Groundwater Contamination potential of agriculture around Lake Naivasha: Comparison of five unsaturated soil zones models

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Groundwater contamination potential of agriculture around Lake Naivasha: Comparison of five different unsaturated soil zone

By

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Abstract

In this study five computer simulation models were evaluated and compared for their ability to predict pesticide leaching in the unsaturated soil zone using experimental field data combined with data from the literature from three agricultural fields in the riparian zone of the Lake Naivasha, Kenya. The selected models were PESTAN (Pesticide Analytical) a simple traditional differential equation (TDE) analytical model, SWAP (Soil-Water-Atmosphere-Plant system) and WAVE (Water and Agrochemical in the soil, crop and Vadose zone) two TDE numerical models and finally SESOIL (Seasonal Soil compartment model) and PRZM-2 (Pesticide Root Zone Model), two compartmental analytical and numerical models.

The purpose of this study was to evaluate critically and qualitatively the behaviour of the models to predict pesticide leaching under three different scenarios likely to occur in the riparian zone of the Lake Naivasha, Kenya. The area is under intensive agriculture, and pesticide is applied on a continuous basis to insure the longevity of the crops. Three scenarios were analysed then, first to simulate a single load of pesticide over a relatively dry year, the second to simulate multiple loads of pesticide with the same dry year and finally the third one to simulate multiple loads of pesticide with a year relatively wet. The evaluation of the models was based on how appropriate the models were for each scenario to simulate the leaching of the pesticides with the available data. The models were calibrated using the recharge data (moisture content) obtained from an experimental infiltration basin realised during the fieldwork.

Only two models SESOIL and SWAP turned out to run all the three scenarios. PESTAN, as a screening model, was able to run only the first scenario with satisfactory results and the capability of WAVE was limited to run only the first and the second scenarios. PRZM-2 was excluded finally due to some numerical problems making the results unreliable. However, this model presents theoretically the capabilities to run three scenarios.

To account for the data scarcity in the process, SESOIL can be suggested as the more suitable model for this environment. It was considered a good tool for assessing groundwater contamination by pesticide via the unsaturated soil zone. This model has the capability to simulate pesticide transport in the soil under a wide range of scenarios at a lower cost than SWAP, because it uses a lower amount of input parameters.

The results of the sensitivity analyses have proved that some parameters are not essentially necessary in the models since their changes do not affect the response of the models in the simulation. Regarding the use of pesticides in the area, the results of this study confirmed indeed the potential risk of groundwater contamination by pesticides.

For the memory of my brother
Jean Claude Jolicoeur

Acknowledgement

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Thanks so much

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Symbol description (Units)

Symbol	Description	Units
C	liquid phase pollutant concentration	(g/cm³)
T	time	(day)
x	distance along the flow path	(cm)
D_{dis}	dispersion coefficient	(cm²/hr)
v	interstitial or pore-water velocity	(cm/hr)
ρb	soil bulk density bulk density	(g/cm³)
θ	volumetric water content	(cm³/cm³)
S	solid-phase concentration	(g/g)
$K1$	first order decay	(/hr)
Kd	the linear Freundlich sorption coefficient.	(cc/g)
W	the water capacity	$(d\theta / dh)$
k	hydraulic conductivity	(cm/d)
h	soil water pressure head	(cm)
A	soil water abstraction rate	(cm³/cm³/d)
θ_{sat}	the saturated water content	(cm³/cm³)
θ_{res}	the residual water content	(cm³/cm³)
α	air entry factor	(/cm)
n	empirical shape factor accounting for	(-)
m	the hysteresis of the soil	(-)
λ	shape constant factor	(-)
ϕ_s	the relative saturation.	(cm³/cm³)
D_{dif}	the diffusion coefficient	(cm²/d)
D_w	the solute diffusion coefficient in free water	(cm²/d)
ϕ_{por}	the soil porosity	(cm³/cm³)
q	the Darcy flux	(cm/d)
J_{dis}	the dispersion coefficient	(g/cm²/d)
K_r	root uptake factor	(-)
r	root water extraction rate	(-)
Δz^*_{i+1}	thickness of compartment i-th compartment	(mm)
Δz_i^*:	the distance between the nodes	(mm)
Δt	the length of time step	(day)
P	Precipitation	(cm)
ET	Evapotranspiration	(cm)
M	Moisture Retention	(cm)
R	Surface runoff	(cm)
I	Infiltration	(cm)
Y	Yield	(cm)
G	Groundwater runoff or Recharge	(cm)
T'	mean monthly soil temperature,	(°C)

T	mean monthly air temperature.	(°C)
P	vertically averaged permeability	(cm²)
P_i	permeability for layer i	(cm²)
x_i	thickness of the layer	(cm)
μ	dynamic viscosity of water	(g/s.cm)
ρ	density of water	(g/cm^3)
g	acceleration of gravity	(cm/s^2)
C_i	The amount of pollutant originally in the soil compartment at time t-1	(µg/cm²)
C_t	The amount of pollutant entering the soil compartment during time step	(µg/cm²)
C_T	The amount of pollutant transferred within the soil compartment at time step.	
.		(µg/cm²)
C_R	The amount of pollutant remaining in the soil compartment at time t	(µg/cm²)
C_M	The amount of pollutant migrating out of the soil compartment during the time	
step		(µg/cm²)
C_{sa}	Pollutant concentration in soil air	(µg/ml)
C_{sw}	Pollutant concentration in soil water	(µg/ml)
H	Henry's law constant	(m³atm/mol)
F	Gas constant	$[8.2*10^{-5}\, m^3 atm/(mol*°v)]$
V	Transmission factor of cloud cover	(-)
n	Freundlich exponent	(-)
D	depth	(cm)
J_w	water velocity	(cm/s)
T_c	Advection time	(sec)
f_a	Air filled porosity (soil porosity –soil water content).	(cm³/cm³)
E	Decayed pollutant mass during time step t	(µg)
$K1l$	Biodegradation rate of the compound in the liquid phase	(/day)
$K1s$	Biodegradation of the compound in the solid phase	(/day)
B	area of pollutant application	(cm²)
N	snowmelt,	(cm)
E	evaporation	(cm)
C_{DW}	mass loss due degradation in dissolved phase	(g/day)
C_{DG}	mass loss due to degradation in the vapor phase	(g/day)
C_U	mass loss by plant uptake of dissolved phase.	(g/day)
C_{QR}	mass loss by removal in runoff	(g/day)
C_{APP}	mass gain due to pesticide deposition on the soil surface	(g/day)
C_{FOF}	mass gain due to washoff from plants to soil	(g/day)
C_{DS}	mass loss due to degradation of sorbed phase chemical	(g/day)
C_{ER}	mass loss by removal on eroded sediments	(g/day)
C_{TRN}	mass gain or loss due to parent/daughter transformation	(g/day)

1 Introduction

1.1 Problem formulation

During the last decades, agriculture has been intensified in the riparian zone of the Lake Naivasha, Kenya. More fertilizers and pesticides are being used in order to keep the crops healthier and more productive. A large variety of pesticides are reported to be in use in the area. They are used on a continuous basis and ranged from slightly toxic to very toxic. Unfortunately, pesticides have side effects; by definition they are poisons and become very hazardous once leaving the root zone where the effects are desired and reaching the groundwater. In the area, people are dependent on groundwater for domestic purposes and also for irrigation. The continuous use of pesticide may have a great deal of impact on the groundwater whether on a long or a short-term basis. Therefore, concern has arisen on how to assess the impact of those agrochemicals on the groundwater, the lake, and ecosystem as a whole.

Being too costly to set up a monitoring system, the use of computer simulation models was another option for assessing the potential for pesticides to leach to the groundwater. Simulation models provide the capability of evaluating the response of natural systems to a range of scenarios in an efficient and cost-effective manner.

In this study, five computer simulation models that predict pesticide leaching in the unsaturated soil zone were compared to one another using the same environmental scenarios. The chosen models were: PESTAN (Pesticide Analytical) a simple Traditional Differential Equation (TDE) analytical model, SWAP (Soil-Water-Atmosphere-Plant system) and WAVE (Water and Agrochemicals in the soil, crop and Vadose zone) two TDE numerical models and finally SESOIL (Seasonal Soil compatment model) and PRZM (Pesticide Root Zone Model), two compartmental analytical and numerical models.

Some of the models have previously been used in the area but at different occasion and under different scenarios.
SESOIL: Tang (1999), PRZM: Anil Upendra De Silva (1998) and
WAVE: Anil Upendra De Silva (1998).

The models vary to some degree with regard to their formulation, assumptions input parameters and output capabilities. Therefore, the magnitude of the predicted leaching will depend partly on the model used. It is however necessary to find out how much they will vary. For this reason, it was decided to compare them in order to determine whether these differences lead to substantially different results when using them to assess potential contamination impact on groundwater in the study area.

** riparian zone: zone situated on the close vicinity of a lake or a river*

1.2 Study objectives

The aim of this research is to critically compare the behaviour of five different unsaturated soil zone models for predicting pesticide leaching in the soil zone around Lake Naivasha.

Besides the main objective of the study we were looking for answers to the following questions:

1- How appropriate are the models for the evaluation of pesticide transport in the unsaturated soil zone in the tropical conditions encountered in the study area such as: climate, chemical type and application, crop type and irrigation practice?

2- What are the minimum field data we need for the different models to adequately simulate pesticide leaching through the unsaturated soil zone?

The second question is important because data scarcity occurs frequently. There may be some field restrictions involved. Some of the models are very data demanding and the collection of the data bears a highly estimated cost. Some of the data are unlikely to be found in the literature. The models may be very sensitive to some parameters, therefore it is worthy to point out those parameters on which emphasis should be given when carrying out further studies.

1.3 Methodological background

The methodology used in this study was designed to fulfil the objectives of the research stated above. The research period has been divided into three phases in order to reach the objectives.

1.3.1 Pre-fieldwork

The major activities in this phase comprised:

- the definition of the problem and research theme,
- study of the different models that were going to be used for the research,
- review of the model parameters and the identification of the source of data acquisition,
- literature review

1.3.2 Fieldwork

The soil has been extensively studied by Siderius and Kwacha (1998). In their report they provide a great deal of data to a depth of 120cm. Groundwater level in the cultivated area is however usually greater than 2 meters. Therefore, more information on the vadose zone properties was needed in order to analyze the potential groundwater contamination risk. The fieldwork was done for three weeks (October 1st to October 23rd) and was mainly devoted to data collection. The most important different data collected in the field were: soil moisture content and saturated hydraulic conductivity. Soil samples were collected from the soil core for laboratory determination of particle size distribution and organic matter content OMC.

During the fieldwork a small infiltration basin was set up in order to collect information on soil moisture distribution for the calibration of the models (more details will be given in chapter 5).

1.3.3 Post-fieldwork

The major activities of this phase were data gathering, data entry, data analysis, models simulations and thesis writing.

1.4 Thesis layout

This thesis consists of seven chapters followed by different appendices to which references are given through the text.

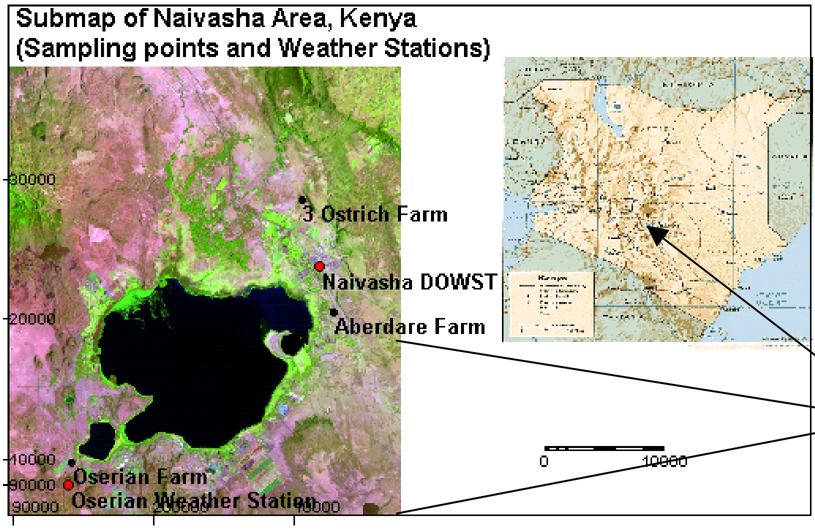
Chapter 1 is the introduction. In this part, the environmental problem is introduced and the objectives of the study are described. The methodological background used to achieve the objectives is also presented in this chapter.
Chapter 2 is the "Description of the study area" in which the study area is presented and described taking account of the various aspects relevant the study topic.
Chapter 3 is the "Background information". In this chapter some relevant environmental studies carried out in the area are presented preceding a brief background definition of factors affecting the potential leaching of pesticide through the unsaturated soil zone.
The different models are presented and described in Chapter 4 and a list of all the required parameters is adjoined to the description.
Chapter 5 is the "Model design". In this chapter, the design of the models is shown defining the different boundary conditions and the soil system.
Chapter 6 is the "Results and discussion". In this chapter, the calibration process is described and the different scenarios are presented. The results of the calibrated models under the different scenarios are given. In the same chapter, they are compared and subsequently analyzed.
Finally, Chapter 7 " Conclusion and recommendation" is a summary of all the results obtained from the different scenarios. In this chapter, the questions asked in Chapter 1 are answered. This chapter is concluded by appropriate recommendations in relation to the study objectives based on the answers to the questions of the first chapter.

2 Description of the study area

2.1 Location

Naivasha is located in the southern part of the Nakuru District, itself located 100 km northwest of Nairobi, the capital of the east African country, Kenya. The map in Figure 1 shows the position of the study area as well as the sampling points and the weather stations:

The study area is located within the UTM zone 37 and lies between the following coordinates:
XY: 19434348, 9938103.5 and
XY: 217537.58, 9902085.28



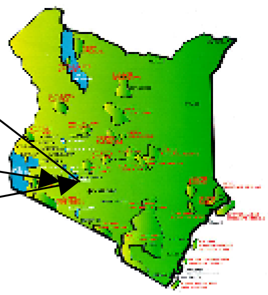


Figure 1. Submap of Naivasha area (sampling points and weather stations)

* DOWST: District Office Weather Station

2.2 Climate of the study area

2.2.1 Rainfall

Rainfall is one of the most important external factors in the assessment of ground-water potential risk to contamination by pesticide, as it induces the leaching of the pesticide through the soil. However, it doesn't imply any automatic leaching as it may be lost either by runoff or by evaporation before reaching the groundwater. The term "lost" is used here because this water does not contribute to the leaching process.

The climate of the study area is a typical equatorial tropical climate with two rainy seasons each followed by a dry season. The first rainy season starts from March and lasts three months and the second is from October to December also three months long. The first season is considered as the long rainy season for bringing more precipitation compared to the second called short season. The dry seasons are from January to February and from June to September. This analysis is based on the climatic data obtained from Ashfaque (1999) provided by the Naivasha District Office (D.O). The average annual rainfall is about 667 mm/year for the period of 1910-1962.

Figure 2 shows the variation of the monthly rainfall over the area for a 42-year period.

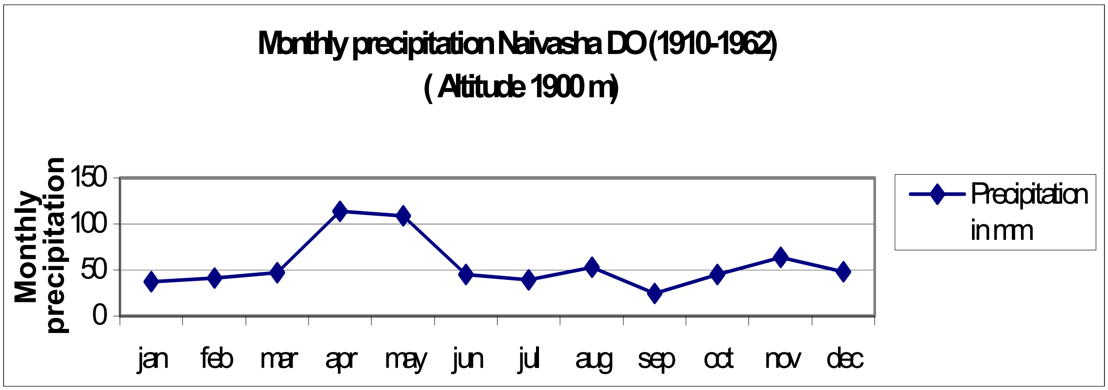


Figure 2. Monthly rainfall (Naivasha D.O)

2.2.2 Temperature

The mean maximum monthly temperature within the area is about 29°C and the mean minimum temperature is about 9°C. The temperature can be as low as 1 or 2° during the night. The warmest months are generally January, February and March whereas the coldest months are July and August. A period of 17 years from 1937 to1954 was considered for this calculation.
The graph in Figure 3 shows the fluctuations in the maximum and minimum temperature over the area.

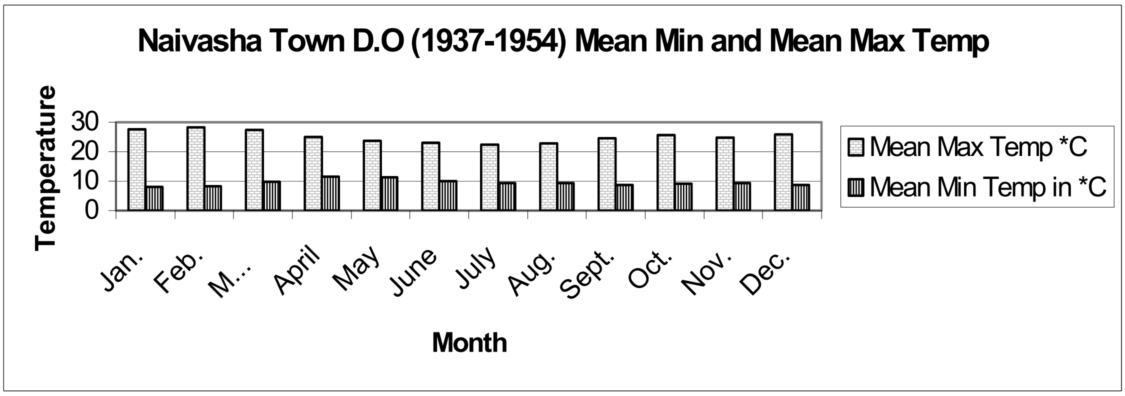


Figure 3. Mean monthly minimum and maximum temperature (Naivasha D.O)

2.2.3 Evaporation

The evaporation rate has been assessed using pan evaporation data from the same station. Result of an average over 33 years of data from 1957 to 1990 is presented in Figure 4. Class A pan was used and the pan coefficient considered is 1. The average monthly evaporation calculated is about 5mm/day (Ashfaque, 1999). The highest evaporation rate occurred in March and the lowest could be observed in November.

The yearly evaporation based on this record is estimated to be 1804.2 mm about 2.7 times greater than the annual rainfall in the area. The tables with the climatic data are given in Appendix A.

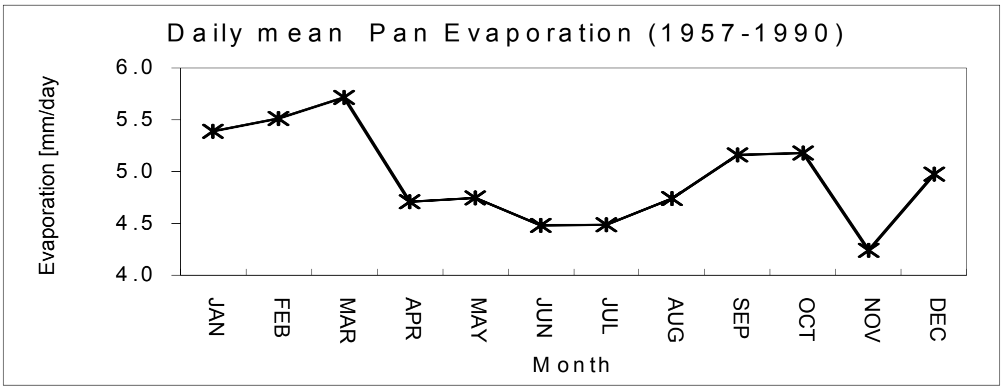


Figure 4. Daily mean pan evaporation (Naivasha D.O)

2.3 Agricultural practices

The farming system is well expanded in the riparian zone of the lake Naivasha which is the only fresh water lake in the Rift valley whereas all it ecological and economical importance in the area. According to Huaccho (1997), the irrigated areas have increased from 981.8 ha in 1988 to 7353 ha in 1998 (cited by Tang, 1999).

2.3.1 Type of crops

The most important products in the area are flowers mainly grown for exportation to European countries specially to the Netherlands, sometimes also in transit to American countries. Their rotation varies according to the type of flowers. Statice and Carnation (Figure 7) remain on the ground for 18 months whereas roses take a maximum of 8 years before being removed completely. The flowers represent about 60% of the cultivated land (De Silva, 1998). The farmers also grow several other types of crops mainly for local consumption, such as vegetables: cabbages, French beans, onions, egg plants, fruits, peas etc and cereal such as corn etc. For French beans the crop rotation is about 3 times a year. Most of the flowers and a small percentage of the food crops such as onions are grown in green houses

2.3.2 Water used and irrigation

Large-scale farmers having large farms use sprinkler or drip irrigation to supply water to their crops. Figure 6 shows a plantation field irrigated using a pivot system. Lake water is used by those living nearby and the farms located at a considerable distance to the lake get their water from the underlying aquifer. The irrigation practice, consequently, raises concerns about the general water balance issue of the lake Naivasha area.

2.3.3 Type of chemicals used

To promote the yield of their crops, the farmers make use of fertilizers. They are aimed to overcome diseases, increase the yield and by providing required nutrients contribute to the full development of the crop. However, fertilizers can be harmful by creating an environment that favours the growth of many insects, which primarily were aimed at destroying diseased crops. Thus it makes the farms dependent on pesticides for economical crop management.

Figure 5. New Pivot system used for irrigation at 3 Ostrich Farm

Figure 6. Plantation of French beans at Aberdare State Farm

De Silva (1998) and Tang (1999) have investigated about sixty different types of pesticides being in use in the area by the riparian farmers. The inventory list is given in Appendix B. In this list can be found Vinclozolin and Gibberilic, two fungicides that are very persistent with a half-life of more than 600 days. Others like

fenamiphos, Aldicarb, and Dimethoate are very toxic however fortunately less persistent. The pesticides are classified in term of their toxicity according to the norms of the World Health Organization (WHO), Kidd (1991) and in term of the persistency according to the U.S Environmental Agency (U.S.E.P.A.), ETA (1993) cited by Tang (1999).

Figure 7. Experimental flower plantation at Oserian Farm (Statice)

2.4 Geology

Naivasha is located within the Rift Valley of East Africa, which starts from Syria and expands to Mozambique through Ethiopia, Kenya and Tanzania successively.

Lars-Erik Ase, (1986) characterized the Rift Valley as one of the most remarkable features of the earth crust . The volcanoes such as the Longonot, Eburu, etc are young and responsible through their eruption for the soils and the rock types around the lake. In general, the study area is covered by 2 types of quaternary deposits: one of lacustrine and the other of volcanic origin (Thompson et al., 1958). Lithologically, the volcanic rocks in the area consist of basalts, phonolites, tephrites, trachytes, rhyolites, comendites, pyroclastic of acidic nature. The lacustrine formations are mainly consolidated tuffs, diatomite, very fine pyroclastics to pumice and occasionally fine sediment from the upland (personal communication with Dr Siderius).

The study of the geology of the area is very relevant to the study of pesticide leaching. It is very important for example to have basic information on the geologic layers between the surface soil and groundwater which control the groundwater flow, the infiltration, and the vertical water movement.

2.4.1 Geomorphology

Morphologically, two main landscapes have been identified by Kwacha, (1998): thelacustrine plains and the volcanic plains. The lacustrine plains occur mainly in the north and northeast part of the lake and formed by a number of terraces due to fluctuations of the lake water levels. Whereas, the volcanic plains, which resulted of the lava flow from eruptions of the Longonot volcano, occur mainly at the southern part and are associated with the lacustrine plains sometimes in as intricate pattern (personal communication with Dr Siderius)

2.4.2 Soil

The soils in the study area are divided into two types according to their occurrence in the landscape and the parent material. The soils developed on lacustrine deposits have been classified by Siderius (1998) as being moderately drained, deep, dark grayish brown to brown soils, sandy loam to sandy clay loam. Kwacha (1998) classified those formed on the volcanic plain as well drained, moderately deep to very deep, dark brown to pale brown soils, defined further by the Kenyan Soil Survey (KSS), as loam to clay loam.

2.5 Hydrogeological settings

2.5.1 Groundwater depth

The aquifers in the sub-catchment of Naivasha occur mainly in the fractured volcanic formations, or along the weathered contacts between different lithological units (Gressando, 1999). These aquifers are often unconfined for those close to the lake and confined or semi confined away from the lake. High permeabilities and high yield are generally found in the vicinity of the lake.

Data from about 67 boreholes were used to assess the depth of the groundwater within the study area. The depths were measured from 1980 to 1999. Additional data could have been collected from other borehole records but unfortunately they had to be discarded due to technical problems (personal communication with Owor).

