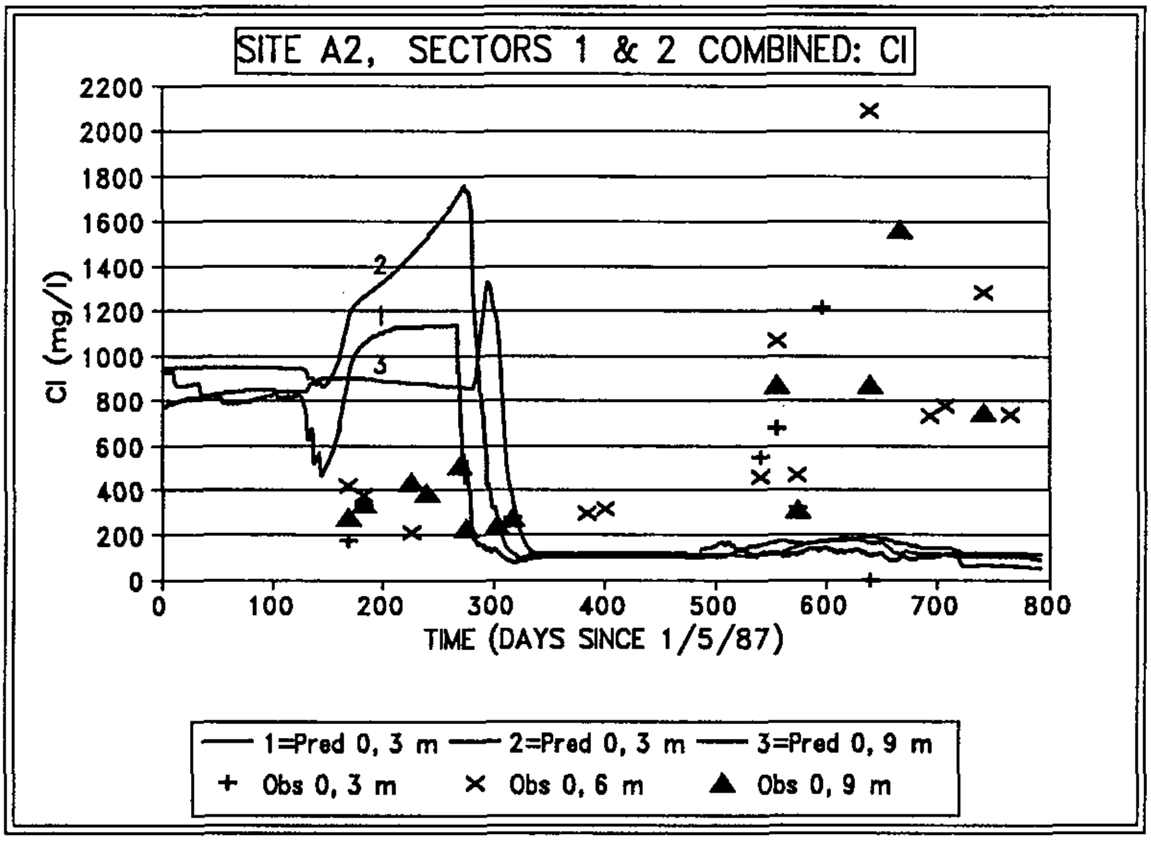
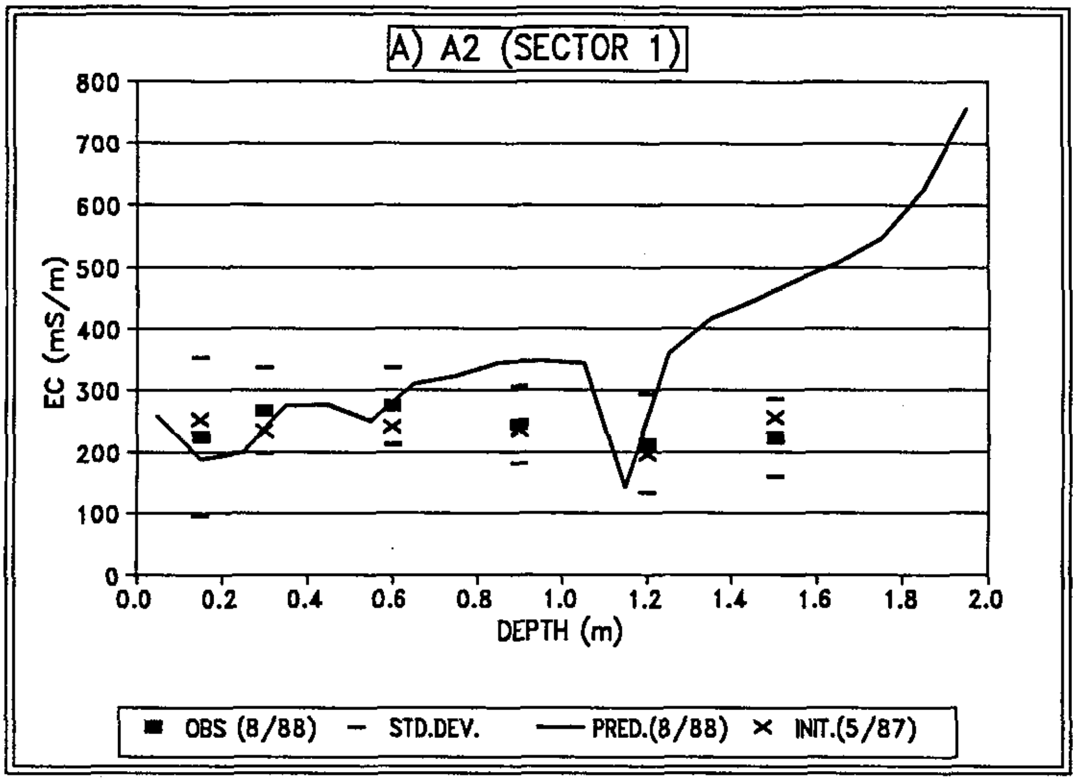


Figure 4.8 Temporal trend of the electrical conductivity and chloride content of the soil solution in the area covered by sectors 1 and 2 of site A2



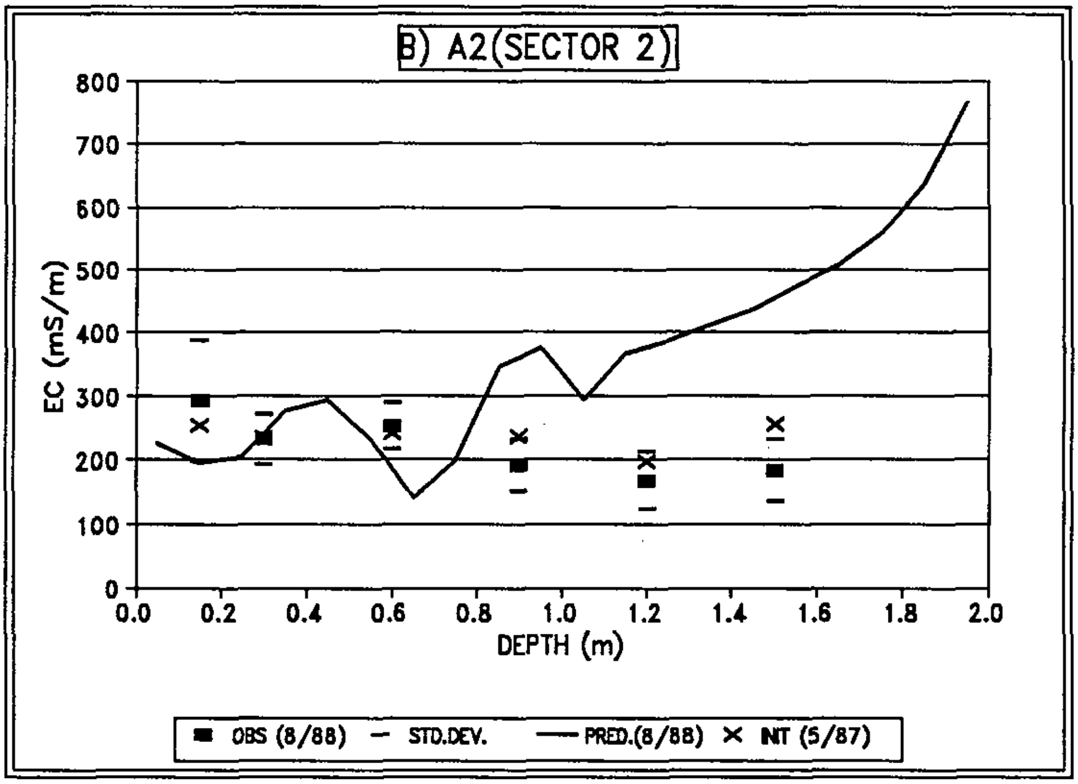
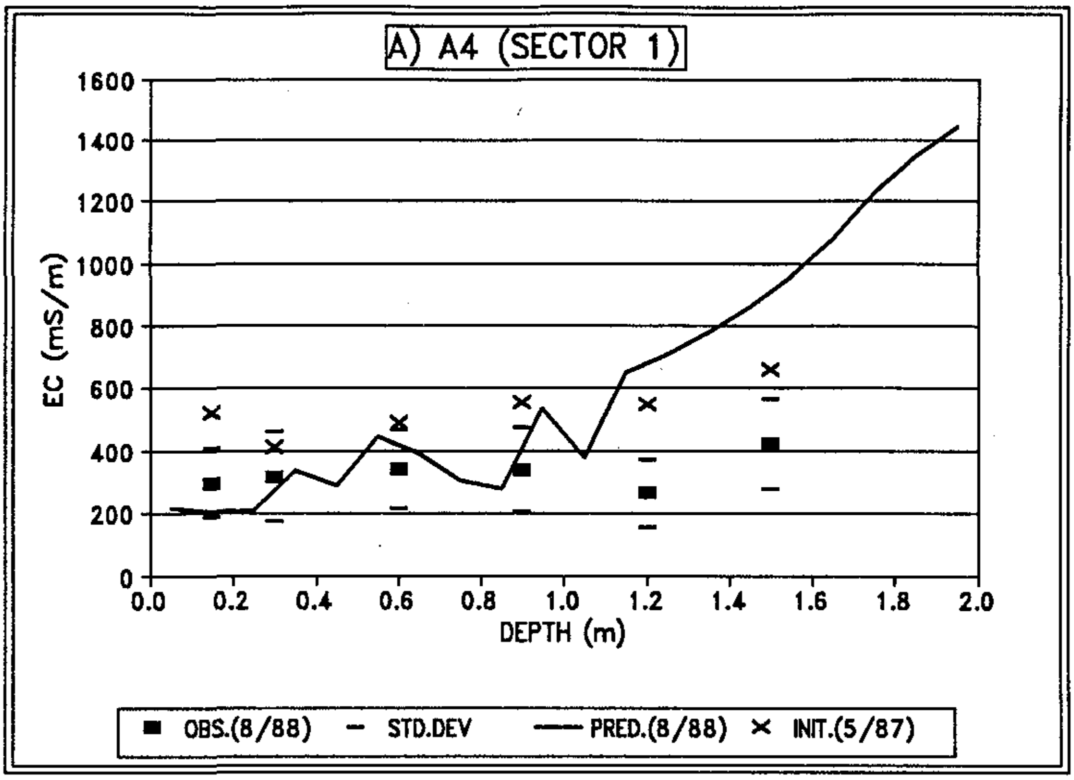


Figure 4.9 Depth distribution of the specific electrical conductivity (EC) of the extract of a saturated soil paste measured and predicted for 23/08/88 in two sectors of site A2. (The horizontal bars represent the standard deviation from the observed mean of four samples. Also indicated are the EC's initially used as input on 01/05/87).
a) Sector 1 (0-0,25 m from emitter),
b) Sector 2 (0,25-0,50 m from emitter).



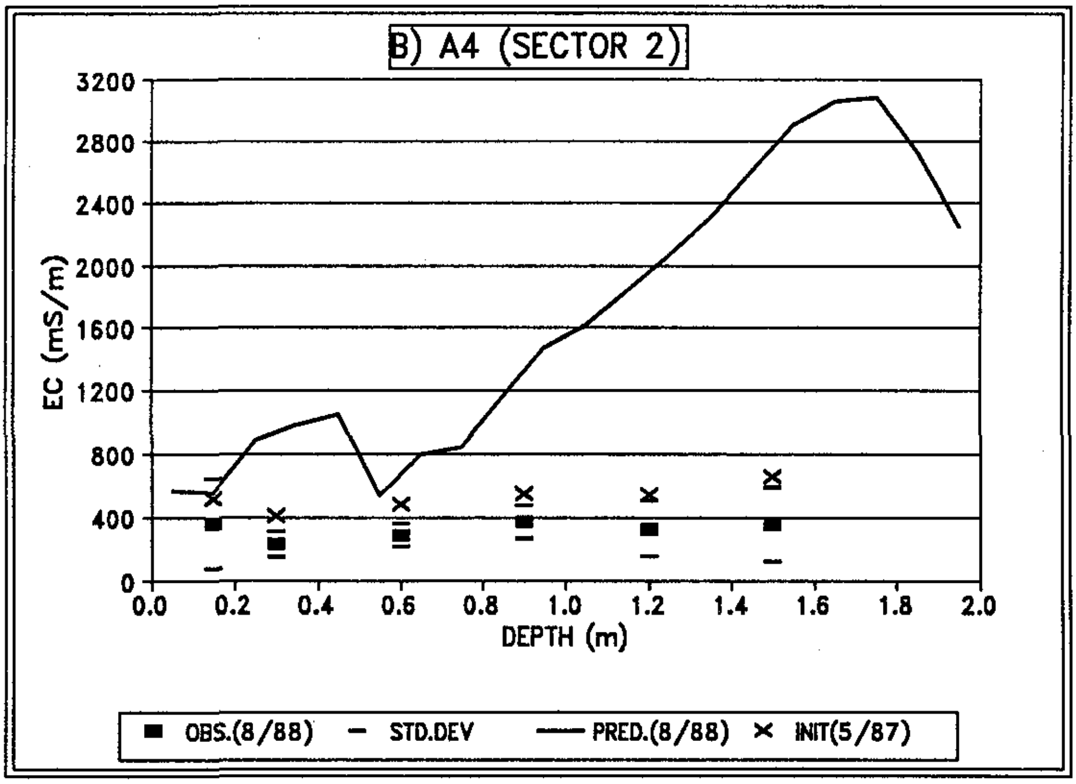


Figure 4.10 Depth distribution of the specific electrical conductivity (EC) of the extract of a saturated soil paste measured and predicted for 23/08/88 in two sectors of site A4. (The horizontal bars represent the standard deviation from the observed mean of four samples. Also indicated are the EC's initially used as input on 01/05/87):
a) Sector 1 (0-0,25 m from emitter),
b) Sector 2 (0,25-0,50 m from emitter).

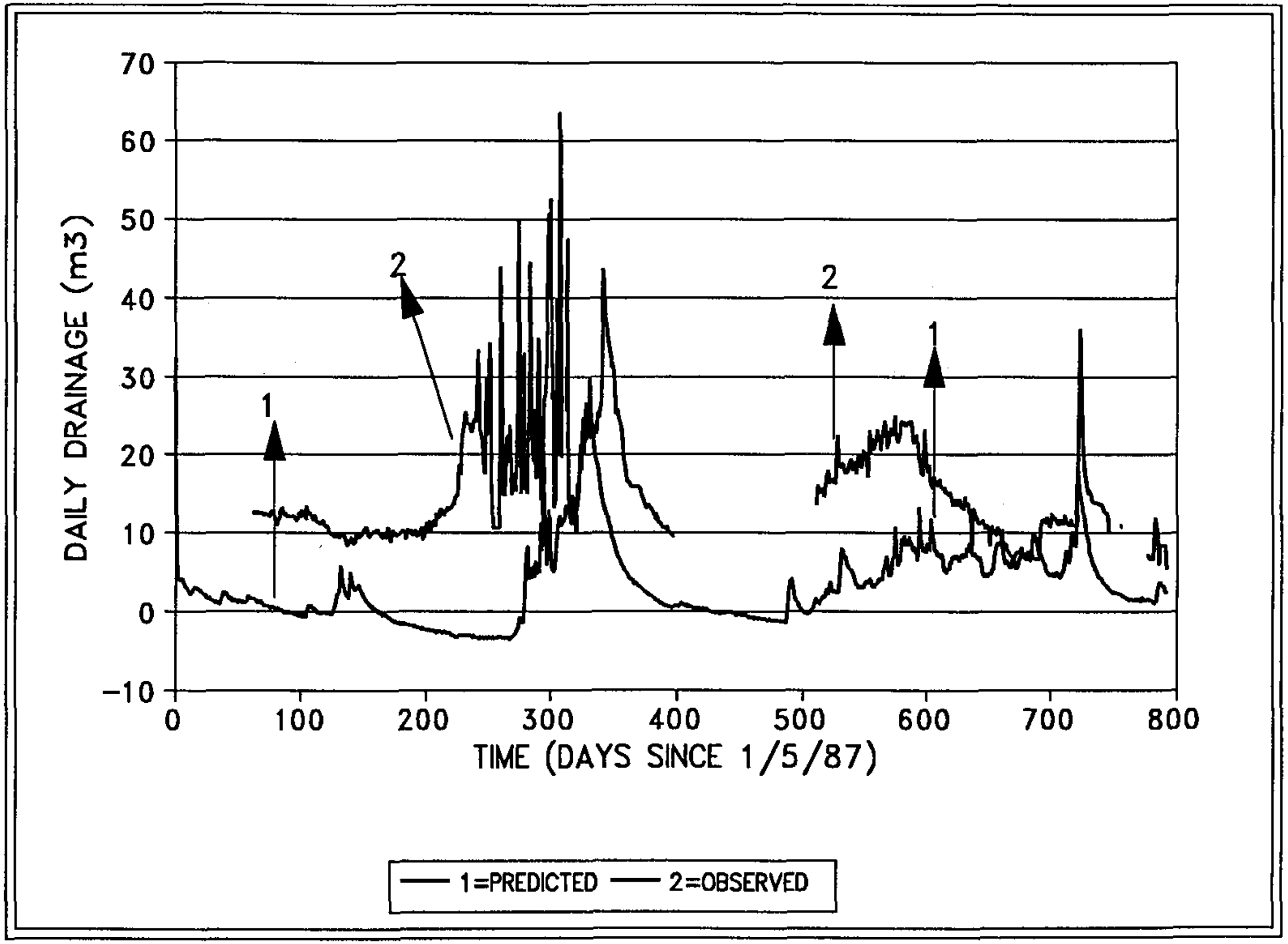


Figure 4.11 Predicted field averaged and measured daily drainage volumes at 2 m depth for the period 1 May 1987 to 30 June 1989.

4.4 DISCUSSION AND CONCLUSIONS

The overriding conclusion that was reached at the end of this study was one of conflicting results. Firstly, in terms of the predicted soil water contents and fluxes, the numerical statistics and graphical comparisons leave contrasting impressions of the adequacy of LEACHM as a modelling tool to calculate accurately the fate of applied water in this drip irrigated vineyard. Based on statistical norms, neither the coefficients of determination (R^2), nor the d-index of Wilmot (1981) justify any confidence in the model at all. The maximum R^2 value and d-index that were obtained are 0,306 and 0,774 respectively. However, judging the adequacy of prediction in terms of visual comparisons only, give a slightly better impression of the predictive ability of LEACHM. Except for marked underpredictions in the soil water content of the shallower soil layers during the summer of 1987/88, the predicted water contents as well as the temporal trends did not deviate too much from the measured values and trends. Also, the visual comparison between the predicted and observed drainage rates supports the latter conclusion. Considering the fact that the predicted daily drainage volumes and rates of a known area are compared with the observed values coming from an unknown area, the calculations of LEACHM can be taken as a fair representation of the conditions and soil water fluxes that prevailed in this vineyard during the study period.

The predicted soil water contents and fluxes should furthermore be judged against the complexity of the three dimensional flow patterns in the drip irrigated field to which this one-dimensional model was applied. In the sensitivity analysis of LEACHM it was established that small changes in the amounts of irrigation water inputs and evapotranspirational losses, have a large effect on the calculated water and salt fluxes. Even a small change in the assumed wetted area hat is used in the conversion of volume of applied water to depth units is therefore likely to result in substantial differences between the measured and predicted water contents and fluxes. Consequently, in this particular application of LEACHM, the statistically poor match between predictions and observations might be related to either model inadequacies, or input errors and it is rather difficult to distinguish between these two.

The numerical problems encountered with the chemistry version of LEACHM, i.e. LEACHC, is disturbing and do little to install confidence in this particular version. It was found that situations where the square root of a negative number, or division by zero, is attempted could not be predicted beforehand. In this study all of these cases were associated with the chemistry of calcium. Sometimes this problem could be overcome by increasing the specified quantity of lime in the soil, but even this was no guarantee of success in all cases. The fact that LEACHC has apparently been used successfully elsewhere (Hutson, 1991, personal communication) confounds the issue even more. One possible reason for the numerical instability found in this study might be related to the fact that:

i) a large amount of non-saline, low salt water was applied to,

ii) a saline soil with a rather low cation exchange capacity (compared to the environments for which it was developed) in a soil with,

iii) small quantities of gypsum and free lime.

Under these conditions the salt content of the soil solution and the chemical composition of the exchange complex could change rapidly from saline to non-saline conditions, with a commensurate decrease in the gypsum and lime contents. This latter condition can then develop into a situation where calcium concentrations become very small. Such circumstances are atypical of semi-arid and arid soils.

The above explanation is supported by the data supplied as input for sectors 1 and 2, which represent the area in close proximity of the emitters, i.e. a large amount of non-saline water percolating through the soil. However, this was not the case in sector 4 situated between two vineyard rows at the maximum distance from the emitters. In this sector, according to the input information, only minor amounts of water were applied on a soil that is highly saline. The possibility that the initially high calcium concentrations in sector 4 could have been reduced to very low values, are very remote. Therefore, the above explanation, although supported by sectors 1 and 2, is refuted by the conditions prevailing in sector 4.

The original aim for conducting this study was to apply and evaluate LEACHM on a microscale to a field where conditions were closely monitored. In terms of soil water transport the study is regarded as inconclusive. The main reason for this is the application of a one dimensional flow model to a complex three dimensional drip irrigated case, which probably constituted an wrong application of LEACHM at the outset. For the same reason, as well as those caused by numerical instabilities, the chemistry version of LEACHM could not be evaluated thoroughly.

The information and experience gained with this study indicate that the application of one-dimensional models to drip irrigated, widely spaced, row cropped fields, by nature of the model construction will be met with poor results. In view of this evidence it is recommended that the development of a three-dimensional flow and salt transport model be investigated. Such a model could then be used to simulate and predict the fate of water and soluble salt in drip irrigated fields. Alternatively, the evaluation of a number of existing three dimensional flow models of the unsaturated zone (e.g. Healy, 1987) should be undertaken.

CHAPTER 5
PREDICTING THE CHANGES IN THE WATER AND SOLUBLE SALT CONTENT OF TWO IRRIGATED FIELDS IN THE SAN JOAQUIN VALLEY, CALIFORNIA: AN EVALUATION OF THREE MODELS ON A MESO SPATIAL SCALE USING LIMITED DATA

5.1 INTRODUCTION

The objective of this part of the research project was to apply one mechanistic research model and three functional management models to field data and to assess their accuracy of prediction at a mesoscale (1 - 10 ha) using limited data. The models used were LEACHC which is the chemistry version of LEACHM (Wagenet and Hutson, 1989), BURNS (Burns, 1974), and TETrans (Corwin and Waggoner, 1990). In the rest of this discussion, the more generally known acronym *LEACHM* will be used. Because no local (South African) data on a meso scale could be found, use was made of the results of two treatments of a 61 ha irrigation experiment conducted in the San Joaquin Valley of California. The two treatments that were used are a 5,7 ha furrow irrigated, and a 2,4 ha drip irrigated plot. In the case of the drip irrigated field the density of emitters was 1 m x 1 m, i.e. one emitter per m^2.

5.2 FIELD DESCRIPTION AND INPUT DATA USED FOR THE THREE MODELS

5.2.1 General

The information that was used in this part of the study, is based on a five year research project (1982-1987), conducted by the AWML* on the Murrieta Ranch which is located in the San Joaquin Valley of California. The irrigation experiment involved different crops, methods of water application as well as different water qualities. In this study, the application was confined to the results of two of the irrigation treatments, and to measurements made between May 1983 and November 1987 only.

This particular evaluation of transport models is representative of circumstances where only limited data are available as input, while the balance of the input must be inferred or calculated from other soil properties. The soil water content and chemical predictions of the three models were evaluated against a) soil water data measured from May 1983 to August 1984, and b) the chemical composition of the saturated soil paste extracts sampled at irregular intervals from March 1984 to November 1987.

The methods that were used to meet the input requirements of the LEACHM model will be outlined in the following paragraphs. The input requirements of the less data demanding Burns and TETrans models are dealt with separately.

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* AWML = Agricultural Water Management Research Laboratory, Agricultural Research Service, 2021 S. Peach Ave, Fresno, Ca 93727.

5.2.2 Input data for LEACHM

5.2.2.1 Irrigation methods and quantities

The irrigation information of two of the experimental fields, i.e. the furrow and drip irrigated plots were used as input. In the case of the furrow irrigated plot, farm records were used to obtain the amount of irrigation water applied between the period 1 May 1983 to 31 August 1986. On the drip plot metered readings, converted to a depth unit by dividing with the area of the plot, were used. In both cases and for most of the years a so-called pre-irrigation was applied (during winter) using gravity techniques, i.e. both the furrow and drip plots received the pre-irrigation as flood irrigation. In some specific instances (e.g. to promote proper germination) the water was sprinkler applied. The actual dates, amounts and methods used to apply the water (if different from the original furrow or drip methods) are indicated in Table 5.1.