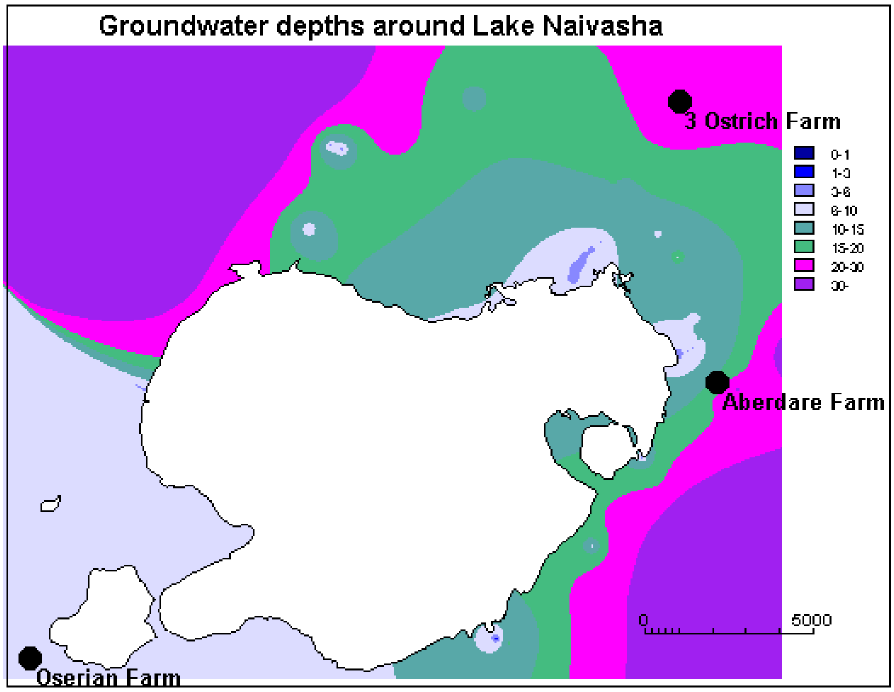


Figure 8. Various groundwater depths around Lake Naivasha

The depth map of Fig. 8 shows a rough presentation of the spatial variation of the groundwater depth around the lake. The map has been calculated using the moving average point interpolation technique.

3 Background Information

3.1 Previous relevant studies

Extensive studies have been carried out in the lake Naivasha area by researchers from different field who have separately highlighted several aspects of the ecosystem.

Clarke, Thompson and Dodson (1958) have studied the geology and geomorphology of the Naivasha area which allowed other soil scientists as mentioned earlier (in soil description) to continue with the study of the soil units in the lake area.

Siderius (1998) and Kwacha (1998) have classified the different soil map units on the basis of the geomorphological units.

Hydrogeologists dealing with environmental issues carry out several studies recently about the water balance, the main concern in the area. In April 1999 and in October 1999, presentations were given by Robert Becht (from ITC, the Netherlands) in Naivasha Town on the long term water balance of the lake Naivasha area relative to the lake fluctuation. This water balance was based on a modified model of M'Bui (1999).

Several studies on the use of agrochemicals in the area have been carried out. Groundwater chemistry has been the focus of the study of Morgan (1998). She explained that the quality of the groundwater in the area is deteriorated by high nitrate level from agriculture and unsewed systems, which contribute to the reduction of potable (drinking) water. According to her, poor water quality for drinking purposes was indicated due to very high fluoride levels too.

Several analysis based on mathematical modelling of pesticide fate processes have been carried about by several environmental hydrologists.

PRZM-2 and WAVE two mathematical modelling packages have been tested and used by Anil Upendra da Silva (Anil, 1998) to simulate the fate of pesticides and fertilizers in the vadose zone. The results of the simulations showed that most of the chemicals were retained in the first 100 cm of the soil depth. Therefore the potential risk of pesticides and fertilizers leaching was found to be relatively low due relatively low rainfall and great soil depth where the experiments have been undertaken. He further explained that the irrigation rate and schedule doesn't have a significant effect on the leaching.

Finally, a similar analysis of the pesticides fate and water quality has been produced by Tang (1999) whose aims were to identify and evaluate the potential pollution of agrochemicals used in the area of Naivasha. She used SESOIL for the simulation.

The results of her assessment revealed that the water quality of the lake Naivasha was suitable for irrigation but not suitable for drinking purposes without treatment. She showed that water quality indicators measured from farm effluents discharging into the lake exceeded the discharge guidelines of Kenya. According to her, the sandy loam area around the lake was the most susceptible soil to pesticide leaching.

De Silva (1998) and Tang (1999) reported an inventory list of all pesticides and fertilizers used in the area.

3.2 Soil - Pesticide Leaching Potential

Most of the studies about pesticide leaching to groundwater are mainly focussed on the unsaturated soil zone. This unsaturated soil zone constitutes the transfer zone between the soil surface and the groundwater by the fact that all solute should reach the groundwater via this medium. Whatsoever applied at the soil surface: water, fertilizers, pesticides etc, would be flushed downward through the unsaturated soil zone with the possible fate of reaching the groundwater whether in the long or in the short term. This downward movement is called leaching and has earned great concerns over the time in term of pesticide pollution considering its potential impact on the groundwater. Therefore, due to the role of the unsaturated soil zone in the leaching process, a thorough understanding of the soil properties and the processes leading to the leaching through the soil will allow to have a clear insight on this matter. Nevertheless, the soil properties alone are insufficient to determine the leaching of the pesticides. The pesticide properties such as its solubility, its volatility, its degradation, etc contribute also greatly to its movement.

The properties of the soil together with the properties of the pesticides determine the soil-pesticide leaching potential into groundwater. Other external factors are also involved in the process such as the depth to the groundwater, or climatic conditions that also influence the leaching of pesticide through the soil by providing or reducing the moisture content of the environment.

3.2.1 Effect of soil properties on pesticide leaching

We know that the soil type is able to affect significantly the likelihood of pesticide leaching into the groundwater. For example, sandy soils allow pesticides to move towards the groundwater more rapidly than soils with significant clay content. If the soil has clay minerals as part of its composition, the positively charged pesticides can adsorb onto the negatively charged clay particles. Soil with a high organic matter content can also adsorb pesticides, thereby inhibit their movement.
The soil physical properties that affect the likelihood of the pesticide leaching into the groundwater are the following:

Soil texture

It is determined by the relative proportion of different sizes of soil particles meaning the relative proportion of sand, clay and silt. Leaching is more rapid in coarse or light (sand textured) soils than in fine or heavy (clay textured) soils. The faster the movement of percolating water, the lower the opportunity for adsorption of pesticides and therefore the greater the chance of a pesticide to reach the groundwater.

Soil structure and porosity

The way soil particles are aggregated also affects water movement. Loosely packed soil aggregates are more likely to allow easy downward movement of water than a compacted soil therefore more pesticide can be carried along. Also, pesticides are more likely to leach through more porous soils.

Soil hydraulic conductivity

It is a measure of how fast water can move downward through the soil. While moving downward the pesticide can be carried along in an advective process. Therefore, the more permeable the higher the potential for the leaching of pesticides.

Soil organic matter (OM)

Pesticides tend to be adsorbed by the OM as it is driven down by water within the unsaturated soil zone. As a matter of fact, soils high in OM tend to be more adsorptive, contrarily to soils low in OM which are less adsorptive.

Soil moisture

It determines the content of water in the soil. The downward transport of pesticides through the soil is achieved ultimately by water driven by the hydraulic gradient; therefore, a dry soil is less likely to transport pesticides than a wet soil.

Depth to the groundwater

The depth of the groundwater table is one important factor to look into the pesticide leaching process because the shallower the depth to groundwater, the less soil there is to act as a filter. There are also fewer opportunities for degradation or adsorption of pesticides due to the little time for those processes to undergo their reactions.

3.2.2 Pesticide leaching potential

Besides the several properties of the soil affecting the leaching of pesticides through the soil into the groundwater, some properties of the pesticides themselves also play an important role in the process. There are several characteristics of pesticides that affect the likelihood of pesticides leaching into the ground water.

Solubility of pesticides in water

It is defined as the tendency for a pesticide to dissolve in water and, hence, be carried down to groundwater. Therefore, the pesticide with a higher solubility has greater potential of being moved downward through the soil, possibly reaching the groundwater.

Pesticide volatility

Volatilisation is identified by the loss of pesticide as it changes from a liquid or a solid to a gas and vaporises from the soil or plant surface into the atmosphere. It is measured in terms of its vapour pressure. The higher the vapour pressure of a pesticide, the faster it is lost to the atmosphere and the less that remains available for leaching.

Pesticide degradation

It is the breakdown of pesticides by processes that do not involve living organisms. This process occurs when the pesticides react with water, oxygen, or other chemicals in the soil. One of the most common pesticide degradation reactions is hydrolysis a breakdown process where the pesticides reacts with water.

Microbial degradation

The predominant means of decomposition mainly in the root zone are biochemical processes carried out by soil microorganisms. The biodegradation is the breakdown of pesticides by microorganisms present in the soil. Microorganisms such as bacteria, fungi, etc are mainly responsible for the degradation of pesticides in soil, sometimes acting singly and sometimes in combination.

Photodegradation

Another process through which pesticides degrade is photolysis, or breakdown caused by exposure to sunlight. Photodegradation can destroy pesticides on foliage, on the soil surface and even in the air.

Therefore, the longer the time before the pesticide is broken down, the longer it is available to leach toward the groundwater.

Pesticide half-life in soils

It is defined as the length of time required for one-half of the amount of applied pesticide to be completely degraded or decompose to other compounds. Therefore, the longer the half-life period, the more likely the pesticide will have time to leach to the ground water.

4 Description of the models

For the study, two types of models were used, they are all capable of simulating transport of pesticide through the unsaturated soil zone. They are ranged from very simple to very complex ones in term of data requirement and chemical and physical processes that they account for. PESTAN is a TDE model (Traditional Differential Equation) using an analytical solution by simplifying the environment, SWAP and WAVE are TDE models using a numerical scheme to solve the main equations and SESOIL, PRZM-2 are compartmental models using both an analytical and a numerical solutions. To ease the understanding of the text structure, they will be presented in the same order however this order doesn't imply their presentation from the simpler model to the more complex ones. Most of the models can simulate not only pesticides but also other chemicals, but the focus of the study is on pesticide.

4.1 Pesticide Analytical (PESTAN)

Developed by Enfield, et al., in 1982, the Pesticide Analytical model (PESTAN) is a computer program for estimating the transport of pollutant through soil to groundwater. It is a very simple model that can be presented by few words. The model is conceptualised in Figure 9.

The model simulates the vertical transport of pollutant through the soil as a slug of contaminated water that migrates into a homogeneous unsaturated soil. The slug is defined (by Collins dictionary) as being a unit of mass.

The following equation describes the vertical transport of a pollutant dissolved with water through the soil.

$$\frac{\partial C}{\partial t} = Ddis\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x} - \frac{\rho b}{\theta}\frac{\partial S}{\partial t} - k1C \qquad \textbf{Eq. 1}$$

Where C = liquid phase pollutant concentration (g/cm³), t = time (day), x = distance along the flow path (cm), $Ddis$ = dispersion coefficient (cm²/hr), v = interstitial or pore-water velocity (cm/hr), ρb = bulk density (g/cm³), θ = volumetric water content (cm³/cm³), S = solid-phase concentration (g/g), $K1$ = first order decay (/hr).

Several assumptions are made in PESTAN:

- First, it assumes the steady state flow conditions through the soil domain.
- All water once infiltrated is assumed to go for the recharge.
- The model also assumes homogeneous soil conditions. It is conceptualised as one single layer.
- Solid degradation is assumed to occur at the surface and hydrolysis degradation is expected within the soil.
- The rate of liquid-phase degradation does not change with soil depth or time
- Once the slug enters the soil, sorption and dispersion influence the pollutant transport.

More assumptions are made in the model; the interested reader is referred to the user manual.

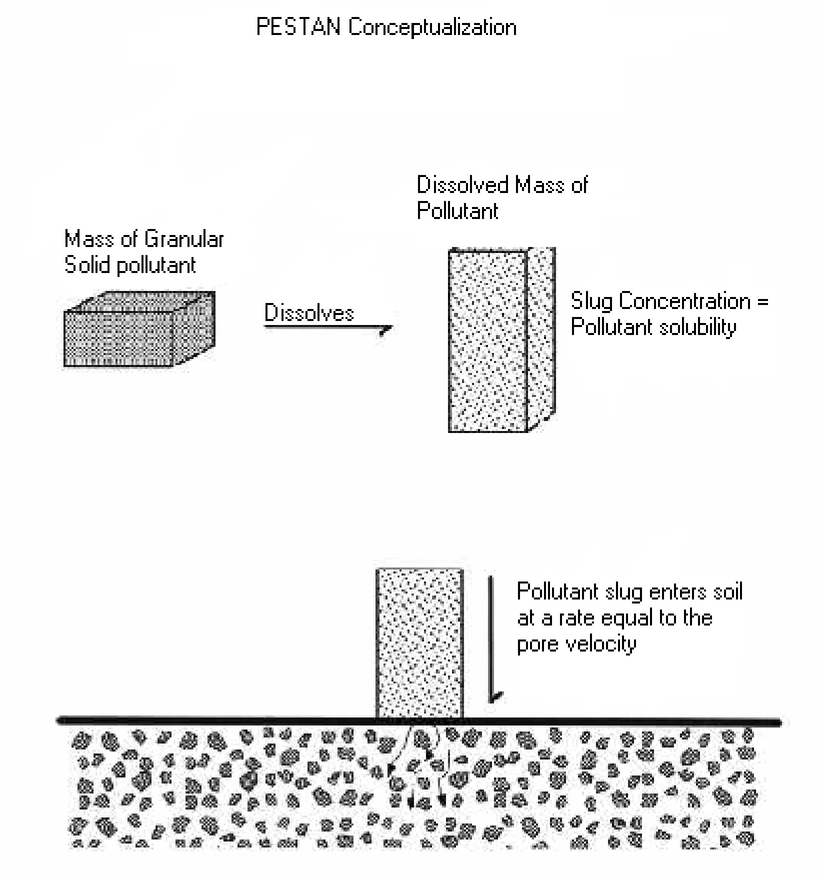


Figure 9. PESTAN conceptualisation of the pollutant migration with the soil system

The term $\frac{\partial S}{\partial t}$ of Equation 1 represents the rate of loss from liquid phase to solid phase due to sorption, which can be written as in Equation 2, assuming linear and instantaneous sorption.

$$\frac{\partial S}{\partial t} = Kd \frac{\partial C}{\partial t} \qquad \text{Eq. 2}$$

where Kd cc/g is the linear Freundlich sorption coefficient.

Due to limitations all applications of pesticide are assumed to happen before the recharge. The upper boundary is defined as a slug of a certain thickness that enters the soil at time Ø. This thickness is calculated using the water solubility when the chemical is applied in a granular form by determining the equivalent depth of water from the soil water content required to dissolve all the available mass of pesticide.

4.2 Soil-Water-Atmosphere-Plant environment (SWAP version 2.0)

The simulation of water flow, solute transport and plant growth in Soil-Water-Atmosphere-Plant environment model (SWAP) has been developed by Wageningen Agricultural University, The Netherlands with close cooperation in DLO Winand Staring Center. It is a computer model that simulates transport of water, solutes and heat in variably saturated top soils. The following diagram (Fig.10) describes schematically the Soil-Water-Atmosphere-Plant system (taken from the SWAP release 2.0.6 manual):

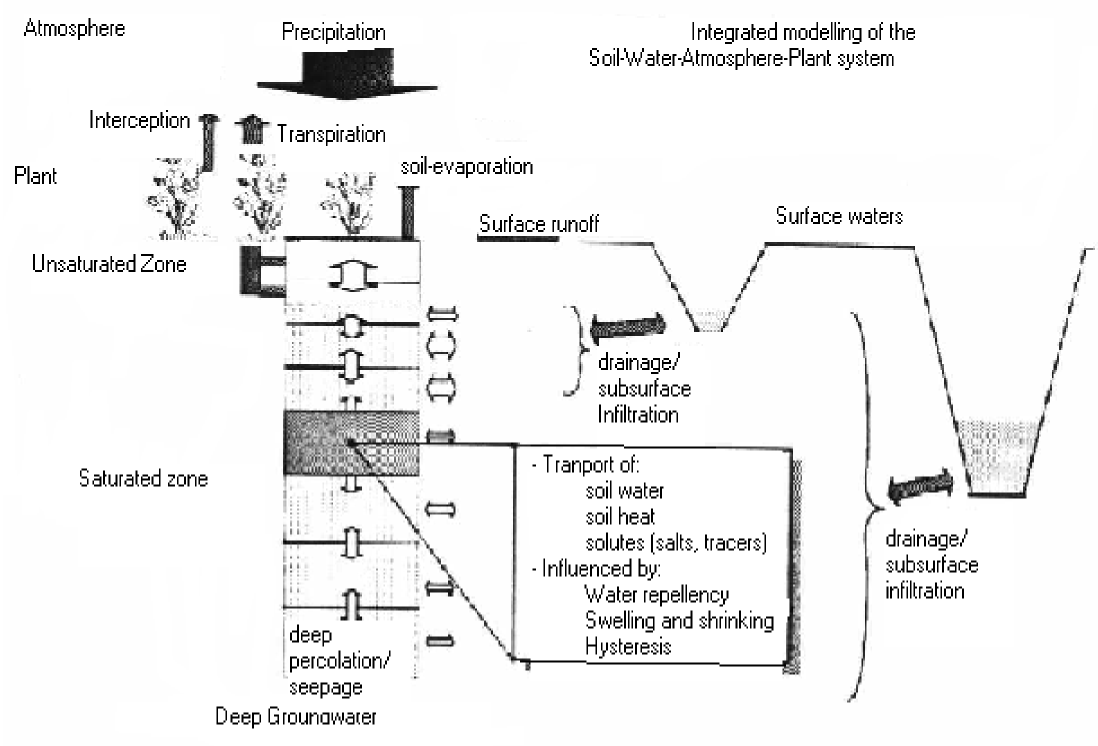


Figure 10. A schematised overview of the modelled system (SWAP release2.0.6)

4.2.1 Soil Water Flow

SWAP is a one-dimensional physical, finite difference numerical model describing water flow in unsaturated soils based on the Richards equation:

$$\frac{\partial\theta}{\partial t} = W(h)\frac{\partial h}{\partial t} = \frac{\partial\left[K(h)\left(\frac{\partial h}{\partial x}+1\right)\right]}{\partial x} - A(h) \qquad \text{Eq. 3}$$

where W is the water capacity $(d\theta / dh)$, K is hydraulic conductivity (cm/d), h is soil water pressure head (cm), A is soil water abstraction rate (cm³/cm³/d),

In SWAP the above one-dimensional partial equation is solved numerically using an implicit finite difference scheme based on a mass balance.
The unsaturated function of Equation 4 describes the soil moisture retention characteristic curve using the empirical function of Van Genuchten.

$$\theta = \theta_{res} + \frac{\theta_{sat} - \theta_{res}}{\left(1 + |\alpha h|^{n}\right)^{m}} \qquad \text{Eq. 4}$$

where θ_{sat} is the saturated water content(cm³/cm³), θ_{res} is the residual water content (cm³/cm³), and α (1/cm), n (-) and m(-) are empirical shape factors accounting for the hysteresis of the soil describing the main drying and the main wetting curve.

The unsaturated hydraulic conductivity K has been calculated applying the predictive model of Mualem (1976):

$$K = K_{sat}\phi_s^{\lambda}\left[1 - \left(1 - \phi_s^{\frac{1}{m}}\right)^{m}\right]^2 \qquad \text{Eq. 5}$$

where ϕ_s is the relative saturation, *Ksat* is the saturated hydraulic conductivity and λ (-)is a shape parameter.

The top and the bottom boundary conditions have to be specified in order to get accurate simulation. Up to 5 layers and 40 sub-layers can be simulated. The boundary conditions at the soil surface are formulated in terms of rainfall, irrigation, interception, transpiration (in case of a cropped soil) and soil evaporation.

Daily evapotranspiration

A two-step-approach of the Penman-Monteith equation is adopted in SWAP. In this approach, the potential evapotranspiration is first calculated and then the actual evapotranspiration is deducted using the root water uptake reduction due to water stress. In the model, the evapotranspiration can be either calculated or specified as reference evapotranspiration ETref. In the present study, ETref is provided and a crop factor is thus specified. In order to partition the potential evapotranspiration into potential transpiration rate and potential soil evaporation rate either the leaf area index LAI or the soil cover fraction as a function of development stage is used. In order to model the crop transpiration, SWAP uses a simple crop model, which represents a green canopy that intercepts precipitation, transpires and shades the ground.

The bottom boundary in the SWAP model is either the unsaturated zone or in the upper part of the saturated zone. Several options are available in SWAP to define the bottom boundary condition:
- groundwater level as a function of time
- bottom flux as a function of time
- pressure head as a function of time
- zero flux at the bottom
- free drainage of soil profile, etc

4.2.2 Solute transport

SWAP simulates diffusion, convection and dispersion, non-linear adsorption, first – order decomposition and root uptakes of solutes. The model is focussed on the transport of salts, pesticides and other solutes, no volatilisation is therefore processed. The solute transport processes are expressed in terms of their fluxes.

The diffusive solute flux (g/cm²/day) is described by Fick's first law of Eq.6:

$$J_{dif} = \theta D_{dif} \frac{\partial C}{\partial x} \qquad \text{Eq. 6}$$

with D_{dif} the diffusion coefficient (cm²/d)

The relation proposed by Millington and Quirk (1961) (Eq. 7) describes the diffusion process in SWAP:

$$D_{dif} = D_w \frac{\theta^{7/3}}{\phi_{por}^2} \qquad \text{Eq. 7}$$

With D_w the solute diffusion coefficient in free water (cm²/d) and ϕ_{por} the soil porosity (cm³/cm³).

The bulk transport described by the convection process is calculated from the average soil water flux (g/cm²/day) represented by the following relation (Eq.8):

$$J_{con} = qC \qquad \text{Eq. 8}$$

with q, the Darcy flux (cm/d)

The dispersion flux is proportional to the solute gradient by the following relation:

$$J_{dis} = -\theta D_{dis} \frac{\partial C}{\partial x} \qquad \text{Eq. 9}$$

Where J_{dis} is the dispersion coefficient (g/cm²/d)

Considering all the above fluxes from the different processes, the total flux can therefore be written as:

$$J = J_{dif} + J_{con} + J_{dis} = qC - \left(D_{dif} + D_{dis}\right)\frac{\partial C}{\partial x} \qquad \text{Eq. 10}$$

The general transport equation applied in SWAP including the pesticide first order decay rate and the root uptake is written as followed:

$$\frac{\partial(\theta C + \rho bS)}{\partial t} = -\frac{\partial qC}{\partial x} + \frac{\partial}{\partial x}\left(\theta\left(D_{dif} + D_{dis}\right)\frac{\partial C}{\partial x}\right) - K1(\theta c + \rho bS) - k_r rC \qquad \text{Eq. 11}$$

Where: K_r is the root uptake factor (-) and r is the root water extraction rate (-).

To solve the above equation a numerical finite difference scheme is used. For more detail refer to the SWAP manual (Technical document 45, Van Dam et al.,1997)

4.3 Water and Agrochemicals in the soil, crop and Vadose Zone model (WAVE)

The WAVE is a software package developed by the Institute for Land and Water Management of the K.U Leuven, Belgium. This is a deterministic model. It uses the finite difference techniques to solve the differential equations describing matter and energy transport in the soil-crop continuum. The model is one-dimensional because it is assumed that governing transport processes of matter and energy in the soil sub-system occur essentially in the vertical direction (Vanclooster et al, 1994).

WAVE deals with several modules such as water transport module, solute transport module, the heat transport module, the crop growth module and the nitrogen fate module. However, for the present study only the water transport module and the solute transport module will be discussed. The flow chart of Figure 11 shows the interaction between the different modules in WAVE.

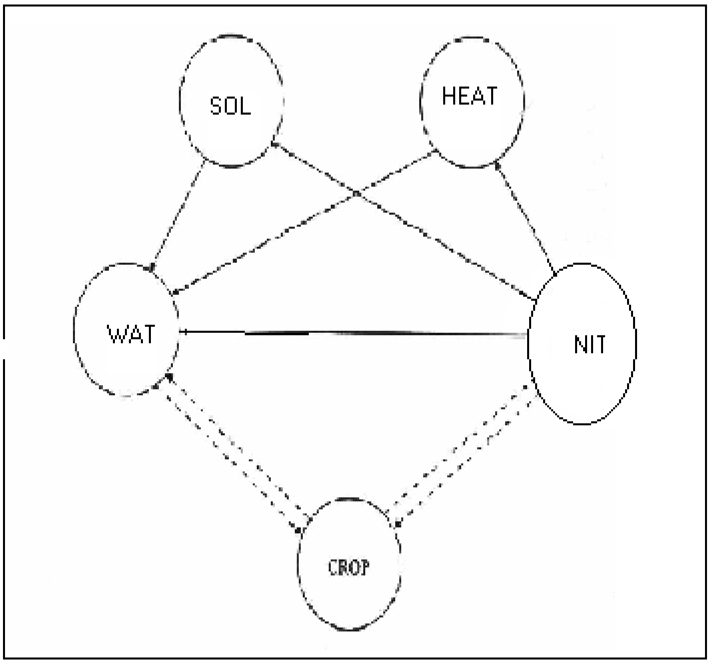


Figure 11. Schematic presentation of the modules in WAVE (WAVE release 2.2).

* Full line arrows Represents obligatory “uses-relations”, dashed lines are optional.
SOL = solute; NIT = nitrate; WAT = water

4.3.1 Water Transport Module

The Richard’s equation is used in WAVE too to describe the one-dimensional water transport in the soil medium as in equation 3. The soil water flow equation (Eq. 3) is solved in WAVE numerically. A discretization of the scheme into a number of compartments is done over a time period and for each of those compartments the parameters of the moisture retention characteristic and hydraulic conductivity curve are given. Those parameters are the following: saturated volumetric soil water content, residual soil volumetric soil water content, inverse of the air entry, etc.

In addition to the widely used retention curve equation of Van Genuchten (Eq.4) some other hysteretic models are available in the WAVE model such as the Mualem model II and the Mualem universal model based on the Mualem model II. As for the moisture retention curve, other models are available in the WAVE model to describe the hydraulic conductivity curve of the soils. They are the Gardner Power function, Gardner exponential function, Gilham, Brooks and Correy and Mualem.

The model uses a numerical implicit difference scheme (Eq. 12) to approximate the Richard's equation (Eq. 3) that is the following:

$$C_i^j \frac{h_i^{j+1} - h_i^j}{\Delta t} = \frac{K_{i-\frac{1}{2}}^j \left[\frac{h_{i-1}^{j+1} - h_i^{j+1}}{\Delta z_i^*} + 1 \right] - K_{i+1/2}^j \left[\frac{h_i^{j+1} - h_{i+1}^{j+1}}{\Delta z_{i+1}^*} + 1 \right]}{\Delta z_i} \qquad \text{Eq. 12}$$

Where:
Δz^*_{i+1} : thickness of compartment i-th compartment (mm)
Δz_i^*: is the distance between the nodes (mm)

Δt : is the length of time step (day)

The bottom and the upper boundary conditions are also defined in order to set the flow situation at the surface and at the bottom of the compartments. The flow situation at the soil surface is determined by the infiltration or the evaporative flux. The potential evapotranspiration of a disease free crop is calculated in the WAVE model by multiplying the potential evapotranspiration of a reference surface (ETref) with a crop coefficient Kc.. Using crop factors such as leaf area index and soil cover fraction, root depth, etc the potential evapotranspiration is partitioned into potential transpiration and potential evaporation which are further split into actual transpiration and actual evaporation. The Penman equation can also be selected.

The bottom boundary can be determined using several options that are presented in the following lines:
- the presence of a groundwater table is considered,
- the pressure head at the bottom is known as a function of time,
- the flux through the bottom is known at each time step or
- a lysimeter with free outflow is present at the bottom.

4.3.2 Solute Transport Module

The Wave-model described numerically the transport of a decaying and sorbing solute in soils. The module assumes the existence of immobile or stagnant soil water regions, situated at the intra-aggregate or dead end pores and mobile soil water regions. In both regions, adsorption is assumed to occur reversibly and linearly.

In WAVE as in the SWAP model, the transport of solutes in the mobile soil region is determined by chemical diffusion, convection and hydrodynamic dispersion; no volatilisation is considered in the process. Those different solute transport processes were described in equations 6 to 11.

To solve those equations, WAVE uses the same finite difference technique as applied for the water flow transport with a time and space discretization. Each compartment or layer is initialised with the required parameters.

4.4 Seasonal Soil compartment model (SESOIL)

SESOIL is an acronym standing for Seasonal Soil compartment model. As indicated by the acronym, it is a seasonal compartment model that simulates long-term pollutant fate and migration in the unsaturated soil zone. It was developed for the U.S. Environmental Protection Agency (USEPA).

4.4.1 Hydrologic cycle

This cycle focuses on the role of soil moisture (or interstitial pore water) in soil compartment. It is an adaptation of the water balance dynamics theory of Eagleson (1978). Equations 13 and 14 describe the water balance equation of the hydrologic cycle.

$$P - ET - M = S + R + G = Y \qquad \text{Eq. 13}$$

$$I = P - R \qquad \text{Eq. 14}$$

Where P is precipitation (cm), *ET is actual e*vapotranpiration (cm), M is moisture retention (cm), R is surface runoff (cm), I is infiltration (cm), Y is yield (cm), G is groundwater runoff or recharge (cm).

The soil temperature, which is used to calculate the concentration in soil air for the different seasons of the year, is obtained from the air temperature according to the following regression equations:

Summer: $T' = 16.115 + 0.856\ T$ Eq. 15

Fall: $T' = 1.576 + 1.023\ T$ Eq. 16

Winter: $T' = 15.322 + 1.656\ T$ Eq. 17

Spring: $T' = 0.179 + 1.052\ T$ Eq. 18

Where: T' is the mean monthly soil temperature (°F) and T is the mean monthly air temperature (°F).

Infiltration is described by the Philip's equation which assumes the medium to be effectively semi-infinite, and the internal soil moisture content at the beginning of each storm, and inter-storm period to be uniform. Surface runoff is derived from the distribution of rainfall intensity and duration by the use of the Philip infiltration equation. Capillary rise from the water table is assumed to be steady throughout the time period.

The soil column may be composed of up to four layers, each layer having different soil properties that affect the pollutant fate. In addition, each layer may be subdivided into a maximum of 10 sublayers. Nevertheless, Eagleson's approach (Equations13 and14) assumes that the soils are homogeneous. Therefore, the entire unsaturated soil zone is conceptualised as a single layer (or compartment) (Figure.12) and the prediction for soil water content is an average value for the entire zone.

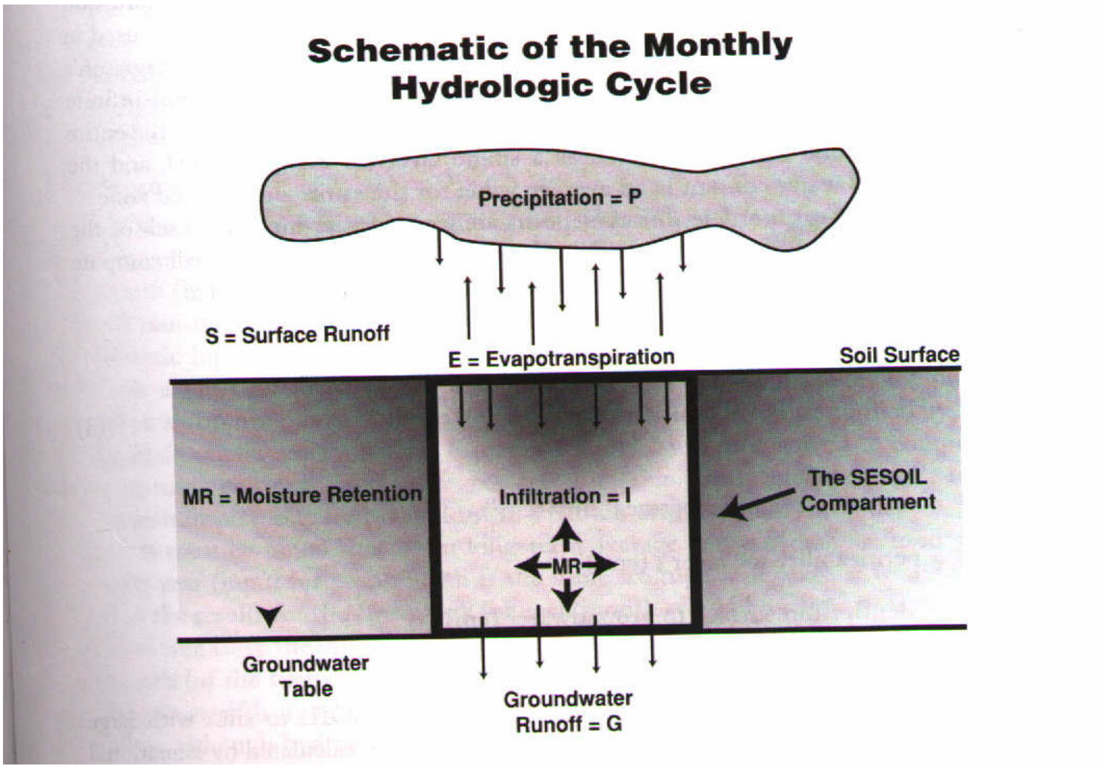


Figure 12. Schematic of the monthly hydrologic cycle in SESOIL after Hetrick et al, 1994. (Bonazountas et al. 1997)

While the user can provide different permeability values as input for each of the four major soil layers, the hydrologic cycle will compute and use the depth-weighted average permeability according to the following equation:

$$P = \frac{x}{\sum_{i=1}^{n} \frac{xi}{Pi}} \qquad \text{Eq. 19}$$

Where: P is the vertically averaged permeability (cm²), P_i is the permeability for layer i (cm²) and x_i is the thickness of the layer (cm).

The intrinsic permeability can be calculated from the hydraulic conductivity using the following formula (Fetter, 1994):

$$P = K_{sat} * \mu / g\rho \qquad \text{Eq. 20}$$

Where μ = dynamic viscosity of water (g/s.cm), ρ = density of water (g/cm^3), g = acceleration of gravity (cm/s^2).

4.4.2 Pollutant fate cycle

The pollutant fate cycle uses the calculated results from the hydrologic cycle. The following pollutant fate processes are accounted for: volatilisation, adsorption, cation exchange, biodegradation, hydrolysis and complexation The last won't be considered any further because heavy metals are not being studied (for more detail refer to the SESOIL manual, Bonazountas et al.). The model can consider only one compound at a time. It is based on a mass balance and equilibrium partitioning of the chemical between different phases (dissolved, sorbed, vapour and pure).

Like the hydrologic cycle, the pollutant fate cycle is based on mass balance (Eq. 21). It tracks the pollutant as it moves in the soil moisture between subcompartments (or sublayers). Contrarily to the hydrologic cycle, each soil layer is considered separately. They are distinctly defined by their own properties. Upon reaching and entering a layer or a sublayer, the model assumes instantaneous uniform distribution of the pollutant throughout that layer (or sublayer). Each layer (or sublayer) has its own mass balance equation (Eq.21) and can receive or release to and from adjacent layers (or sublayers).

$$C_i + Ct = C_T + C_R + C_M \qquad \text{Eq. 21}$$

Where:
C_i = The amount of pollutant originally in the soil compartment at time t-1 (µg/cm²)
C_t = The amount of pollutant entering the soil compartment during time step (µg/cm²)
C_T = The amount of pollutant transferred within the soil compartment at time step. (µg/cm²)
C_R = The amount of pollutant remaining in the soil compartment at time t (µg/cm²)
C_M = The amount of pollutant migrating out of the soil compartment during the time step (µg/cm²).

The fate of the pollutant in the soil column includes both transport and transformation processes, which depend on the chemical's partitioning among the three phases: soil air, soil moisture, and soil solids. The concentration in the soil air is calculated from the Henry's law as stated in Eq. 22.

$$C_{sa} = \frac{C_{sw} H}{F(T + 273)} \qquad \text{Eq. 22}$$

Where: C_{sa} is the Pollutant concentration in soil air (µg/ml), C_{sw} is the Pollutant concentration in soil water (µg/ml), *H* is the Henry's law constant (m³atm/mol), *F is the* gas constant $[8.2*10^{-5}\, m^3 atm/(mol*°v)]$, *T* is the soil temperature (°C), *V is the* Transmission factor of cloud cover (-).

SESOIL employs the general Freundlich equation to model the soil sorption process.

$$S = Kd * C^{1/n} \qquad \text{Eq. 23}$$

Where *n* is Freundlich exponent (-).

SESOIL assumes that the dissolved chemical will travel to another layer or to the ground-water at the same speed as the moisture mass originating in the same soil layer. This movement is however assumed to be retarded by volatilisation, partitioning and adsorption of the chemical on the soil particles. The following equation (Eq. 24) expresses the depth reached by a chemical with a linear equilibrium partitioning between its vapour, liquid, and adsorbed phases (Jury et al., 1984) cited by Bonazountas et al.,(1997):

$$D = \frac{J_w t_c}{\theta + \rho b + \frac{f_a H}{F(T+273)}} \qquad \text{Eq. 24}$$

Where *D is* the depth (cm), *Jw* is the water velocity (cm/s), t_c is the Advection time (sec), f_a is the Air filled porosity (-).

SESOIL simulates a process, which is not included in the above described models: the volatilisation. In SESOIL, volatilisation includes movement of the pollutant from the soil surface to the atmosphere and from lower soil layer to upper. It operates only in the upward direction. The following equation describes the vapor phase diffusion flux through the soil:

$$Ja = -D_{dif}\left(\frac{f_a^{\frac{10}{3}}}{\phi^2}\right)\frac{\partial C_{sa}}{\partial x} \qquad \text{Eq. 25}$$

J*a (*µg/cm²/s)

Two degradation processes are considered in SESOIL: biodegradation and hydrolysis. The biodegradation in SESOIL is handled as a primary degradation, which is defined as any structural transformation in the parent compound, which results in a change of the chemical's identity. The biodegradation algorithm in the soil uses the following first order equation rate equation:

$$E = (C*\theta*K1l + S*\rho b*K1s)*B*\partial xi*\partial t \qquad \text{Eq. 26}$$

Where *E* is the decayed pollutant mass during time step t (µg); *K1l* is the biodegradation rate of the compound in the liquid phase (/day); *K1s* is the biodegradation of the compound in the solid phase (/day) and *B* is the area of pollutant application (cm²).

4.5 Pesticide Root Zone Model (PRZM-2)

The Pesticide Root Zone Model, PRZM-2, was developed for the U.S. Environmental Protection Agency (EPA). It was selected as a program to simulate the transport and transformation of agriculturally applied pesticides in the crop root zone and the vadose zone which are both described by the PRZM and Vadoze Zone Flow and Transport Model (VADOFT). Due to the limitations of the present study, only the PRZM module is described here. The following diagram (Figure13) shows the link between both components of the PRZM-2 model.

PRZM is a one-dimensional, compartmental model that simulates chemical movement in the unsaturated soil systems within and immediately below the plant root zone. It allows the user to perform simulations of potentially toxic chemicals particularly pesticides, those are applied to the soil or to the plant foliage. The soil properties such as bulk density, field capacity, etc have to be specified by each horizon. PRZM-2 can be schematized as in figure 14.

PRZM has two main modules: the hydrology module and the chemical transport module.

4.5.1 Hydrologic module

In this module the movement of water is simulated by the use of general soil parameters, including field capacity, wilting point and saturated water content. In general, the water movement is described using the well-known Richards's equation as given in equation 3.

The potential evapotranspiration (ETo) is determined from daily pan evaporation data or is estimated using daily air temperature and average daily hours of sunshine. Actual ET is then calculated considering evaporation from canopy, ponded surface water, soil evaporation and crop transpiration. Soil evaporation occurs to a user specified depth, and plant transpiration is extracted from the active root zone.

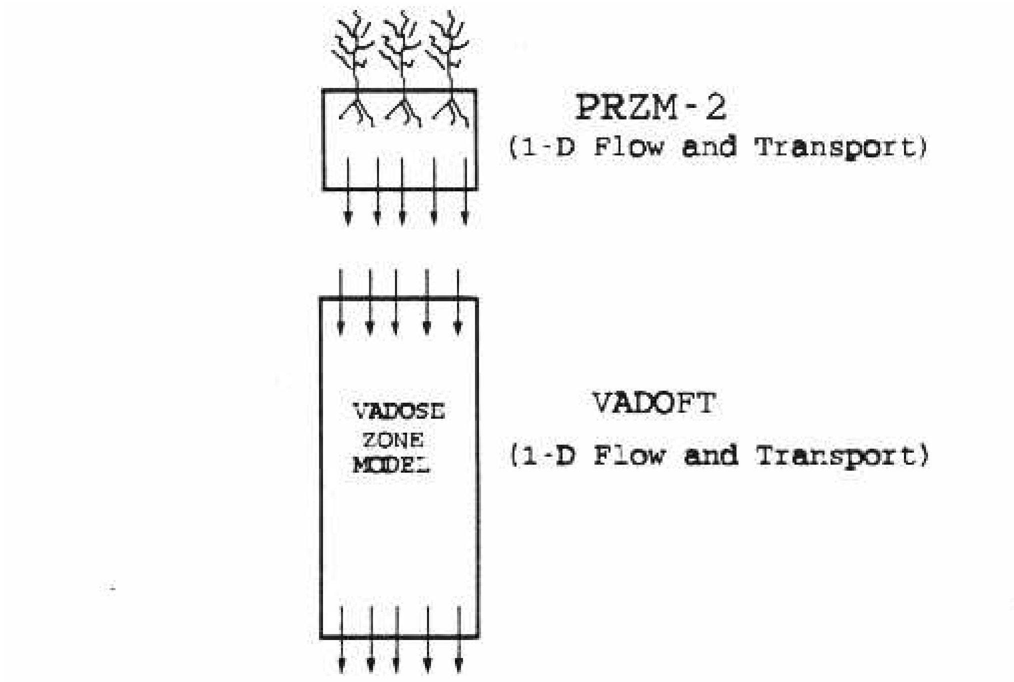


Figure 13. Schematic representation of the linked modeling system configuration.

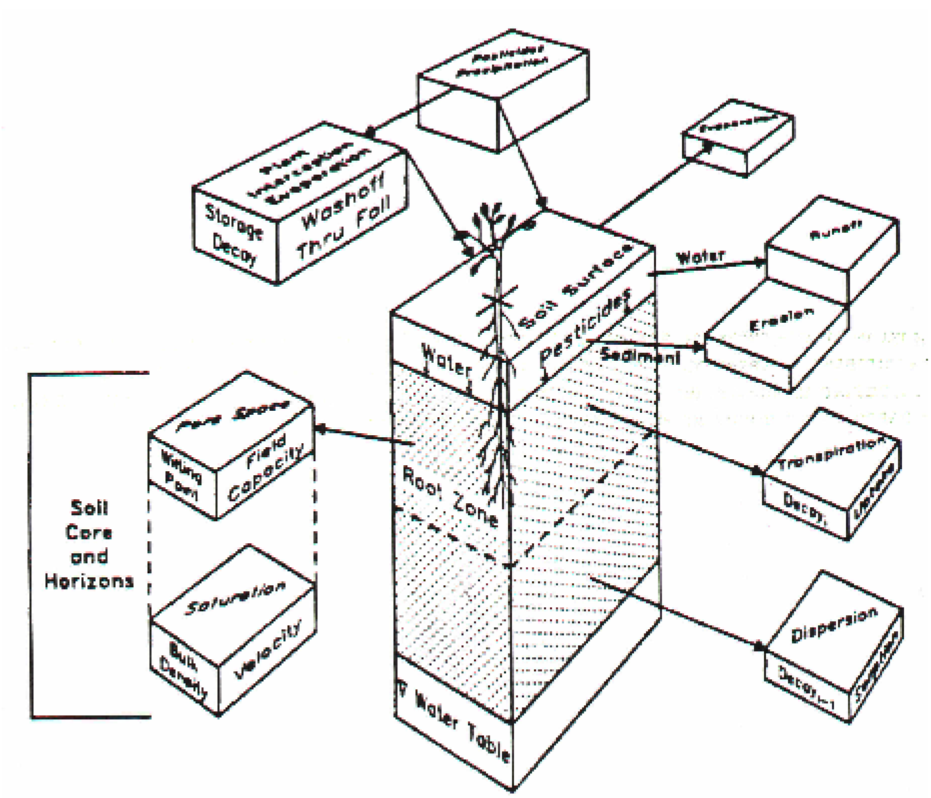


Figure 14. Schematization of the PRZM component

Infiltration is calculated as:

$$I = P + N - R - ET \qquad \text{Eq. 27}$$

Where N is the snowmelt (cm/d) and ET is the evapotranpiration (cm/d)

To partition the precipitation and the irrigation between infiltrating water and runoff PRZM made use of the USDA Soil Conservation Service curve number approach according to Haith et al. 1979 (cited by the manual of PRZM-2, Mullins et al. 1993). The curve numbers are functions of soil type, soil drainage properties, crop type and management practices.

4.5.2 Chemical transport component

PRZM uses the Advection-Dispersion equation to simulate chemical transport in the soil. The surface zone expressions for the dissolved, adsorbed, and vapor phases can be written as in equations 28, 29, and 30:

$$\frac{B\Delta x\partial(C\theta)}{\partial t} = J_{Dif} - J_{con} - C_{DW} - C_U - C_{QR} + C_{APP} + C_{FOF} \pm C_{TRN} \qquad \text{Eq. 28}$$

$$\frac{B\Delta x\partial(C_s\rho b)}{\partial t} = -C_{DS} - C_{ER} \qquad \text{Eq. 29}$$

$$\frac{B\Delta x\partial(C_{sa}f_a)}{\partial t} = J_{Dis} - C_{DG} \qquad \text{Eq. 30}$$

Where :
C_{DW} = mass loss due degradation in dissolved phase (g/day)
C_{DG} = mass loss due to degradation in the vapor phase (g/day)
C_U = mass loss by plant uptake of dissolved phase. (g/day)
C_{QR} = mass loss by removal in runoff (g/day)
C_{APP} = mass gain due to pesticide deposition on the soil surface (g/day)
C_{FOF} = mass gain due to washoff from plants to soil (g/day)
C_{DS} = mass loss due to degradation of sorbed phase chemical (g/day)
C_{ER} = mass loss by removal on eroded sediments (g/day)
C_{TRN} = mass gain or loss due to parent/daughter transformation (g/day)

A plant uptake coefficient is also included to calculate the amount of dissolved solute transported to the plants during the transpiration. The user can specify the degradation rate and the linear adsorption distribution coefficient (Kd) for each soil horizon
The model allows the simulation of chemical transport in runoff, in erosion, in percolating water, equilibrium adsorption, and first order decay in foliage as well as soil.

Dissolved, adsorbed, and vapor-phase concentrations in the soil are estimated by simultaneously considering the processes of pesticide uptake by plants, surface runoff, erosion, decay, volatilization, foliar washoff, advection, dispersion, and retardation. Dispersion and diffusion in both the dissolved and vapor phases are described by Fick's law and Millington and Quirk as given in equations 6, 7, 8, 9, and 10.

PRZM-2 uses two different techniques to solve the discretized chemical transport equation:
- a backward difference method to simulate all chemical transport processes.
- a method of characteristics (MOC) algorithm.

For additional information the reader is referred to the PRZM-2 user manual (Mullins et al.1993).Table 1 presents a list of required input parameters for the different models.

Table 1. Model input parameters

	PESTAN	SWAP	WAVE	SESOIL	PRZM-2
Climate					
Temperature		*	*	*	*
Precipitation		*		*	*
EvapoTranspira tion		*	*	*	
Recharge	*				
Pan factor					*
Pan Evaporation					*
Mean storm duration				*	
Number of storms per months				*	
Length of rainy seasons within M				*	
Irrigation rate		*	*		*
Crop related parameter					
Root water upake		*	*		
Interception		*	*		*
Root depth		*	*		*
Soil cover fraction		*	*		*
Leaf area Index		*	*		
Canopy height		*	*		*
Crop factor		*	*		
Solute water uptake					*
Pressure head at wilting point		*	*		
Pressure head at field capacity		*	*		
Root density distribution		*	*		
Soil Water Parameter					
Hydrodynamic dispersivity			*		
Initial groundwater level		*	*		
Curve coefficient	*				
Residual Moisture Content		*	*		
Saturated Moisture Content		*	*		
Ksat	*	*	*		
Alpha main drying curve		*	*		
Exponent lambda function		*	*		

Parameter n		*	*		
Parameter m		*	*		
P sand		*			
P silt		*			
P clay		*			
P org matter		*			
P org carbon		*			
Wilting point					*
Field capacity					*
Bulk density	*		*		*
Intrinsic permeability				*	
Disconnectedness				*	
Effective porosity				*	
Initial soil water in the layer					*
Runoff CN					*
Chemical Parameters					
Air Dif Coef		*	*		*
Molecular Df coef				*	*
Henry'Law const				*	*
A coefficient			*		
B coefficient			*		
Dispersion length			*		
Mobile total Moisture Content					
Mass transfer Coefficient			*		
Adsorbed Fraction in the mobile zone			*		
Vapor Enthalpy					*
Adsorbed Phase Decay				*	*
Dissolved Phase Decay	*			*	*
Vapor Phase decay	*	*	*	*	*
Initial Pest Level		*	*	*	*
Solubility	*			*	
Koc		*		*	
Freunlich Expon Kd	*		*		*
Freundlich exponent		*		*	
Molecular weight				*	
Reference solute concentration		*			
Factor reduction decomposition rate due to temperature		*			
Minimum water content for potential decomposition		*			
Exponent in reduction decomposition due to dryness		*			
Dispersion Coefficient	*				*

As we can see from Table 1 a huge amount of data are required for the simulation of pesticide fate in the unsaturated soil zone using those five models. SWAP, WAVE, and PRZM use a great amount of data whereas PESTAN uses only eight of them. The gathering of these parameters will be discussed in detail in the next chapter.

5 Model design

This section describes the design and parameter estimation for the modelling of the unsaturated soil zone model in the selected site of the Naivasha area, using the above described model. The calculations with the different models were carried out on a daily and/or a monthly basis (some of the models do not have the capability to provide daily outputs). In order to be able to compare accurately the results of the different simulation models, the same upper and bottom boundary conditions, soil and chemical parameters were taken for all the models. Parameter values were based on site-specific data, user manuals, and values from the literature.

5.1 Climatic data

5.1.1 Precipitation and irrigation

Input data of daily precipitation were obtained from the Oserian weather station (Figure1) located about 500 meters away from the experimental site, for the period of October 1998-September 1999. Data was also available from Naivasha District Office (D.O.) located in the township of Naivasha for the period of October 1989 to September 1990. In the modelling the period of October1998-September 1999 was considered as a dry year (yearly precipitation is 502.8 mm) and the second period of October 1989 to September 1990 with a yearly precipitation of 916 mm, was considered as a wet year according to the dependable rainfall analysis carried out by De Silva (1998). The dry year was taken from the probability over a 36-year period of exceeding rank at 90% and the wet year was considered from the probability of exceeding at 10% of the same period. Unfortunately, meteorological data for the month of October 1999 for the period of the fieldwork was not yet available.

In Naivasha, as was mentioned above, the crops depend strongly on irrigation. The application rate and the schedule vary from crop to crop and also with the prevailing climatic condition. For Statice, for example, one of the flower types grown in the farm (Figure 7), an amount of 80 m^3/ha/day is applied, which gives a depth of 8 mm/day. Since it was applied as drip irrigation, which means that the water is applied directly at the roots of the crops, which are arranged into rows of 80 cm wide and separated by a space of about 80 cm, the net irrigation rate is practically higher than 8 mm/day at the crop. In fact, the effective area covered by the crops is about 50%, and the spacing between the rows remains dry during or after the irrigation. Nevertheless, for the sake of the modeling, the area can not be divided between irrigated area and non-irrigated one. Therefore, an average value of 8 mm/day is considered to be equally distributed over the area. Less irrigation water is used whenever there is rain for the day.