All of the irrigation quantities were taken from farm records. In the case of the furrow irrigation applications for the wheat crop of 1985 and the cotton crop of 1985/86, both the frequency and amount of water applied seemed to be suspect. Inspection showed that the frequency was in all probability correct but that the amount per application could have been an overestimate of the actual infiltrated water. The furrow field was operated as a tail water recovery system, with the result that the difference between applied and infiltrated water could have been substantial. In order to minimise the effect of this overestimate of infiltrated water, the applications of 1985 and 1986 were reduced by the empirical ratio of total seasonal applied drip irrigation water to applied flood irrigation water. For example, during the 1985 wheat growing period the ratio of drip to furrow applied water was 377/532 = 0,71. Consequently the applications of the furrow plot taken from the farm records, were reduced by 0,71 e.g. the 147 mm supposedly applied on Jan 28, 1985 (Table 5.1) becomes 147 * 0,71 = 104 mm. The ratio for the 1985/86 cotton season that was used is 807/948 = 0,85. It should be stressed that this approach is entirely empirical.

Table 5.1 Dates, amounts and methods of irrigation applications, Murrieta Ranch, May 1983 to November 1987

Date	Quantity (mm) Furrow	Drip	Method[1]	Adjusted Furrow (mm) '85-'86
830523	60	60	Spr	60
830708	80	80		80
830727		84		
830731		30		
830803	135			135
830808		54		
830823		15		
830824		15		
831229	170	170	Spr/Fur	170
840510	20	20		20
840705	109	78		109
840719		30		
840724		29		
840725	109			109
840730		29		
840802	109			109
840803		24		
840808		30		
840815		42		
840816	109			109
840820		54		
840905	109			109
850128	85	85	Spr	85
850303		35		
850306	147			104
850310		48		
850327		45		
850408	150			106
850418		118		
850427	150			106
850502		46		
850816	40	40	Spr	40
850929	40	40	Spr	40
851007	115	115	Spr	98
860411	119			101
860501		73		
860505	119			101
860515		49		
860520		26		
860523		39		
860524	119			101
860529		92		
860603		109		
860606	119			101
860611		30		
860622		48		
860624	119			101
860625		39		

contd.

Table 5.1 (contd.)

Date	Quantity (mm) Furrow	Drip	Method[1]	Adjusted Furrow (mm) '85-'86
860701	119			101
860707		40		
860711		62		
860715	119			101
860718		41		
860728		44		
861220		170	Spr/fur	
870702		24		
870706		65		
870720		9		
870722		3		
870724		58		
870726		57		
870728		42		
870806		16		
870809		56		
870816		52		
870823		58		
Total	**2570**	**2718**		**2296**

1. Indicates the irrigation method applicable to the drip plot for that particular date.

5.2.2.2 Chemical composition of the irrigation water

The furrow plot was irrigated with good quality water (EC = 20 mS m^{-1}) from the Westlands Water District throughout the period of 1983 to 1986. The chemical composition of the water is indicated in Table 5.2. With the exception of the pre-irrigation application, the drip plot was for the most part irrigated with saline drainage water (EC = 507 to 913 mS m^{-1}) from adjacent fields. The actual chemical analyses of this water varied between the range of concentrations listed in Table 5.2. The analytical information was taken directly from the records of the Water Management Research Laboratory and no attempt was made to modify the analytical data in order to secure ionic charge balance.

Table 5.2 Chemical composition of irrigation water used as input for LEACHM

Ca	Mg	Na	K	Cl	SO_4	HCO_3
<-----		mmol dm^{-3}				---->
Furrow	(all dates 1983-1986)					
0,30	0,20	0,80	0,04	0,70	0,30	0,54
Drip						
Minimum concentration						
21,11	14,93	45,84	0,29	17,55	60,16	0,00
Maximum concentration						
25,35	18,34	58,29	0,31	33,60	76,00	0,00

5.2.2.3 Meteorological data and crop water requirements

Daily rainfall and class A-pan evaporation information recorded on site at the Murrieta Ranch during the period May 1983 to November 1987 were available. Only rainfall in excess of 5 mm per event was used as input and the total amount of rainfall used in the model is summarized in Table 5.3. It should be stressed that the figures given in Table 5.3 refer to two different periods, i.e. 1 May 1983 to 31 August 1986, and 1 May 1983 to 30 November 1987 for the furrow and drip irrigated plots respectively.

Crop specific coefficients were used to convert the pan evaporation data to weekly totals of actual evapotranspiration. The total potential- and actual evapotranspiration for the two different periods (i.e. furrow and drip plots) are summarized in Table 5.3 while the temporal relationship between PET and AET is given in Figure 5.1.

Table 5.3 Total rainfall, irrigation, potential-, and actual evapotranspiration for the furrow and drip irrigated plots

	Furrow (mm)	Drip (mm)
Irrigation	2296	2718
Rain	630	760
PET	5370	7105
AET	2992	3620

5.2.2.4 Textural composition

The particle size distribution of the furrow and drip irrigated soil was determined using an abbreviated version of the hydrometer method (Gee & Bauder, 1982). No pretreatment for organic material removal was done and the soluble salts only were removed. The analytical results are given in Table 5.4. As indicated in Table 5.4, the texture varied between loam and clay loam. The soil of the furrow plot showed a distinct increase in the sand content between the 0,9 and 1,2 m depths.

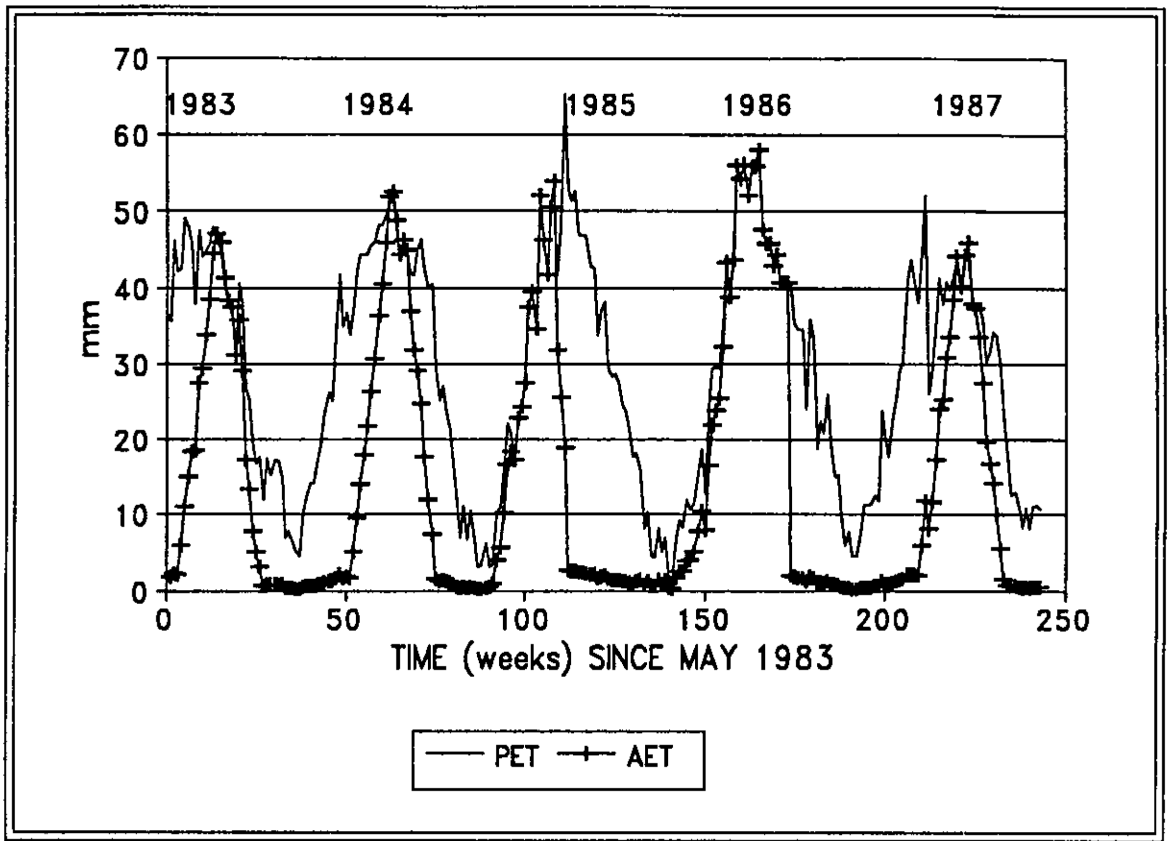


Figure 5.1 Weekly totals of the estimated potential- and actual evapotranspiration for the period May 1983 to November 1987

Table 5.4 Particle size analyses of the furrow- and drip irrigated plots at Murrieta Ranch

Plot	Depth (m)	Sand	Silt	Clay	Class
Furrow	0,3	34,4	26,2	39,4	ClLm
	0,6	42,9	25,8	31,3	ClLm
	0,9	36,4	27,1	36,5	ClLm
	1,2	44,1	28,7	27,2	Lm
	1,5	45,6	31,1	23,3	Lm
	1,8	46,5	31,4	22,1	Lm
	2,1	46,1	31,2	22,7	Lm
Drip	0,3	29,3	25,0	45,7	Cl
	0,6	25,6	28,7	45,7	Cl
	0,9	21,6	29,8	48,6	Cl
	1,2	22,8	28,7	48,5	Cl
	1,5	23,0	35,2	41,8	ClLm
	1,8	24,2	36,6	39,2	ClLm
	2,1	20,1	46,0	33,9	ClLm

Sand = 2,0-0,05 mm; Silt = 0,05-0,002 mm; Clay = <0,002 mm.

5.2.2.5 Estimation of air entry potential and water retention properties

No information about either the soil water characteristic curve of undisturbed soil cores, or the air entry potential of the experimental soil was available. Little information about the air entry potential of soils is found in literature and the field determination thereof is rarely reported, the work of Bouwer (1966) being the exception. However several methods exist that can be used to infer the water characteristic from particle size distribution data (e.g. Rawls & Brakensiek, 1982). This method and the subsequent procedure to obtain estimates for the Campbell *a* and *b* coefficients form the soil water characteristic is described in greater detail on page 4.10 (Chapter 4). The same approach was used here, i.e. the soil water characteristic was inferred from the particle size distribution data, from which the *a* and *b* coefficients were obtained. The values are listed in Table 5.5.

Table 5.5 Calculated values of the airentry potential and slope of the soil water retention curve used as input for LEACHM

Depth (m)	*a* (kPa)	*b*
Furrow plot		
0,3	2,46	8,5
0,6	8,58	7,8
0,9	1,50	8,4
1,2	6,05	7,2
1,5	6,93	6,8
1,8	6,45	6,6
Drip plot		
0,3	4,51	9,1
0,6	4,58	9,0
0,9	6,98	9,4
1,2	5,77	9,5
1,5	6,33	8,7
1,8	5,05	8,3
2,1	4,81	7,3

5.2.2.6 Bottom boundary condition and hydraulic conductivity

LEACHM can be used to simulate four different bottom boundary conditions, i.e. a fixed depth water table, a free- draining profile, zero flux or a lysimeter tank condition. Field observations suggests that neither of the first three conditions of LEACHM is applicable to the Murrieta fields because the water table has been observed to fluctuate substantially on an annual basis. The presence of the water table furthermore negates the free draining or zero flux boundary conditions. As both the furrow irrigated and the drip irrigated fields are underlain by a tile drain, LEACHM was run using the lysimeter tank option as input. In this case water can drain from the soil (i.e. lysimeter) when the bottom layer is saturated or has a pressure potential greater than that of the suction drainage system. No water can move into the soil by capillary action when the matric potential is lower than the drainage system potential. This is similar to the situation where, once water has been removed by the drains, it cannot get back into the root zone through capillary rise. On the furrow plot, the tile drain is located at 1,7 m and on the drip plot at 2,0 m depth.

No information on *in situ* determined saturated hydraulic conductivity or any other hydraulic properties of the Murrieta soil were available. In view of the results of the sensitivity study where it was established that the hydraulic conductivity is of minor importance in determining the quality and quantity of salt leaving the root zone, it was decided to use a single value of 200 mm d^{-1} to represent the saturated hydraulic conductivity of the soil profile. The exception was the surface layer (0-0,15 m) where a value of 50 mm d^{-1} was used. This was done to suppress evaporation of water at the soil surface. Previous experience with LEACHM (unpublished data) has indicated that the rate and quantity of surface evaporation are greatly influenced by the hydraulic conductivity of the surface node. Increasing the conductivity led to an increase in surface evaporation, sometimes to the extent that the ratio of evaporation to transpiration was unrealistic.

In a previous study with LEACHM Hutson *et al* (1988) found that changing the hydraulic conductivity of the soil by several orders of magnitude had an insignificant effect on the distribution of the applied chemical. However, in that particular study no mention is made of the bottom boundary condition that was used. In the present case of the lysimeter tank condition, it is conceivable that the rate at which water can be removed by the drains for a given and constant drain spacing, is dependent on the saturated hydraulic conductivity of the soil, especially the soil layer in which the drains are located. Consequently, the observed maximum drainage flow rate were used as a first estimate of the hydraulic conductivity at the bottom of the soil profile. The maximum flow rate translated to an estimated conductivity value of 1,0 mm d^{-1}. For the rest of the soil profile a conductivity value of 200 mm d^{-1} was used.

5.2.2.7 Soluble salt content and composition

The analytical data of all the soil samples collected on the furrow and drip irrigated plots in March 1983 were used to obtain arithmetic mean chemical compositions. These means values served as input for the LEACHM model and are listed in Table 5.6. Also indicated (where available), are the associated standard errors. Before being used as input, the salt concentrations of the saturated soil paste (Table 5.6) were adjusted (i.e. concentrated) to field water content.

5.2.2.8 Exchangeable cation composition

The cation exchange capacity (CEC) of the two areas that were used (furrow and drip plots) were not available. However, at the onset of the irrigation experiment in March 1982, the whole experimental area (61 ha) was sampled and on some of these samples the CEC was determined. The results displayed a large amount of variability which was seemingly not related to the observed textural differences. In view of this, it was decided to pool all the information of the samples on a depth basis to obtain a set of arithmetic mean values per depth. The same set of mean CEC values was then used as input for both the furrow- and drip irrigation plots (Table 5.7).

No information on either the exchangeable cation composition or the cation selectivity coefficients were available for the two particular plots under consideration. However, a total of 32 samples from all of the Murrieta fields on which both the soluble salt content and ammonium acetate extractable cation composition were determined in 1985/86 and September 1987, were available. The exchangeable cation composition of these 32 samples could thus be calculated (i.e. exchangeable = extractable - soluble). The six Gapon selectivity coefficients for a Ca, Mg, Na & K exchange system were calculated by assuming that the chemical composition of the soil solution and adsorbed phases represent equilibrium conditions. This was done by using CHEMEQ, the stand alone version of the chemical subroutine CHEM of LEACHM. No apparent differences were discernable with depth and consequently pooled mean values only were used for both the furrow and drip irrigated plots. The selectivity coefficients are listed in Table 5.8. Also listed are the mean values of cation selectivity coefficients of Robbins (1986).

Once the selectivity coefficients were known, the soluble salt compositions of March 1983 (Table 5.6) and cation exchange capacities (Table 5.7) could be combined, again using CHEMEQ, to determine the exchangeable cation composition of the soil samples collected in March 1983. These exchangeable cation concentrations were used to represent the conditions at the start of the simulation period and served as input for LEACHM (Table 5.9). This procedure serves as an example of how input requirements can be inferred from other analytical soil data.

A fixed value of 0,001 and 0,01 for the lime and gypsum contents respectively (given as mass fractions) were used throughout for all depths of the drip- and furrow-irrigated plots (Table 5.9).

Table 5.6 Mean concentrations of the soluble salt in the saturated soil paste extracts of the furrow and drip irrigated plots (sampled March 1983)

Depth	Sat	BD	EC		Cl		HCO_3
			Mean	SE	Mean	SE	Mean
m		Mg m^{-3}	mS m^{-1}		mmol dm^{-3}		mmol dm^{-3}
Furrow plot (n=3)							
0,15	56	1,30	280	93	4,2	2,4	nd
0,45	54	1,34	526	334	10,4	8,9	nd
0,75	51	1,38	857	344	29,0	24,3	nd
1,05	44	1,40	919	249	37,3	17,4	nd
1,35	40	1,40	822	292	34,5	16,4	nd
1,65	41	1,45	757	182	27,6	12,2	nd
Drip plot (n=2)							
0,15	59	1,30	128	12	1,5	0,1	4,4
0,45	62	1,34	291	189	1,8	0,5	4,3
0,75	58	1,38	538	418	8,8	6,9	3,3
1,05	55	1,40	567	404	16,4	13,4	3,5
1,35	50	1,40	900	328	38,3	28,0	2,6
1,65	50	1,50	900	na	38,3	na	2,6

Depth	Ca		Mg		Na		SO_4	
	Mean	SE	Mean	SE	Mean	SE	Mean	SE
m	mmol dm^{-3}		mmol dm^{-3}		mmol dm^{-3}		mmol dm^{-3}	
Furrow plot (n=3)								
0,15	5,5	1,6	1,5	0,4	19,3	8,3	9,0	4,0
0,45	5,9	4,7	1,8	1,3	54,5	36,3	21,9	16,4
0,75	7,9	3,7	2,7	1,2	81,6	30,8	30,6	8,0
1,05	8,1	3,4	4,1	1,8	87,4	20,8	29,9	5,8
1,35	7,4	3,5	3,2	2,0	75,0	24,9	24,6	8,2
1,65	7,7	3,5	3,1	1,5	74,5	14,3	34,6	8,0
Drip plot (n=2)								
0,15	6,3	0,2	1,6	0,1	8,9	1,3	7,2	0,4
0,45	6,9	6,5	3,2	na	30,7	18,9	25,2	19,3
0,75	24,4	na	7,2	na	61,7	48,4	56,8	50,8
1,05	12,9	12,5	8,4	na	63,3	45,4	54,8	45,8
1,35	25,8	3,3	7,2	3,2	89,4	31,5	67,4	9,4
1,65	25,8	na	7,2	na	89,4	na	67,4	na

n=number samples, SE=standard error, sat=saturation percentage of paste (g $100g^{-1}$), nd=not determined; na=not available.

Table 5.7 Means of measured CEC values as determined in March 1982

Depth (m)	CEC (mmol(+) kg^{-1})
0,3	294
0,6	277
0,9	211
1,2	175
1,5	165
1,8	160
2,1	162

Table 5.8 Calculated selectivity coefficients for the furrow and drip irrigated fields

Combination	Murrieta Mean	Murrieta S.Dev	Robbins (1986)
Mg/Ca	0,84	0,40	0,39
Ca/Na	4,07	2,85	3,84
Ca/K	0,30	0,16	0,27
Mg/K	0,24	0,14	0,14
Mg/Na	2,85	2,04	1,61
K/Na	16,04	12,61	15,48

S.Dev=standard deviation, n=32

5.2.2.9 Crop information

The crop rotation cycle for the period 1983 to 1987, and other pertinent dates required as input by the LEACHM model, are listed in Table 5.10. The same data were used for both modes of irrigation, with the exception of the 1986 to 1987 period where the details about the cotton crop applies to the drip plot only. The maximum rooting depths for the various crops, as required by the LEACHM model, are also listed in Table 5.10.

5.2.3 Input data for the Burns and TETrans models

5.2.3.1 Hydrological soil properties

Both the BURNS and TETRans models focus on the capacity of a soil to retain its water and therefore requires as input the field capacity for each soil depth. The field capacity used as input for these two models was estimated using the LEACHM model to predict the water content of a soil profile that is in equilibrium with a water table at the 1,65 m depth. The calculated values are listed in Table 5.11. The two models furthermore require a soil water content that resembles the so-called "evaporation limit", i.e. the water content below which evapotranspiration stops. A constant, but arbitrary value of 0,15 m^3 m^{-3} was used for each soil segment.

Table 5.9 Exchangeable cation composition and lime and gypsum content of the furrow- and drip irrigated plots during March 1983

Depth	Ca	Mg	Na	K	Lime	Gypsum
m	<------------	mmol(+) kg^{-1}	------------->		<---fraction--->	
Furrow plot						
0,3	180,8	83,0	23,9	6,3	0,001	0,01
0,6	152,0	72,6	45,7	6,7	0,001	0,01
0,9	111,3	57,3	39,2	3,2	0,001	0,01
1,2	87,8	53,5	29,4	4,3	0,001	0,01
1,5	86,9	50,0	25,1	2,9	0,001	0,01
1,8	83,2	46,6	26,4	3,9	0,001	0,01
2,1	87,6	50,8	19,2	4,5	0,001	0,01
Drip plot						
0,3	183,4	79,3	16,1	15,1	0,001	0,01
0,6	141,4	84,1	38,8	12,7	0,001	0,01
0,9	117,1	56,2	35,7	1,9	0,001	0,01
1,2	80,9	57,8	33,8	2,4	0,001	0,01
1,5	87,8	40,8	34,6	1,8	0,001	0,01
1,8	83,8	38,9	35,4	1,9	0,001	0,01
2,1	84,4	39,3	36,4	1,9	0,001	0,01

Table 5.10 Crop rotation and other phenological information

Crop	Dates (yy,mm,dd) 1	2	3	4	5	Dens	Depth
Cotton	830503	830513	830731	830807	831015	11	0,825
Cotton	840409	840419	840710	840701	841110	11	0,825
Wheat	841214	850107	850315	850301	850617	175	0,975
Sug.beet	851003	851017	860421	860320	860820	15	1,125
Cotton	870416	870430	870715	870722	871123	11	0,825

1=planting; 2=emergence; 3=root maturity; 4=plant maturity; 5=harvest; dens=plant density (.m^{-2}); depth=maximum rooting depth (m)

5.2.3.2 Irrigation, rainfall and evapotranspiration

The same irrigation, rain, and evapotranspiration amounts for the period 1 May 1983 to 31 August 1986 that were used in the LEACHM study, were used as input for the BURNS and TETrans models, the only exception being that the input formats were slightly different. In the case of the Burns model, the irrigation and rainfall, as well as the actual evapotranspiration were supplied on a daily basis in units of cm day^{-1}. Also supplied was the amount of chloride, in units of kg ha^{-1}, applied with the irrigation water. The evapotranspiration, furrow applied irrigation water, and chloride additions of May 1983 serve as an example of the input format required by the two models (Table 5.12).

The input format of the TETrans model differs slightly from the Burns format. Instead of daily evapotranspiration amounts, it uses the total depth of evapotranspiration between two consecutive irrigation/rainfall events. Consequently, the model does not calculate daily soil water and solute fluctuations, but rather the depth distribution of water and solute immediately following, and immediately prior to an irrigation event. The soil water content will therefore be at its maximum (at or close to field capacity), and the salt concentration at its lowest just after an irrigation event. The opposite condition holds for the day preceding the next irrigation. An example of the structure of the input file, as used for the furrow plot simulation, is given in Table 5.12.

5.2.3.3 Soluble salt content (Chloride)

Also required for each soil segment is the initial soluble salt content, in units of kg ha^{-1} for the Burns model, and in mg dm^{-3} for the TETrans model. The Burns model cannot simulate chemical exchange and adsorption processes, while TETrans offers the option to partition a reactive solute into solution and adsorbed phases using appropriate adsorption isotherms. For comparative purposes this study confined itself to the conservative chloride ion only. The concentrations used are the same as that of the LEACHM study and reflect the soil conditions in May 1983. These concentrations are listed in Table 5.11.

5.2.4 Statistical methods

Four different methods were used to evaluate the predicted soil water contents and chemical composition of the soil solution, namely graphical interpretation, linear regression analysis, the root mean square error, and Wilmot's coefficient of agreement (see page 2.14 Chapter 2). The root mean square error, RMSE, is calculated as:

$$RMSE = [1/n\ \Sigma(P-O)^2]^{0.5}$$

where P=predicted and O=observed value.