Precipitation and irrigation are entered differently in the models. In SESOIL, there is no separate module for irrigation, therefore it is added up with the precipitation and aggregated as monthly input considering the days with rainfall. When it has rained lower than 8 mm for the day, irrigation is added until reaching 8 mm but if it has rained more than that value, irrigation is not supplied according to the explanations of the farmers. In addition, three parameters have to be defined in the model: storm duration, number of storms and length of rainy seasons. They should be given for each month of the year. These parameters are the basis of the model of Eagleson describing the water balance equation used in the model (equations 13, 14). Unfortunately, they were not available since there is no digital recorder at the site. Therefore they were assumed using a qualitative approach. As irrigation was added to the precipitation, every event is considered as a storm and the duration of the irrigation is the storm duration regardless any other rainfall events during the month. The table below shows the values taken for each month. In this approach, the number of storms and the storm duration is obviously higher but as we do not have any other information about them we keep these values as estimation.

Table 2. SESOIL climatic file

Month	Storm duration (day)	# of storms	Length of rainy season (days)
Oct	0.083	31.00	31.00
Nov	0.083	30.00	30.00
Dec	0.083	31.00	31.00
Jan	0.083	31.00	31.00
Feb	0.083	28.00	28.00
Mar	0.083	31.00	31.00
Apr	0.083	30.00	30.00
May	0.083	31.00	31.00
Jun	0.083	30.00	30.00
Jul	0.083	31.00	31.00
Aug	0.083	31.00	31.00
Sep	0.083	30.00	30.00

In SWAP, the irrigation and the rainfall events are added up daily, because the model does not allow for more than 50 fixed irrigation applications in the irrigation module. In PRZM, a fixed irrigation rate per hour can be specified which is applied by the model, based on the calculation of the soil moisture deficit. In the WAVE model precipitation and irrigation are entered separately on a daily basis.

5.1.2 Temperature

Mean monthly air temperatures are required only in SESOIL to calculate the concentration in soil air. The air temperature is converted to soil temperature according to regression equations 15, 16, 17 and 18. The other models do not require the temperature to calculate the pollutant cycle.

5.1.3 Evapotranspiration and crop-related parameters

Daily pan evaporation data were collected for the same modelled period. They were multiplied by a pan coefficient to obtain the reference evapotranspiration ETref. A pan coefficient of 0.85 was taken for the modelled crop (flowers) according to the FAO guidelines for crop water requirements.

SWAP and WAVE use daily ETref while PRZM uses daily pan evaporation. The simulated mean daily actual evapotranspiration were taken from SWAP as an input to SESOIL for the simulation.

Crop-related parameters need to be specified for the simulation such as crop factor, leaf area index, rooting depth, soil cover fraction, crop height, interception, root water uptake. The first six parameters are given as a function of the maturity stage and the last as a function of depth. However, those parameters are difficult to be found in literature specifically for flower type crop. Therefore, they were either estimated or assumed but it remains clear that those parameters have to be chosen accurately considering their sensitivity in the leaching process.

The parameters are used in SWAP and WAVE to partition potential evapotranspiration rate into potential transpiration rate and potential soil evaporation those are further reduced to the actual evaporation and actual transpiration. The height of the canopy was estimated at about 80 cm and the rooting depth is 60 cm (De Silva, 1998). The interception was put to 0 because of the limitation of the models. A constant crop factor of 1.1 was taken considering the maturity stage of the crop for the whole simulation period. Soil cover fraction was assumed 0.5 considering the spacing between the rows of crops, and a value of 3 was suggested for the leaf area index considering the density of the layers leaves of the statice (Figure 7). The root water uptake of grass was taken as a reference from the compilation of literature data given by Diels (1994), (cited by Vanclooster et al.1994). The root water uptake is taken from 0.026 at the surface to 0.005 down at the root depth. The ponding depth was set to 40 cm according to the depth of applied water in the infiltration basin during the field work. The results of these in-situ measurements were used for the calibration of the hydrological cycle of the models.

The upper and the lower limits of the root water extraction function are specified in the models. The pressure heads defined the root water extraction function. The wilting point and the field capacity were suggested at -16000 cm and –100 cm suctions respectively and the starting point of extraction water from the soil at –10cm (taken from the WAVE and SWAP manual).

For PESTAN, only the recharge value is necessary because the water applied at the surface is assumed to infiltrate at a constant rate. Therefore, recharge values from the other applied models were taken to PESTAN for the simulation.

The bottom of the soil profile is assumed to drain freely since the groundwater table is below the modelled profile, therefore free drainage is taken as the bottom boundary condition.

5.2 Soil data

The soil data were divided between those collected in the field and those estimated from literature. Data collected in the field are used either separately by the models (e.g. % of sand, silt and clay used by SWAP) or used to calculate other parameters (e.g. θ_{sat}, θ_{res}, etc) required by the different models. The data collected in the field were: saturated hydraulic conductivity and soil moisture content. Soil samples were taken at different depths for the determination of particle size distribution. In order to reduce the cost of the laboratory analysis to determine the particle size distribution and the OM content, the samples were sent to a laboratory in Poland, which offered a significant relief in the cost.

5.2.1 Field measurement of parameters

During the soil investigation that has been carried out from October 2nd to October 23rd 1999 in the Lake Naivasha area, disturbed soil samples were collected at the three sites using an 8-cm diameter hand auger (No undisturbed samples were then collected due to the lack of appropriate equipment). Using the Munsel color chart and a manual technique, the different layers were described. For different layers, the hydraulic conductivity was measured and soil moisture content were obtained on the soil coring using the theta probe at various depths. More details are given further below (section 5.2.1.2).

Particle size allows the determination of the soil texture classes. The different soil texture classes are given in tables 2, 3 and 4. They indicate soils varying from clay to loamy sand even to fine sand. At Oserian, a volcanic ash layer was found at 4 meters in some bore holes but this layer was quite variable in thickness and in depth. Though this layer was found also to be silt loam in the texture triangle, the same as the material it is embedded into, it was considered as a separate layer based the in-situ judgement of its bulk density and wetness. The results of the laboratory analysis of particle size distribution is given in Appendix D

5.2.1.1 Hydraulic conductivity

Hydraulic conductivity (K) is one of the main parameter of the flow of water in the soil zone. Above the water table, this parameter was determined using the inverse auger-hole method. This method is described by the French physicist called Porchet whereas the name of the method of Porchet.

Considering a multi-layer unsaturated soil zone, the value of K is determined for each separate layer. Therefore, a hole of a certain radius r is augered down to the specified layer at a depth D and filled with water up to a required height in order to remain within the layer. The drawdown h'(ti) of the water-level is measured at each time step and recorded successively. Subsequently, h(ti) is obtained by subtraction from the total depth D. Therefore [h(ti)+r/2] is plotted against the time t on a semi-log paper so to obtained the slope ε. The expression of the hydraulic conductivity is given by Eq. 32. The results are given in tables 3, 4 and 5. The different graphs are given in Appendix C.

$$K = 1.15 r \operatorname{tg} \varepsilon \text{ (meter/day)} \qquad \text{Eq. 31}$$

Table 3. Hydraulic conductivity and soil types at Aberdare

Depth Range (in cm)	Saturated Hydraulic conductivity in cm/day	Soil types
0-80	37.2	Loam to clay
80-600	26.6	Sandy loam

Table 4. Hydraulic conductivity and soil types at 3 Ostrich farm

Depth range (in cm)	Saturated Hydraulic conductivity in cm/day	Soil types
0-40	4	Clay
40-80	8.9	Loam
80-150	41.6	Silt loam
150-600	46.4	Sandy loam to loamy sand

Table 5. Saturated Hydraulic conductivity and soil types at Oserian farm

Depth range (in cm)	Saturated Hydraulic Conductivity (in cm/day)	Soil types
0-80	161	Sandy loam
80-400	29	Silt loam
400-530	41	Silt loam (ash)
530-600	29	Silt loam

5.2.1.2 Infiltration basin experiments

The purpose of the infiltration basin was to obtain the recharge characteristics in order to calibrate the models. As the fieldwork was carried out for a short time and considering it was not possible to collect any meteorological data for the month of October 1999, any natural soil moisture to be measured would not be the response of the actual meteorological conditions. Therefore, a small hydrologic scenario was designed in order to obtain the soil moisture content at various depths based on the known antecedent hydrologic (meteorological) situation.

Figure.15 Infiltration basin for the collection of soil moisture content (Oserian farm)

A small plot of 2m*2m (Figure15) was isolated in each selected spot and was filled with 40 cm of water and covered after with a plastic sheet in order to avoid evaporation and the soil moisture content was to be measured at successive days for 10 days. The soil moisture was measured at various depths using a theta probe from the soil cores. The experiment was carried out in the three sites (Figure 1). At 3 Ostrich Farm it was not possible to add 40 cm of water in one day because the top layer is very impermeable with a hydraulic conductivity of 4cm per day (tables 2-4). The water would remain at the surface for 10 days. Therefore only 10 cm of water was applied. However, the site was abandoned finally due to some handling failure. At Aberdare the experiment was also abandoned after the second day because the plot was no longer available to carry on the experiment. It was needed for ploughing. At Oserian farm authorization was given to carry out the soil study only 9 days prior the end of the field work, therefore the experiment was limited to that period. The soil moisture content was assessed at various depths of four days at Oserian Farm. Figure 16 shows the time series of soil moisture profiles at various depths at the farm.

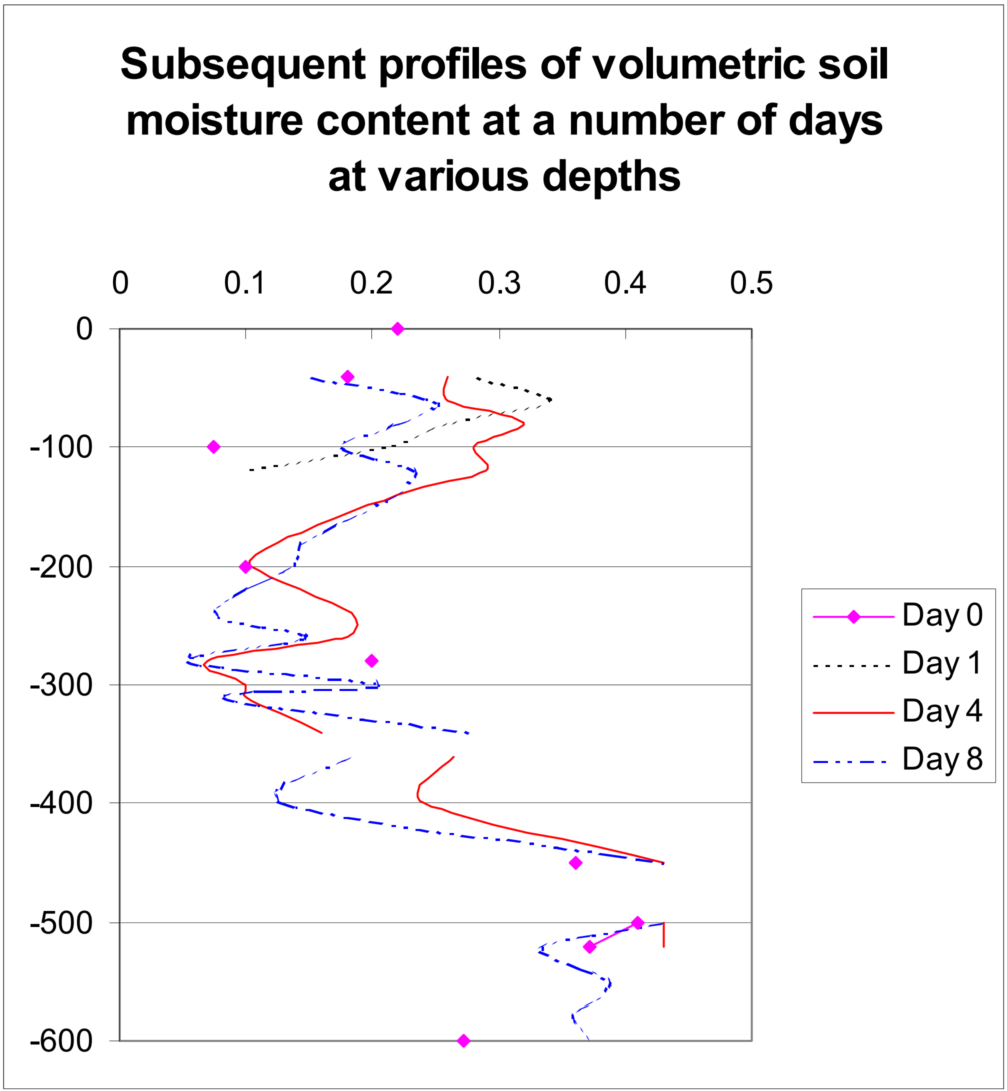


Figure.16 Subsequent profiles of volumetric

The soil moisture content on day 0 represents the initial soil moisture condition at the beginning of the experiment. On day 1 of the experiment, the soil water content increases down to a depth of 180 cm. On day 4, the soil moisture content is higher down to 4 meters and on day 8 it increases down to 8 meters. At the same time, the water content at the top layers starts decreasing. At day 8, the water content down to 60 cm was already almost the same as at the initial day (day 0). The variation of the moisture content is higher in the first 180 cm.

5.2.2 Parameter estimation

Since it was not possible to collect undisturbed samples, the soil hydraulic properties required in the models were estimated from literature based on the soil textural classes. After intense literature review, most of the parameters were gathered but it remains clear that they are specific soil properties, they should be accurately related to the soil site. The soil parameters are introduced in the following, according to their respective models.

5.2.2.1 PESTAN

The discretization in PESTAN is simple. Only one layer is specified for the whole depth (600 cm), therefore an average depth value of the parameters is entered for the whole profile. Bulk density was taken as suggested by Rawls (1982) and the porosity was calculated based on the following formula:

$$\phi_{por} = (1 - \rho b / \rho p) * 100 \qquad \text{Eq. 32}$$

where ρp is the particle density taken 2.67 g/cm³.

The characteristic curve constant *b* was taken from Li et al (1976, cited by Ravi et al.), the dispersion coefficient is calculated from the hydrodynamic dispersivity and the pore water velocity from Beven et al (1993, cited by Vanclooster et al, 1994).

Table 6. Input soil parameters for PESTAN model

Depth	ρb g/cm³	ϕpor (cm³/cm³)	B (-)	Ddis Cm²/h	Ksat cm/h
600 cm	1.17	0.55	5.2	1.09	1.46

5.2.2.2 SWAP model

The unsaturated soil zone was discretized into 4 layers and subdivided into 40 sublayers. The depth division of the soil layers is based on the soil texture classes provided by the particle size distribution. Soil sublayers of the upper layer were taken smaller (1-7 cm) than in the deeper layer (10-32 cm).

From the collected samples, 23 soil water retention curves (from the three sites) were obtained by laboratory measurements on disturbed soil samples taken at different depths. Because of the disturbed state of the samples, the pF curves provided qualitative assessment of the soil retention parameters. Only the parameters of the ash

layer were obtained directly from the curves because it was difficult to find related parameters for ash in the literature and the values from the pF strongly correlated with the in situ estimation.

The Van Genuchten parameters were estimated using the USDA texture classes whereas the lambda parameter was estimated based on the Dutch texture classes. No hysteresis and no preferential flow were assumed because of data limitation.

Table 7. Input soil parameters for SWAP model

Layer #	θres cm/cm	θsat cm/cm	α 1/cm	n (-)	m (-)	$Ksat$ cm/d	λ (-)	% sand	% silt	% clay	% OM	Soil types
1	0.065	0.41	0.075	1.89	0.47	161	1.40	51	43	6	0.71	Sandy loam
2	0.067	0.45	0.020	1.41	0.29	29	1.24	42	53	5	0.58	Silty loam
3	0.100	0.39	0.020	1.41	0.29	41	1.15	14	65	21	0.58	Silty loam
4	0.100	0.39	0.020	1.41	0.29	29	1.15	39	55	6	0.58	Silty loam

5.2.2.3 WAVE

Contrarily to the SWAP model, in the WAVE model the soil layers can not be discretized into sublayers of different thicknesses. Giving the sublayers a small thickness would result in a large amount of compartments that is not accepted by the model because the computation requirements are too high, whereas the assignment of a large thickness to the sublayers would increase the uncertainty in the calculation. Therefore, a thickness of 10 cm was assumed for all compartments.

The hydraulic parameters of the Van Genuchten functions are the same as for the SWAP model.

5.2.2.4 SESOIL

According to the soil profile in the Oserian Farm, the same number of physical layers was used in all the models. However, the maximum number of sublayers for each layer in SESOIL can not be greater than 10, therefore, the thickness of each sublayer is determined according to the thickness of the modelled physical layer.

The intrinsic permeability values and were calculated according to equation 20 and entered for each layer together with the organic carbon (OC) values whereas the disconnectedness b , the bulk density and the effective porosity were depth averaged for the whole profile.

Table 8. Input soil parameters for the SESOIL model

Depth ranges cm	*Thickness cm*	*P (cm^2)*	*b (-)*	*ρb (g/cm^3)*	*ϕpor (cm^3/cm^3)*	*%OC*
0-112	80	1.9E-08				0.41
112-400	320	3.57E-09				0.34
400-530	130	1.77E-09				0.34
530-600	600	2.7E-09				0.34
Average	600	3.20E-09	5.6	1.17	0.55	0.36

5.2.2.5 PRZM-2

In the PRZM-2 model, the profile was discretized into 4 layers, as in the other models, and the thickness of the sublayers of the upper layer is as low as 1 cm, whereas from the second layer the thickness values of the sublayers were taken as 20 cm. A value of 83 was taken for the runoff curve number after simulation of annual surface runoff with the Agriculture Non-Point Source pollution model, AGNPS (personal communication with Mai). Field capacity, wilting point, and bulk density were taken from from the field measurement and from the literature (Table 9) as suggested by Rawls (1983) and the initial soil moisture in each layer was measured in the field.

Table 9. Input soil parameters for PRZM-2 model

Depth range	*FC (cm^3/cm^3)*	*WP(cm^3/cm^3)*	*ρb (g/cm^3)*	*θ initial (cm^3/cm^3)*
0-112	0.27	0.950	1.49	0.20
112-400	0.33	0.133	1.32	0.12
400-530	*0.74*	*0.289*	*0.55*	*0.38*
530-600	0.33	0.133	1.32	0.32

** the value in italic are field measurement*

5.3 Chemical parameters

Four types of pesticides were chosen for the simulations according to their level of toxicity. Those pesticides are: chlorpyrifos, dimethoate, fenamiphos and oxamyl.

Chlorpyrifos, also known as Brodan, Cross fire (trade name), is an insecticide used to control insects in the soil and in some foliar insects on a wide range including indoor or outdoor ornamental flowers. This pesticide has a half-life varying from 60 to 120 days. Chlorpyrifos is toxicity class II- moderately toxic by the EPA.

Dimethoate is also known commercially as BAS152J or Chemathoate. It is an insecticide also used to control insects in ornamental flowers. Its hydrolysis leads to dimethyl-phosphorodithoate and the oxydation of the phosphorodithoate gives the corresponding oxone which is highly toxic. Dimethoate is a moderately toxic compound in EPA toxicity class II.

Fenamiphos also known as Nemacur is used in the control of ectoparasitic, root-knot nematodes in ornamental flower, fruit, vegetables etc. It has a half-life of about 4 months. Fenamiphos is an highly toxic compound in EPA toxicity class I. It is a restricted use pesticide.

Thioxamyl or Blade are trade name for Oxamyl. It is considered as an insecticide, an acaricide and a nematicide. It is used in the control of chewing and sucking insects (including soil insects, spider mites and nematodes) in ornamental, fruit trees and vegetables. It is degraded rapidly in soil with a half-life of 7 days. Oxamyl is highly toxic compound in EPA toxicity class I. It is also a restricted use pesticide.

Most of the chemical properties were estimated from the literature as for the soil properties. Some of them were not found though, therefore they are assumed within the range of the range suggested as default by the models. The applied chemical input parameters are presented in table 10.

Table 10. Chemical properties input parameters

Parameters	Fenamiphos	Chlorpyrifos	Dimethoate	Oxamyl	Units
Solubility	700	2	25000	280000	Mg/l
Air diffusion coef	0.036	0.031	0.0476	0.0497	cm^2/s
Henry's Constant	5.87 E-10	4.45E-6	1.15E-9	0.24E-09	m3.atm/mole
Koc	169.82	6026	19.95	25.12	g/ml
Molecular weight	303.4	422.9	229.3	219.40	g/mole
Liquid Phase Biodegradation	0.005775	0.0231	0.03465	0.05	/day
Solid phase Biodegradation	0.005775	0.0231	0.03465	0.05	/day
Molecular diffusion coefficient	0.012	0.012	0.012	0.012	cm^2/day
Freundlich exponent	1	1	1	1	(-)
Vapor enthalpy	20	20	20	20	Kcal/mole

6 Results and discussion

Model simulations were conducted for a one-year period from 1st October 1998 to 30th September 1999 and from 1st October 1989 to 30th September 1990. Pesticide leaching through the unsaturated soil zone was simulated during those period using the five models described in detail in chapter 4. The leaching depth over the time and the solute concentration in the soil profile simulated by the different models were the basis of the comparison between the models. The comparison allowed us to determine the level of applicability of the models for evaluating specific environmental scenarios. For the fairness of the comparison, the parameters were taken equal as already explained in the model design of chapter 5.

First, the models were calibrated hydraulically and then simulations were performed creating three different scenarios with the calibrated models. A detailed chemical calibration of the models was beyond the possibilities of the present study. Therefore, the chemical and physical properties of the pesticides were taken from the published literature, and the sensitivity of the models to some of the most important parameters was analysed to assess the consequences of possible inaccuracies in the determination of the parameter values. Then, the results of the different simulations were compared to each other and subsequently discussed and analyzed.

6.1 Hydraulic calibration

The purpose of the calibration was to better represent the unsaturated soil system and the movement of the soil water, which carries the pesticide in a manner similar to that of the actual system. The basis of the calibration was the infiltration test carried out during the fieldwork (Subsection 5.2.1.2). A trial-and-error procedure was used to improve the fit between simulated and observed soil moisture content. Soil moisture content measurement of the eighth day along the profile was taken as the calibration target for this study. Because of limited accuracy of the soil moisture measurement with the theta probe, the strict fit of the observed and calculated soil moisture content was not pursued. A qualitative calibration of the overall soil moisture profile was targeted and achieved.

The infiltration test was considered as a precipitation event of 40 cm falling in one day (the first day of the simulation), followed by 8 days of ø rainfall and ø evaporation. All the water was assumed to infiltrate.

After reviewing the models it was realised that only SWAP was suitable to simulate the scenario involving the infiltration basin. WAVE does not allow an application of greater than 5 cm for precipitation and more than 10 cm per day of irrigation. PRZM-2 does not simulate this amount properly. Due to the limited output capability (monthly and annual basis) of the SESOIL model, it can not be used to make a simulation over 9 days. Therefore, SWAP was calibrated and the adjusted parameters were taken to the other models in order to run them comparably.

6.1.1 Parameter selection for adjustments

Many parameters can in principle be used to adjust the simulation to the measurements. Two main groups of parameters related to the hydrologic processes can be distinguished: soil parameters and those related to the boundary conditions (Gehrels, 1999). The saturated hydraulic conductivity was optimised, because the calculated soil moisture content and the recharge appeared to be quite sensitive to this parameter. The soil discretization was also modified in order to achieve the fit. The process is described in detail in the next subsection.

6.1.2 Calibration of the selected parameters

The predicted soil water content of the uncalibrated model runs were in general higher than the observed values in the second and in the third layer. Therefore values of Ksat were lowered to 30 cm/d in the second layer, to 15 cm/d in the third and to 22.89 cm/d in the fourth layer. Further improvement was achieved when modifying the soil discretization. In fact, there was no sharp boundaries observed in the field between the fist and the second layers, so the discretization could be changed. The thickness of the first layer in the model was modified from 80 cm to 112 cm reducing the second layer to 288 cm while keeping the other layers with the same thickness. Figure 17 shows the observed and the calculated soil moisture content after the calibration, down to 6 meters. However, from 4 meters downward the soil moisture changes do not appear to be the response of the water applied 8 days prior to the measurement. Table 11 shows the adjusted parameter values for the calibration.

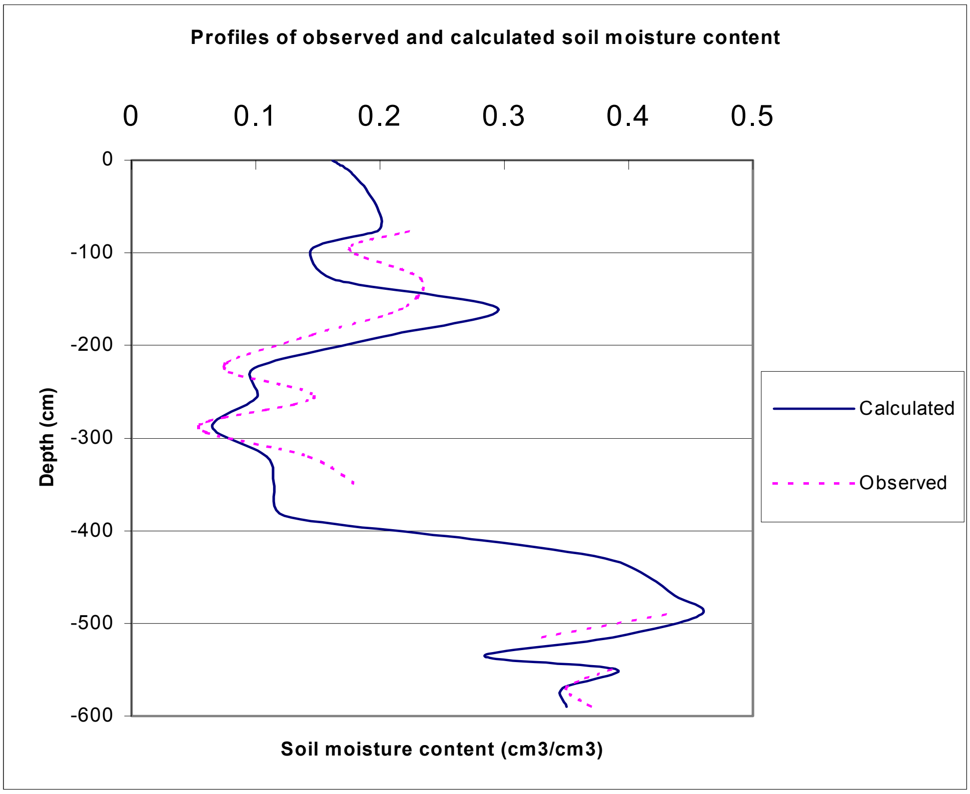


Figure 17. Observed and calculated soil moisture content at various depths in the soil at the eighth day

Table 11. Adjusted soil properties

Layer thickness (cm)	*Ksat (cm/day)*
0-112	161.00
112-400	30.30
400-530	15.00
530-600	22.90

6.2 Simulations with the hydraulically calibrated models

In this part, the hydraulically calibrated models were used to simulate pesticide leaching through the soil zone. The target of the simulation is to evaluate qualitatively the leaching of pesticide through the unsaturated soil zone via the different models under different circumstances. As presented above, the adjusted parameters from SWAP were taken to the other models in order to have the same soil properties.

There were three main scenarios:
- One scenario was run with a dry meteorological year of October 1998-September 1999 with the application of a single load of pesticide.
- The second scenario was performed with the same meteorological year, but this time with multiple loads of pesticide.
- The last scenario was performed with a wet year Oct 1989-September 1990 with an annual precipitation of 918 mm.

The leaching of the pesticides presented in the previous chapter was simulated for every scenario. The results of the different runs was compared and analyzed. The models were selectively taken according to their capability to run under the given scenario. The simulation breakthrough curves of the different scenarios are given in Appendix E.

6.2.1 Scenario 1 An average dry year with the application of a single load of pesticide

For this scenario, we considered that one load of pesticide was applied on the first day of the year. This day was taken for the application because PESTAN can not simulate any load within the simulation period. The simulations were performed first with SWAP in order to obtain annual recharge value that is required in PESTAN and also the mean daily actual evapotranspiration required in SESOIL as there was no other mean to estimate them with the available data. The total annual recharge calculated by SWAP was about 162.11 cm for an average yearly actual evapotranspiration of 102.68 cm. Those two values were used in PESTAN and SESOIL on an hourly and on a monthly basis respectively. Depths of pesticide penetration can be seen in table 12 as well as in figure 18.

Table 12. Leaching depths of the pesticides in scenario 1

Penetration (cm)	Chlorpyrifos	Dimethoate	Fenamiphos	Oxamyl
PESTAN	32.5	525	200	480
SWAP	20.5			
WAVE	65	505	385	255
SESOIL	8.8	600	278	575

Only four models were able to run this scenario. Due to some numerical problems PRZM-2 was unable to run the different scenarios. Concentration values of Ø were simulated by this model for all the pesticides. Different values were obtained only when the decay rates were put to Ø. Obviously this is unacceptable because each pesticide has a decay value more or less known and all the other models could handle the decay process. Therefore, it was unacceptable to modify the decay rate values so PRZM-2 was left out from the analysis of this scenario. Nevertheless, it was not the only model that turned out to perform improperly. SWAP could run only the simulation of chlorpyrifos leaching in the scenario. For the other pesticides, it has produced concentration values of Ø everywhere in the soil column. The low partition coefficient associated with the application of one load of pesticide for the whole year may have caused the pesticides to be either dispersed or flushed down quickly, leaving a very small concentration of the pesticide in the soil column that the model can not simulate.

Unfortunately, there was not sufficient time available to modify the source code of the different models in order to adjust the precision criteria. Therefore, they only could be discarded from the analysis whenever they turned out to have difficulty to perform in the proper way.

The penetration depths vary from one model to another and from one pesticide to another. PESTAN and SESOIL generally predict a high leaching depth for the most soluble pesticides such as dimethoate and oxamyl. Whereas those with a relatively high partition coefficient such as chlorpyrifos and fenamiphos have a higher predicted leaching depth in SWAP and WAVE (for SWAP it is only for chlorpyrifos) (Figure 18).

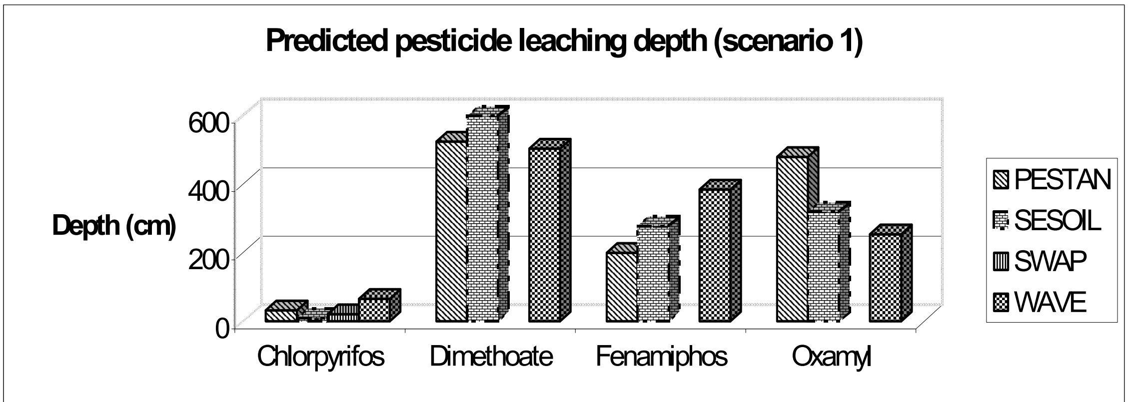


Figure 18. Leaching depths of the pesticides with the different models

The reason could be found in the fact that SESOIL and PESTAN both use the pesticide solubility (which is the amount of the pesticide that can be dissolved in water and thus carried down by water) to process the leaching of pesticide in the soil column.

6.2.2 Scenario 2 An average dry year with the application of multiple loads of pesticide

In this scenario, the same meteorological year was considered with a regular application of pesticide load on a monthly basis, as it is the case in the Naivasha area.

PESTAN can not simulate more than one load of pesticide during the simulation period. All load of pesticides is assumed to be applied prior to the recharge. Consequently, the pesticide would start degrading at the surface at the same decay rate indicated. Therefore, it was discarded. PRZM-2 remained the most problematic model. Since it was not possible to provide any values for the pesticide concentration in the soil column it was discarded for the remaining simulations. Only leaching fluxes were shown down to a maximum depth of 7 cm. Therefore, three models were selected for the simulations: SESOIL, WAVE and SWAP. Table 13 shows the predicted penetration depths for this scenario of the different pesticides by the different models.

Table 13. Penetration leaching depths of the pesticides in scenario 2

Penetration depth (cm)	Chlorpyrifos	Dimethoate	Fenamiphos	Oxamyl
SWAP	65	256	224	256
WAVE	65	585	395	515
SESOIL	8.8	600	278	575

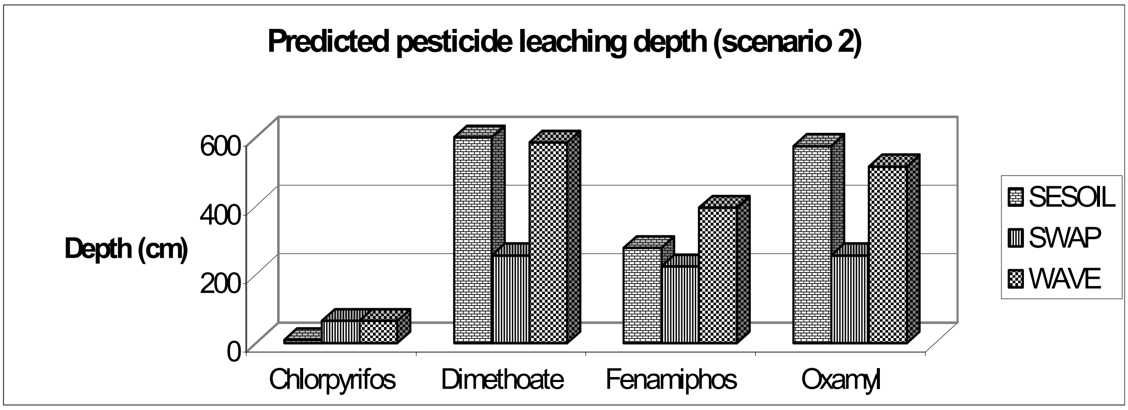


Figure 19. Pesticide penetration depth in the second scenario with the different models

All three models predicted lower leaching depth for chlorpyrifos that can be explained by the tendency of this pesticide to be adsorbed onto the soil particles, especially by organic matter (OM). The pesticide application routine does not appear to affect much the predicted leaching depths in SESOIL, since they remained the same as in the first scenario. Only the predicted concentrations of the different pesticides in the soil column vary (see further discussion of the concentration distributions in Subsection 6.2.4). SESOIL and WAVE predict both dimethoate and oxamyl almost similarly. For SWAP, the difference between the penetration depths of dimethoate, fenamiphos and oxamyl is within a range of 20 cm. As it can be observed from figure 19, the penetration depth of chlorpyrifos predicted in SWAP and WAVE are equal.

6.2.3 Scenario 3 An average wet year with the application of multiple loads of pesticide

The year of 1989 was considered as a relatively wet year with a total annual rainfall of 916 mm. Therefore, it was necessary to know how the models would predict the behavior of the pesticide in such circumstances. To run the wet year scenario the pan evaporation and the precipitation data of this year were used in the models. Table 14 and Figure 20 show the predicted values of pesticide penetration depths obtained from the simulation.

Table 14. Predicted penetration depths of pesticide with SESOIL and SWAP

Penetration depth (cm)	Chlorpyrifos	Dimethoate	Fenamiphos	Oxamyl
SWAP	65	256	224	256
SESOIL	8.89	600	284	579

Only two models were able to perform the simulation of this scenario. They are SESOIL and SWAP. PESTAN and PRZM have been discarded for the same reasons as described above. WAVE could not run this simulation because for some days it has rained more than 5 cm in one day that is beyond the capacity of the model. However, the wet year does not appear to have great effect on the leaching of the pesticide. The predicted leaching depths are the same both in SWAP and SESOIL except the last one with only a slight difference observed for fenamiphos and oxamyl of barely 5 cm deeper.

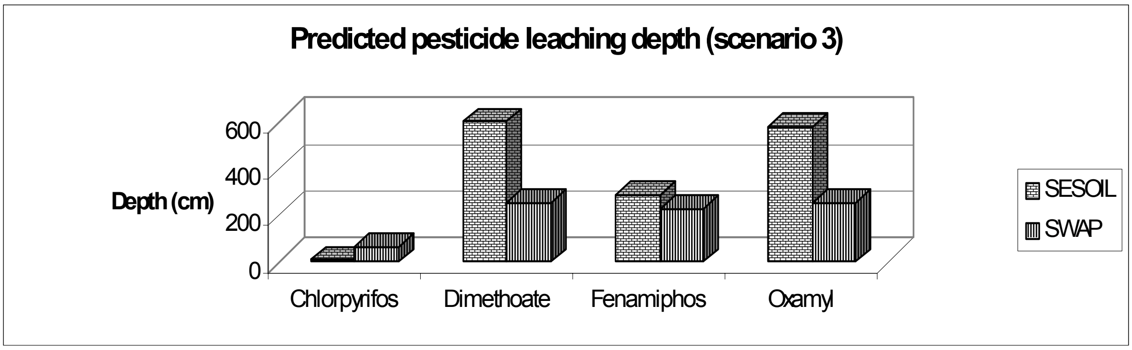


Figure 20. Predicted penetration depths of the pesticides with SESOIL and SWAP.

The reason is that the crops depend mainly on irrigation. They are supplied by irrigation water according to their need, which is calculated to be 8 mm of water per day. As mentioned earlier in chapter 5, irrigation depends on the prevailing weather conditions. In case of a wet year the irrigation routine is merely adjusted to fit the situation. Therefore, the farmers provide less irrigation water that gives at the end of the year the same amount of water supplied to the surface as by rainfall. The difference observed in the predicted leaching of pesticide would have been more significant if daily rainfall values were excessively high but this was not the case for this year. Nonetheless, this scenario showed that due to the irrigation practice the leaching of pesticides is not dependent on the actual weather.

6.2.4 Chemical concentration distribution

Though the interest was mainly to know how deep a specific pesticide would leach down in the soil, it was also important to know the concentration distribution of that pesticide that is either in the solid, liquid or vapor phases of the soil. A pesticide is considered to be harmful when it is found at a concentration higher than a standard. Below a certain level, a pesticide is not even detectable. This level is called the detection level and is the basis to find whether it is still a threat after a certain time at a certain depth. The detection level was found in the literature only for chlorpyrifos and dimethoate, therefore, the lowest values were considered for the other pesticides in order to remain within a safety margin. For chlorpyrifos a value of 0.20 *μg/l* was suggested and for dimethoate a higher value of 0.50 *μg/l* was given.

The concentration of the different pesticide at the end of the modelled year from PESTAN (only scenario 1) SESOIL, SWAP and WAVE are given in tables 15, 16 17 and 18. The values in the tables 15, 16, 17 and 18 represent the concentration values at the lowest depths that the pesticide has reached at the end of the simulation year of each scenario (Tables 12,13 and 14)

Table 15. Concentration of pesticide in the soil as predicted by PESTAN at the end of the year.

Pesticide concentration in different phases	Chlorpyrifos	Dimethoate	Fenamiphos	Oxamyl
Concentration in water *μg/l*	13	1.4E-3	0.79	0.0088
Concentration in soil *mg/kg*	1300	4.6E-4	2.2	0.0037
Total Concentration soil *μg/l*	1500	1.1E-3	2.9	0.0078

Table 16. Concentration of pesticide in the soil as predicted by SESOIL at the end of the year.

Solute concentration in different phases	Chlorpyrifos			Dimethoate			Fenamiphos			Oxamyl		
	Sce 1	Sce 2	Sce 3	Sce 1	Sce 2	Sce 3	Sce 1	Sce 2	Sce 3	Sce 1	Sce 2	Sce 3

Dissolved phase *µg/l*	110	110	110	1E-3	4E-3	5.5E-3	0.8	7	8	1E-5	2.5E-5	4E-5
Adsorbed phase *µg/g*	110	4E3	4E3	4E-4	1.5E-3	2E-3	2.5	20	25	5E-7	1.2E-5	1.2E-5
Air in pore *µg/cm³*	0	0	0	0	0	0	0	0	0	0	0	0

** Sce = scenario*

Table 17. Concentration of pesticide in the soil as predicted by SWAP at the end of the year.

	Total solute concentration in the soil in *µg/l*		
	Scenario 1	Scenario 2	Scenario 3
Chlorpyrifos	110	550	600
Dimethoate		10000	11000
Fenamiphos		11000	1100
Oxamyl		11000	11000

Table 18. Pesticide concentration in the soil column as predicted by WAVE at the end of the year in the lowest soil layer.

	Total solute concentration in the soil (*µg/l*)	
	Scenario 1	Scenario 2
Chlorpyrifos	1	3
Dimethoate	1	1
Fenamiphos	1	1
Oxamyl	1	1

It is difficult to compare the concentration of the pesticide all together because they concentrations are given either by phase or in total. Therefore PESTAN and SESOIL were compared because they present the same phases whereas SWAP and WAVE were grouped because they both display total solute concentration.

PESTAN predicted lower concentrations in water than SESOIL in the first scenario but the concentration in soil is predicted higher in PESTAN than in SESOIL. Both models have predicted more or less the same concentration for dimethoate and fenamiphos in both liquid and solid phases. Oxamyl is predicted at higher concentration in PESTAN than in SESOIL by an order of magnitude of 100.

The concentration of the pesticides predicted by SESOIL in the second and in the third scenario is ten times higher than in the first scenario. It can be observed also in both models that the solid phase con-centration of chlorpyrifos and fenamiphos is higher than the liquid phase as expected due to the relatively high adsorption of those pesticides. It is also important to point out that the concentration in the vapor phase predicted by SESOIL is null despite the fact that this model includes volatilization in the leaching process. This piece of evidence is a fact that this process is not significant for those pesticides with such a low Henry's law constant and air diffusion coefficient.

SWAP predicted very high pesticide concentration for almost all scenarios except for chlorpyrifos for which the total concentration is the same as the concentration in the liquid phase in SESOIL. Similarly to the SWAP model, WAVE predicted the same concentration for dime-thoate, fenamiphos and oxamyl which is very suspicious because the pesticides have their own properties different from each other. This analysis allows us to determine though two models are conceptually based more or less on the same theory, they may behave different differently due to the inherent properties of each one of them. That is the case for SWAP and WAVE though both are TDE numerical models they behave differently in the leaching of pesticide through the soil.

6.3 Sensitivity analysis

Every model input parameter should be subjected to sensitivity analyses to test model response to the potential range of parameters, especially when not all the model parameters can be calibrated. These analyses permit the evaluation of the effects on model outputs of varying hydrogeologic properties, dispersivities, source loading rates, etc. (Bonazountas et al., 1997).

Uncertainties in the fate and transport assumptions were studied by performing a sensitivity analysis on SESOIL and SWAP. These two models were chosen because of their capability to run extreme scenarios. The sensitivity analysis was performed only with fenamiphos to examine the effects of varying selected parameters on the resulting penetration depths. Several soil or pesticide related properties were included in the sensitivity analysis such as the soil disconnectedness, Freundlich exponent, dispersion length and the volatilization related properties such as Henry's constant and air diffusion coefficient, permeability and leaf area index. Indeed, as mentioned in the beginning, every model input parameter should have been chosen for the sensitivity analysis. However, as a matter of limited time, the runs were done only with those few. Low and high values for each parameter were selected to account for the range of reasonably possible values. Only one parameter was adjusted in each sensitivity analysis run while keeping the others constant. Since in the third scenario the leaching did not show any significant difference to the second scenario the sensitivity analysis was carried out for the third scenario.

The initial parameters were modified using a selected multiplier. This multiplier is aimed to reduce, or to increase the parameter according to a certain range. The ranges were taken as a magnitude of order of ±10 % and ±20 % about the initial calibrated value (considered as base value).

Table 19 lists the values used in the sensitivity analysis and the resulting penetration depths. From the table we can observe that the ±10 and ±20% changes of most of the parameters do not affect much the leaching of the pesticide in the soil. No changes have been observed in the penetration depths simulated by SWAP. The values remain the same as the base value. SESOIL exhibits few changes with the changes of the increase or decrease of some parameters. The calculated leaching depths associated with the sensitivity analysis runs are summarized in table 20 and also shown in figure 21.

The change in the disconnectedness index values produced a symmetrical change in the leaching depth of fenamiphos whereas the change in the permeability values showed a different curve. It is completely asymmetrical up to +10% and from that value to + 20 %, the changes are no longer significant where the curve looks to have reached an asymptote. This pattern suggests that the error would be larger when a value of the disconnectedness index is taken in the positive direction than when it is taken in negative direction. However in the negative direction the curve does not look to have yet reached an asymptote at –20% as in the reverse case. That also suggests that the changes may continue if the decrease of that value persists while in the positive direction no further changes are expected.

To summarize we can say that the SWAP model is not sensitive to this range where the values of the dispersion length, the Freundlich coefficient and the LAI were taken as regarding to this scenario and this set of parameters. It is important not to generalize by saying that the model is not sensitive to changes of these parameters because the changes in the simulation depends on other parameters and also on the range. The change observed with SESOIL was not substantial either to draw any considerable conclusion. However, the figures indicate that this model is more sensitive to changes in the permeability and the disconnectedness index.

Table 19. Sensitivity analysis input parameters

Sensitivity parameter	Multiplier	**Layer 1**	**Layer 2**	**Layer 3**	**Layer 4**	Penetration depth (cm)
Soil disconnectedness SESOIL	-20%	4.496				287.7
	-10%	5.058				286.6
	Base value	5.62				284
	+10%	6.182				282
	+20%	6.744				281
Freundlich exponent SWAP	-20%	0.8				192
	-10%	0.9				192
	Base value	1				192
	+10%	1.1				192
	+20%	1.2				192
Freundlich exponent SESOIL	-20%	0.8				284
	-10%	0.9				284
	Base value	1				284
	+10%	1.1				284
	+20%	1.2				284
Dispersion length SWAP	-20%	12.8				192
	-10%	14.4				192
	Base value	16				192
	+10%	17.6				192
	+20%	19.2				192
Henry's constant SESOIL	Base value	1.15E-09				284
	0	0				284
Air diffusion coefficient SESOIL	Base value	0.036				284
	0	0				284
Permeability SESOIL	-20%	**1.52E-8**	**2.86E-9**	**1.42E-9**	**2.16E-9**	281
	-10%	**1.71E-8**	**3.21E-9**	**1.59E-9**	**2.49E-9**	283
	Base value	**1.90E-8**	**3.57E-9**	**1.77E-9**	**3.70E-9**	284
	+10%	**2.09E-8**	**3.93E-9**	**1.95E-9**	**2.97E-9**	291.7
	+20%	**2.28E-8**	**4.28E-9**	**2.12E-9**	**3.24E-9**	292
Leaf area index SWAP	-20%	2.4				192
	-10%	2.7				192
	Base value	3				192
	+10%	3.3				192
	+20%	3.6				192

** The values in bold represent the corresponding layer permeability values used only in SESOIL*

Another piece of evidence was obtained supporting the interpretation of the air-in-pore pesticide concentration when the volatilization pathway was turned off using a ø value for the Henry's law constant and the air diffusion coefficient. When this was done no changes have been observed either in the soil pesticide concentration or in the leaching depth. Therefore we can conclude that, indeed, the difference in the penetration depth or concentration observed between SESOIL and the other models is not due to the use of the vapor phase transport included in the model, because both parameters (Henry's law constant and air diffusion coefficient) are not significant to induce any upward movement of the pesticide. The vapor phase depends on the pesticide used.

Table 20. Sensitivity analysis results in %

Penetration depth variation in %	Soil disconnectedness index	Freundlich exponent	Permeability
-20%	1.3	0	-1.05
-10%	0.81	0	-0.35
0	0	0	0
+10%	-0.7	0	2.71
+20%	-1.05	0	2.81

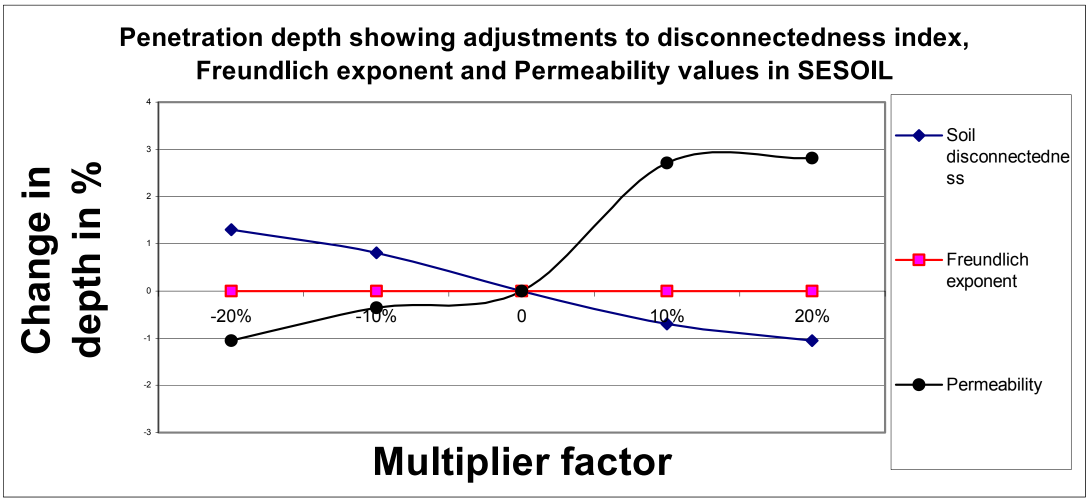


Figure 21. Sensitivity analysis results in %

7 Conclusions and recommendations

The computer simulation models PESTAN, SWAP, WAVE, SESOIL, and PRZM-2 were evaluated and compared for their ability to predict the leaching of pesticides in the unsaturated soil zone using experimental field data combined with data from the literature.

The study was carried out in the riparian zone of the Lake Naivasha, Kenya (Figure 1) in three agricultural farms (Oserian, Aberdare and 3 Ostrich) located on two different soil units: sandy loam in the northeastern part and clay loam in the southwestern part. The soil units have been identified from previous study by Kwacha (1998), and by Siderius (1998).

The comparison of the above mentioned models was pursued first in order to find out how appropriate the models are for the evaluation of pesticide transport in the unsaturated soil zone in tropical conditions. Secondly, it was necessary to determine the minimum field data needed for the different models to adequately simulate the leaching of selected pesticides.

In order to collect more information about the unsaturated soil zone, a short fieldwork was done during which several field experiments were carried out. The soil profile was assessed from the soil core down to 6 meters. The different layers were determined using a simple manual technique and also using the Munsell color chart. Soil samples were collected in the field and sent for laboratory analysis of particle size distribution and organic matter content. For each layer the soil hydraulic conductivity was assessed using the inverse auger hole method. After having reviewed the different sites regarding the soil properties, the site of Oserian, which is located on the sandy loam soil unit was selected to conduct the simulations. The selection of this site was based on the soil characteristics affecting the likelihood for pesticide leaching such as the soil type, the depth to the groundwater table and the soil hydraulic conductivity (Figures 1 and 8, Tables 3, 4 and 5).