Table 5.11 Hydrological soil properties and chloride content used as input for the BURNS and TETrans models

Depth (m)	FC (m^3 m^{-3})	EL (m^3 m^{-3})	MC (m^3 m^{-3})	BD (Mg m^{-3})	Cl (mg dm^{-3})	Cl (kg ha^{-1})
a) Furrow plot						
0,15	0,439	0,150	0,299	1,300	425,3	190,7
0,30	0,442	0,150	0,367	1,320	425,3	234,1
0,45	0,387	0,150	0,447	1,340	813,3	545,3
0,60	0,394	0,150	0,451	1,360	813,3	550,2
0,75	0,441	0,150	0,457	1,380	1617,0	1108,5
0,90	0,465	0,150	0,465	1,390	1617,0	1127,9
1,05	0,472	0,150	0,469	1,400	1814,1	1276,2
1,20	0,472	0,150	0,470	1,400	1814,1	1278,9
1,35	0,472	0,150	0,471	1,400	1725,7	1220,2
1,50	0,453	0,150	0,453	1,450	1725,7	1171,5
1,65	0,434	0,150	0,434	1,500	1596,4	1038,8
b) Drip plot						
0,15	0,446	0,15	0,299	1,30	137,4	61,6
0,30	0,444	0,15	0,367	1,32	137,4	75,6
0,45	0,443	0,15	0,447	1,34	116,1	77,8
0,60	0,442	0,15	0,451	1,36	116,1	78,5
0,75	0,463	0,15	0,457	1,38	543,9	372,8
0,90	0,464	0,15	0,465	1,39	543,9	379,3
1,05	0,461	0,15	0,469	1,40	953,5	670,8
1,20	0,465	0,15	0,470	1,40	953,5	672,2
1,35	0,469	0,15	0,471	1,40	2013,9	1424,0
1,50	0,452	0,15	0,453	1,45	2013,9	1367,3
1,65	0,434	0,15	0,434	1,50	2268,5	1476,1
1,80	0,434	0,15	0,434	1,50	2268,5	1476,1
1,95	0,434	0,15	0,434	1,50	2346,6	1526,9
2,10	0,434	0,15	0,434	1,50	2346,6	1526,9

FC=field capacity; EL=evaporation limit; MC=initial water content; BD=bulk density; Cl=chloride content

Table 5.12 Example of the input format for the irrigation, evapotranspiration and salt quantities required by the BURNS and TETrans models

	BURNS format			TETrans format		
Day	Irrig (cm)	Evapot. (cm)	Cl (kg ha^{-1})	Irrig (cm)	Evapot (cm)	Cl (mg dm^{-3})
430	0,0	0,742	0,0			
431	0,0	0,742	0,0			
432	10,9	0,742	27,1	10,9	13,51	24,9
433	0,0	0,742	0,0			
434	0,0	0,742	0,0			
435	0,0	0,749	0,0			
436	0,0	0,749	0,0			
437	0,0	0,749	0,0			
438	0,0	0,749	0,0			
439	0,0	0,749	0,0			
440	0,0	0,749	0,0			
441	0,0	0,749	0,0			
442	0,0	0,698	0,0			
443	0,0	0,698	0,0			
444	0,0	0,698	0,0			
445	0,0	0,698	0,0			
446	0,0	0,698	0,0			
447	0,0	0,698	0,0			
448	0,0	0,698	0,0			
449	0,0	0,634	0,0			
450	0,0	0,634	0,0			
451	0,8	0,634	0,0			
452	10,9	0,634	27,1	11,7	5,19	24,9
453	0,0	0,634	0,0			
454	0,0	0,634	0,0			
455	0,0	0,634	0,0			
456	0,0	0,663	0,0			
457	0,0	0,663	0,0			
458	0,0	0,663	0,0			
459	0,0	0,663	0,0			
460	10,9	0,663	27,1	10,9	8,60	24,9

5.3 RESULTS

5.3.1 Soil Water Content

The predicted depth distribution of the soil water content of the furrow and drip irrigated plots for three dates during 1983 are given in Figures 5.2 and 5.3 and show a rather poor accord between measured and predicted values. This is especially true for the Burns and TETrans models, where depending on the depth, the predicted soil water content deviated markedly from the observed data. For example, on 20 October 1983, both the Burns and TETrans models severely underestimated the soil water content of the 0-1,0 m depth. TETrans predicted that the soil water content will increase abruptly from about the 1,0 m depth, while the BURNS model predicted a similar, but less abrupt increase to occur below the 1,4 m depth (Figure 5.2). The information depicted in Figures 5.2 and 5.3 also reveal a tendency for the two functional models to either consistently underpredict (shallower depths) or overpredict (deeper depths) the soil water content.

It is possible that the poor performance of the two functional models was caused by the field capacity and evaporation limits that were chosen. A more likely explanation for the sharp discontinuities and consistent under- and overprediction of the soil water content, is the way in which evapotranspiration and redistribution is handled in the Burns and TETrans models. On any specific day all of the water required to meet the ET demand is drawn from the first soil layer (or layers) in which sufficient water is available. Water uptake is not handled according to root distribution. This, as well as the fact that the two models do not make sufficient provision for redistribution during the process of water uptake, can result in sharp discontinuities as shown by the data in Figures 5.2 and 5.3.

In the case of the furrow plot, the LEACHM predicted values accorded better with the observed data (Figure 5.2). However, on the drip plot, LEACHM overpredicted the soil water content at the depths shallower than 1,2 m (Figure 5.3). Although only three dates are shown in Figure 5.3, similar poor agreements were observed at other dates.

The predicted temporal fluctuations in the soil water content at three depths of the furrow plot for the period 1983 to 1986, are given in Figure 5.4a. These values were used to calculate the quantitative statistics, i.e. the Wilmot d-indices and root mean square error (RMSE) values for the LEACHM predicted soil water content of the furrow- and drip irrigated plots. In these calculations all the comparisons of measured and predicted soil water content for the respective simulation periods (i.e. 1983 to

1986 for the furrow, and 1983 to 1987 for the drip plots) were used. The results of the 0,45 m, 0,75 m and 1,35 m, as well as the profile water content are listed in Table 5.13. The root mean square error (RMSE) for the profile water content is 98 mm per 1,65 m profile, and 137 mm per 2,10 m profile for the furrow and drip irrigated fields respectively. The d-values in all cases are less than 0,7 which is indicative of a poor predictive capability.

Table 5.13 Statistics summarizing the comparison of LEACHM -predicted and measured soil water content for the furrow (1983-1986 data) and drip (1983-1987 data) irrigated plots

Depth (m)	n	d	RMSE	Units
Furrow plot				
0,45	37	0,666	0,050	$m^3\ m^{-3}$
0,75	37	0,508	0,067	$m^3\ m^{-3}$
1,35	37	0,402	0,083	$m^3\ m^{-3}$
0-1,65	37	0,595	98	mm
Drip plot				
0,45	36	0,480	0,089	$m^3\ m^{-3}$
0,75	36	0,492	0,084	$m^3\ m^{-3}$
1,35	36	0,652	0,062	$m^3\ m^{-3}$
0-2,10	36	0,585	137	mm
n=sample size; RMSE=Root mean square error; d=Wilmot's index of agreement				

Table 5.14 Root mean square error and Wilmot's d-index for the predicted and measured soil water content during the period May 1983 to July 1984

Depth (m)	n	d	RMSE	Units
Furrow plot				
0,45	23	0,891	0,030	$m^3\ m^{-3}$
0,75	23	0,759	0,042	$m^3\ m^{-3}$
1,35	23	0,595	0,054	$m^3\ m^{-3}$
0-1,65	23	0,816	65	mm
Drip plot				
0,45	18	0,463	0,098	$m^3\ m^{-3}$
0,75	18	0,473	0,084	$m^3\ m^{-3}$
1,35	18	0,622	0,042	$m^3\ m^{-3}$
0-2,10	18	0,517	118	mm

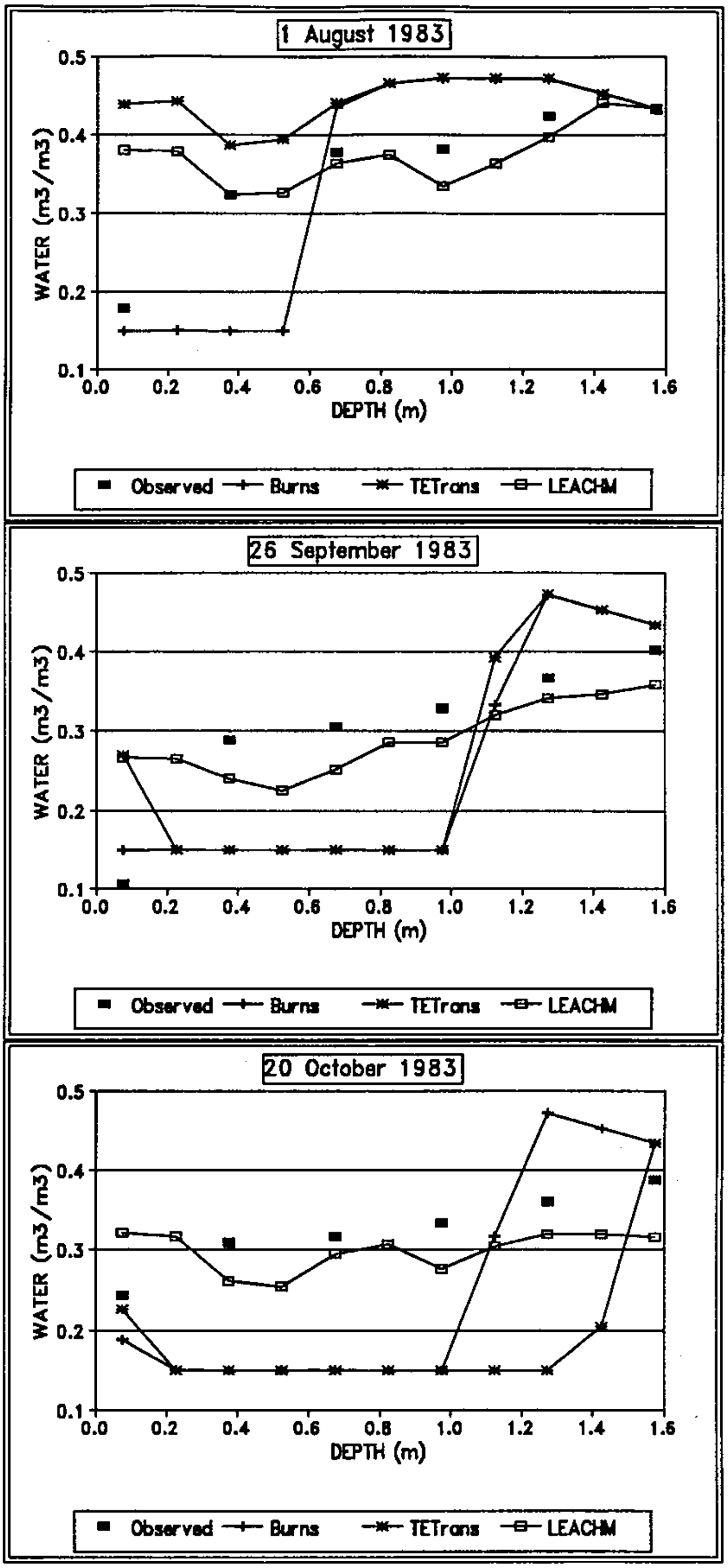


Figure 5.2 Observed and predicted soil water content of the furrow irrigated plot on three dates during the 1983 season

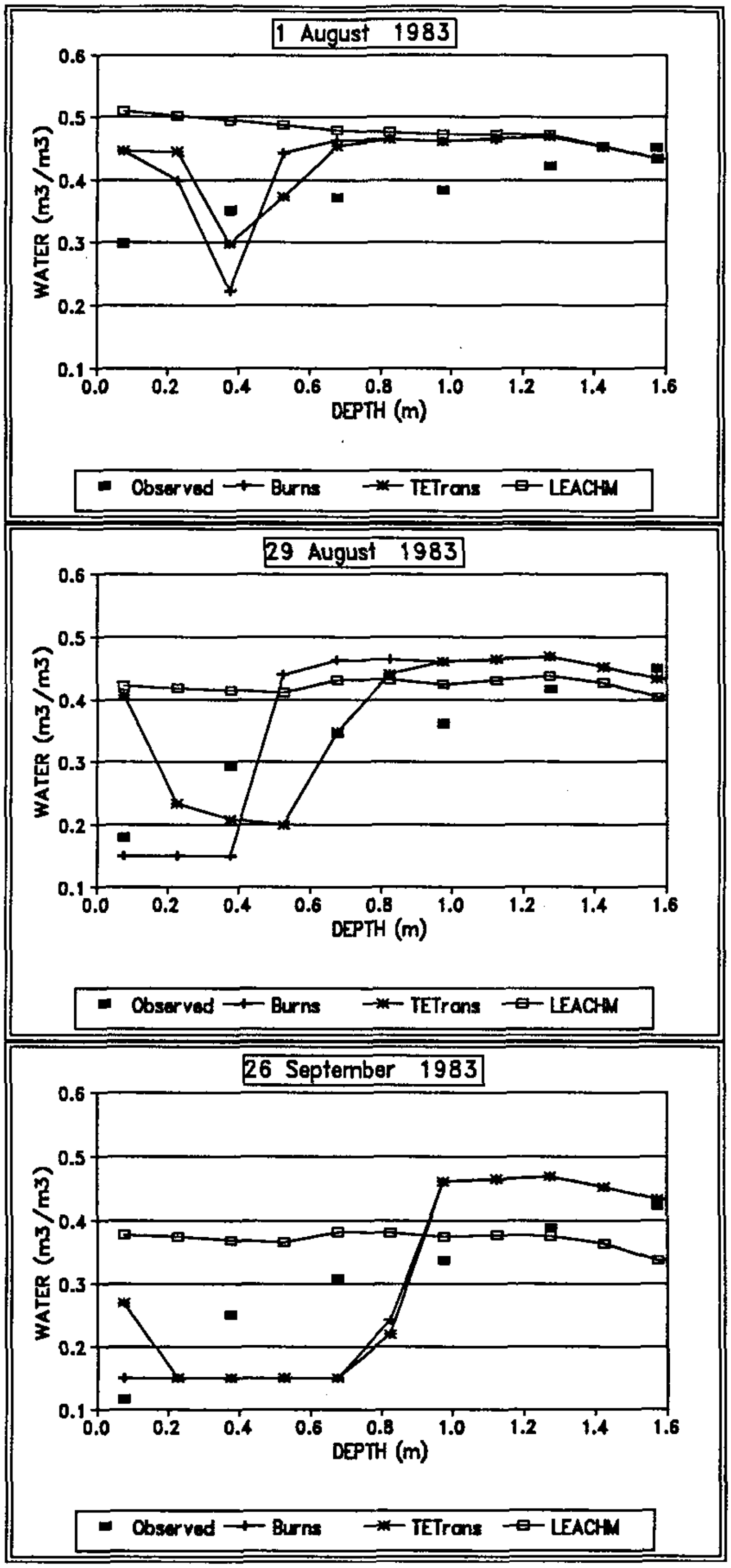


Figure 5.3 Observed and predicted soil water content of the drip irrigated plot on three dates during the 1983 season

The observed temporal distribution of the measured soil water content of the furrow irrigated plot for the period 1983 to 1987 offer a possible explanation for the poor agreement (Figure 5.4b). The soil water content for the period 1983 to October 1984 on the whole is substantially higher than the 1985, 1986 and 1987 water contents. Despite comparable irrigation applications and weather conditions for the different seasons, the soil water content apparently never got back to the values initially measured during 1983 and the early part of 1984. (The water content of the drip irrigated plot show a similar trend). No soil physical or hydrological explanation could be offered for this, i.e. the porosity of the soil, and the depth and fluctuation of the water table did not change during the period 1983 to 1986. A possible explanation for this observation is the fact that two different neutron probes (i.e. a Troxler and a CPN) with different radioactive sources and probe diameters were used during the course of the irrigation experiment. It is not certain when the change to the larger diameter probe was made but apparently it happened during the second half of 1984. Furthermore, during the course of 1984 when the new CPN probe was being put into use, it was not calibrated using *in situ* collected gravimetric samples from Murrieta, but against another, previously calibrated CPN probe. The accuracy and statistical measures of neither of the two calibration equations were reported or recorded.

These long term changes in the soil water content were not detected during the course of the irrigation experiment, because short term water balances and crop water uptake quantities only were calculated. It was only when the data required for this particular modelling study were assembled, that the long term temporal drift in the soil water content became apparent. Against this background it seems justifiable not to use the soil water content that has been measured since July 1984 as values against which the predicted results can be compared. When only the 1983 to 1984 data is considered, the RMSE and d-indices improve considerably (Table 5.14).

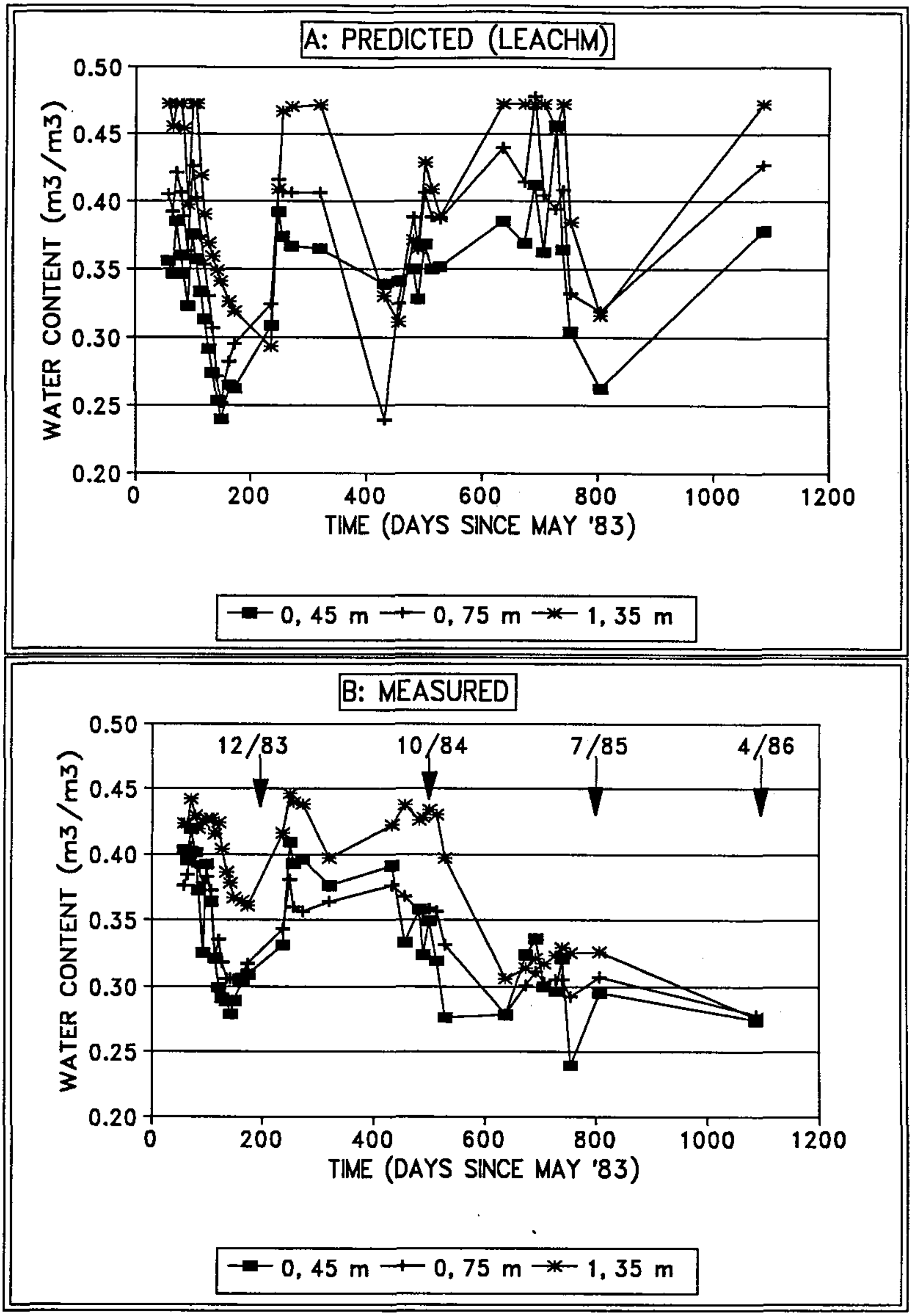


Figure 5.4 **Fluctuations in the soil water content between 1983 and 1986 at three depths of the furrow irrigated plot; a) Predicted with LEACHM, b) Measured with a neutron probe**

5.3.2 Soil Chemistry

5.3.2.1 General

The chemical composition of the soil solution was measured on a few occasions only with the result that a limited amount of data were available to evaluate the accuracy of the predicted chemical composition of the two experimental fields. In the case of the furrow irrigated field, the soil was sampled and analyzed on four occasions, i.e. during March and November 1984, March 1985, and August 1986 when the original experiment on the furrow plot was terminated. The drip plot was sampled at the following eight times: during March and November 1984, March and October 1985, March and October 1986, and March and November 1987.

The chemical concentrations calculated by all three simulation models are at field water content. Consequently, for the purpose of comparison, the predicted concentrations had to be adjusted to reflect those of a saturated soil paste. In the case of chloride, which is a conservative anion, this adjustment was a simple dilution, but for all the other ions, both a simple dilution as well as chemical reactions such as dissolution of gypsum at the higher saturated paste water content were also considered. This was done by using CHEMEQ, the standalone chemistry programme of LEACHM.

The Burns model can simulate the chemistry of conservative salts like chloride only and, although TETrans can simulate some chemical exchange reactions, in this study the simulation was restricted to the transport of the non-reactive chloride ion. The LEACHM-simulation included the chemistry of the other major cations and anions of the soil solution as well. Consequently, the results pertaining to the chloride ion, and the other more reactive ions, will be dealt with separately.

5.3.2.2 Chloride: Burns, TETrans and LEACHM predictions

The predicted chloride concentrations at the end of the simulation period, adjusted to the soil water content of a saturated paste extract, are given in Figures 5.5 and 5.6 for the furrow and drip plots respectively. The chloride concentration at the end of the experiment correspond to the August 1986 (furrow plot) and November 1987 (drip plot) sampling events. It is quite clear that the depth distribution of chloride predicted with the Burns and TETrans models bear no resemblance to the observed data. The accordance between the LEACHM predictions and observed data are substantially better than the Burns and TETrans predictions. The LEACHM simulation of the drip plot furthermore seems to be better than that of the furrow plot. This latter result is the opposite of a previous observation where the quantitative statistics suggested a more accurate prediction of soil water content in the furrow irrigated plot than on the drip irrigated plot (Tables 5.13 and 5.14).

The superior predictive ability of the LEACHM model over the Burns and TETrans models is supported by the root mean square error (RMSE) and d-index values which indicate a smaller error and better accordance between predicted and observed chloride concentrations at all depths (Table 5.15). (The predicted chloride concentrations used in the statistical analyses were adjusted to the water content of a saturated soil paste).

Table 5.15 Statistics of the comparison between predicted and observed chloride concentration of a saturated soil paste

Depth (m)	LEACHM RMSE	d	Burns RMSE	d	TETrans RMSE	d
Furrow irrigated plot						
0,225	10,54	0,42	12,75	0,35	12,49	0,36
0,525	15,45	0,49	24,94	0,31	24,31	0,32
0,825	20,23	0,42	41,57	0,24	37,25	0,27
1,125	9,15	0,39	33,12	0,37	26,76	0,00
1,425	16,93	0,33	15,97	0,04	33,43	0,30
0-1,650	16,80	0,76	31,08	0,43	31,50	0,52
Drip irrigated plot						
0,225	3,6	0,97	11,5	0,62	11,6	0,74
0,525	15,1	0,77	30,6	0,37	10,3	0,76
0,825	14,6	0,72	47,7	0,11	27,9	0,52
1,125	20,5	0,59	57,7	0,12	35,0	0,25
1,425	29,1	0,56	53,0	0,11	31,4	0,17
0-1,650	41,5	0,79	97,4	0,32	56,8	0,53

Units of RMSE (root mean square error) = mmol dm^{-3}

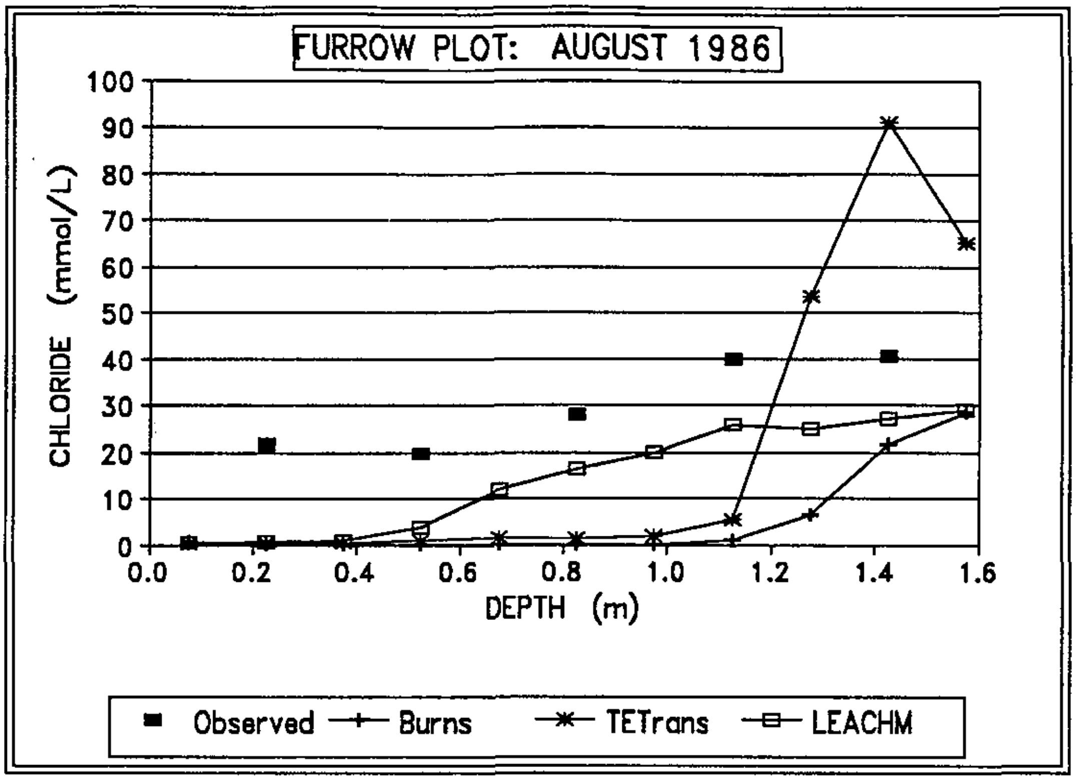


Figure 5.5 Observed and predicted chloride content of the furrow irrigated plot at the end of the irrigation experiment in August 1986

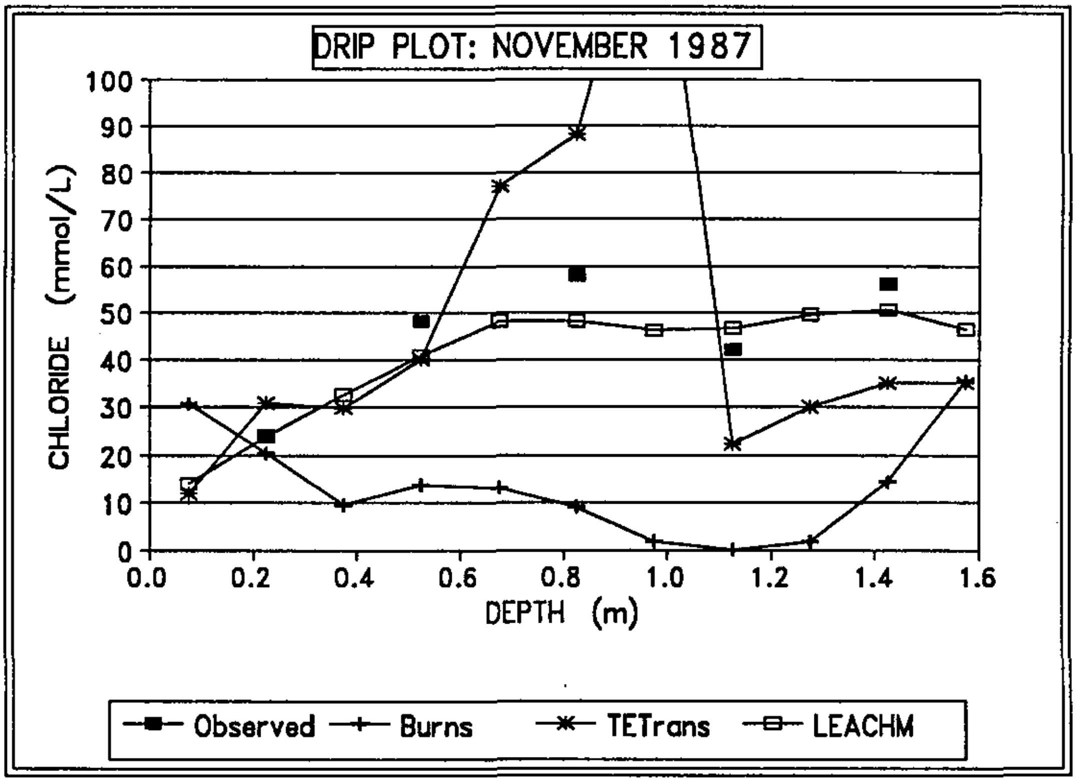


Figure 5.6 Observed and predicted chloride content of the drip irrigated plot at the end of the drip irrigation experiment in November 1987

5.3.2.3 LEACHM-predicted Ca, Mg, Na, SO_4 and EC

As previously mentioned, the concentrations calculated by LEACHM reflect the equilibrium chemical composition of the solution and adsorbed phases at the prevailing soil water content. When the predicted concentrations are diluted to that of a saturated soil paste, the solution and adsorbed phases will not be in equilibrium any more. The equilibrium concentrations at the higher soil water content (i.e. saturated paste water content), were calculated with the simulation model CHEMEQ. In the following paragraphs, the results of both the simple dilution, i.e. non-equilibrium condition, and CHEMEQ adjusted equilibrium condition will be illustrated and statistically analysed.