One important field experiment carried out during the fieldwork was the infiltration basin (Figure 15) whose purpose was to obtain the recharge characteristics (soil moisture content) in order to calibrate the models. Based on the moisture content distribution obtained from the infiltration basin on the selected site, the models were calibrated and simulations were performed creating three main scenarios with the calibrated models. The scenarios were the following:

- One scenario was run with a dry meteorological year of October 1998-September 1999 with the application of a single load of pesticide.
- The second scenario was performed with the same meteorological year, but this time with multiple loads of pesticide.
- The last scenario was performed with a wet year observed in Oct 1989-September 1990 with multiple loads.

The models were compared and evaluated on the basis of the leaching depths over the time and the solute concentration in the soil profile in order to determine their applicability to evaluate specific environmental scenarios. In order to allow a fair comparison of the models, the parameters were taken equal. Finally sensitivity analyses were done with selected parameters in order to assess the consequences of possible inaccuracies in the determination of the parameter values.

The results of this study indicate clearly that only two models, SESOIL and SWAP (Figure 20), were capable to simulate the given range of scenarios occuring in the Naivasha area. The other models can also do a good job but for a limited range of purposes. For example, though the simplistic characteristics of PESTAN to represent the soil system and the processes involving the transport of pesticide, the results of the simulations were found very close to those of other more complex models in the first scenario. It was proved that we can also get good results for assessing the leaching depth with a simple model such as PESTAN (Figure 18). This simple model can be useful as a screening tool in case of data scarcity.

Generally speaking, SWAP and WAVE present the same features (almost the same input parameters, the same processes and equations) to describe the water flow and pesticide transport within the soil. The hydrologic cycle in both models is described by the well known Richard's equation while the solute transport processes are governed in both by the Fick's first law and the relation proposed by Millington and Quirk. Nonetheless, WAVE has exhibited some limitations. The runs failed when the rainfall is greater or equal to 5 cm or the irrigation is greater or equal to 10 cm per day. Being in a tropical country, the rainfall is affected by a high variability. Even during a normal year or a dry year the rainfall in one day may be heavy, more than 5 cm of rainfall per day can be expected and the model has proven it is incapable to handle this situation. PRZM-2 was discarded along the study due to numerical problem.

SESOIL and SWAP have shown their ability to simulate several kinds of scenarios from very simple scenario to more complex ones. On the other hand, picking any of the two would be just a matter of how much data is available. In this way, SESOIL would be more preferable since it requires less data but yet some of the data are not easy to find. The model requires for the hydrologic cycle the time distribution of climatic data such as number and duration of storms in a month, which are only obtainable from a digital recorder (logger). This equipment is rarely available over the whole catchment and their readings (if they exist) are not consistent. Another parameter in the hydrologic cycle of SESOIL is the actual evapotranspiration that the model calculates using temperature, humidity and albedo. As the last parameter was not available, the actual ET was directly provided to the model. In this study it was taken directly from SWAP as this model can calculate this parameter and for the sake of the comparison it was necessary to have the data sets as similar as possible. Nevertheless, if SESOIL has to be used independently, this parameter can also be calculated separately using some known method such as the Penman and the Bowen ratio.

In case of data scarcity, SWAP would be the least recommendable model for the study area since it requires a larger amount of input data (Table 1). Some parameters are also hardly available in the literature. Usually the soil related parameters obtained from the literature are based on series of soils from different climate, region and depth of which a mean is given with a range of expected deviation. However, only the validation of the model could prove whether the data taken from literature present certain reliability in case of field data scarcity or total absence of historical data.

The results of the sensitivity analyses showed that indeed some parameters are not necessary in the models (Tables 19, 20). For instance, the SWAP model is not sensitive to the changes of the parameters such as the LAI, the dispersion coefficient and the Freundlich coefficient and the change in the Freundlich exponent does not affect the leaching process in SESOIL.

Meanwhile, the SESOIL model has shown slightly different patterns. Figure 21 indicates a certain asymmetry in the response that suggest that the error would be more important whenever the value of the permeability would be taken greater than the base value up to a maximum of 10%. This value constitutes a certain asymptote where no significant change is expected with any further increase of the permeability. Meanwhile when decreasing the permeability to –20%, a linear decrease can be observed in the response, which also suggests that changes are still expected when decreasing the permeability further. Therefore, extreme care should be taken when estimating the hydraulic conductivity in the field.

The results of the different simulations show that the threat of potential groundwater contamination is obviously present in the area and depend indeed on the pesticide type used, although different results were obtained by the different models. Pesticides such as dimethoate and oxamyl appear more likely to leach deeper and to reach faster the groundwater than chlorpyrifos and fenamiphos, due to their high solubility. Chlorpyrifos and fenamiphos would not leach too deep after one year of application due to the high adsorption. However, it is difficult to draw a conclusion about the potential risk of the pesticides because of the large variability in the model predictions. All the model predictions agreed more or less about the threat of fenamiphos in the soil. Such a pesticide with relatively high solubility compared to chlorpyrifos and a relatively low adsorption compared to dimethoate and oxamyl, a low decay rate and a long half-life is more likely to be in the soil for a long term threatening the groundwater. Therefore, a real management care should be considered in order to limit the use of such pesticide.

Finally the results of this study must be viewed in the scope of its purposes. The focus was on comparing the five models in running the same environmental scenarios. It should also be considered that the evaluation is based on a short-term field study so, several assumptions had to be used. Therefore, only limited quantitative comparative analysis could be done. However, it was not the intent of this study to conduct comparison of predicted results to field measurements. Such field validation should be the basis of further studies that should also include the spatial variability of the field parameters throughout the area such as vertical and spatial soil variability, different crop types, etc.

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Appendix A.

Climatic data

	Pan data 1957-1990	Temperature in ºC (1937-154)		Rainfall (1910-1960)
	(mm/day)	Mean Max Temp	Mean Min Temp	Mm
January	5.39	22.7	8.1	37
February	5.51	28.3	8.2	41
March	5.72	27.3	9.8	47
April	4.71	25.1	11.5	114
May	4.74	23.8	11.3	109
June	4.48	23.0	9.9	45
July	4.49	22.5	9.3	39
August	4.74	22.9	9.4	53
September	5.16	24.5	8.8	25
October	5.18	25.6	9.1	45
November	4.24	24.7	9.3	64
December	4.97	25.8	8.7	48

Appendix B

Table of pesticides used in the Riparian area of the Lake Naivasha from Tang (1999)

Number	Common name	Trade name	Toxicity		Persistence
			WHO	EPA	Half lIfe
1	Acrinathrin	Rufast	III	IV	52
2	Acephate	Orthene	III	III	7-10 days
3	Aldicarb	Temik	Ia	I	10 weeks
4	Alfa-cypermethrin	Fastac	II	II	13 weeks
5	Amitraz	Mitac	III	III	<1
6	Azocyclotin	Peropal	Ib	II	3 weeks
7	Bacillus thuringiensisi	Dipel	III	III	-
8	Benomyl	Benlate	-	IV	6-12 months
9	Bifenthrin	Brigade	II	II	62
10	Bitertanol	Bayor	-	IV	-
11	Bupirimate	Nimrod	-	III	6-7 weeks
12	Cadusafos	Rugby	III	III	45 days
13	Captan	Captan	-	IV	-
14	Carbosulfan	Marshal	II	I or II	2-3 days
15	Carboxin	Vitavax	-	III	24 hours
16	Chloropyrifos	Pyrinex	II	II	30-60 days
17	Chlorothalonil	Bravo	-	IV	1.5-3 months
18	Clofentezine	Apollo	-	III	28-56 days
19	Copper oxychloride	-	III	III	-
20	Cymoxanil	Milraz	III	III	<2 weeks
21	Cypermethrin	Ripcord	II	II	16 week
22	CyproConazole	Alto	-	IV	3 months
23	Cyromazine	-	-	III	-
24	Dichlofluanid	Euparen	-	IV	-
25	Dicofol	Kelthane	III	II	-
26	Dienochlor	Pentac	III	III	-
27	Diflubenzuron	Dimili	-	III	<7 days
28	Dimethoate	-	II	II	7-120 days
29	Dodemorph	Meltatox	-	IV	-
30	Endosulfan	Thiodan	II	I	Plant 3-7 days
31	Fenamiphos	Nemacur	Ia	I	4 months
32	Fenaznquin	Pride	III	III	-
33	Fenbutatin	Oxide	-	III	-

34	Flusilazole	Nustar	-	III	-
35	Fosetyl	Alliette	-	III	-
36	Hexaconazole	Anvil	-	IV	-
37	Imidacloprid	Gaucho	-	IV	-
38	Iprodione	Rovral	-	IV	20-160 days
39	Lambda-cyhalothrine	Icon	-	-	4-12 weeks
40	Mancozeb	Dithane M-45	-	IV	-
41	Metaxyl	Ridomil	III	III	70-90 days
42	Methiocard	Mesurol	II	II	-
43	Methomyl	Lannate	Ib	I, IV	-
44	Metiram	Polyram-combi	-	IV	-
45	Oxamyl	Vydate	Ib	I	7 days
46	Oxycarboxin	Plantvax	-	III	-
47	Pirimiphos-methyl	Actellic	III	III	<30 days
48	Polyoxins	Polyoxin	-	IV	-
49	Procymidone	Sumilex	-	-	4-12 weeks
50	Propancarb	Previcur N	-	IV	3-4 weeks
51	Propargite	Omite	III	III	2-4 weeks
52	Propineb	Antracol	-	IV	-
53	Pyrethrins	Py-mark	II	II	-
54	Quintozene	Brassicol	-	-	4-10 months
55	Sulphur	-	-	IV	-
56	Tetradifon	Tedion	-	III	-
57	Thiocyclam	Evisect	II	II	1
58	Thiophanate-methyl	Cercobin	-	IV	-
59	Thiram	Thiram	III	III	-
60	Triforine	Saprol	-	IV	3 weeks

* WHO toxicity classification:

Ia: extremely hazardous
Ib: highly hazardous
II: moderately hazardous
III: slightly hazardous
Table5: product unlikely to Present acute hazard in normal use.

* EPA(USA) persistence classification (ETN, 1993)

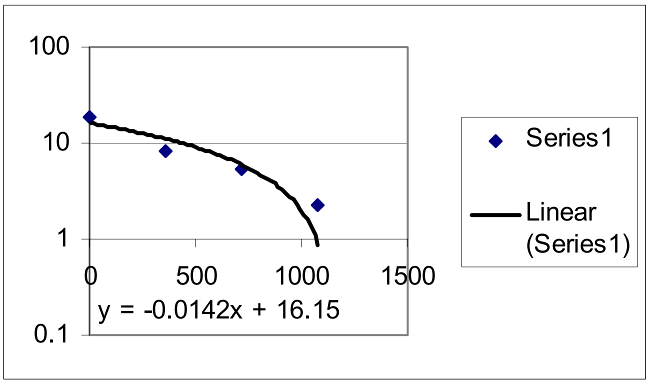
Low: 0-30 days
Medium: 30-60 days
High: >100 days

* (-) for missing information

Appendix C

Layer hydraulic conductivity at Oserian Farm

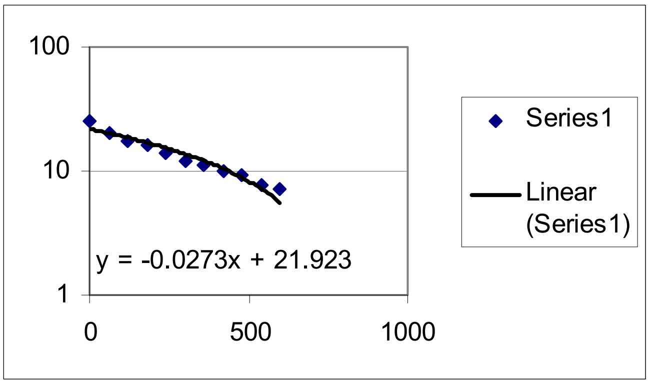
Depth: 16 cm



ti	h'ti	hti	hti+r/2
0	0	16	18.25
360	10	6	8.25
720	13	3	5.25
1080	16	0	2.25

K= 110.8cm/d

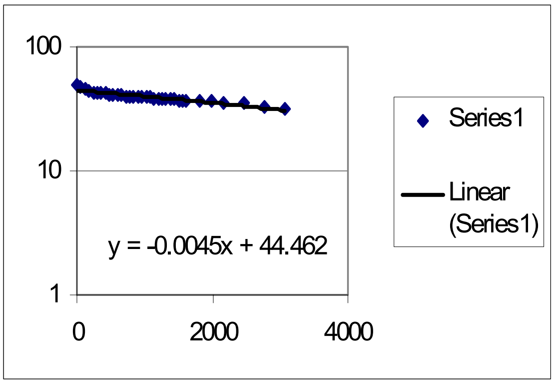
Depth: 53 cm



ti	h'ti	hti	hti+r/2
0	30	23	25.25
60	35	18	20.25
120	37.5	15.5	17.75
180	39.3	13.7	15.95
240	41.2	11.8	14.05
300	43	10	12.25
360	44	9	11.25
420	45.1	7.9	10.15
480	46.1	6.9	9.15
540	47.5	5.5	7.75
600	48	5	7.25

K = 213 cm/d

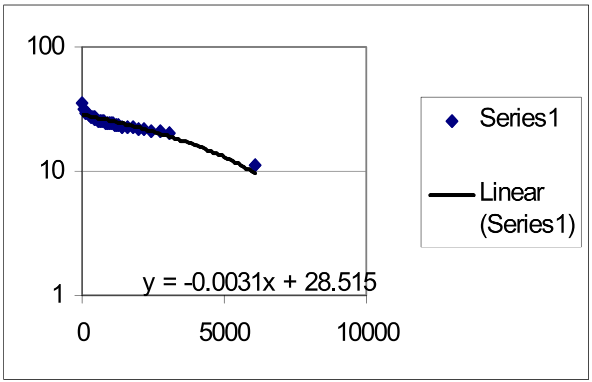
Depth: 260 cm



K = 35.11 cm/d

ti	h'ti	hti	hti+r/2
0	212	48	50.25
60	215	45	47.25
120	216.7	43.3	45.55
180	218	42	44.25
240	219	41	43.25
300	219.5	40.5	42.75
360	220	40	42.25
420	220.2	39.8	42.05
480	220.8	39.2	41.45
540	221	39	41.25
600	221.5	38.5	40.75
660	221.8	38.2	40.45
720	222.2	37.8	40.05
780	222.4	37.6	39.85
840	222.9	37.1	39.35
900	223.1	36.9	39.15
960	223.1	36.9	39.15
1020	223.2	36.8	39.05
1080	223.3	36.7	38.95
1140	223.7	36.3	38.55
1200	223.9	36.1	38.35
1260	224	36	38.25
1320	224.2	35.8	38.05
1380	224.5	35.5	37.75
1440	224.8	35.2	37.45
1500	225	35	37.25
1560	225.1	34.9	37.15
1620	225.2	34.8	37.05
1800	225.5	34.5	36.75
1980	226.1	33.9	36.15
2160	226.5	33.5	35.75
2460	227.2	32.8	35.05
2760	229	31	33.25
3060	230.7	29.3	31.55

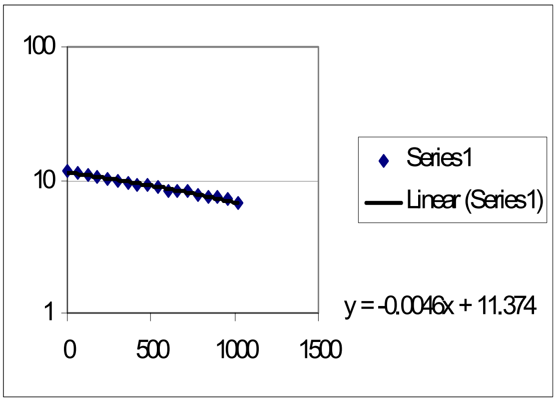
Depth: 353 cm



K = 24.19 cm/d

radius	4.5		
ti	h'ti	hti	hti+r/2
0	320.5	32.5	34.75
60	324	29	31.25
120	325.5	27.5	29.75
180	326	27	29.25
240	327	26	28.25
300	327.8	25.2	27.45
360	328	25	27.25
420	328.2	24.8	27.05
480	328.5	24.5	26.75
540	329	24	26.25
600	329.5	23.5	25.75
660	329.5	23.5	25.75
720	330	23	25.25
780	330.2	22.8	25.05
840	330.5	22.5	24.75
900	330.6	22.4	24.65
960	330.7	22.3	24.55
1020	331	22	24.25
1080	331.2	21.8	24.05
1140	331.5	21.5	23.75
1200	331.6	21.4	23.65
1260	331.8	21.2	23.45
1440	332.3	20.7	22.95
1620	332.4	20.6	22.85
1800	332.6	20.4	22.65
1980	333.2	19.8	22.05
2160	333.5	19.5	21.75
2460	334.2	18.8	21.05
2760	334.5	18.5	20.75
3060	335.2	17.8	20.05
6060	344	9	11.25

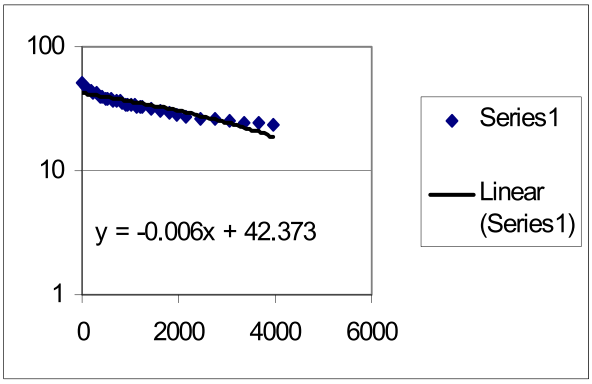
Depth: 428.5 cm



ti	h'ti	hti	hti+r/2
0	419	9.5	11.75
60	419.4	9.1	11.35
120	419.8	8.7	10.95
180	420.2	8.3	10.55
240	420.6	7.9	10.15
300	421	7.5	9.75
360	421.3	7.2	9.45
420	421.5	7	9.25
480	421.7	6.8	9.05
540	422	6.5	8.75
600	422.4	6.1	8.35
660	422.5	6	8.25
720	422.6	5.9	8.15
780	423	5.5	7.75
840	423.2	5.3	7.55
900	423.4	5.1	7.35
960	423.5	5	7.25
1020	424	4.5	6.75

K = 35.89 cm/d

Depth: 475 cm



K = 46.82 cm/d

ti	h'ti	hti	hti+r/2
0	426	49	51.25
60	429	46	48.25
120	431	44	46.25
180	432.5	42.5	44.75
240	434.2	40.8	43.05
300	435.2	39.8	42.05
360	437	38	40.25
420	438	37	39.25
480	438.6	36.4	38.65

540	439	36	38.25
600	439.3	35.7	37.95
660	440	35	37.25
720	440.6	34.4	36.65
780	441.1	33.9	36.15
840	442.2	32.8	35.05
900	442.6	32.4	34.65
960	443	32	34.25
1020	443.3	31.7	33.95
1080	443.7	31.3	33.55
1140	444.1	30.9	33.15
1200	444.7	30.3	32.55
1260	445	30	32.25
1440	446	29	31.25
1620	447	28	30.25
1800	447.8	27.2	29.45
1980	448.8	26.2	28.45
2160	449.5	25.5	27.75
2460	450.5	24.5	26.75
2760	451.4	23.6	25.85
3060	452	23	25.25
3360	452.5	22.5	24.75
3660	453	22	24.25
3960	453.5	21.5	23.75

Appendix D

Nr.	Depth	Sand	Silt	Clay
Sample		2 - 0,05	0,05 - 0,002	<0,002
1				
1	Aberdare 25 m, 60	38.6	48	14
2	Aberdare 70	41.7	45	13
3	Aberdare 100	71.2	22	7
4	Aberdare 168	72.3	23	5
5	Aberdare 270	64.9	29	6
6	Aberdare 380	62.7	31	6
7	Aberdare 480	67.5	28	5
8	Oserian 40 cm	50.9	43	6
9	Oserian 70	50.6	43	7
10	Oserian 100	41.9	50	8
11	Oserian 230	46.4	50	4
12	Oserian 280	38.0	58	4
13	Oserian 450	12.2	63	25
14	Oserian 520	16.1	66	18

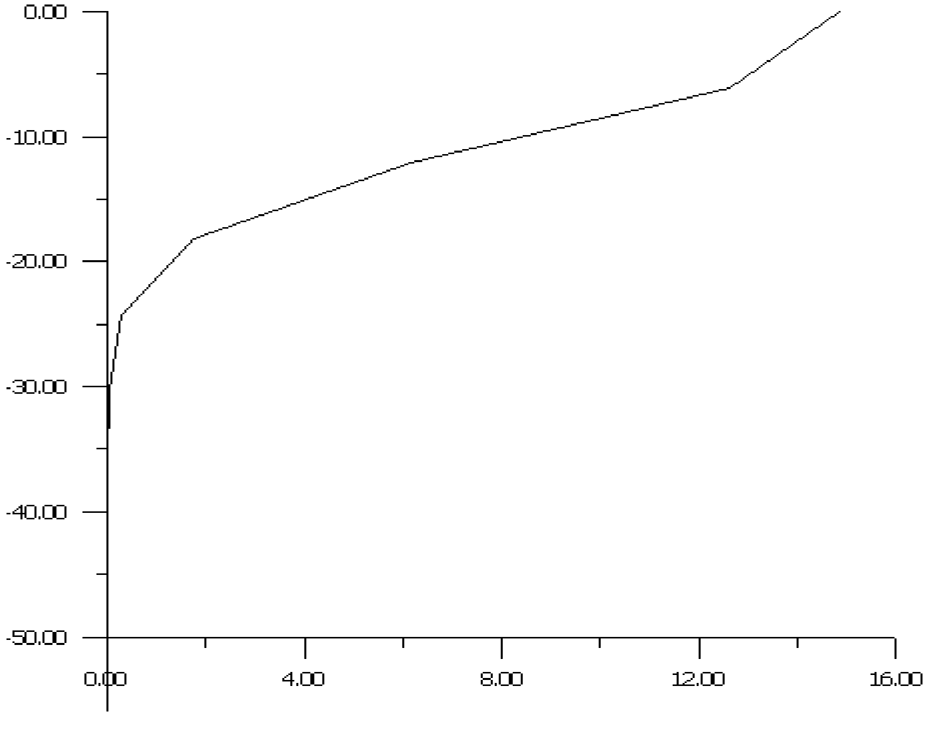
15	Oserian 550	87.2	11	2
16	Oserian 600	39.0	55	6
17	Ostrich 60	50.9	32	17
18	Ostrich 100	37.0	43	20
19	Ostrich 150	31.0	62	7
20	Ostrich 230	65.6	29	6
21	Ostrich 300	80.4	16	4
22	Ostrich 380	83.6	13	4
23	Ostrich 600	87.2	10	3

Appendix E.

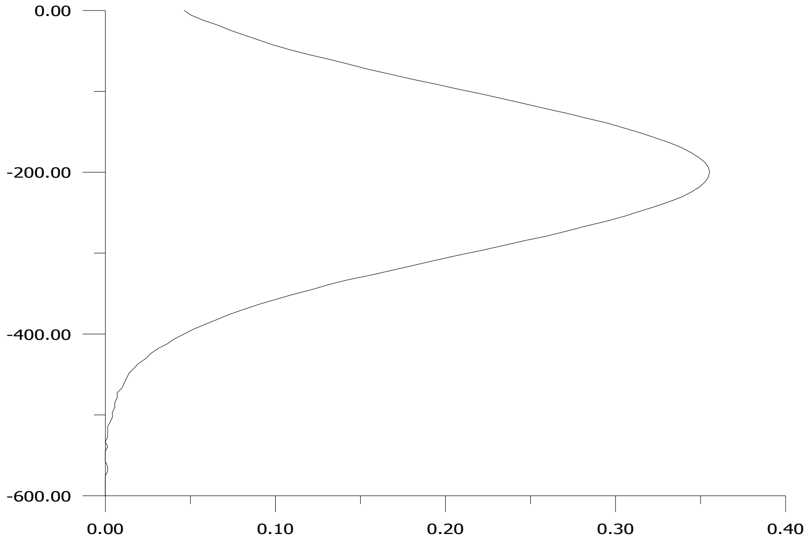
Breakthrough curves

Scenario 1

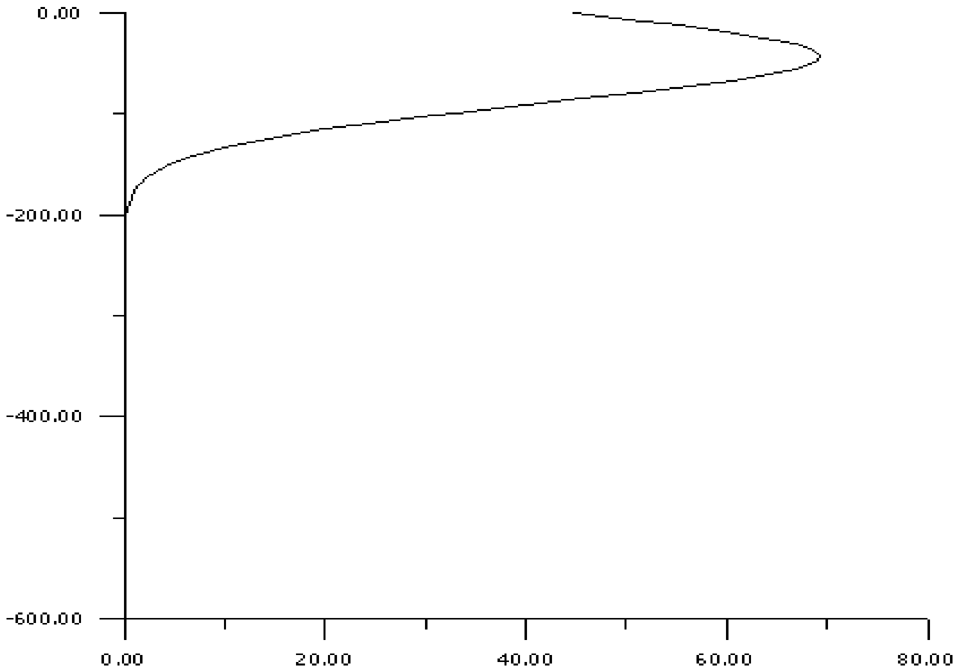
PESTAN



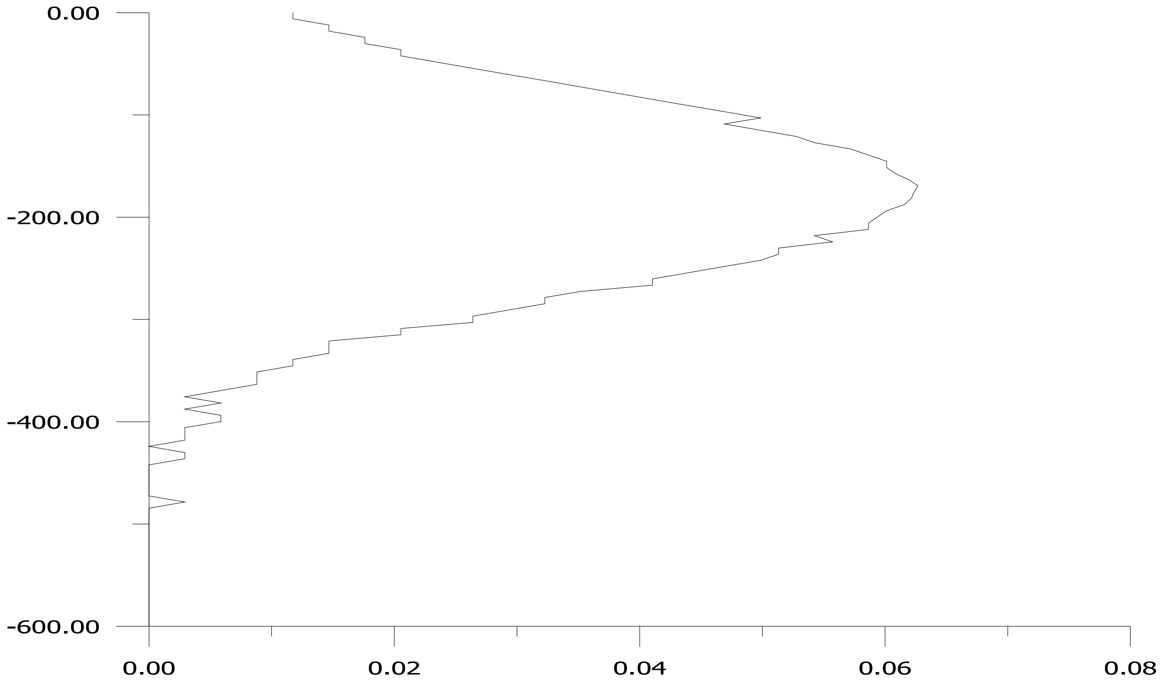
Chlorpyrifos



Dimethoate

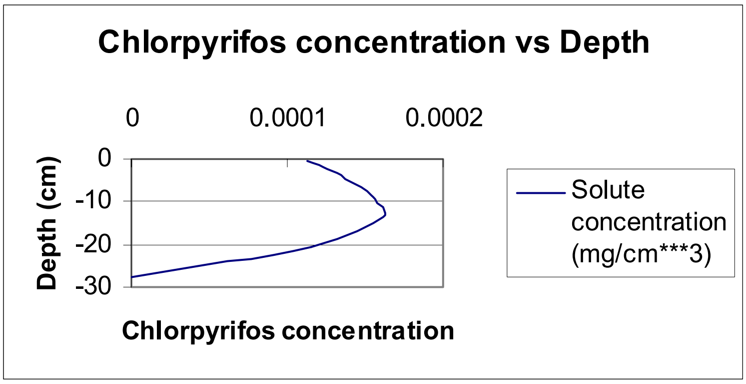


Fenamiphos

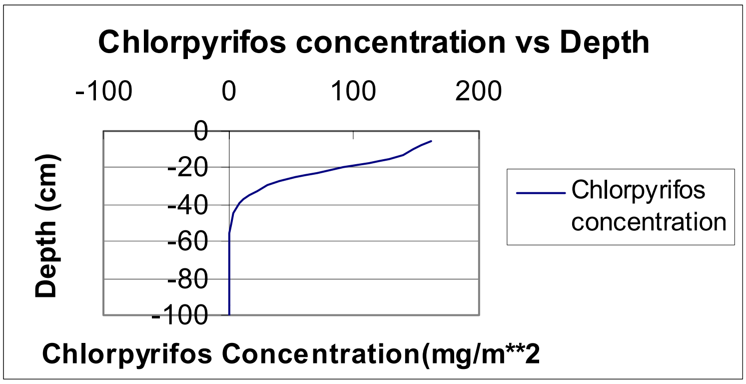


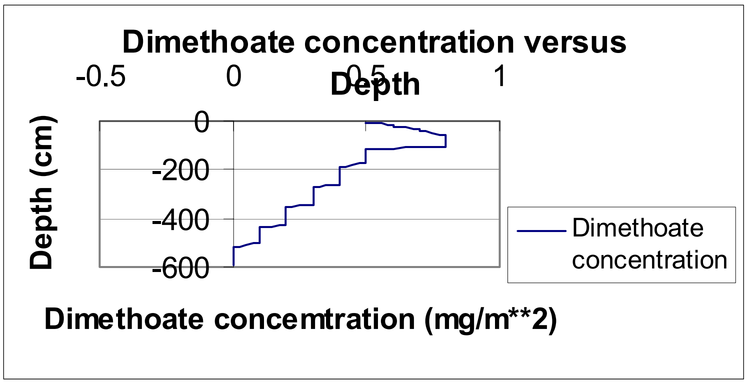
Oxamyl

SWAP

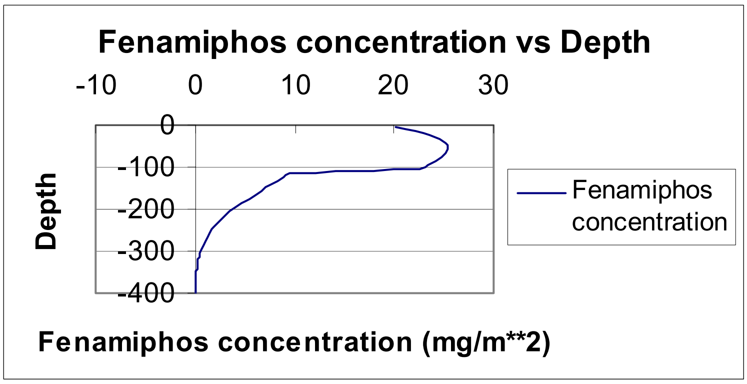


WAVE

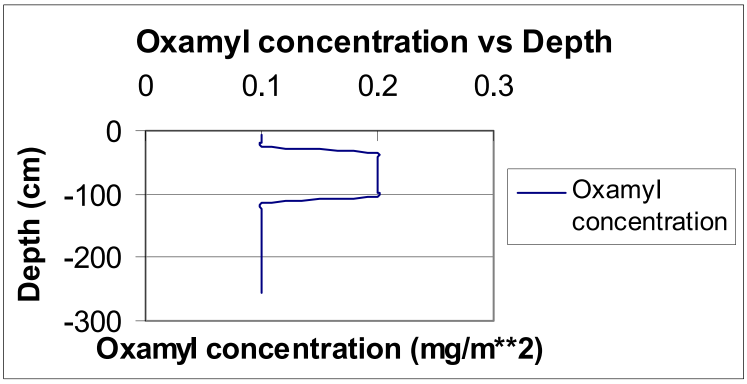




Dimethoate concentration versus Depth
-0.5
0
0.5
1
0
-200
-400
-600
Depth (cm)
Dimethoate concentration
Dimethoate concemtration (mg/m**2)

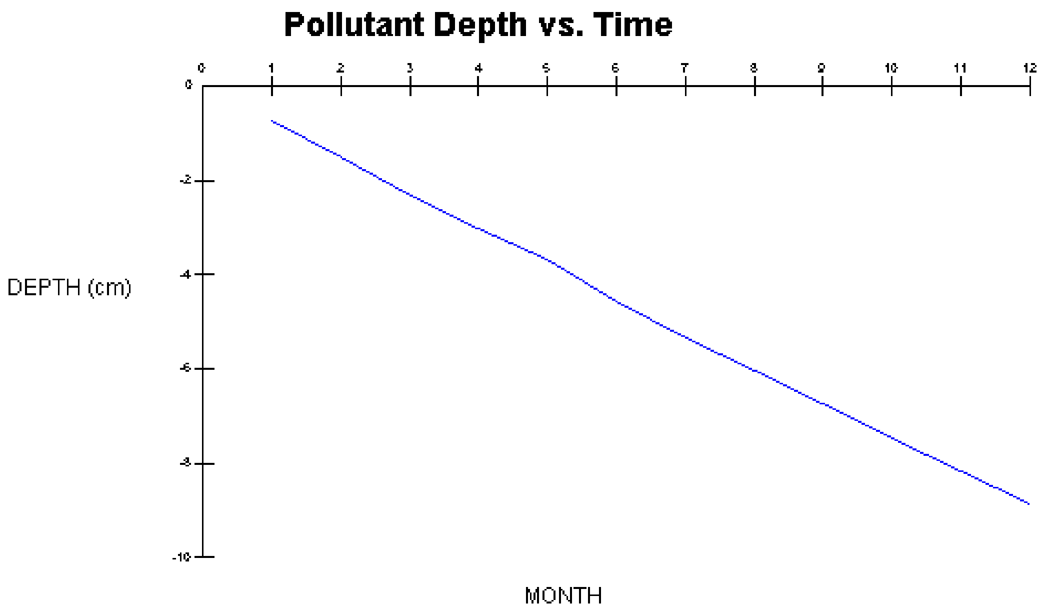


Fenamiphos concentration vs Depth
-10
0
10
20
30
0
-100
-200
-300
-400
Depth
Fenamiphos concentration
Fenamiphos concentration (mg/m**2)

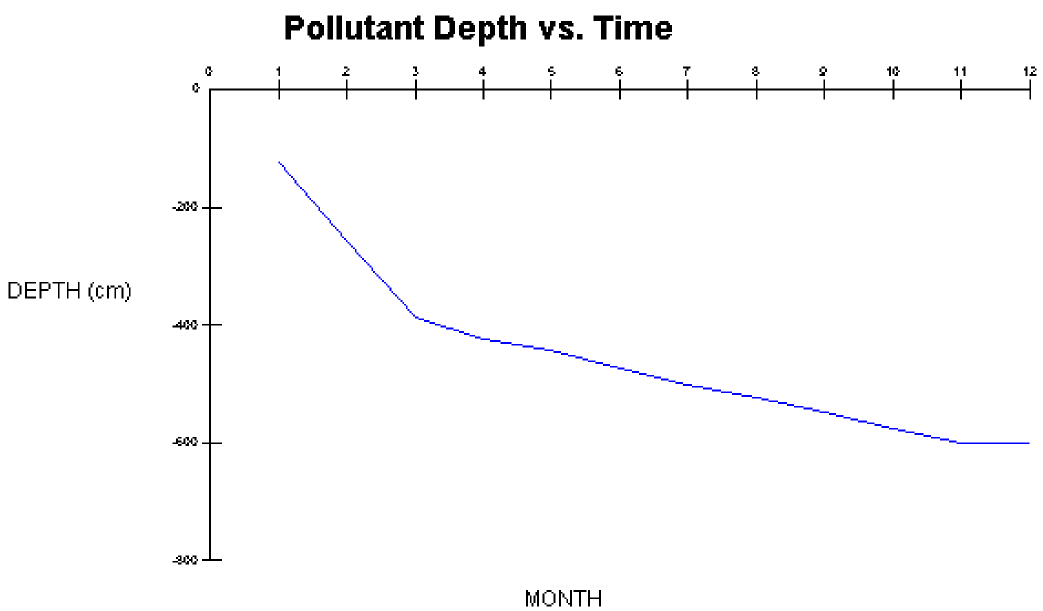


Oxamyl concentration vs Depth
0
0.1
0.2
0.3
0
-100
-200
-300
Depth (cm)
Oxamyl concentration
Oxamyl concentration (mg/m**2)

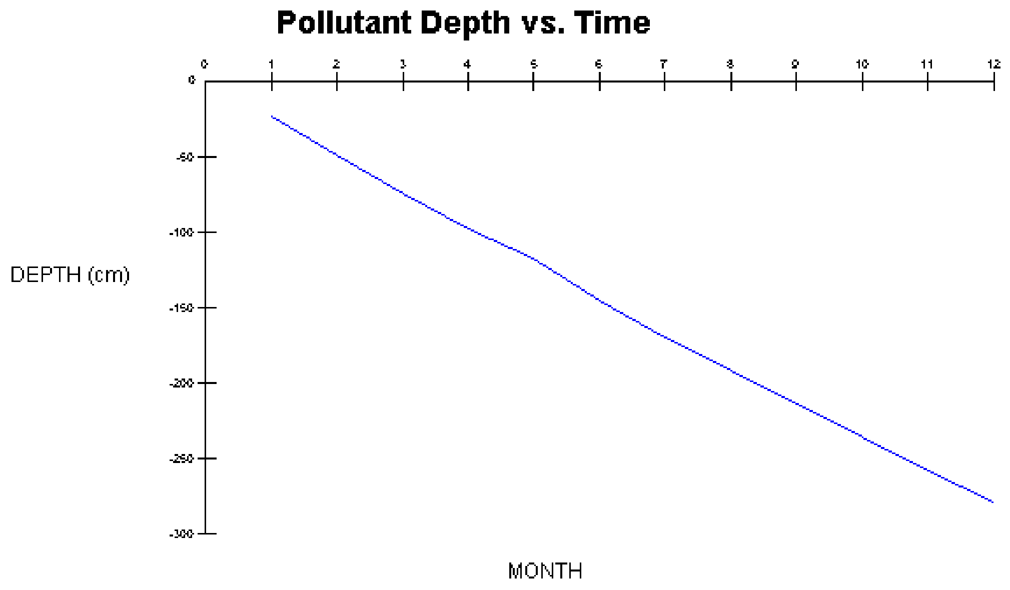
SESOIL



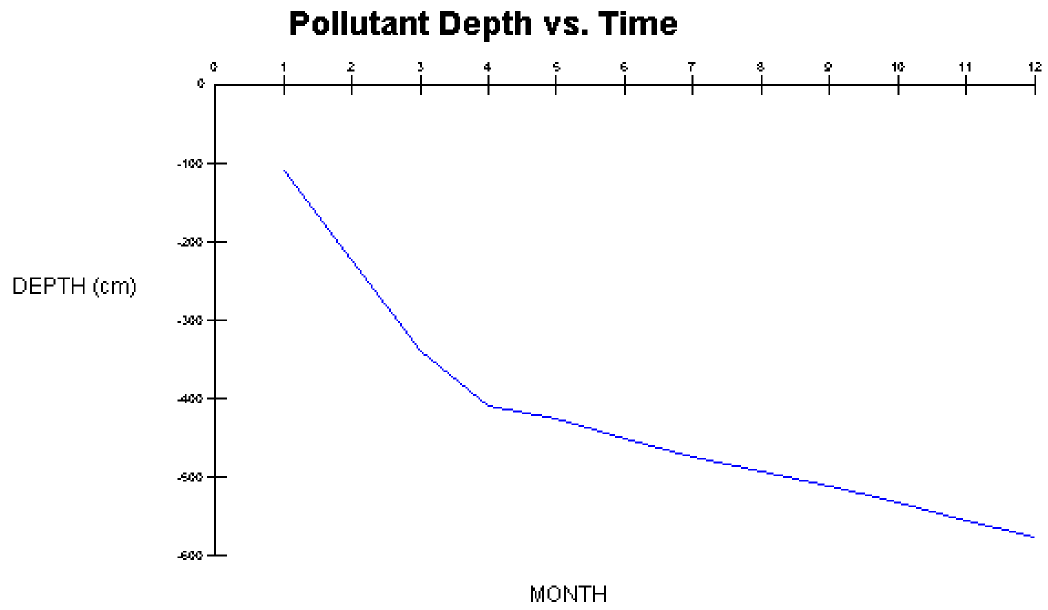
Chlorpyrifos



Dimethoate



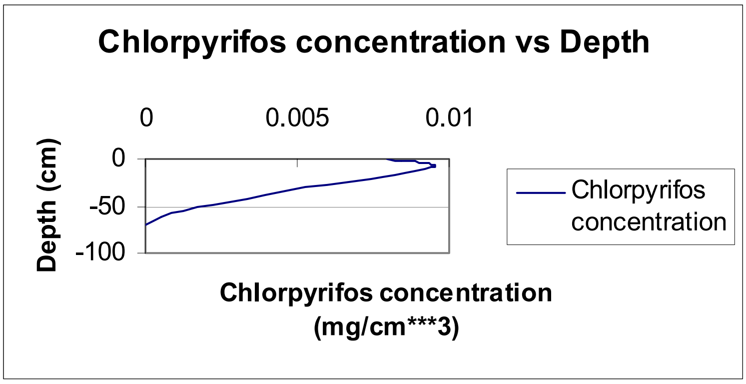
Fenamiphos

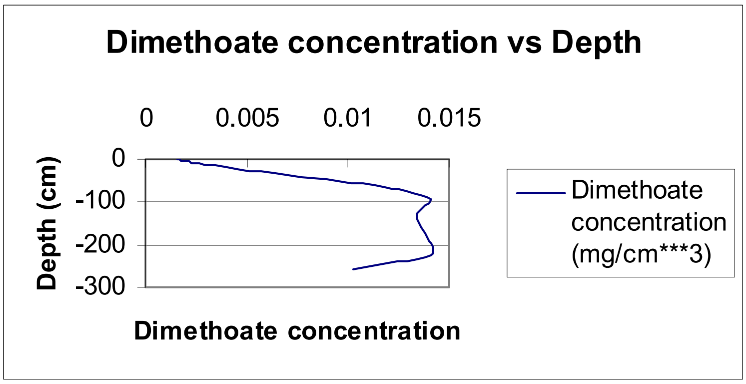


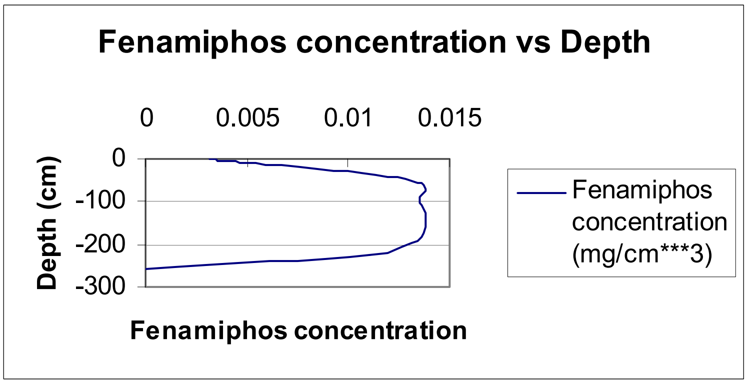
Oxamyl

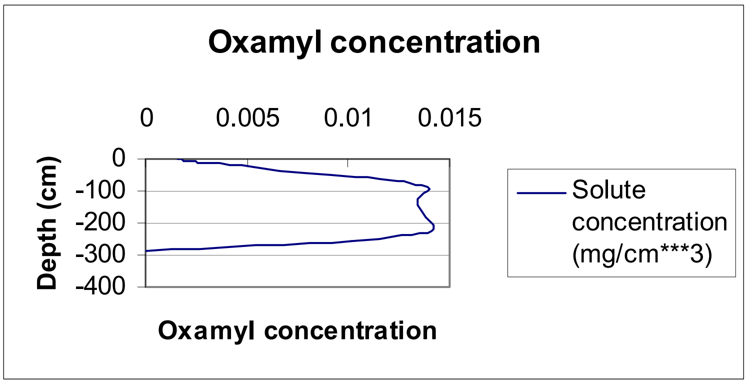
Scenario 2

SWAP

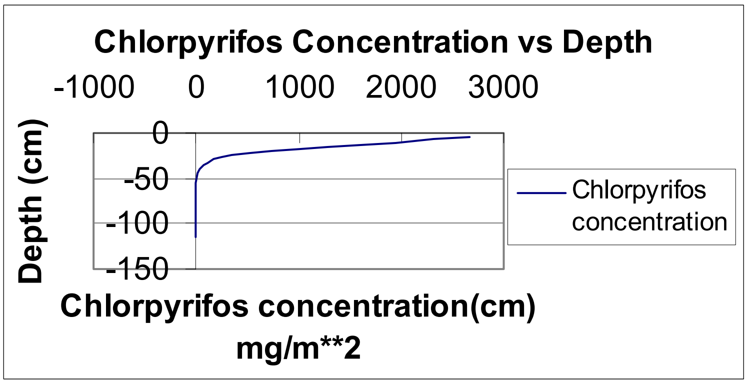


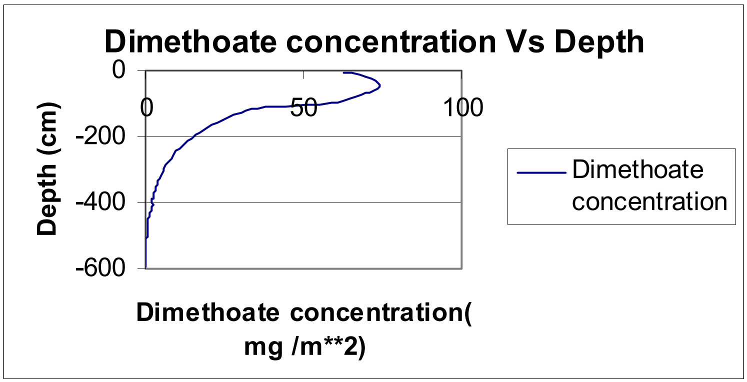


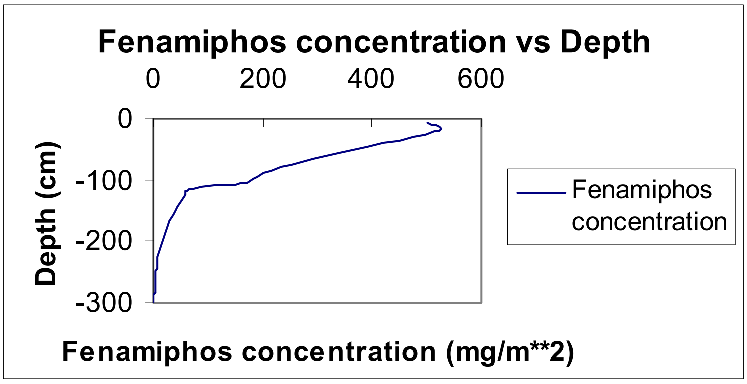


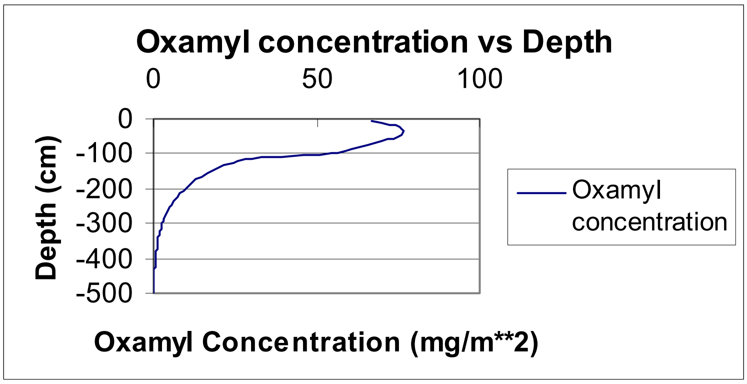

Oxamyl concentration
0
0.005
0.01
0.015
0
-100
-200
-300
-400
Depth (cm)
Solute concentration (mg/cm***3)
Oxamyl concentration

WAVE

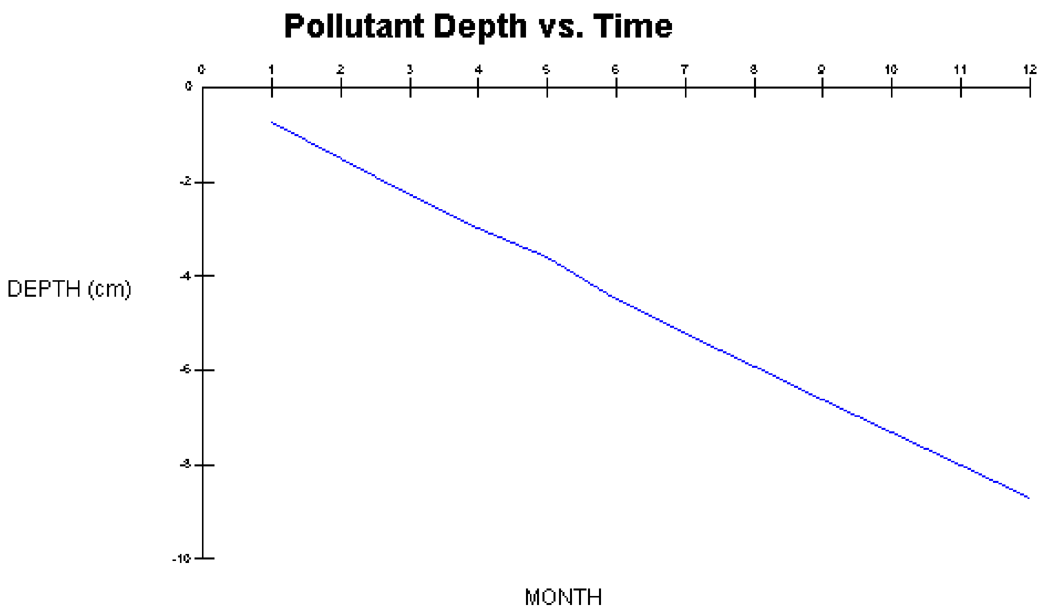

Chlorpyrifos Concentration vs Depth
-1000
0
1000
2000
3000
0
-50
-100
-150
Depth (cm)
Chlorpyrifos concentration
Chlorpyrifos concentration(cm) mg/m**2