Table 5.16 Linear regression statistics of the comparison over time and depth between the predicted and measured chemical composition of the furrow irrigated plot, 1983-1986 data (4 sampling events, n=20)

	a	Std Err	b	Std Err	R^2
Without chemical equilibrium					
EC	274	263,3	0,94	0,22	0,510
Cl	13,99	13,06	0,65	0,19	0,388
SO_4	0,42	14,77	2,23	0,53	0,383
Ca	14,63	11,62	0,28	0,84	0,006
Mg	3,07	1,86	0,34	0,19	0,143
Na	22,31	23,05	0,82	0,14	0,642
With chemical equilibrium					
EC	4,63	16,75	1,29	0,41	0,356
Cl	13,99	13,06	0,65	0,19	0,388
SO_4	4,63	16,75	1,29	0,41	0,356
Ca	11,04	11,56	0,45	0,86	0,015
Mg	2,92	1,90	0,30	0,20	0,109
Na	14,42	20,92	0,79	0,12	0,706
a=intercept, b=slope; concentration in mmol dm^{-3}; EC in mS m^{-1}					

The intercept, slope and coefficient of determination of a linear regression analysis on the data of all the sampling events and depths, with and without considering the new chemical equilibria at the saturated paste water content, are listed in Tables 5.16 and 5.17 for the furrow and drip irrigated plots respectively. The results indicate a lack of a 1:1 relationship as well a poor prediction. Consideration of the chemical equilibrium at the higher water content, in general yielded slightly higher R^2 values. It also seems as if the predicted chloride and sodium concentrations accord better with the measured data than is the case with calcium, magnesium and sulphate ions. These statistics give the impression that LEACHM failed to simulate the chemical processes in the soil accurately. The scatterplots of the 'best' and 'worst' comparisons (in terms of the R^2 values), for the furrow and drip irrigated plots are given as Figures 5.7 and 5.8. These graphs visually confirm the lack of agreement between the predicted and observed results, which is particularly evident in the case of Ca. The actual magnitude of the errors produced by LEACHM is given by the root mean square error values (RMSE) listed in Tables 5.18 and 5.19. Also indicated are Wilmot's indices of agreement for each ion and depth.

The d-indices calculated for the whole soil profile, i.e. 0-1,65 m, suggests a better prediction of total salt content, (i.e. EC_e), chloride and sodium than is the case with sulfate, calcium and magnesium. However, in spite of the higher d-indices, the RMSE values for EC, Cl, SO_4 and Na are much larger than for Ca and Mg. For some of the ions and depths, the errors are in excess of 20 mmol dm^{-3} which in many real world cases will be unacceptable.

Based on the results given in Tables 5.18 and 5.19 the following additional deductions can be made:

i) Adjusting the chemical composition of the soil solution to obtain chemical equilibrium at the higher water content, did not necessarily resulted in higher d-values.

ii) The magnitude of the RMSE and d-values were not influenced by the method of irrigation, i.e. they are more or less the same for both the furrow and drip irrigated plots.

Table 5.17 Linear regression statistics of the comparison over time and depth between the predicted and measured chemical composition of the drip irrigated plot, 1983-1986 data (8 sampling events, n=40)

	a	Std Err	b	Std Err	R^2
Without chemical equilibrium					
EC	58,59	293,39	1,38	0,19	0,590
Cl	2,95	15,70	1,23	0,16	0,597
SO_4	11,29	13,22	0,97	0,27	0,253
Ca	26,47	4,12	-2,21	0,68	0,218
Mg	1,74	1,89	0,48	0,20	0,136
Na	6,70	27,32	1,15	0,16	0,585
With chemical equilibrium					
EC	-432,24	288,96	1,29	0,17	0,602
Cl	2,95	15,70	1,23	0,16	0,597
SO_4	-11,57	11,85	1,12	0,22	0,400
Ca	25,63	4,59	-1,11	1,01	0,031
Mg	1,96	1,93	0,31	0,15	0,101
Na	-4,82	25,84	1,04	0,13	0,629

a=intercept, b=slope; concentration in mmol dm^{-3}; EC in mS m^{-1}

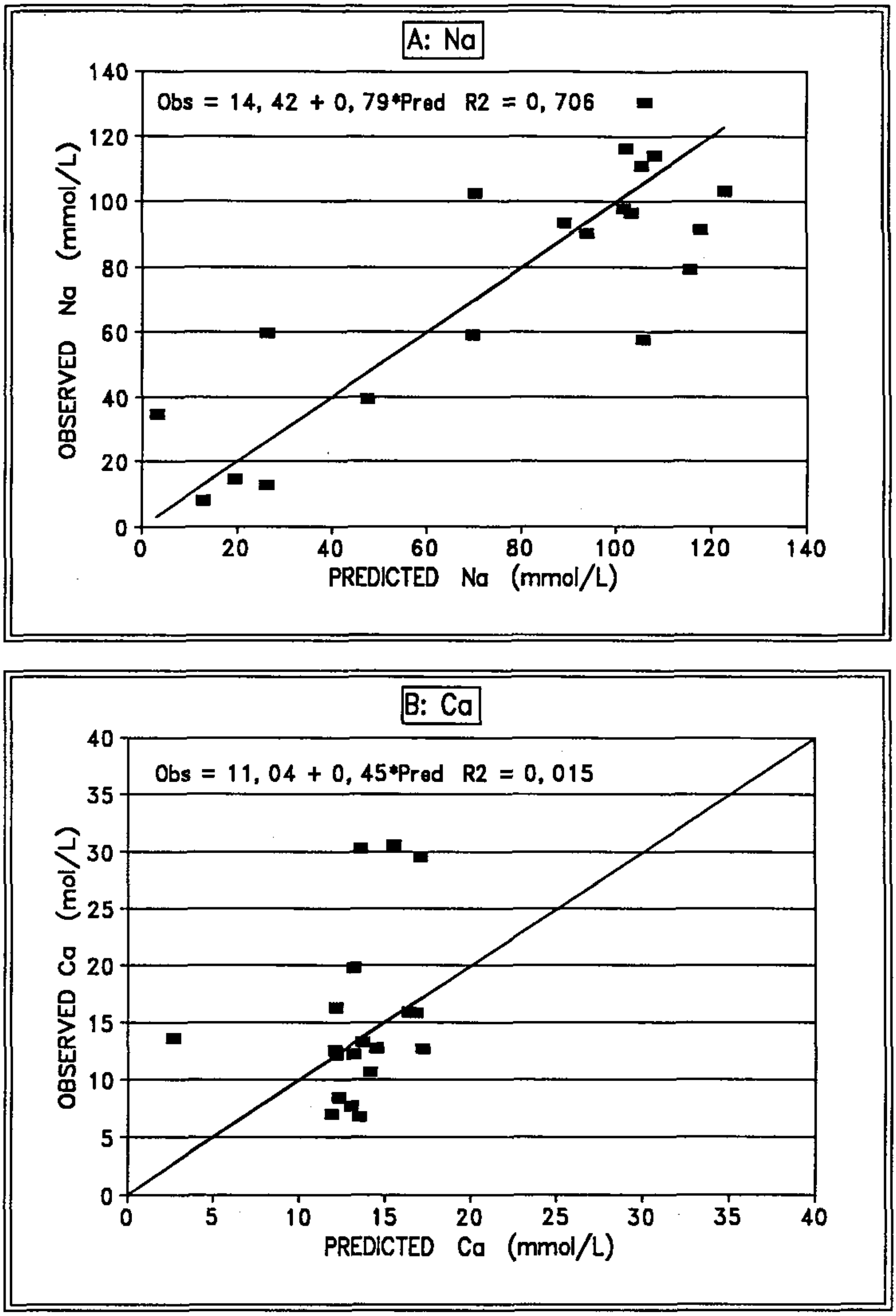


Figure 5.7 Scatterplot and the 1:1 relationship between predicted and observed sodium (a) and calcium (b) concentrations over time and depth for the furrow irrigated plot (1983-1986 data)

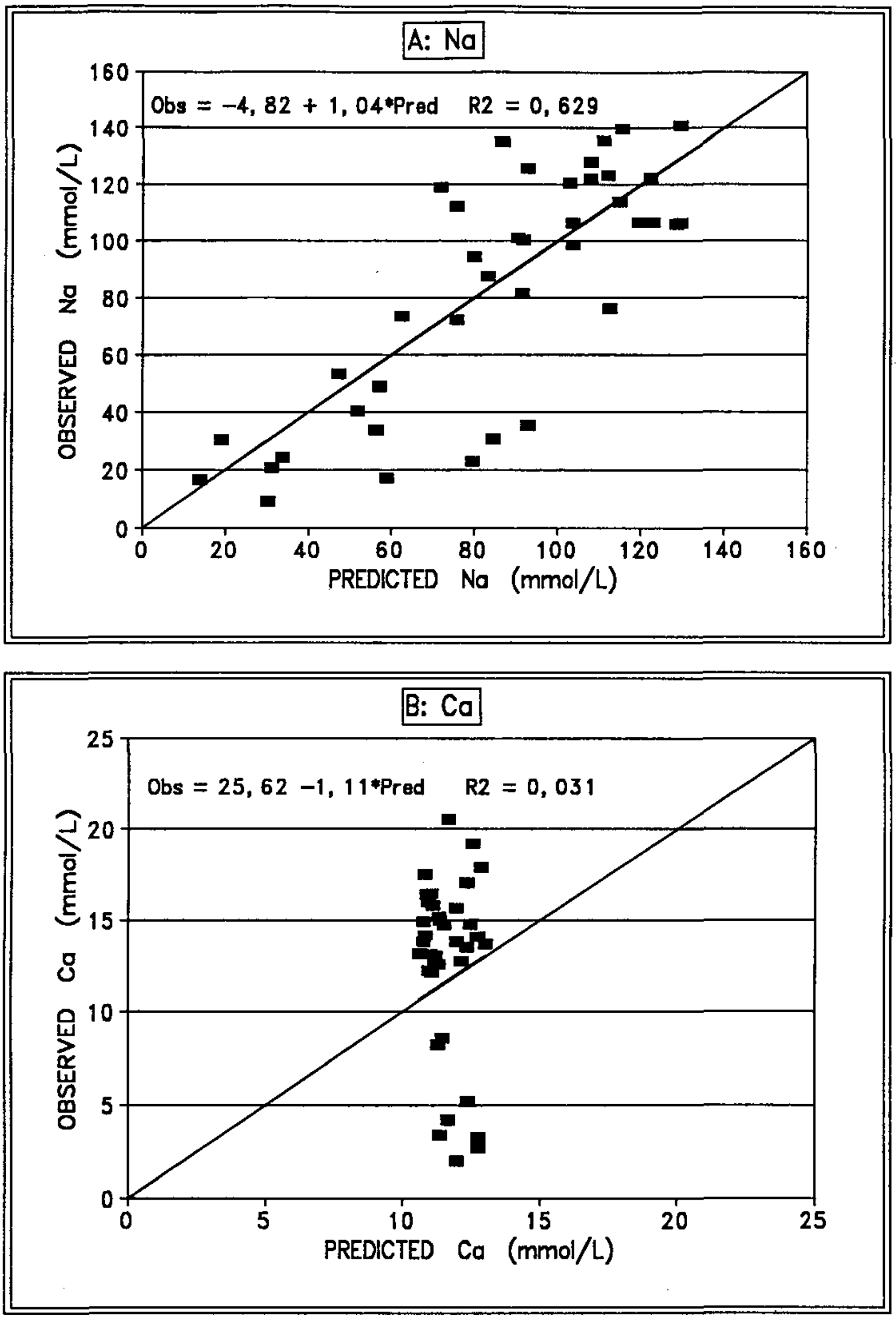


Figure 5.8 Scatterplot and the 1:1 relationship between predicted and observed sodium (a) and calcium (b) concentrations over time and depth for the drip irrigated plot (1983-1987 data)

Table 5.18 Root mean square error and Wilmot's index of agreement between the predicted and measured chemical composition of the furrow irrigated plot, 1983-1986 data (n=4)

a) Dilution without chemical equilibrium reactions

DEPTH m	EC ($mS\ m^{-1}$) RMSE	d	Cl ($mmol\ dm^{-3}$) RMSE	d	SO_4 ($mmol\ dm^{-3}$) RMSE	d
0,225	248	0,30	10,54	0,42	9,71	0,08
0,525	461	0,41	15,45	0,49	28,59	0,38
0,825	333	0,25	20,23	0,42	36,43	0,40
1,125	383	0,38	9,15	0,39	32,79	0,32
1,425	274	0,32	16,93	0,33	34,11	0,31
0-1,65	389	0,73	16,80	0,76	33,46	0,53

DEPTH m	Ca ($mmol\ dm^{-3}$) RMSE	d	Mg ($mmol\ dm^{-3}$) RMSE	d	Na ($mmol\ dm^{-3}$) RMSE	d
0,225	8,1	0,35	2,5	0,37	16,6	0,23
0,525	24,0	0,44	2,8	0,54	34,6	0,48
0,825	12,0	0,46	2,3	0,31	22,3	0,54
1,125	10,5	0,49	1,6	0,56	20,6	0,28
1,425	8,1	0,49	2,1	0,61	27,7	0,23
0-1,65	15,5	0,42	2,6	0,63	28,1	0,88

b) Dilution with chemical reactions

DEPTH m	EC ($mS\ m^{-1}$) RMSE	d	Cl ($mmol\ dm^{-3}$) RMSE	d	SO_4 ($mmol\ dm^{-3}$) RMSE	d
0,225	339	0,00	10,54	0,42	13,25	0,00
0,525	271	0,57	15,45	0,49	17,51	0,35
0,825	267	0,37	20,23	0,42	23,38	0,47
1,125	402	0,42	9,15	0,39	21,99	0,39
1,425	564	0,36	16,93	0,33	27,09	0,34
0-1,650	430	0,76	16,80	0,76	23,70	0,62

DEPTH m	Ca ($mmol\ dm^{-3}$) RMSE	d	Mg ($mmol\ dm^{-3}$) RMSE	d	Na ($mmol\ dm^{-3}$) RMSE	d
0,225	7,7	0,14	2,46	0,05	17,6	0,12
0,525	21,1	0,38	1,92	0,50	24,3	0,59
0,825	8,8	0,42	2,46	0,01	5,0	0,93
1,125	7,6	0,48	2,51	0,42	20,7	0,07
1,425	6,7	0,36	2,71	0,52	30,8	0,36
0-1,650	13,1	0,33	2,71	0,58	24,0	0,91

RMSE=root mean square error; d=Wilmot's index of agreement.

Table 5.19 Root mean square error and Wilmot's index of agreement between the predicted and measured chemical composition of the drip irrigated plot, 1983-1987 data (n=8)

a) Dilution without chemical reactions

DEPTH m	EC ($mS\ m^{-1}$) RMSE	d	Cl ($mmol\ dm^{-3}$) RMSE	d	SO_4 ($mmol\ dm^{-3}$) RMSE	d
0,225	185,8	0,75	3,6	0,97	10,1	0,43
0,525	328,7	0,62	15,1	0,77	16,0	0,48
0,825	492,3	0,55	14,6	0,72	18,5	0,52
1,125	491,2	0,53	20,5	0,59	18,6	0,50
1,425	578,4	0,49	29,1	0,56	18,3	0,44
0-1,650	980,2	0,70	41,5	0,79	37,1	0,59
DEPTH m	**Ca ($mmol\ dm^{-3}$) RMSE**	**d**	**Mg ($mmol\ dm^{-3}$) RMSE**	**d**	**Na ($mmol\ dm^{-3}$) RMSE**	**d**
0,225	7,0	0,42	1,8	0,74	10,6	0,76
0,525	9,7	0,34	1,7	0,74	23,0	0,65
0,825	8,9	0,31	2,1	0,63	37,8	0,54
1,125	8,3	0,29	2,1	0,54	37,4	0,49
1,425	7,2	0,30	2,6	0,50	39,6	0,46
0-1,650	18,5	0,35	4,7	0,59	71,0	0,80

b) Dilution with chemical reactions

DEPTH m	EC ($mS\ m^{-1}$) RMSE	d	Cl ($mmol\ dm^{-3}$) RMSE	d	SO_4 ($mmol\ dm^{-3}$) RMSE	d
0,225	325,7	0,66	3,6	0,97	17,3	0,50
0,525	286,7	0,68	15,1	0,77	12,8	0,47
0,825	312,9	0,67	14,6	0,72	14,1	0,59
1,125	299,4	0,61	20,5	0,59	11,1	0,66
1,425	333,3	0,54	29,1	0,56	9,4	0,61
0-1,650	697,8	0,80	41,5	0,79	29,6	0,67
DEPTH m	**Ca ($mmol\ dm^{-3}$) RMSE**	**d**	**Mg ($mmol\ dm^{-3}$) RMSE**	**d**	**Na ($mmol\ dm^{-3}$) RMSE**	**d**
0,225	5,1	0,25	4,0	0,53	13,5	0,75
0,525	5,1	0,38	3,6	0,50	21,2	0,68
0,825	5,1	0,21	3,2	0,52	28,7	0,61
1,125	4,7	0,12	2,9	0,52	29,3	0,56
1,425	4,1	0,06	2,1	0,55	29,7	0,54
0-1,650	10,8	0,17	7,2	0,47	56,5	0,87

RMSE=root mean square error; d=Wilmot's index of agreement

Another method to evaluate the model predictions, is a visual comparison between the observed and predicted ion concentrations at the end of the simulation period, i.e. when the irrigation experiment was terminated. This comparison differs from the previous methods in that the measurements of one sampling event only are used. In the case of the furrow plot the final concentrations refer to the sampling event of August 1986, while those of the drip plot refer to the samples collected in November 1987. The results are represented in Figures 5.9 to 5.13, and include both the equilibrium and non-equilibrium conditions. With the exception of the calcium and magnesium contents of the drip irrigated plot, the predicted results seem to be a fair to good representation of actual soil conditions. For example, the concentrations and depth distributions of the chloride and sodium ions on both the furrow and drip irrigated plots are for all practical purposes exact copies of the observed values and depth trends. However, this is true only when the new chemical equilibrium are considered. If the LEACHM results are just diluted to the water content of the saturated paste, underpredictions are obtained.

The predicted depth trends in the concentrations of calcium and magnesium on the drip plot are not in agreement with the observed data. In the case of magnesium, the concentration was observed to increase slightly with depth, while LEACHM predicted a decrease from approximately 11,5 mmol dm^{-3} at the surface to 4,5 mmol dm^{-3} at the 1,60 m depth. Similarly, LEACHM calculated that the calcium concentration will not change with depth, as opposed to the slight increase (albeit erratic) that was observed. A possible explanation for this results is that the cation exchange capacities and cation selectivity coefficients that were used as input do not apply to the drip plot. However, the sensitivity analysis of LEACHM (Chapter 3) suggests that the exchange properties will have a minor effect on the predicted chemical composition of the soil solution. Also, the calculation of the sodium content was good and this gives some support for the selectivity coefficients that were used. Therefore, no explanation for this result can be offered at this stage other than the possible effect of spatial variability (discussed below) and possible analytical errors.

Despite the poor prediction of calcium and magnesium on the drip plot, the overall impression given by the results contained in Figures 5.9 to 5.13 is in contrast with the quantitative statistics listed in Tables 5.16 to 5.19, i.e. R^2, RMSE and d-indices. This anomaly might be explained by the influence of spatial variability on the estimate of the true mean, i.e. the way in which the experimental plots were sampled. Apparently the samples were not taken at exactly the same positions within each plot every year. Furthermore, only a limited number of samples were collected each time. These two factors make it difficult to get reliable estimates of the mean salt content of each plot and to detect temporal trends which can be used to evaluate the predicted values. A good example of this is given in Table 5.20 where the coefficients of variation for the initial (March 1983) and final (August 1986; November 1987) sampling events for some of the ions are listed. The coefficients of variation vary substantially between the different ions, depths and times. It is not clear why the CV's of the March 1983 samples are so much larger than those of the final sampling event. It is unlikely that the applied irrigation water could have reduced the spatial variability of the soluble salt content to the extent that is suggested by the smaller coefficients of variation indicated in Table 5.20.

The final attempt to evaluate the adequacy of the LEACHM predictions was to use only the results at the end of the two simulation periods and to pool all the data, irrespective of the various ions (Cl,SO_4,Ca,Mg,Na) and depths, and to compare them with the observed data of the final sampling events. This comparison was quantified by using linear regression techniques, Wilmot's d-index, and RMSE values. The visual result of this comparison is illustrated as scatter plots in Figure 5.14 and suggests a very good accord between observed and predicted salt contents. This impression is supported by the d-indices and R^2 values which for both plots are in excess of 0,90. The statistics also indicate that the simulation of the drip plot is better than that of the furrow plot inasmuch that the slope of the regression line is closer to 1, the intercept is smaller, and the d-index larger. It is granted that the validity of this statistical technique might be questioned especially as the R^2-values of the regression statistics are greatly influenced by the few very high concentrations indicated in Figure 5.14.

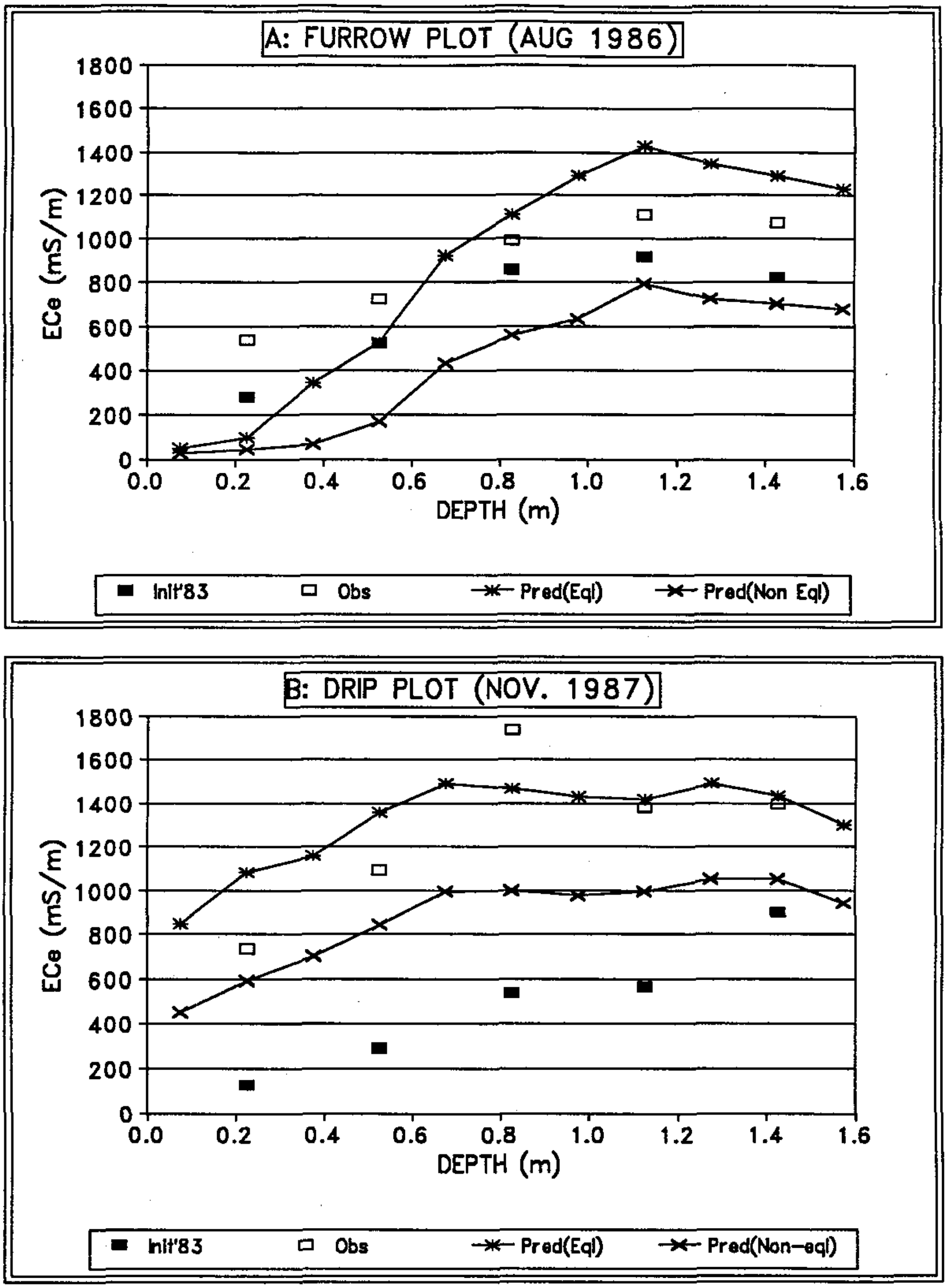
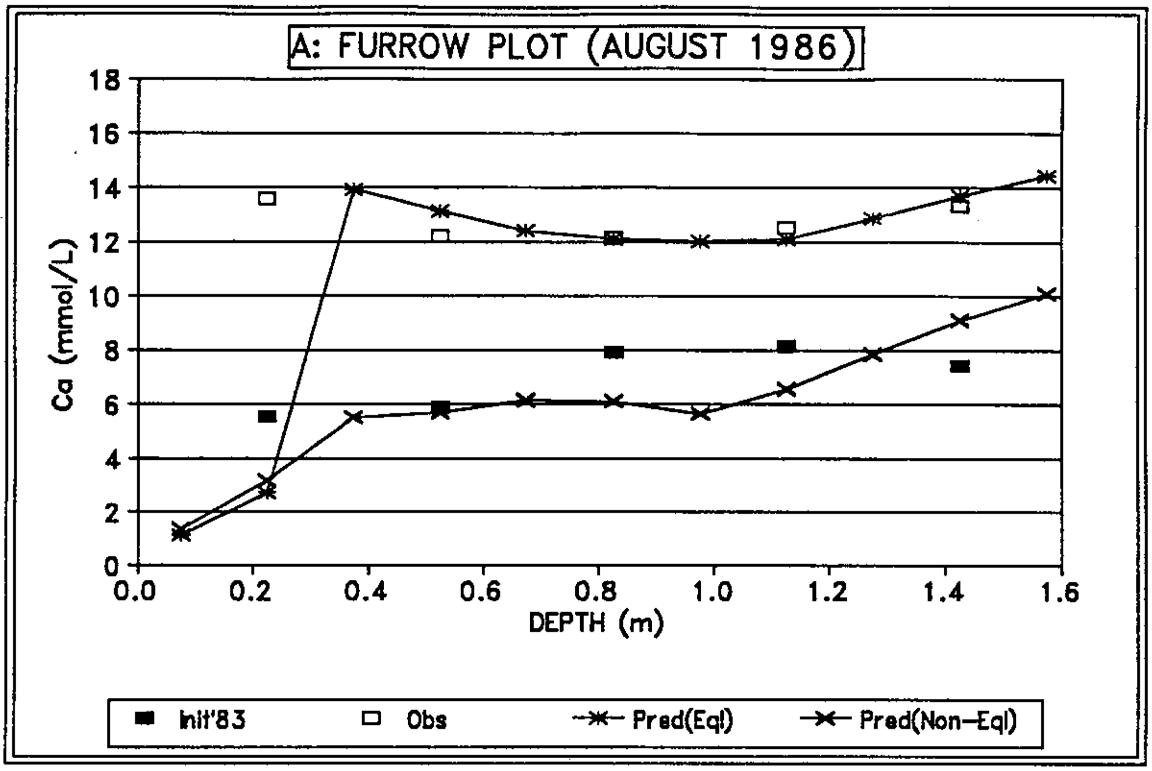


Figure 5.9 Predicted and observed electrical conductivity at the end of the irrigation experiment, with and without adjustment for a new chemical equilibrium at the water content of a saturated soil paste: a) furrow irrigated, and b) drip irrigated plot



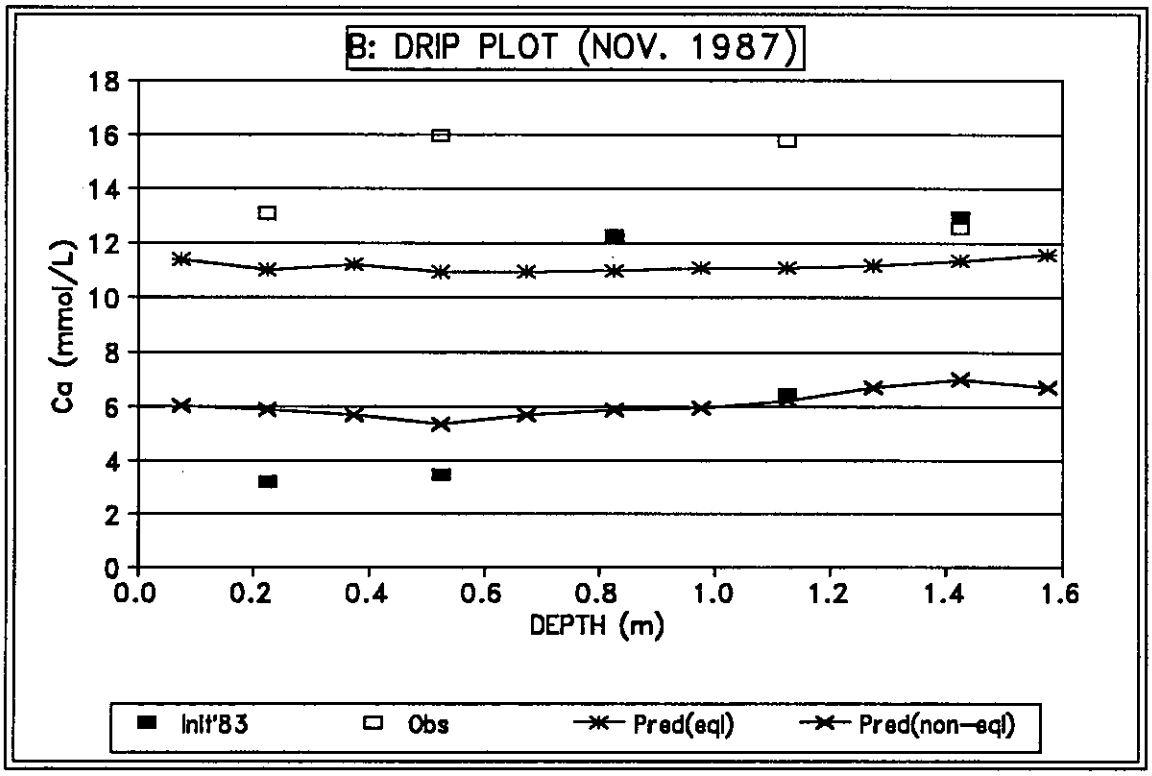


Figure 5.10 Predicted and observed Calcium concentration at the end of the irrigation experiment, with and without adjustment for a new chemical equilibrium at the water content of a saturated soil paste: a) furrow irrigated, and b) drip irrigated plot

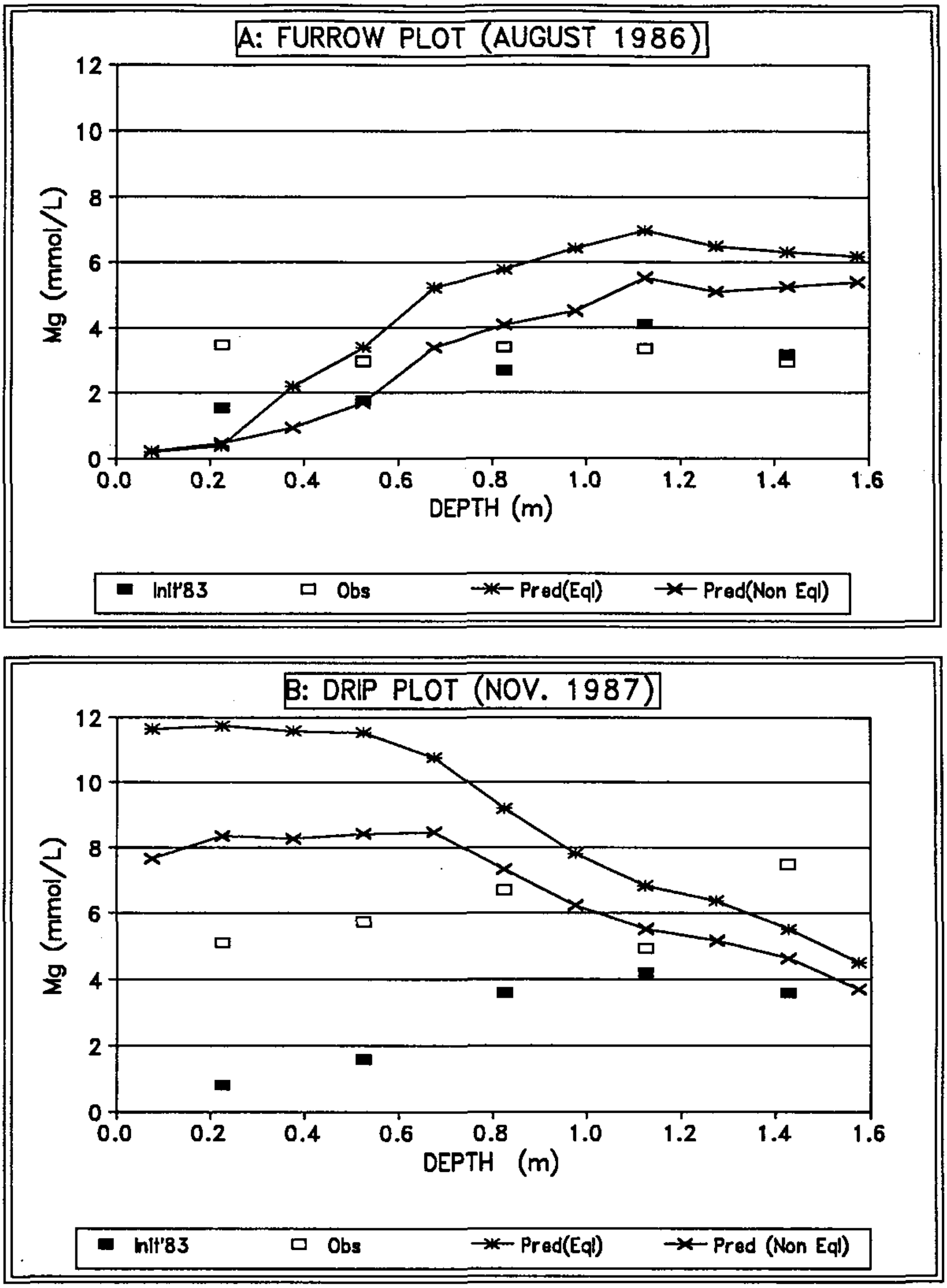
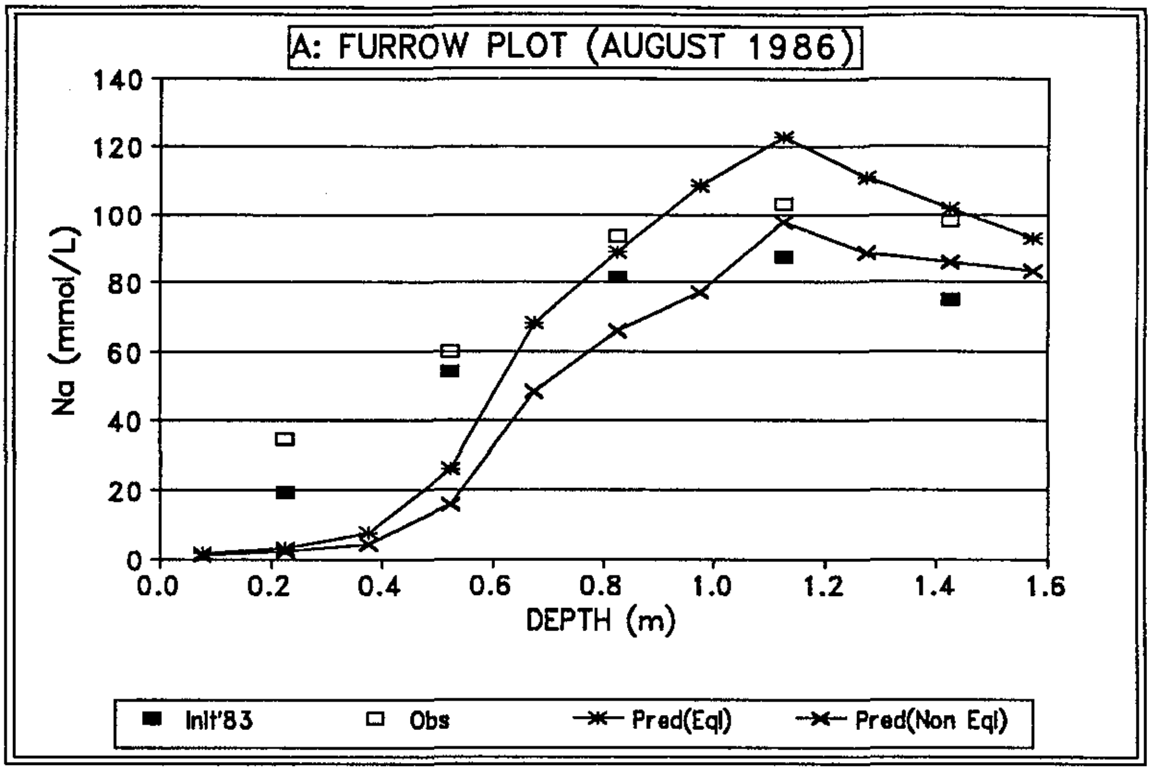


Figure 5.11 Predicted and observed Magnesium concentration at the end of the irrigation experiment, with and without adjustment for a new chemical equilibrium at the water content of a saturated soil paste: a) furrow irrigated, and b) drip irrigated plot



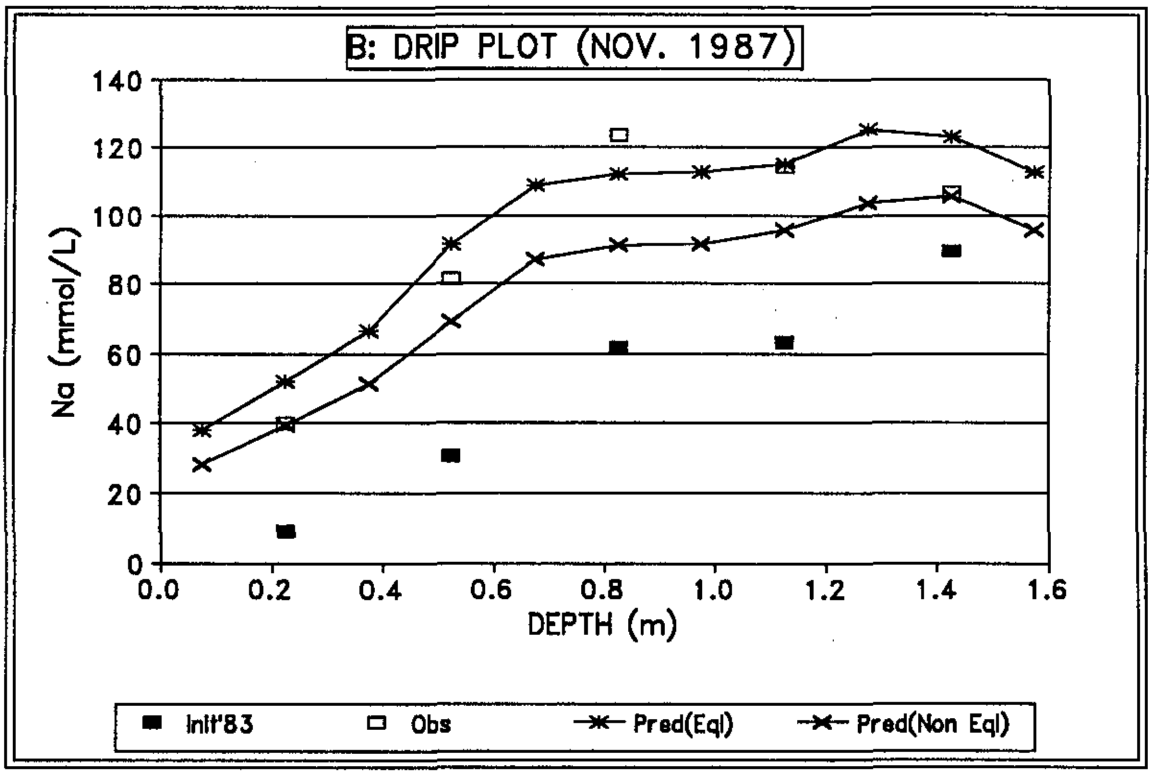
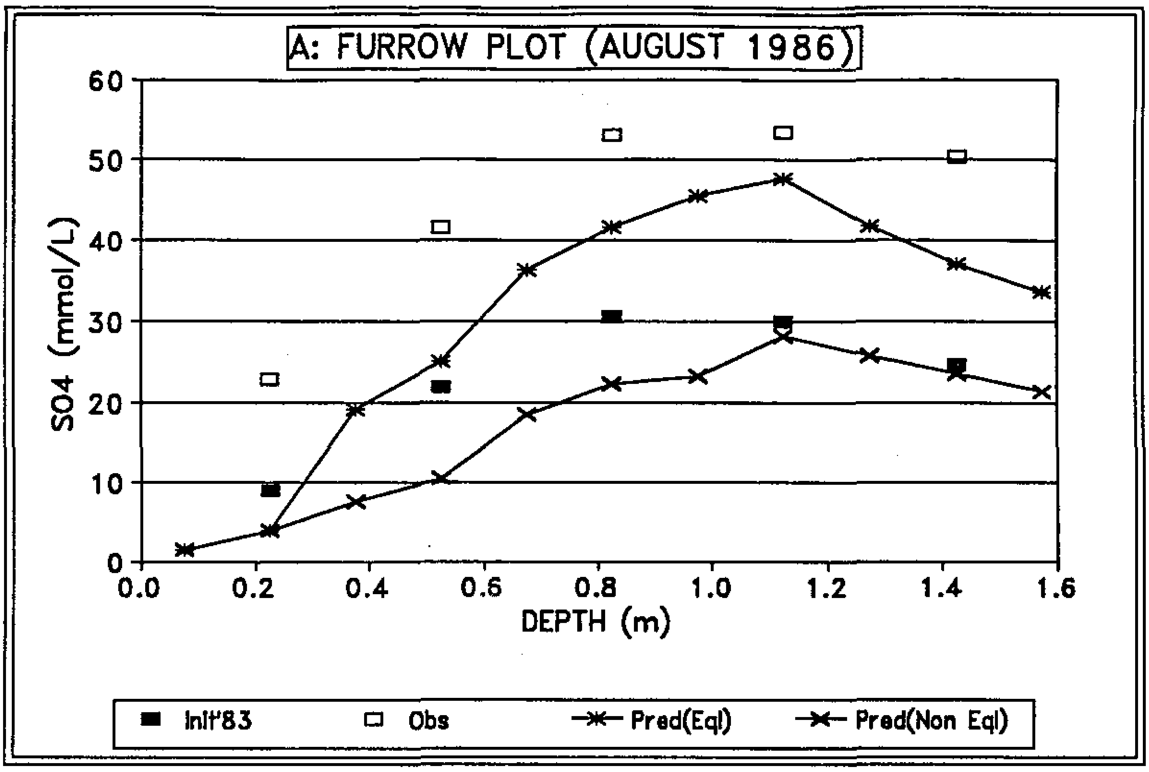


Figure 5.12 Predicted and observed Sodium concentration at the end of the irrigation experiment, with and without adjustment for a new chemical equilibrium at the water content of a saturated soil paste: a) furrow irrigated, and b) drip irrigated plot



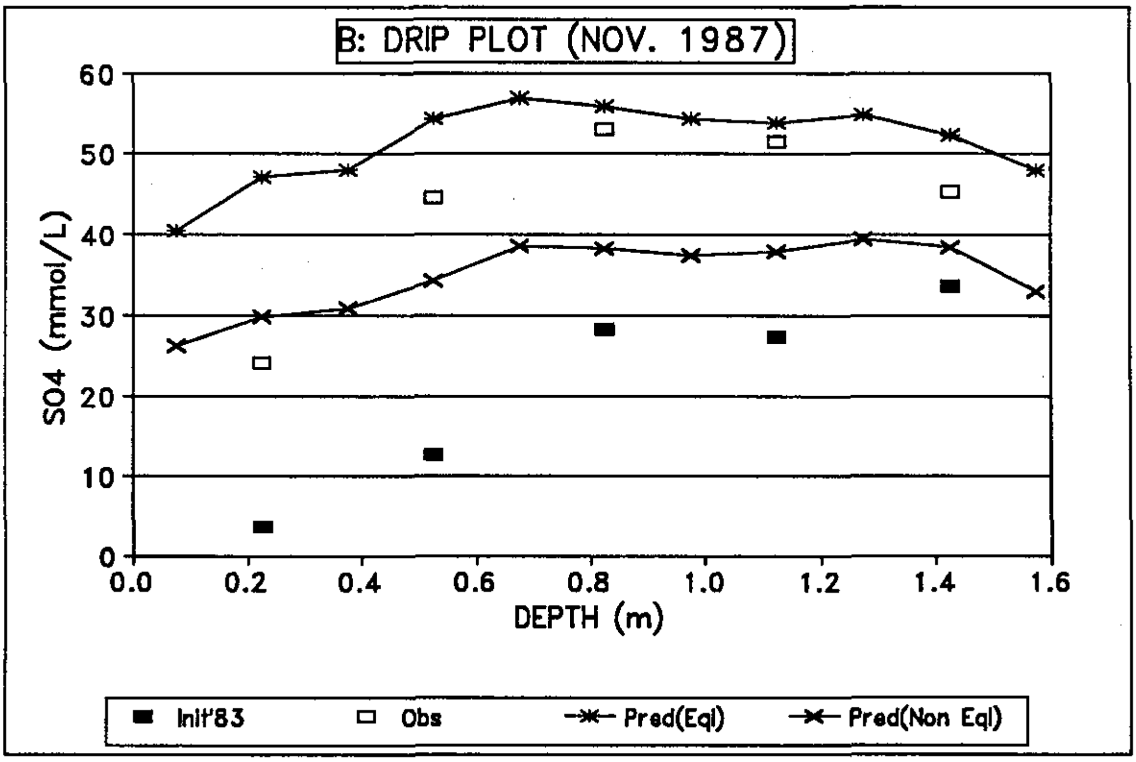
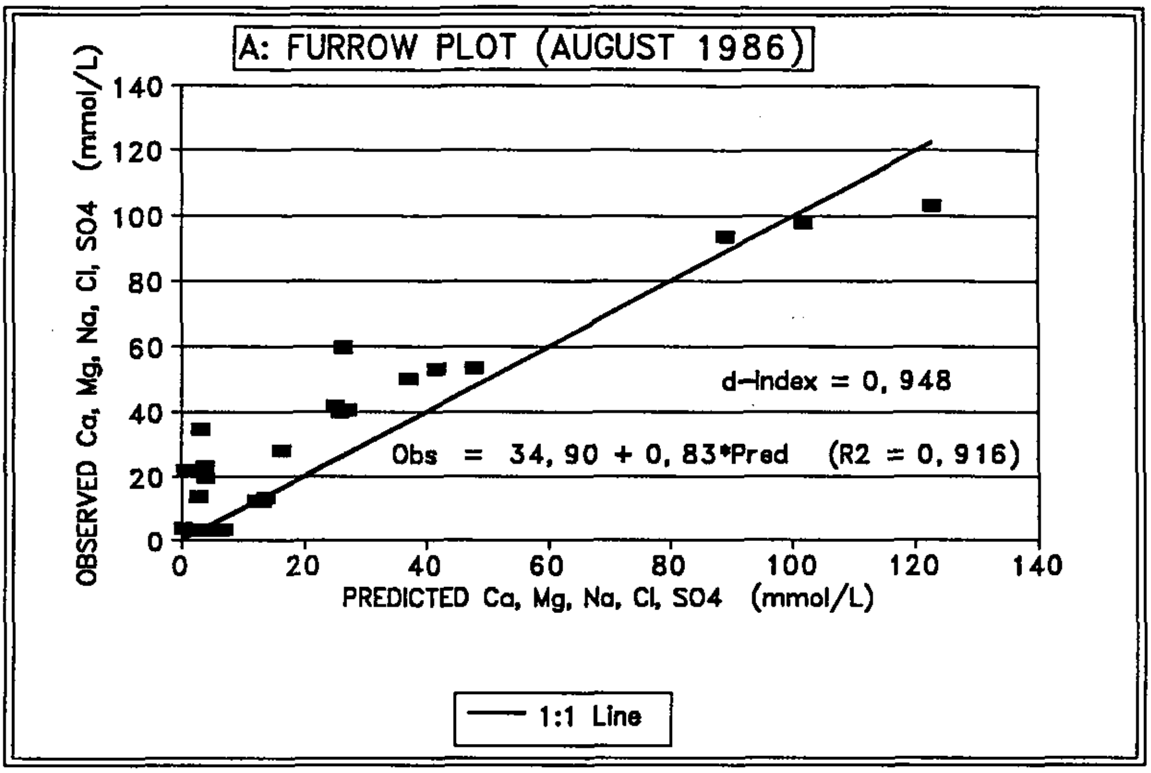


Figure 5.13 Predicted and observed Sulphate concentration at the end of the irrigation experiment, with and without adjustment for a new chemical equilibrium at the water content of a saturated soil paste: a) furrow irrigated, and b) drip irrigated plot

Table 5.20 Coefficients of variation of the analytical data for the samples collected in March 1983, August 1986 (furrow plot), and November 1987 (drip plot)

Depth(m)	EC	Cl	SO_4	Ca	Mg	Na
Drip plot 1983 (n=2)						
0,15	0,09	0,09	0,05	0,03	0,09	0,15
0,45	0,65	0,28	0,77	0,94	NA	0,61
0,75	0,78	0,79	0,89	NA	NA	0,78
1,05	0,71	0,82	0,84	0,98	NA	0,72
1,35	0,36	0,73	0,14	0,13	NA	0,35
Drip plot 1987 (n=2)						
0,15	0,13	0,16	0,20	0,04	0,09	0,21
0,45	0,06	0,34	0,14	0,03	0,01	0,13
0,75	0,18	0,29	0,13	0,09	0,08	0,04
1,05	0,01	0,21	0,10	0,04	0,03	0,07
1,35	0,01	0,09	0,04	0,05	NA	0,03
1,65	0,07	0,27	0,06	0,04	0,09	0,02
Furrow plot 1983 (n=3)						
0,15	0,33	0,58	0,45	0,29	0,28	0,43
0,45	0,63	0,86	0,75	0,80	0,72	0,67
0,75	0,40	0,84	0,26	0,47	0,43	0,38
1,05	0,27	0,47	0,19	0,42	0,43	0,24
1,35	0,36	0,47	0,33	0,47	0,63	0,33
1,65	0,24	0,44	0,23	0,45	0,47	0,19
Furrow plot 1986 (n=4)						
0,15	0,06	0,08	0,06	0,07	0,05	0,06
0,45	0,08	0,03	0,09	0,07	0,08	0,10
0,75	0,03	0,07	0,04	0,04	0,14	0,02
1,05	0,03	0,07	0,03	0,03	0,09	0,06
1,35	0,01	0,10	0,04	0,02	0,10	0,02
1,65	0,04	0,14	0,04	0,05	0,02	0,03

NA = not available



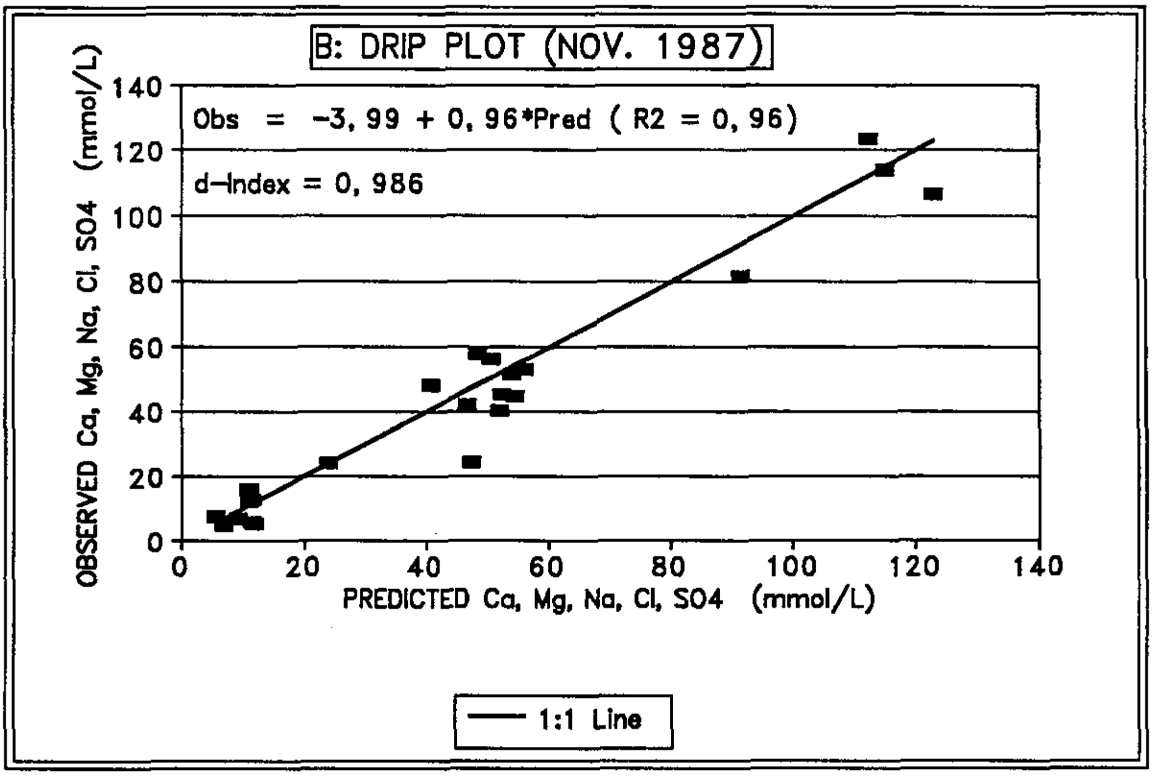


Figure 5.14 Comparison of the predicted and observed salt concentrations, irrespective of ions and depth, at the end of the simulation period: a) furrow, and b) drip irrigated plot

5.4 DISCUSSION AND CONCLUSIONS

At first glance, and based on the quantitative statistics, it seems as if the predictive capability of the leaching model LEACHM when applied on a mesoscale, is rather poor. For example, i) the predicted soil water contents could not adequately match the observed data; and ii) very low R^2 values and d-indices were obtained when the predicted and observed results are compared on a temporal scale.

The fact that some of the temporal predictions and depth trends were inadequately predicted by LEACHM might be related to measurement errors, especially if the large variability and the few samples that were taken are considered. The mean salt concentrations that were used as input, had very high standard errors, e.g. for the furrow plot at the 0,75 m depth: Cl = 29,0 mmol dm^{-3} $\pm$ 24,3 (Table 5.6). In the case of the 5,7 ha furrow plot the number of samples taken at any one of the four sampling dates, was never more than three. Previous studies on sampling strategies in saline soils, have demonstrated the effect of spatial variability on the estimate of the mean salt content (e.g. Miyamoto & Cruz, 1986; Moolman, 1989). The studies also proved that a large number of spatially distributed samples is required in order to detect trends and calculate means. Also, because of the effect of spatial variability, care should be taken to use exactly the same sampling strategy whenever temporal trends in saline soils are to be detected. This was not the case in the irrigation experiment that was simulated here. Notwithstanding the inadequacies of the measured data that were used in the present study, indications are that the chemistry of calcium and magnesium are not satisfactorily dealt with by LEACHM.

However, a graphical comparison between the observed and predicted results at the end of the simulation period, i.e. the final ion concentrations, indicate the opposite, namely a good predictive capability. Supported by these graphical representations and considering some of inadequacies associated with the actual measurements that were made in the field, the leaching model LEACHM seems to hold promise as a method that can be used on a meso spatial scale to predict trends in water and salt movement on irrigated fields. For example, in this study, LEACHM predicted that the soluble salt content of soils that are irrigated with saline drainage water, will increase appreciably. In the field experiment this was observed to be the case. A similar result was obtained even when good quality water was used with furrow irrigation as an application method.

In the sensitivity analysis of two solute transport models (Chapter 3) it was established that the flux of water through the soil had a profound effect on the predicted salt concentrations within the root zone as well as in the deep percolate.

Determining the amount of applied, as well as infiltrated water is considerably easier with drip irrigation than with furrow irrigation. It is therefore reasonable to assume that in the simulation of the drip plot, the amount of applied irrigation water that was used as input will be a more accurate account of the actual field infiltrated water than is the case with the furrow applied water. It is thus logical to expect the drip simulation to be more accurate than the furrow plot simulation. This was proved by the drip plot's higher d-indices and R^2 values calculated using the pooled data of all the ions and depths at the end of the simulation period.

All in all it thus seems justified to conclude that, in this particular meso scale experiment, LEACHM was capable of not only predicting the correct trends in time and depth, but also to yield relatively accurate salt concentrations.

CHAPTER 6
SIMULATING THE EFFECT OF DIFFERENT LEACHING STRATEGIES ON THE SALT LOAD OF THE DEEP PERCOLATE OF IRRIGATED LANDS

6.1 INTRODUCTION

Solute and water transport models attempt to simulate natural processes active in the soil-plant-atmosphere system. Numerical models are not only used to analyze field data or field scale problems (Wierenga, 1988) but also as research tools to aid the testing of hypotheses and the exposure of areas of incomplete understanding (Addiscot and Wagenet, 1985). Jury (1982) states that a "*solute transport model has its greatest utility as a tool for predicting relative behaviour of different irrigation waters, different soil types, or different water management strategies when a scenario for drainage ion composition is produced*". For example, Jury and Pratt (1980) used a dynamic solute transport model which considers chemical reactions to estimate the salt burden of four different irrigation drainage waters as a function of different leaching fractions. Depending on the chemical composition of the irrigation water and the leaching fraction (LF) that was simulated, the TDS and salt load of the drainage waters differed greatly. The salt load of the drainage water of soil irrigated with water from the Feather River which is low in TDS and undersaturated with $CaCO_3$, increases from 0,79 to 3,73 t ha^{-1} a^{-1} (i.e. with a factor of 4,72) as the LF increases from 0,10 to 0,40. Equivalent salt loads for irrigation water from the Colorado River which has a high salt content and close to saturation with respect to $CaCO_3$, were 5,01 and 10,98 t ha^{-1} a^{-1} respectively (i.e. with a factor of 2,19 only). The reason for the smaller increase in salt load of the latter water is attributed to the fact that $CaCO_3$ in the deep percolate will precipitate when concentrated, while the former water will pick up substantial quantities of minerals from the soil by dissolution as it percolates through the root zone (Jury and Pratt, 1980).

Van Rooyen and Moolman (1980) used the model of Shaffer *et al* (1977) to predict the effect of the water table depth and irrigation frequency on the salinization of soils. Their predictions revealed a definite benefit derived from a heavy irrigation at the beginning of the growing season, both with regard to soil moisture and salt buildup. Similar results were obtained when comparing short and long irrigation frequencies, favouring the former.

These and other studies suggest that hydrosalinity models are potentially useful tools that can be used to design minimum leaching irrigation management systems to conserve water and to combat detrimental salinity affects on the salt loading of groundwater and river systems. The purpose of this particular study was therefore to illustrate how a solute transport model can be used to change surface water management strategies in order to decrease the salt load of the deep percolate. The water and solute transport model that was used for this purpose is LEACHM (Wagenet & Hutson, 1989).

In a recently conducted survey of a 1074 ha of irrigated land in the Breede River Valley it was found that sprinkler- and drip irrigation are the two most common irrigation methods used. Drip and sprinkler irrigation accounted for 55% and 32% of the area surveyed (Bruwer, 1990). The irrigation frequencies varies between daily applications (drip systems) to applications every two weeks (sprinkler irrigation). According to the guidelines of the Department of Water Affairs and Forestry, the Brandvlei Dam (which is the principal storage dam in the valley), is operated in such a way that for 30% of the time during an irrigation season, the electrical conductivity of the water at the lower end of the river system, may exceed 70 mS m^{-1} but not 120 mS m^{-1}. This information, soil properties, irrigation water composition and irrigation management strategies that are all common to the Breede River (South Western Cape, South Africa), were used as the basis for the different leaching strategies that were investigated.

6.2 DESCRIPTION OF LEACHING SCENARIOS AND INPUT DATA

6.2.1 Leaching scenarios and time scale

The effect of six different salinity control measures as affected by using various leaching strategies, simulated for three consecutive years, on the salt and water flux of a hypothetical irrigated soil were investigated. For each year and leaching strategy (with the exception of one scenario), the same rainfall and actual evapotranspiration (AET) data were used throughout. In the discussions to follow, the following codes will be used when referring to these six scenarios:

S = summer, W = winter; 0, 5 or 20 = leaching fraction as a percentage;
/1 or /7 = irrigation frequency in units of days; X = increase in AET.

The six leaching strategies were:

a) Daily applications of irrigation water equal to 100% of the previous day's actual evapotranspiration from September to March; no winter leaching (code **0S0W/1**).

b) The same as a) but apply a single irrigation during the winter equal to 20% of the total evapotranspiration during summer (September to March); (code **0S20W/1**).

c) The same as a) but apply 105% of the previous day's AET with every irrigation event on a daily basis from September to March, i.e. a 5% excess of water (LF=0,05) was applied with every irrigation throughout the summer period; no winter leaching; (code **5S0W/1**).

d) The same as c) but apply 120% of the previous day's AET with every irrigation event on a daily basis from September to March, i.e. a 20% over-irrigation per event (LF=0,20) was used during the summer period; no winter leaching; (code **20S0W/1**).

e) The same as d) but decrease the irrigation frequency from daily to weekly applications, i.e. 120% of the previous week's AET was irrigated once a week; no winter leaching; (code **20S0W/7**).

f) The same as scenario b) but increase AET by the empirical amount of 10%. This was done to evaluate the effect of an increase in the soil surface evaporation component due to the high frequency of water application; (code **0S20W/1X**).

Although the actual years and dates have no particular significance, the starting and termination dates of each simulation run were September 1, 1987 and August 30, 1990 respectively. As will be shown later, LEACHM again could not be successfully used (due to mathematical instabilities) to simulate the whole three-year period.

6.2.2 Irrigation and meteorological data

The rainfall and pan evaporation depths and temporal distribution recorded in a 0,5 ha irrigated vineyard near Robertson, Breede River Valley during 1988 and 1989 were used to construct a representative climatic year (see sections 4.1 and 4.2.2.3 of Chapter 4 of this report). A common rainfall and AET record were used with every salinity control scenario that was simulated. For those scenarios where a daily irrigation frequency was simulated, all rainfall events from September to March that was less than 5 mm were assumed to be "ineffective" and were ignored. Only rainfall events in excess of 5 mm were considered to be effective substitutes for irrigation, i.e. whenever it rained more than 5 mm and if the daily AET was less than 5 mm, no irrigation was applied the following day. For the weekly irrigation frequency (i.e. scenario e above), rainfall of less than 5 mm falling on consecutive days were assumed to be effective. As a consequence of this arbitrary guideline, the weekly irrigation scenario received 19 mm more rain as input compared to the daily irrigation frequencies. In the case of strategy **b** (0S20W/1) above, 119 mm of water was applied in June, i.e. a single large quantity of water is applied during winter to affect leaching of accumulated salt as opposed to more smaller quantities applied more regularly (daily) during summer.

The class A-pan evaporation depths were converted to AET values by using the following set of crop factors for vines (see also Chapter 4, section 4.2.2.3): October

0,27; November 0,37; December & January 0,42; February 0,46; March 0,44; April to September 0,20. A summary of the annual irrigation, rainfall and actual evapotranspiration data that were used for each of the six different leaching strategies, are given in Table 6.1.

Table 6.1 Summary of the annual total of irrigation, effective rainfall and actual evapotranspiration that were used as input for each of the leaching strategies

Strategy	Leaching Fraction		Irrig	Annual totals (mm)		
	Summer	Winter	Freq	Irrig	Rain	AET
0S0W/1	0,00	0,00	1	607	251	694
0S20W/1	0,00	0,20	1	724	251	694
5S0W/1	0,05	0,00	1	635	251	694
20S0W/1	0,20	0,00	7	715	270	694
20S0W/1	0,20	0,00	1	724	251	694
0S20W/1x	0,00	0,20	1	724	251	753

The chemical composition of the irrigation water (in mmol dm^{-3}) was assumed to remain constant and were:

Ca = 1,35; Mg = 1,88; Na = 3,53; K = 0,11; Cl = 5,25; SO_4 = 1,82; HCO_3 = 1,20; TDS (mg dm^{-3}) = 618; EC (mS m^{-1}) = 96.

6.2.3 Description of a hypothetical soil profile

For each modeling run used to simulate a particular salinity control measure, the same chemical and hydrological soil properties and crop information were used. The hypothetical soil had a constant water table at 2 m depth. The soil profile was divided into 20 x 0,1 m deep segments.

a) Chemical properties

The depth distribution of the soluble salt and exchangeable cation concentrations of the hypothetical soil are similar to those of profile A2 discussed in Chapter 4. The soluble salt composition at field water content are listed in Table 6.2 while the exchangeable cation concentrations, lime and gypsum fractions for each of the 0,1 m depth segments, are given in Table 6.3. The set of six Gapon type selectivity coefficients used as input are (see also profile A2, Table 4.10): Mg/Ca = 1,89; Ca/Na = 3,05; Ca/K = 0,08; Mg/K = 0,13; Mg/Na = 4,71 and K/Na = 37,02.

b) Hydrological properties

The soil was assumed to be isotropic and the same soil hydrological properties were used for each depth segment. The initial volumetric soil water content and matric potential were in equilibrium with the water table at 2 m depth and are given in Figure 6.1.

Table 6.2 Soluble salt composition at field water content used as input for each of the leaching strategies

Depth m	EC $mS\ m^{-1}$	pH	Ca	Mg	Na	K	HCO_3	Cl	SO_4
			<----			mmol(+) dm^{-3}§			---->
0,1	512,4	7,76	26,83	10,13	22,75	1,04	11,19	18,95	33,78
0,2	513,0	7,76	26,83	10,13	22,75	1,04	11,19	18,95	33,78
0,3	687,2	7,97	10,43	9,06	35,30	0,37	7,20	27,07	20,19
0,4	687,5	7,97	10,43	9,06	35,30	0,37	7,20	27,07	20,19
0,5	687,8	7,97	10,43	9,06	35,30	0,37	7,20	27,07	20,19
0,6	870,4	8,09	4,20	5,16	49,71	0,18	7,20	26,44	17,48
0,7	869,2	8,09	4,20	5,16	49,71	0,18	7,20	26,44	17,48
0,8	867,8	8,09	4,20	5,16	49,71	0,18	7,20	26,44	17,48
0,9	851,1	7,97	4,06	5,46	48,43	0,16	6,59	21,44	19,80
1,0	851,2	7,97	4,06	5,46	48,43	0,16	6,59	21,44	19,80
1,1	848,2	7,97	4,06	5,46	48,43	0,16	6,59	21,44	19,80
1,2	929,6	7,92	4,09	2,54	44,02	0,12	3,64	21,03	16,37
1,3	925,3	7,92	4,09	2,54	44,02	0,12	3,64	21,03	16,37
1,4	920,9	7,92	4,09	2,54	44,02	0,12	3,64	21,03	16,37
1,5	905,5	8,06	4,73	5,67	55,17	0,13	5,12	23,32	23,84
1,6	901,5	8,06	4,73	5,67	55,17	0,13	5,12	23,32	23,84
1,7	901,4	8,06	4,73	5,67	55,17	0,13	5,12	23,32	23,84
1,8	901,6	8,06	4,73	5,67	55,17	0,13	5,12	23,32	23,84
1,9	898,6	8,06	4,73	5,67	55,17	0,13	5,12	23,32	23,84
2,0	898,1	8,06	4,73	5,67	55,17	0,13	5,12	23,32	23,84

§ mmol(+) dm^{-3} = meq dm^{-3}

c) Crop information

The phenological growth stages, harvesting dates and planting density of vines were used and are similar to those listed in Table 4.11.

Table 6.3 Lime, gypsum and exchangeable cation contents of the hypothetical soil used as input for each of the leaching strategies

Depth m	Lime fraction	Gypsum fraction	CEC	Ca	Mg	Na	K
			<----------	----------	mmol(+) kg^{-1}	----------	---------->
0,1	0,011	0,007	89,18	50,20	32,59	2,53	3,86
0,2	0,011	0,007	89,18	50,20	32,59	2,53	3,86
0,3	0,011	0,008	92,50	38,85	46,66	4,83	2,16
0,4	0,011	0,008	92,50	38,85	46,66	4,83	2,16
0,5	0,011	0,008	92,50	38,85	46,66	4,83	2,16
0,6	0,011	0,009	86,70	27,42	45,88	12,17	1,23
0,7	0,011	0,009	86,70	27,42	45,88	12,17	1,23
0,8	0,011	0,009	86,70	27,42	45,88	12,17	1,23
0,9	0,011	0,010	71,25	20,66	39,27	10,27	1,06
1,0	0,011	0,010	71,25	20,66	39,27	10,27	1,06
1,1	0,011	0,010	71,25	20,66	39,27	10,27	1,06
1,2	0,011	0,011	70,00	18,40	38,09	12,73	0,79
1,3	0,011	0,011	70,00	18,40	38,09	12,73	0,79
1,4	0,011	0,011	70,00	18,40	38,09	12,73	0,79
1,5	0,011	0,012	59,03	15,53	32,32	10,49	0,69
1,6	0,011	0,012	59,03	15,53	32,32	10,49	0,69
1,7	0,011	0,012	59,03	15,53	32,32	10,49	0,69
1,8	0,011	0,013	59,03	15,53	32,32	10,49	0,69
1,9	0,011	0,013	59,03	15,53	32,32	10,49	0,69
2,0	0,011	0,013	59,03	15,53	32,32	10,49	0,69

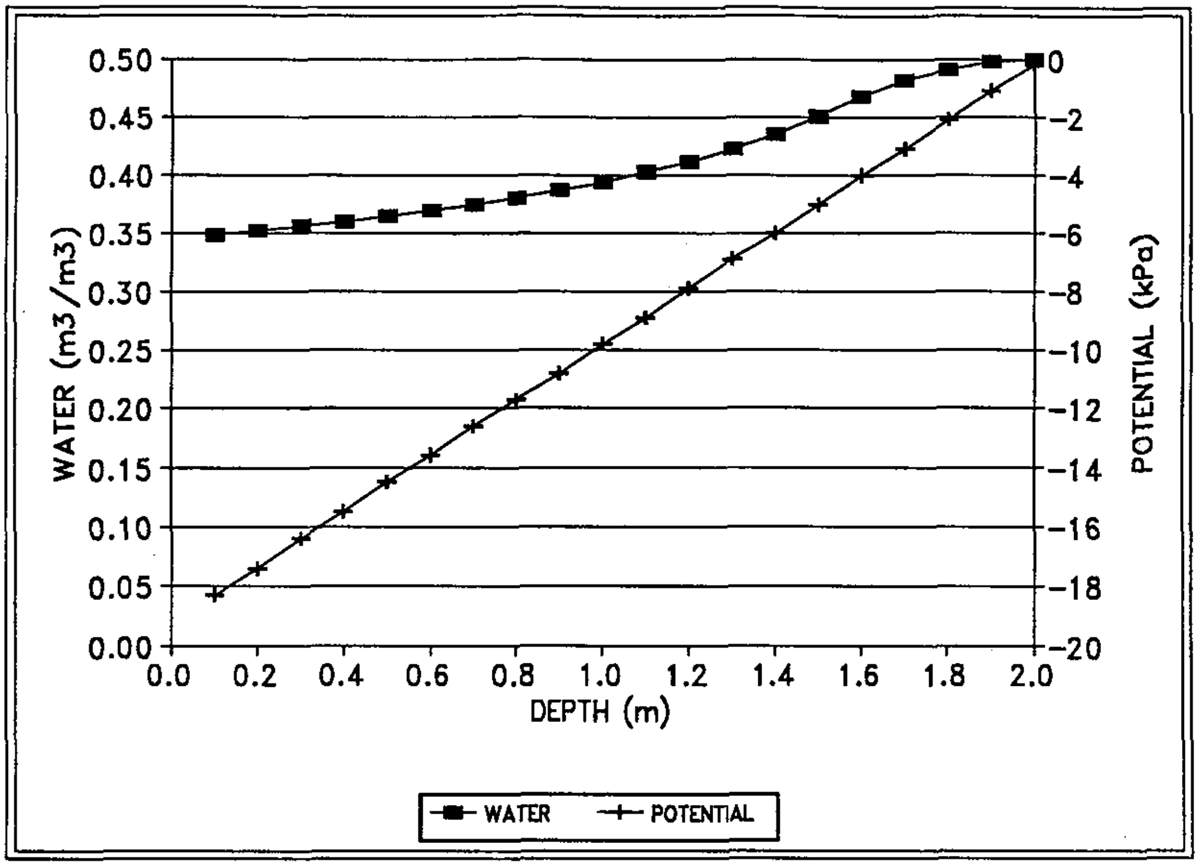


Figure 6.1 Depth distribution of the initial volumetric soil water content and associated matric potential of the hypothetical soil as used at the start of each simulation run

6.3 RESULTS

6.3.1 General

As was the case in Chapter 4 where LEACHM was used to simulate the water and salt distribution in a drip irrigated vineyard, numerical instabilities were also encountered in this study. The weekly irrigation frequency (20SOW/7) was the only salinity control measure that could be simulated for a full three year period, i.e. for 1095 days. In all the other cases the numerical instability of LEACHC, the chemistry version of LEACHM aborted the particular simulation attempt before the full three year period could be successfully completed. The number of completed days and the fictitious date corresponding to the day when the run was terminated for the different salinity control management strategies are listed in Table 6.4.

Table 6.4. Number of successful simulated days per salinity control management strategy and the fictitious date relative to 1 September 1987 when the modelling run was prematurely terminated

Strategy	Number of days	Fictitious date
0S0W/1	595	17/04/89
0S20W/1	658	19/06/89
5S0W/1	728	28/08/89
20S0W/1	567	20/03/89
20S0W/7	1095	30/08/90
0S20W/1x	553	06/03/89

The minimum number of completed days that could be simulated was 553 days and occurred with strategy 0S20W/1x, i.e. a daily irrigation frequency with a single leaching irrigation of 0,20 applied during winter, with a 10% elevated AET during summer. This time period is equivalent to about two complete irrigation seasons (1 September - 30 March) which means that the information of two irrigation seasons can be used to compare the results of the different options that were evaluated. However, a comparison on this basis will exclude the irrigation application of 119 mm during June of each winter which formed part of strategies 0S20W/1 and 0S20W/1x. Consequently, for comparative purposes, it was decided to use the results of the first 365 days only.

It should be obvious that the real values of the predicted water fluxes and salt loads for the different strategies are primarily controlled by the respective input quantities of rain, evapotranspiration, the quantity and chemical composition of the irrigation water and the initial conditions of the hypothetical soil (see Chapter 3). Other irrigation quantities or a soil with different chemical and hydrological properties will produce different fluxes and salt loads. Therefore, in order to focus more on the salinity control measures themselves and to get a better impression of the outcome of the different leaching strategies that were simulated, it was decided to present the results using relative scales. In the case of the water flux and salt load of the deep percolate, the quantities were expressed as ratios of the irrigation management strategy where no controlled leaching is practised, i.e. strategy 0S0W/1. Therefore, on this scale, the water flux and salt load when no leaching is practised, will have a relative value of 1. The effect of the leaching treatments on the salt content of the soil was expressed relative to the initial salt content specified as input in Table 6.2.

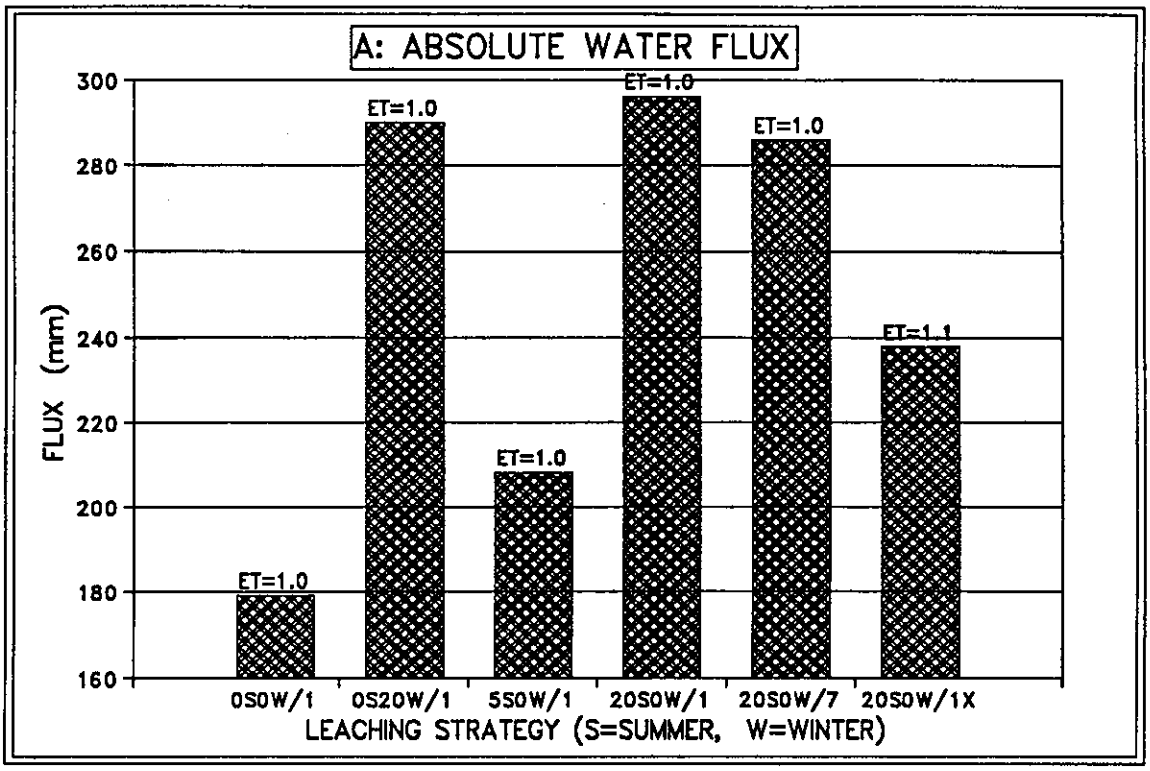
6.3.2 Water flux

The absolute and relative values for the annual water flux at 2 m depth for the different scenarios, are given in Figure 6.2 a & b while the temporal distribution of the cumulative flux, given as relative values, are given in Figure 6.3. At the end of 365 days the total downward flux of water varied from a minimum of 175 mm (option 0S0W/1) to a maximum of 292 mm (option 20S0W/1), which, on a relative scale (Fig 6.2b), ranged from 1,0 to 1,62.

Of particular importance is the difference between options 0S20W/1, 20S0W/1 and 20S0W/7. With these three strategies the total annual irrigation applications are the same, but the timing of the leaching applications are different. The difference in the total water flux of these three leaching options is less than 10 mm per year (Figure 6.2a). However, the temporal distribution of the amount of water leaving the root zone differs markedly (Figure 6.3). At the end of the irrigation season (day 230) the relative cumulative fluxes for options 0S20W/1, 20S0W/1 and 20S0W/7 were 1,00, 1,72 and 1,68 respectively. On the relative scale, the application of the 20% leaching water during winter (on day 304), increases the water flux of option 0S20W/1 from 1,00 to a value 1,60 within a matter of 40 days. At the end of a full summer and winter cycle, the total deep percolate of these three strategies is predicted to sum to approximately the same relative value. These three relative fluxes are 1,6 times more than where no leaching is practised.

LEACHM furthermore predicts that the temporal distribution of the water flux for the daily (20S0W/1) and weekly (20S0W/7) irrigation frequencies will, for all practical purposes, be the same (Figure 6.3). It can be argued that smaller quantities of water applied more frequently will produce less macropore flow (or "short-circuiting") than when larger amounts of water is applied less often, especially if the rate of application also increases as the irrigation frequency decreases. Consequently, in practice one would expect that the water flux of a leaching and irrigation strategy such as option 20S0W/7 (irrigation once a week) will have a larger water flux across the bottom of the root zone than with strategy 20S0W/1 (irrigation every day). The small difference between these two options as predicted with LEACHM, therefore seems rather strange (Figure 6.2 a & b). However, LEACHM cannot simulate macropore flow. In view of this shortcoming, this particular result should be treated with caution.

An increase in the amount of surface evaporation (because of the high frequency of irrigation, i.e. daily applications) will tend to decrease the water flux compared to a weekly frequency: compare for example the results of scenarios 0S20W/1, 0S20W/7 and 0S20W/1x (Figures 6.2 and 6.3).



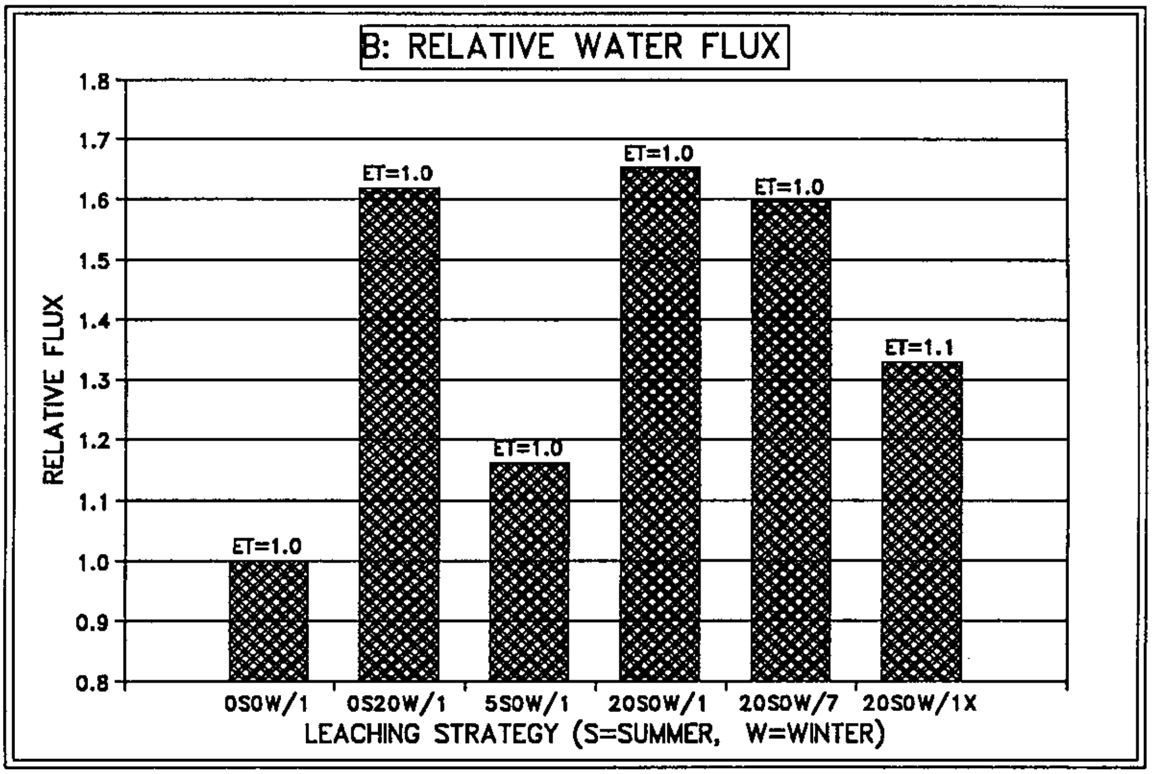


Figure 6.2 Total annual water flux as a function of different salinity control measures: a) absolute; b) relative

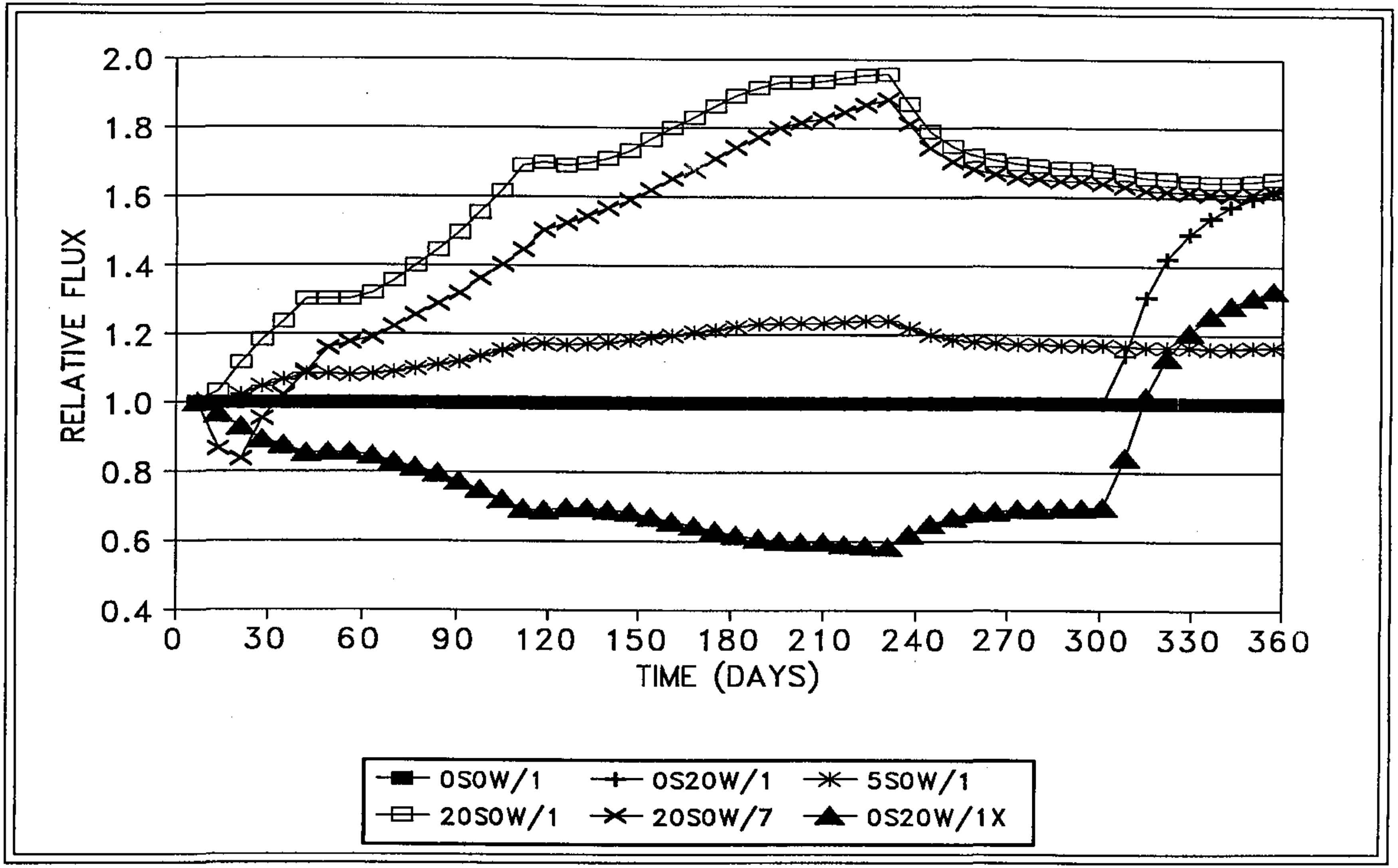


Figure 6.3 Temporal distribution of the cumulative water flux at 2 m depth expressed as ratios relative to the option where no leaching is practised.

6.3.3 Salt load

The total salt load, absolute and relative, at the end of the first annual cycle of irrigation are given in Figures 6.4a & b. The temporal distribution of the cumulative load is indicated in Figure 6.5. Because of the very good positive correlation between water flux and salt load, the trends depicted in Figures 6.4 and 6.5 (load) are similar to those shown in Figures 6.2 and 6.3 (water flux).

The maximum difference in the annual salt load as brought about by the different leaching options is about 6 ton ha^{-1} a^{-1}; compare for instance option 0S0W/1 with 20S0W/7 (Figure 6.4a) which, on a unit area basis, might seem to be insignificant. However, on the relative scale, the salt load of option 20S0W/7 is 1,7 times that of option 0S0W/1 (Figure 6.4b). Such a big difference, when multiplied with the total irrigated area, can have a noticeable effect on the salt burden of a receiving river.

According to the predictions made with LEACHM, the annual salt load of the deep percolate will be nearly the same irrespective of whether a strategy of continuous leaching with every irrigation is followed, *viz.* 20S0W/1 where the relative load is 1,61, or whether leaching is deliberately withheld during summer with a single large amount of water being applied during the winter period *viz.* 0S20W/1 where the relative load is 1,69 (Figure 6.4b). Although the total annual load is the same, the temporal distribution produced by the latter option suggests that it will be more beneficial for the control of the salinity levels in the receiving river (Figure 6.5). A continuous flow of solutes out of the root zone, being the result of frequent leaching applications during the growing season (summer), will increase the salt load and therefore salt concentration of the irrigation return flow. If the receiving river is used both for distribution and drainage (as is the case for example, in the Breede River and Great Fish River systems), this in turn will call for measures to decrease the concentration of salts in the river to within acceptable limits. Currently this is accomplished by releasing additional dilution water from the storage dams. If on the other hand, little or no leaching is practiced during summer, followed by large applications of irrigation water during winter, the salt concentration in the river will be substantially less at the time when it matters most, i.e. during the irrigation season. For example, on a relative scale, the cumulative load at the end of the irrigation season (day 230) is 1,00 for option 0S20W/1, but 1,95 for option 20S0W/1 (Fig. 6.5). This means that a strategy of frequent leaching during summer, will yield 1,95 times more salt than when no controlled leaching is practised.

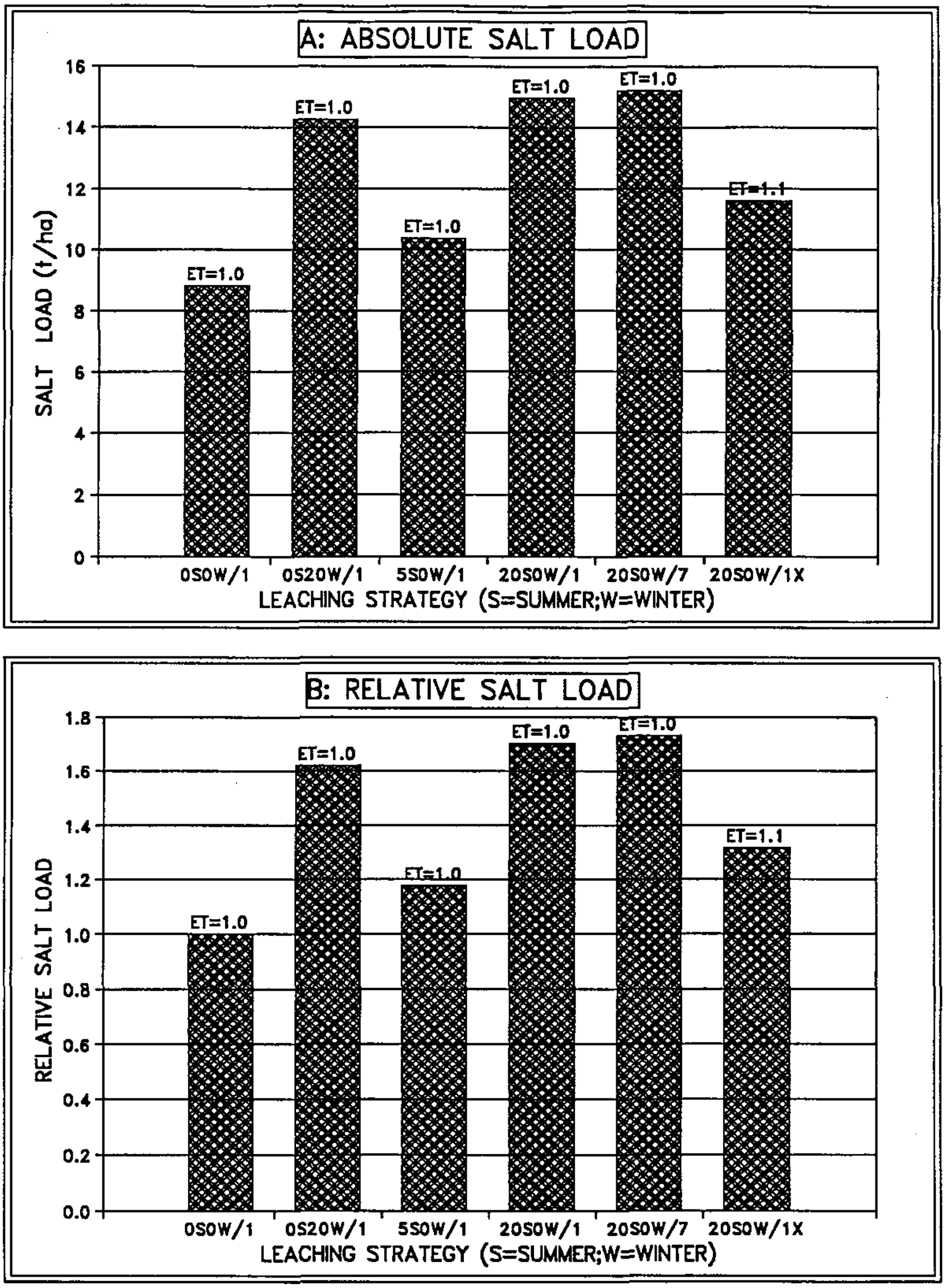


Figure 6.4 Total annual salt load as a function of different salinity control measures: a) absolute (t ha^{-1} a^{-1}); b) relative to the results of option 0S0W/1

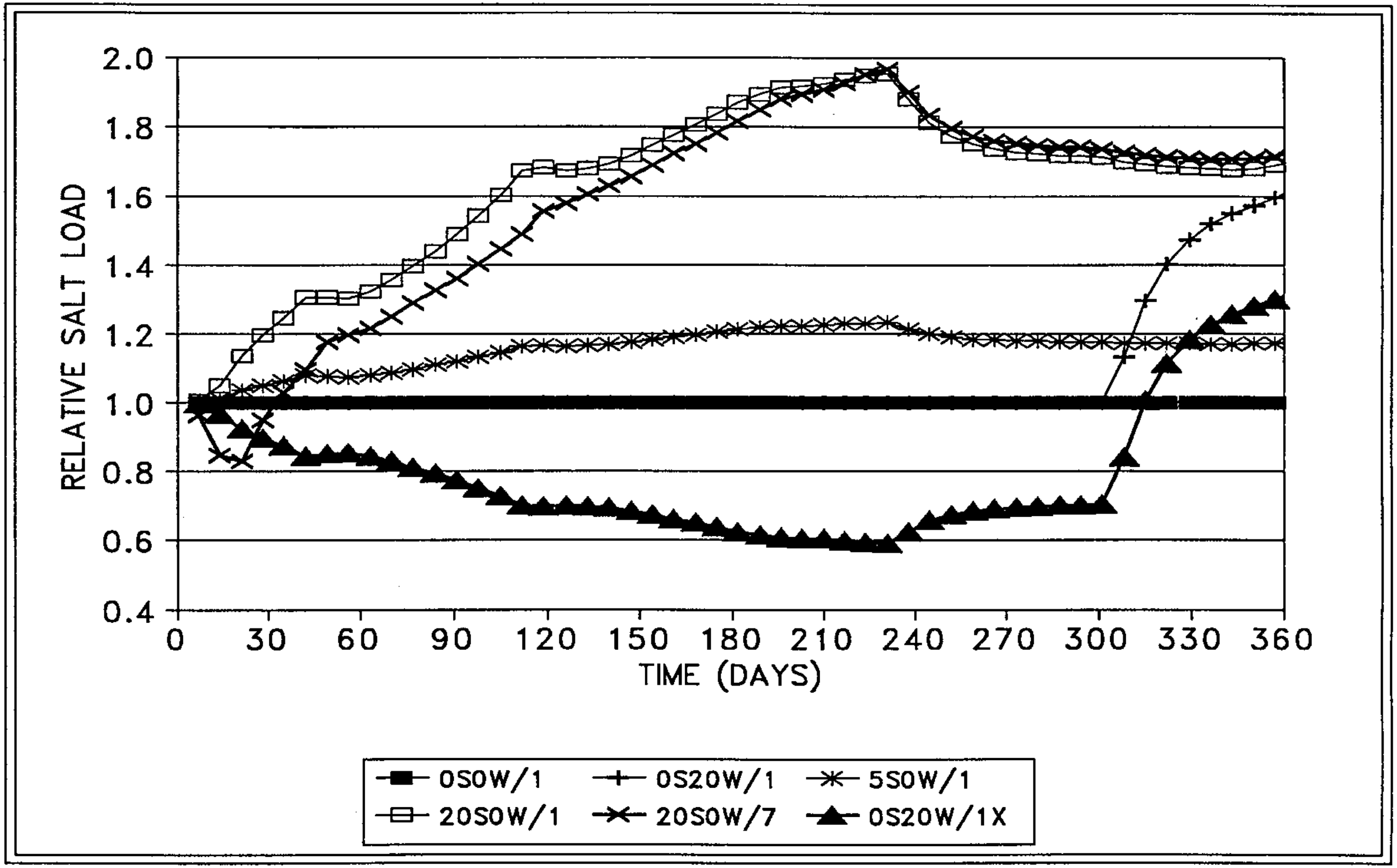


Figure 6.5 Temporal distribution of the cumulative salt load of the deep percolate expressed as ratios relative to the option where no leaching is practised, i.e option 0S0W/1.

(**Note**: The decrease in the cumulative load from day 230 for options 20S0W/1 and 20S0W/7, is due to the capillary movement of salt from the water table into the lower half of the root zone during winter).

Another noteworthy result is the difference in the salt load when a 5% *vs*. 20% leaching is practised, i.e. options 5S0W/1 and 20S0W/1. On a percentage basis the increase in the load is much more than the increase in the additional water that is required with the higher leaching fraction. In this hypothetical study, the 20% leaching strategy required 14% more water during the irrigation season than the 5% leaching strategy: [14% = (724-635 mm) x (100/635 mm)] (Table 6.1). However, the 20% leaching strategy yielded 45% more salt than the 5% strategy: [45% =(14,5-10,0 t/ha) x (100/10,0 t/ha)] (Figure 6.4a). The reason for this disproportionate increase in the salt load as the leaching fraction increases, is the increased dissolution of minerals (e.g. gypsum and lime) in the soils.

As was found with the water flux, a bigger surface evaporation component (because of an increased irrigation frequency), will tend to decrease the salt load of the deep percolate: compare for example the relative loads of options 20S0W/1, 20S0W/7 and 20S0W/1x (Fig. 6.4b).

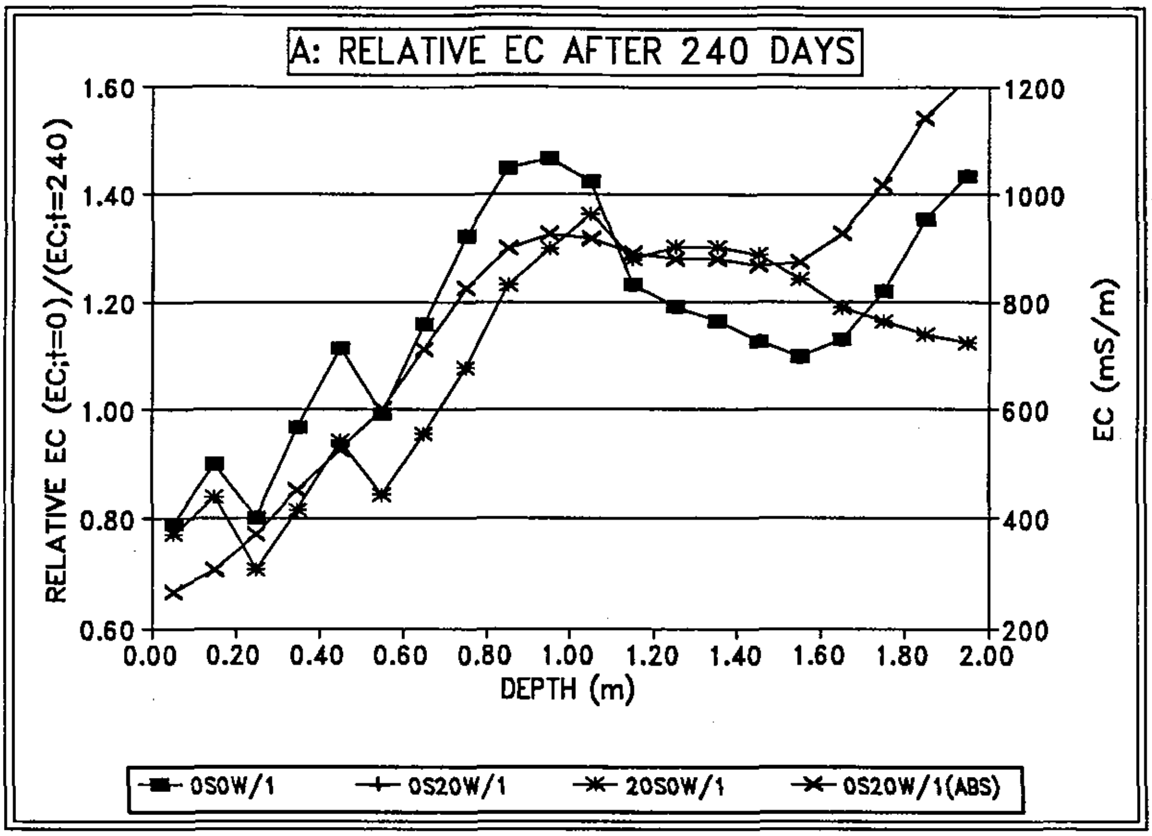
6.3.4 Salt concentration in the root zone

A salinity control measure that favours winter *vs*. summer leaching, can only be employed if the salt buildup within the root zone during summer is not harmful to the crop. The depth distribution of the electrical conductivity (EC) of the soil solution of options 0S0W/1, 0S20W/1 and 20S0W/1 at the end of the irrigation season (240 days) and at the end of a 365 day cycle is given in Figure 6.6. Because of different soil water contents, the EC values were adjusted to a constant 40% gravimetric water content throughout and expressed as ratios of the initial EC (the initial values listed in Table 6.2 were also adjusted to a 40% water content).

According to the model predictions, during the first irrigation season a considerable accumulation of salt below the 0,6 m depth will occur if no leaching is applied; e.g. options 0S0W/1 and 0S20W/1. For example, at the 1,0 m depth the EC had increased from the initial relative value of 1 to a relative value of 1,45. (For the sake of clarity, the absolute EC values in mS m^{-1} for option 0S20W/1 are also indicated in Figure 6.6a. These absolute values ranged from about 250 mS m^{-1} in the surface layer to 1100 mS m^{-1} at the bottom of the profile). LEACHM furthermore predicts, as expected, that a continuous leaching of 20% in summer will result in a decrease in EC for depths < 1 m with slightly increased EC values below that (see for example 20S0W/1 in Figure 6.6a).

The winter leaching application employed with strategy 0S20W/1 resulted in a significant reduction in the relative EC, both in comparison to the values at the end of the irrigation season, as well as when compared to the no-leaching- and summer-leaching options, i.e. 0S0W/1 and 20S0W/1 (Fig 6.6b). The most significant reduction in the relative EC occurred in the shallower layers. Although, if no leaching is practised during summer, the salt content within the root zone at the end of the irrigation season will be considerably higher than when leaching is applied, the practice of a winter leaching reduces the salt content in the upper section of the soil to such an extent that at the onset of the second irrigation season (day 360), option 0S20W/1 actually have less salt than option 20S0W/1 (Figure 6.6b).

The steep increase in the relative and absolute EC values with depth at the end of the irrigation season (Fig 6.6a) and at the end of a full summer and winter cycle (Fig 6.6b), might suggest that even the relatively high leaching fraction of 0,20 as simulated here, is still not enough to prevent an accumulation of salt within the 2 m soil profile. Unfortunately this inference could no be verified because LEACHM was not successful in simulating a full three year cycle for the daily irrigation frequencies (Table 6.4). The only case where LEACHM completed successfully three consecutive years, was when a weekly irrigation frequency with a 20% leaching strategy was simulated, i.e. option 20S0W/7. The depth distribution of the EC values at the end of the first and third years, expressed as ratios of the initial salt contents, is given in Figure 6.7. After three years of irrigation the predicted EC varied between 0,15 and 0,60 of the original values for the depths < 0,6 m. For the depths deeper than 1 m the relative EC values were about 0,60. The absolute EC of the soil solution in mS m^{-1} for the particular soil and irrigation water composition is also indicated in Figure 6.7 and ranged from 40 mS m^{-1} to 500 mS m^{-1} down the soil profile. These salt concentrations are considerably less than the original values. This suggests that, given sufficient time, a 20% leaching application might be adequate to decrease the soluble salt content throughout the soil.



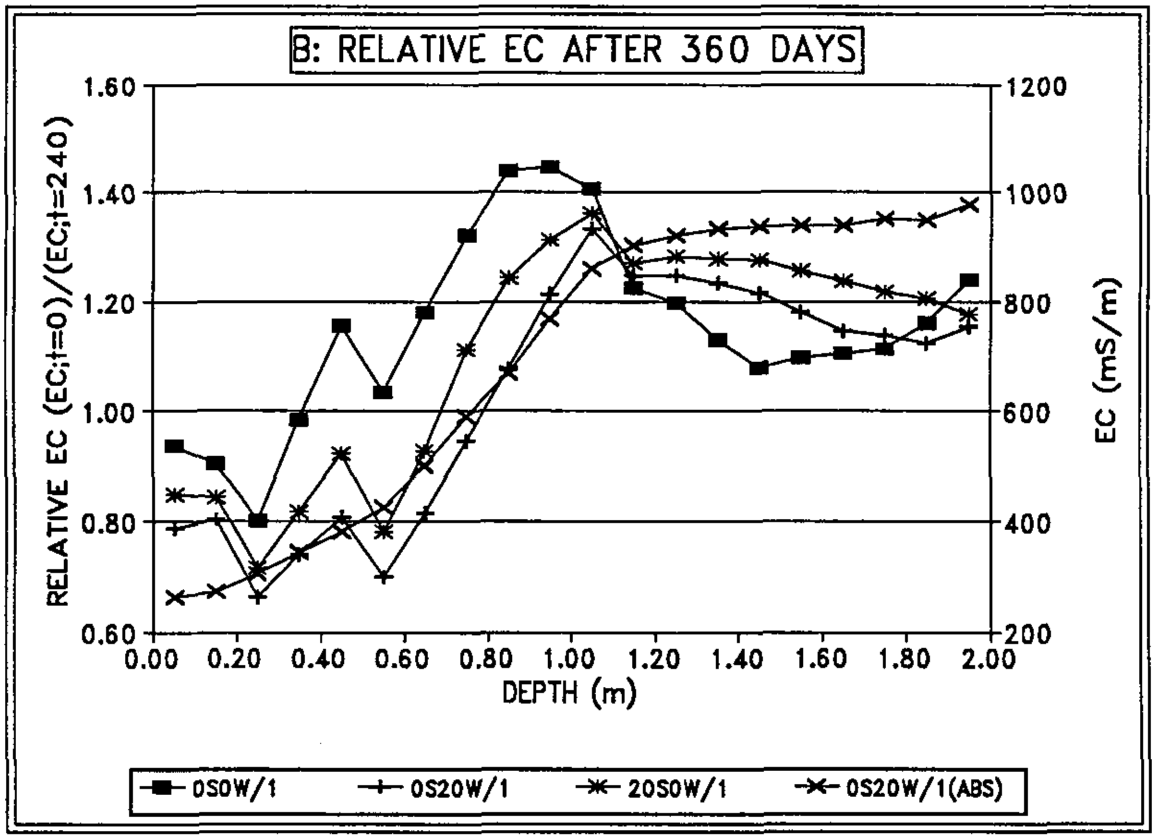


Figure 6.6 Salinity profiles of relative EC values of the soil solution predicted for the options where no leaching (0S0W/1), a 20% winter leaching (0S20W/1) and a continuous 20% leaching during summer (20S0W/1) is used after: a) 240 days and b) 360 days. Also indicated are the absolute EC values of option 0S20W/1

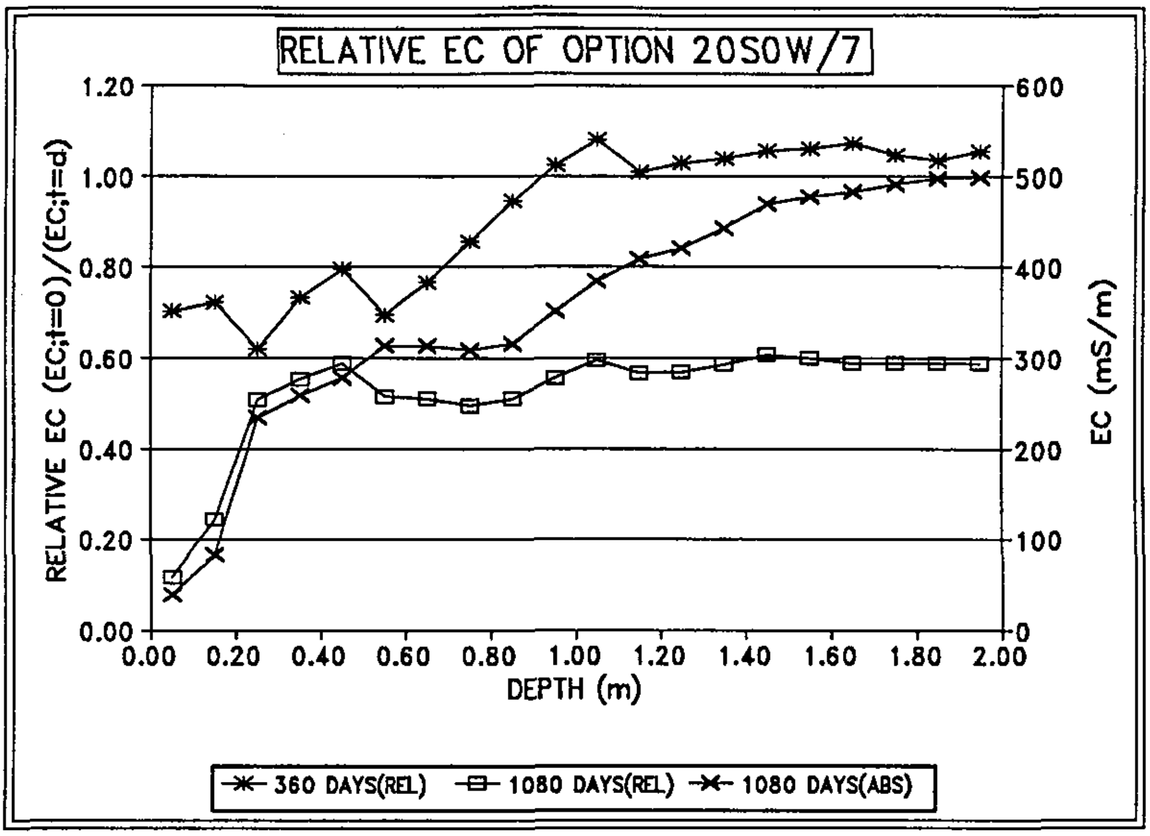


Figure 6.7 Salinity profiles of relative EC values of the soil solution predicted for the option where no leaching is applied during summer followed by a 20% leaching during winter (0S20W/1) after 1 and 3 years of irrigation. The absolute EC values after three years can be read from the secondary Y-axis.

6.4 CONCLUSIONS

Against the background of the particular circumstances that were used in this study (rain, irrigation, evapotranspiration and soil) and based on the results of the first summer and winter cycle, the following conclusions can be made regarding the effect of different leaching strategies that can be used to minimise the salt load of the deep percolate of irrigated lands:

a For a particular leaching fraction, the total flux of water at the bottom of the root zone at the end of a summer and winter cycle will be nearly the same, irrespective of whether: i) a daily or weekly irrigation frequency is used during summer, and ii) the leaching water is applied with every irrigation during summer, or as a single application during winter.

b Although only to a degree, the total salt load of the deep percolate will increase in the order: no leaching during summer, with a single leaching in winter < leaching during summer on a daily frequency < leaching during summer on a weekly frequency.

c The temporal distribution of the salt load and water flux suggests that controlled leaching of salts during winter is more beneficial for the control of the salt concentration of receiving rivers.

d For the irrigation water that was used (EC $\approx$ 100 mS m^{-1}), an irrigation practice where no leaching is employed during the summer period, will result in a considerable accumulation of salts in the bottom half of the root zone during the irrigation season. If a winter leaching is applied, a significant portion of these salts will be leached and the predictions suggest that the salt content within the root zone at the onset of the second irrigation season, will be less than the initial values.

e The fact that LEACHM predicted similar water and salt fluxes for a daily and a weekly irrigation frequency should be treated with caution. This result, in all likelihood stems from the fact that LEACHM can handle D'Arcian type flow only and not macropore flow. In practice, low irrigation frequencies involving large amounts of irrigation water applied at greater rates than smaller quantities at higher frequencies but lower rates, will yield larger water fluxes and salt loads.

f In spite of the general shortcoming of the presently used water and salt transport models not being able to simulate non-D'Arcian type of water flow (e.g. macropore flow), they still are useful tools that can be used to evaluate and design different salinity control strategies. Simulation studies such as the one reported on in this Chapter, are far cheaper to conduct than expensive field trials. The results of simulation studies can then be used to select, test and verify certain salinity control strategies under field conditions. Unfortunately, the particular model that was used in this study, LEACHM, under certain unknown and unpredictable circumstances, turned out to be numerically unstable.

CHAPTER 7
SUMMARY AND CONCLUSIONS

7.1 GENERAL

The purpose of this project was to evaluate a range of computer models that can simulate the transport of solutes and chemicals in the root zone of irrigated soils. The three models that were included in this study were LEACHM (Wagenet and Hutson, 1989), Burns (1974) and TETrans (Corwin and Waggoner, 1990). The study was conducted in different phases with each phase being an independent investigation of a certain aspect.

In the first phase (Chapter 3), the sensitivity of the LEACHM and Burns models to changes in the input values of selected variables was investigated. In the second phase (Chapter 4), LEACHM was used to simulate the water and salt transport for a period of 2,5 years on a microscale in a drip irrigated vineyard. In this case spatially and temporally distributed soil water- and salt contents and daily drainage rates, were available for model validation. With phase 3 (Chapter 5), all three models were applied to a mesoscale field study comprising furrow and drip irrigated fields of which a limited amount of information only were available for input and validation purposes. Finally, in phase 4 (Chapter 6), LEACHM was used to demonstrate the effect of different leaching strategies on the salt load of the deep percolate from irrigated lands. Summaries and conclusions have been given at the end of each chapter in this report. In this particular chapter, a more generalised discussion on model validation, the overall performance of the three models that were evaluated, the choice of models for a particular application, and input requirements will be dealt with.

7.2 VALIDATION

One of the more serious problems encountered in this study was how to decide on the adequacy of the predictions, i.e. are the predicted water and salt contents and fluxes valid? In the two field studies, the norms that were used were quantitative statistics and graphs. In most of the cases, the quantitative statistics that were used, i.e. R^2, root mean square error and Wilmot's d-index, left the impression that none of the three models under study can accurately predict the precise fate of water and solutes in the soil. For example, in the microscale application of LEACHM to a drip irrigated field (Chapter 4), the best temporal relationship between predicted and observed water content had a coefficient of determination (R^2) as low as 0,51 and a d-index of 0,774. In the case of the mesoscale application the best d-index that was achieved was 0,891. However, in the latter case, this particular d-value could be achieved only once the observed data had been screened and limited to information of one season only (see Tables 5.13 and 5.14). The quantitative statistics of the predicted and observed chemical composition of the soil solution were equally poor. Based on these statistics, it would border on conjecture to declare the predicted results as valid and true representations of the field scale processes.

In contrast, the visual comparison of predicted and observed results by means of graphs, generally gave a more favourable impression of the predictive abilities of the models. This is especially true for LEACHM. In the case of the mesoscale study, the predicted depth distribution of the total salt content in the root zone of the drip irrigated plot after four years of continuous irrigation was a very good representation of the observed values (see for example Figure 5.9).

Another observation was that predictions of the soil water content and the chemical composition of the soil, were not equally accurate. In normal soils (i.e. where macropores do not dominate the flow process) it is reasonable to assume that the calculated salt content and fluxes cannot be predicted more accurately than the temporal water content and fluxes. However, this was not always the case in this study. For example, in the microscale study, the temporal trend of the predicted soil water content at a distance 0,25 m from an emitter accorded rather poorly with the observed results (see for example Figure 4.5, page 4.30). Yet, after 18 months of simulated irrigation, the predicted EC of the soil solution of the soil segments to a depth of 1,0 m was within one standard deviation from the observed spatial mean (Figure 4.11, page 4.39).

These rather contrasting results are confusing and raise the following questions:

a) When is a model validated and which criteria should carry the most weight when making this decision - classical statistical norms or graphical representations and temporal trends?;

b) Is an adequate prediction of soil water content sufficient guarantee that the same level of accuracy will be achieved with the prediction of the chemical constituents (and *vice versa*);

c) Does a comparison of predicted and observed data on a continuous temporal scale but insufficient spatial scale, necessarily constitute a more rigorous test of validation, as opposed to limited or point data (in the temporal and spatial sense) only, e.g. should all data for the particular period under study (for instance 1983 to 1987) be used or only the observed results at a specific point in time and space (for instance at the end of the simulation period) ?

I am of the opinion that classical statistical indices alone should not be the only criteria when validating models. In all cases visual comparison should also be used. In some cases a good visual comparison with graphs alone, even if it include limited data only, will be sufficient proof of validation.

With these considerations in mind, and if the primary goal of the two field applications of this study was only to prove that the predictions of the mechanistic deterministic model LEACHM (Wagenet and Hutson, 1989), are *realistic representations of field processes*, it can be concluded that the calculated results are valid. This conclusion can then be extrapolated to the more general statement that water and solute transport models are useful tools to predict water and solute movement and chemical reactions in the unsaturated zone of irrigated soils. If on the other hand accuracy, rather than trends, is important, the conclusion will be the opposite, namely that all three models were unsuccessful in predicting accurately the water and salt contents within the root zone of the two fields to which the models were applied.

Another factor which confounded the issue of model validation was the spatial variability of the soil environment and the method in which samples were collected. McLaughlin, (1988) stress that validation should encompass the entire modelling process, e.g. sampling, input estimation, and prediction and not just the simulation model alone. In the microscale study on the drip irrigated vineyard, an adequate number of samples were collected to compensate for spatial variability at all stages of the field investigation. However, input estimation of variables such as the depths of applied irrigation water and evapotranspiration at different distances from the emitter, could have influenced the predictions to a very large extent. Therefore, although spatial variability was taken care of, the conversion of volume to depth of applied water was the limiting factor in the validation process. The mesoscale study suffered from the same uncertainty.

7.3 OVERALL PERFORMANCE OF MODELS

Of the three models that were used in this study, i.e. Burns, LEACHM, and TETrans and in terms of runtime computer errors, LEACHM proved to the most unreliable. Because of numerical instabilities in the code of this model, a number of computer runs were prematurely terminated. This was particularly evident in the microscale study (Chapter 4) and as well as when the model was used to demonstrate the effect of different leaching strategies (Chapter 6) on the salt load of the deep percolate. The common denominator between these two studies was that relatively low salinity irrigation water was applied to a soil with a relatively low cation exchange capacity, gypsum and lime content. Whether, and if true, why, these conditions will always result in runtime computer errors, could not be ascertained. The problem of numerical instability, furthermore, was always associated with the chemistry and transport of Ca in the soil. Although numerical instabilities did not occur during the mesoscale study (Chapter 5) the predicted Ca concentration at different times over a period of three to four years varied between a minimum of 11 and a maximum of 13 mmol dm^3, irrespective of whether the soil was irrigated with non-saline or saline water (see Figures 5.7 and 5.8). These concentrations are more or less equal to the concentration of a solution that is saturated with $CaSO_4$. LEACHM thus predicted that the soil solution at all stages during the course of the irrigation experiment would have been saturated with gypsum. The field measurements did not confirm this. It therefore seems as if the particular section of LEACHM that deals with the chemistry of Ca needs to be improved.

In the case where the two functional models (Burns, and TETrans) were compared with a mechanistic deterministic model (LEACHM), the former two models yielded results that bore no resemblance with the actual observed water and chloride contents. Very low water contents and sharp discontinuities with depth were predicted. This was not observed in the measured data. LEACHM, on the other hand, although not always very accurate, yielded results that were more in accordance with the observed concentrations and temporal trends. Therefore, it is seems reasonable to conclude that, despite its problem of numerical instability, the predictive ability of the mechanistic deterministic model LEACHM, is superior to that of the two functional models.

7.5 MINIMUM INPUT REQUIREMENTS

In Chapter 3 of this report, the results of a sensitivity study showed that irrigation and evapotranspiration amounts, but more specifically the difference between irrigation and evapotranspiration which constitutes the theoretical flux of water through the root zone, are by far the most important two variables that will determine water and salt movement within the soil profile. Other variables such as the hydrology and cation exchange capacity of the soil had only a secondary influence on the water and salt fluxes. In view of this finding it can be concluded that in any modelling exercise which attempts to predict the fate of water and soluble chemicals in the soil and where runoff is not a factor, accurate information on rainfall, irrigation and evapotranspiration quantities are of the utmost importance. Other hydrological soil properties such as the soil water characteristic and saturated hydraulic conductivity are of lesser importance and in many cases, can be inferred from texture.

7.4 CHOICE OF MODELS

Based in the results of the mesoscale study, supported by the literature review (Chapter 2), it was concluded that the more mechanistic deterministic models are superior to the more simple functional type of models. It can be argued that this statement should depend on the scale of application. If a model has to be applied to large areas (macroscale), obtaining information for all the input variables of a data demanding model such as LEACHM, might be a very expensive exercise. However, the key variables that should receive most attention have been found to be rainfall, irrigation and evapotranspiration quantities. These variables are common to all three models that were evaluated in this study and it is inconceivable to think of a water and solute transport model where this will not be the case. Therefore, although mechanistic models might be more data demanding, the influence of those variables that allegedly are difficult and expensive to get information on, will be secondary to rainfall, irrigation and evapotranspiration.

The salt fluxes from irrigated lands will also depend on the soluble salt content, composition and the supply- and assimilative capacity of the soil. This type information are required, in one form or another, by both deterministic functional and deterministic mechanistic models. These models differ only in the way in which the soil processes and input data are handled -- mechanistic or functional. Consequently, unless for a very specific reason (such as inadequate computing facilities), it is recommended that in any study where water and salt fluxes from irrigated lands are to be predicted or calculated, mechanistic models be used rather than the simpler functional type models.

In this study LEACHM was applied to drip irrigated fields, both on a micro- (Chapter 4) and meso- (Chapter 5) scale. The results (statistics and graphs) suggest that the mesoscale application was more successful. The soil and water in the latter case were both very saline while in the former case only the soil was saline. There is no proof that any of the input information of the mesoscale study were more accurate than those of the microscale study. If anything, the opposite will be true. Consequently, it is unlikely that erroneous soil chemistry and -physical input data were the cause of the poor predictions obtained with the microscale study. The only real difference was the density of emitters per surface area. In the microscale study it was 1 emitter per 2,5 m^2 (drip irrigated vineyard), and 1 emitter per m^2 for the mesoscale application. The greater density of emitters obviously influenced the redistribution of applied water. Because of its greater density of surface coverage, the mesoscale drip irrigated plot could be treated as a fully wetted surface with equal wetting of the whole surface area with one-dimensional flow dominating the redistribution of the water. In the microscale study only a fraction of the surface was wetted and, as a consequence, in the real field condition the applied water would have redistributed three-dimensionally. LEACHM, as is the case with most mechanistic models, can deal will vertical, one-dimensional flow processes only. In order to overcome this problem, the total volume of applied irrigation water and the evapotranspiration were converted to depth units, with the depths decreasing with distance from the emitter. This approach was entirely empirical and could have been the cause for the poorer performance of LEACHM in the microscale field study. In can thus be argued that the application of LEACHM to this field study, was wrong from the outset. In conclusion then, models that can deal will one-dimensional flow processes only, should not be used where the applied irrigation water is known to redistribute three-dimensionally.

Finally, as stated by Wagenet (1988): "*At present, only approximate prediction of water movement and chemical distributions can be made. The reliability of these predictions, whether made by simplified or more mechanistic and data intensive approaches, however remains obscure*".

7.5 RECOMMENDATIONS

a) Investigate and rectify the cause of the numerical instability of LEACHM.

b) Investigate and improve all parts of the code of LEACHM that deals with the chemistry of calcium.

c) Evaluate a number of existing three dimensional water flow models.

d) Develop a simplified version of a three dimensional water flow model that can simulate chemical processes as well.

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