Dimethoate concentration Vs Depth
0
50
100
0
-200
-400
-600
Depth (cm)
Dimethoate concentration
Dimethoate concentration(mg /m**2)

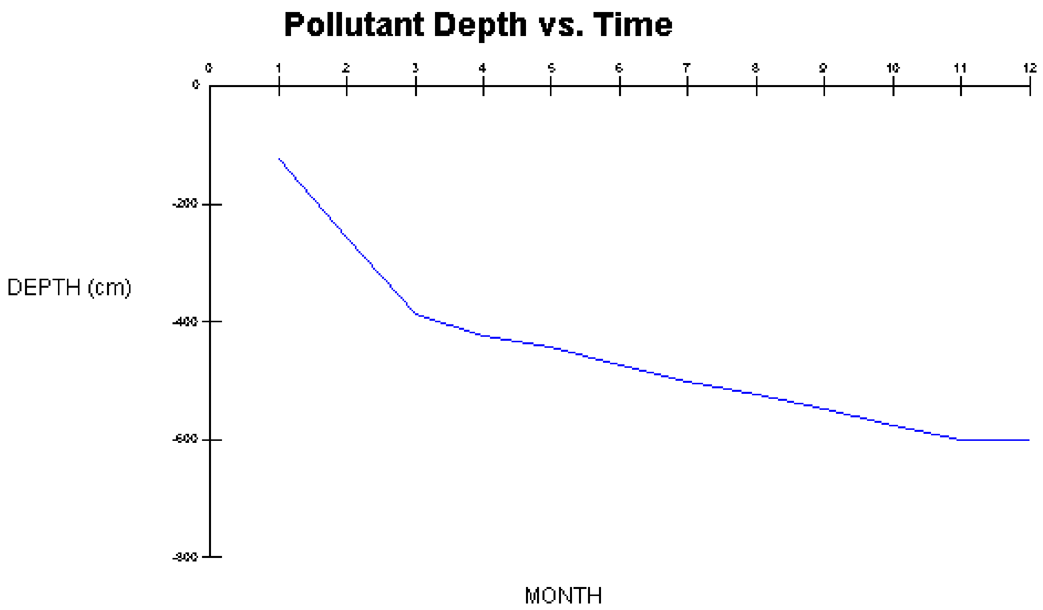




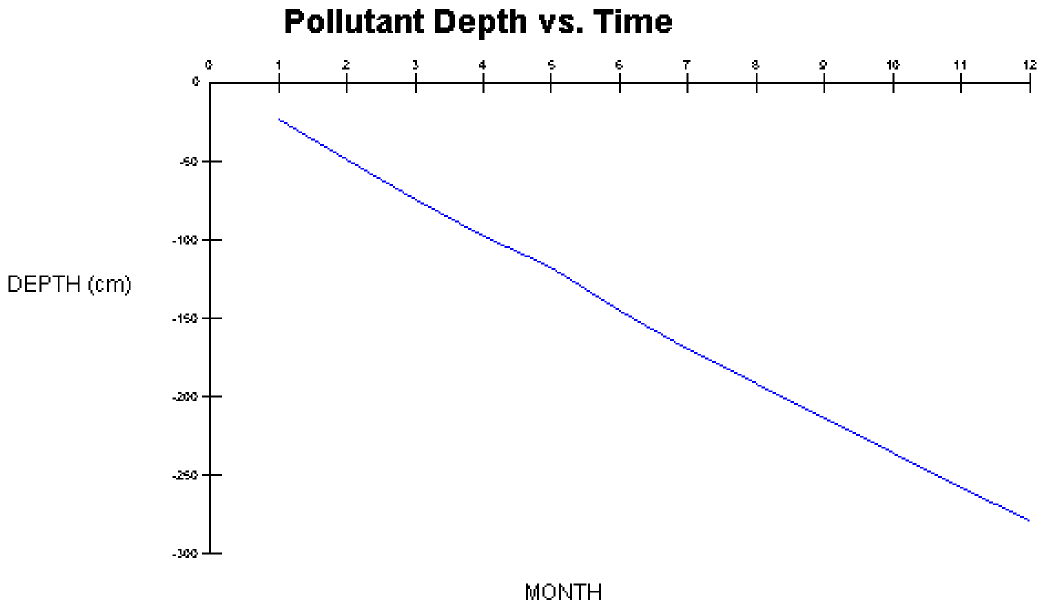
SESOIL



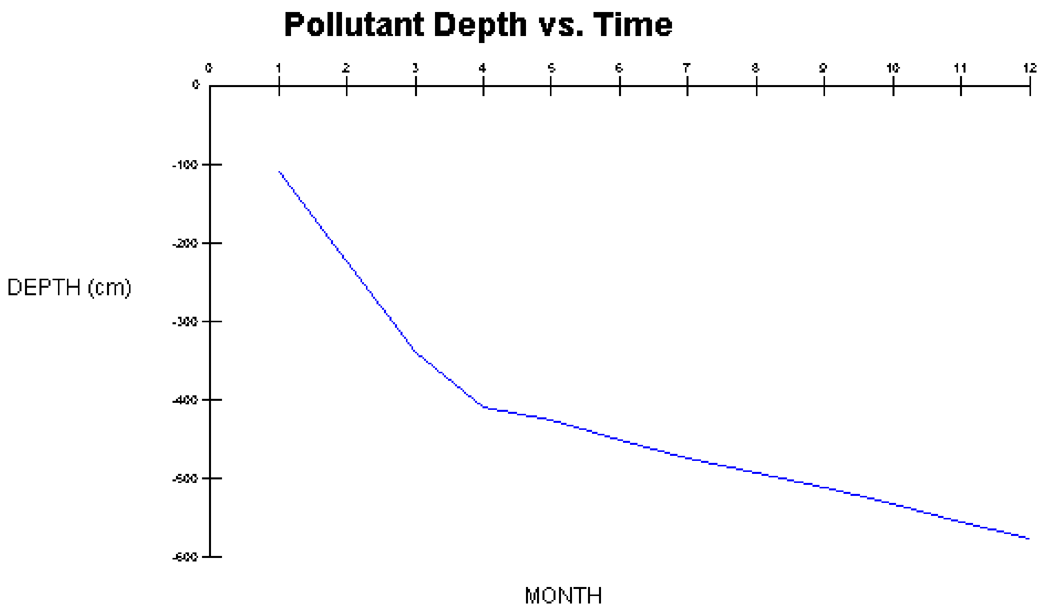
Chlorpyrifos



Dimethoate



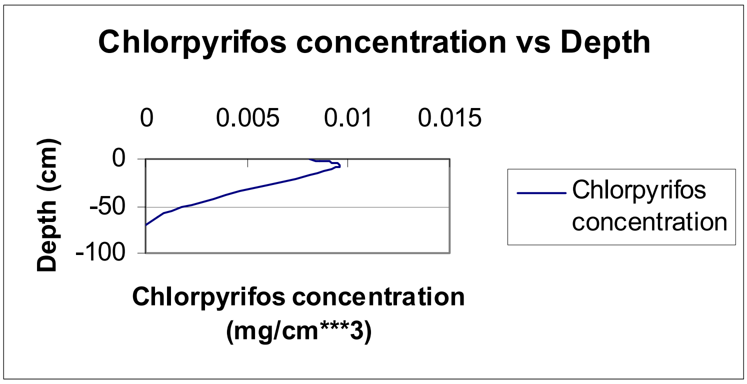
Fenamiphos

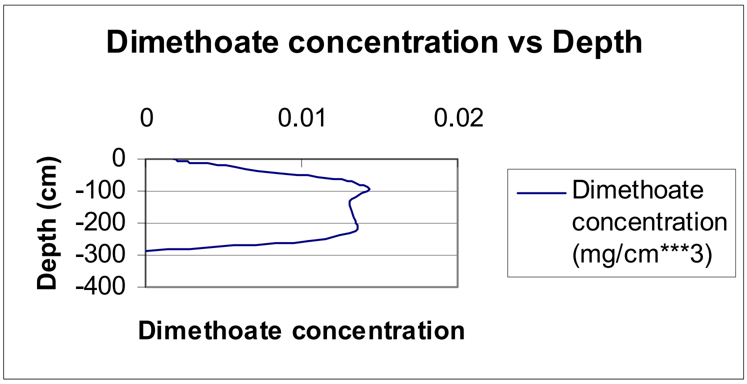

Pollutant Depth vs. Time
DEPTH (cm)
MONTH
0
1
2
3
4
5
6
7
8
9
10
11
12
0
-100
-200
-300
-400
-500
-600

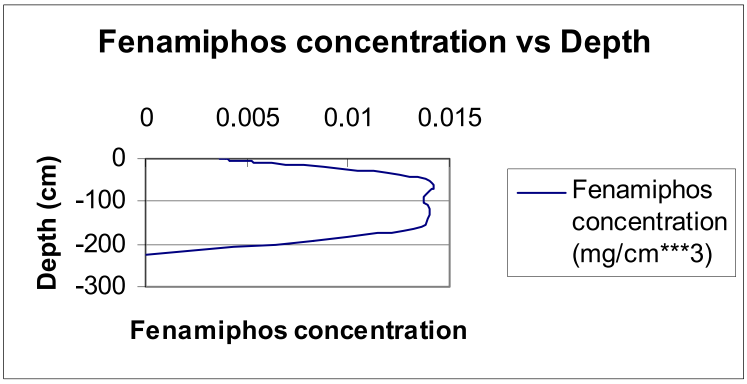
Oxamyl

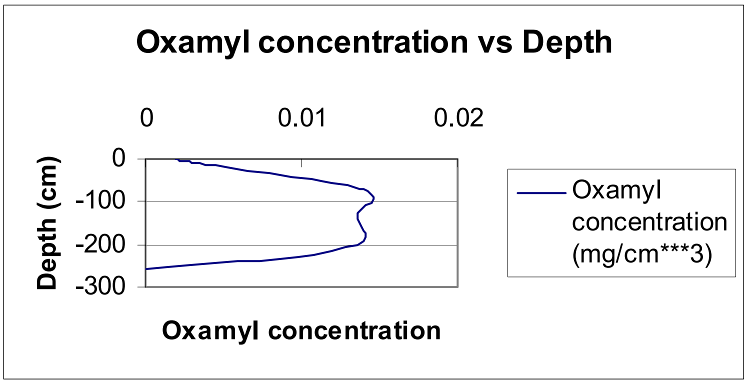
Scenario 3

SWAP

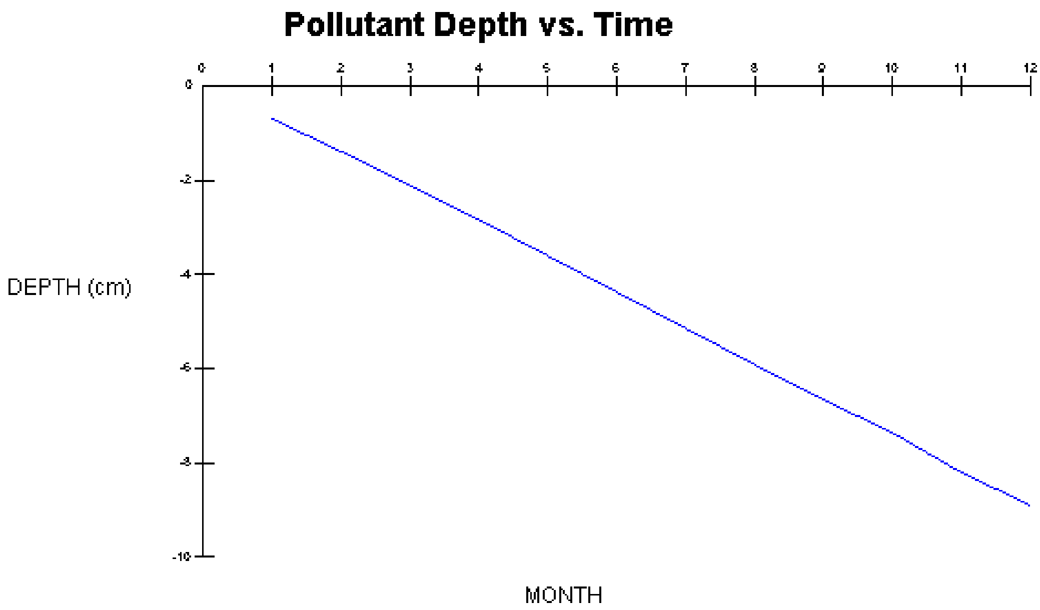




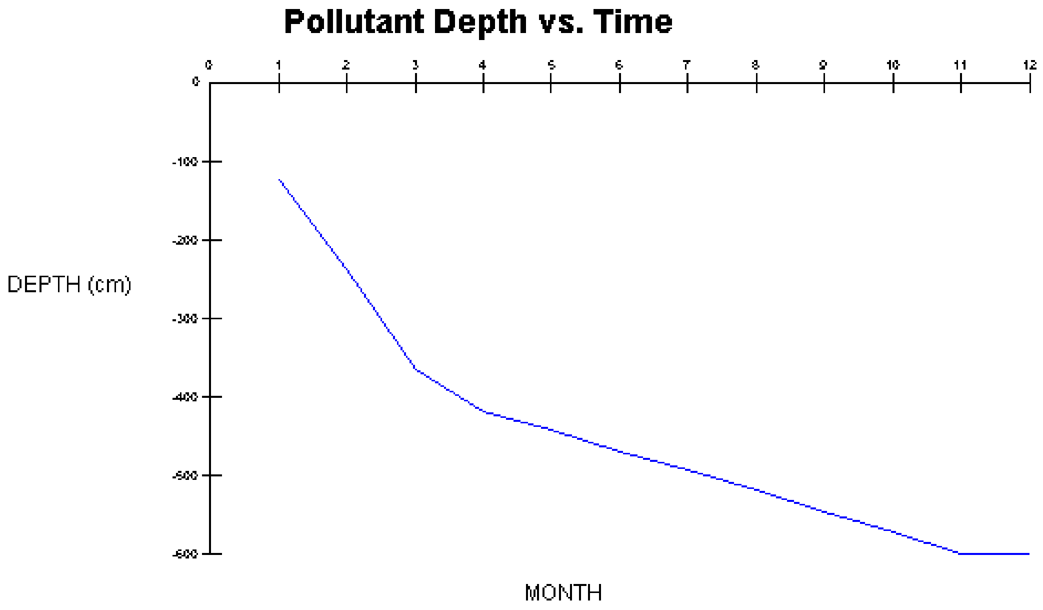




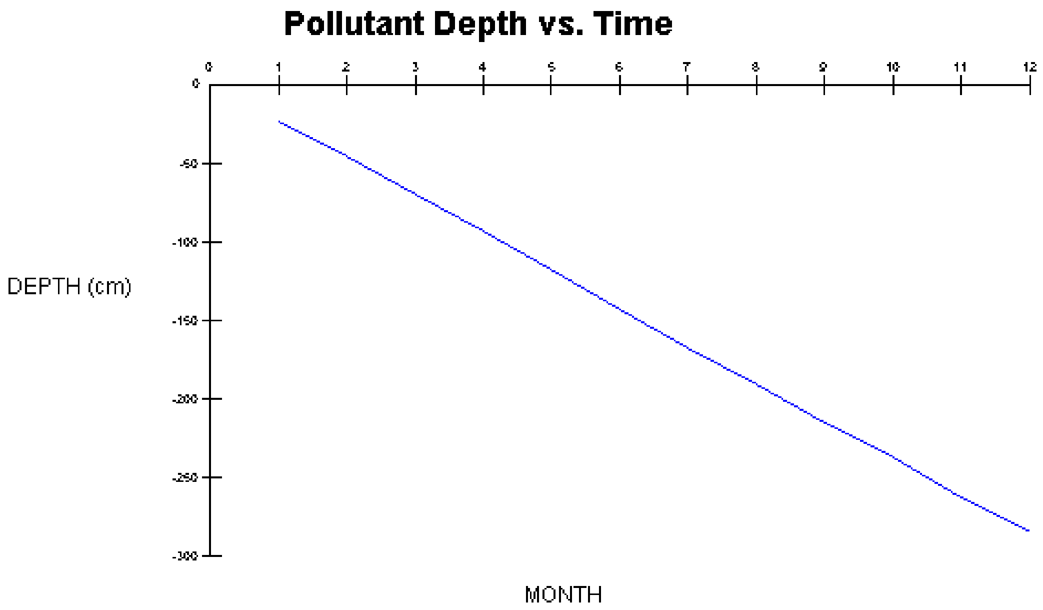
SESOIL



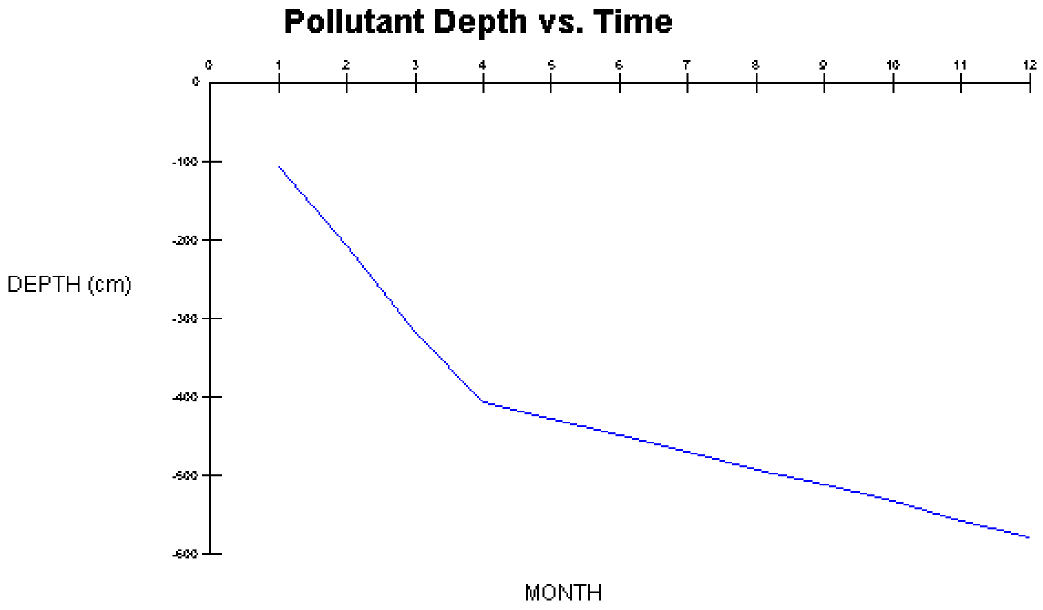
Chlorpyrifos



Dimethoate



Fenamiphos


Pollutant Depth vs. Time
DEPTH (cm)
MONTH
0
1
2
3
4
5
6
7
8
9
10
11
12
0
-100
-200
-300
-400
-500
-600

Oxamyl

Appendix F

File location

File location	File description
C:\MSc thesis\Final Thesis	Thesis
C:\MSc work 1999\subna543	Fig 1
E:\Ashfaque\Naivasha data 98\data analysis.xls	Fig 2
E:\Ashfaque\Naivasha data 98\data analysis.xls	Fig 3
E:\Ashfaque\Naivasha data 98\data analysis.xls	Fig 4
C:\MSc work 1999\GIS\waterl	Fig 8
C:\MSc work 1999\soil file\soil moisture profile.xls	Fig 16
C:\ESM\simulation results.xls	Fig 18,19,20
C:\ESM\sensitivity analysis results.xls	Fig 21
C:\MSc work 1999\Ksat1.xls \Ksat2.xls \Ksat3.xls	Table 3 Table 4 Table 5

The files from the different scenarios are presented in the following order:

List of different Simulation files

PESTAN

INPUT FILES

	Chemical Name	Soil Type
C\ESM\PESTAN\sandch\sandch.INP	Chlorpyrifos	Sandy Loam
C\ESM\PESTAN\sanddi\sanddi.INP	Dimethoate	Sandy Loam
C\ESM\PESTAN\sandfe\sandfe.INP	Fenamiphos	Sandy Loam
C\ESM\PESTAN\sandoxa\sandoxa.INP	Oxamyl	Sandy Loam

OUTPUT FILES	Results of Simulations
C\ESM\PESTAN\sandch\sandch.OUT	General output
C\ESM\PESTAN\sandch\leachbtc.dat	Pollutant Concentration versus Time array for specified depth
C\ESM\PESTAN\sandch\leachflx.dat	Pollutant Flux versus Time array for specified depth
C\ESM\PESTAN\sandch\soilcon.dat	Pollutant Concentration versus depth array for specified time
C\ESM\PESTAN\sanddi\sanddi.OUT	General output

C\ESM\PESTAN\sanddi\leachbtc.dat	Pollutant Concentration versus Time array for specified depth
C\ESM\PESTAN\sanddi\leachflx.dat	Pollutant Flux versus Time array for specified depth
C\ESM\PESTAN\sanddi\soilcon.dat	Pollutant Concentration versus depth array for specified time
C\ESM\PESTAN\sandfe\sandfe.OUT	General output
C\ESM\PESTAN\sandfe\leachbtc.dat	Pollutant Concentration versus Time array for specified depth
C\ESM\PESTAN\sandfe\leachflx.dat	Pollutant Flux versus Time array for specified depth
C\ESM\PESTAN\sandfe\soilcon.dat	Pollutant Concentration versus depth array for specified time
C\ESM\PESTAN\sandoxa\sandoxa.OUT	General output
C\ESM\PESTAN\sandoxa\leachbtc.dat	Pollutant Concentration versus Time array for specified depth
C\ESM\PESTAN\sandoxa\leachflx.dat	Pollutant Flux versus Time array for specified depth
C\ESM\PESTAN\sandoxa\soilcon.dat	Pollutant Concentration versus depth array for specified time

WAVE

	INPUT FILES	Chemical Name	File name	Description	Output files name
		Chlorpyrifos	GENDATA.IN	General Information	WAT_SUM.OUT
			CLIMDATA.IN	Climatic data	SOL_SUM.OUT
Scenario1	C:\ESM\WAVE\Mscfile\SaCh1\		WATDATA.IN	Soil Water Flow Parameters	MC.OUT
Scenario2	C:\ESM\WAVE\Mscfile\SaCh2\		SOLDATA.IN	Solute transport parameters	PH.OUT
		Dimethoate	GENDATA.IN	General Information	
			CLIMDATA.IN	Climatic data	
Scenario1	C:\ESM\WAVE\Mscfile\SaDi1\		WATDATA.IN	Soil Water Flow Parameters	
Scenario2	C:\ESM\WAVE\Mscfile\SaDi2\		SOLDATA.IN	Solute transport parameters	
		Fenamiphos	GENDATA.IN	General Information	
			CLIMDATA.IN	Climatic data	
Scenario1	C:\ESM\WAVE\Mscfile\SaFe1\		WATDATA.IN	Soil Water Flow Parameters	
Scenario2	C:\ESM\WAVE\Mscfile\SaFe2\		SOLDATA.IN	Solute transport parameters	
		Oxamyl	GENDATA.IN	General Information	
			CLIMDATA.IN	Climatic data	
Scenario1	C:\ESM\WAVE\Mscfile\SaOXa1\		WATDATA.IN	Soil Water Flow Parameters	
Scenario2	C:\ESM\WAVE\Mscfile\SaOXa2\		SOLDATA.IN	Solute transport parameters	

List of different Simulation files

SWAP

	INPUT FILES	Chemical Name	Soil Type	Key file	Bot Bound	Water Soil Properties
		Chlorpyrifos	Sandy Loam	Swap.key	Naivasha.BBC	Naivasha.SWA
Scenario1	C:\ESM\SWAP\SwapSaCh1\examples\Exercice\					
Scenario2	C:\ESM\SWAP\SwapSaCh2\examples\Exercice\					
Scenario3	C:\ESM\SWAP\SwapSaCh3\examples\Exercice\					
		Dimethoate	Sandy Loam	Swap.key	Naivasha.BBC	Naivasha.SWA
Scenario1	C:\ESM\SWAP\SwapSaDi1\examples\Exercice\					
Scenario2	C:\ESM\SWAP\SwapSaDi2\examples\Exercice\					
Scenario3	C:\ESM\SWAP\SwapSaDi3\examples\Exercice\					
		Fenamiphos	Sandy Loam	Swap.key	Naivasha.BBC	Naivasha.SWA
Scenario1	C:\ESM\SWAP\SwapSaFe1\examples\Exercice\					
Scenario2	C:\ESM\SWAP\SwapSaFe2\examples\Exercice\					
Scenario3	C:\ESM\SWAP\SwapSaFe3\examples\Exercice\					
		Oxamyl	Sandy Loam	Swap.key	Naivasha.BBC	Naivasha.SWA
Scenario1	C:\ESM\SWAP\SwapSaOxa1\examples\Exercice\					
Scenario2	C:\ESM\SWAP\SwapSaOxa2\examples\Exercice\					
Scenario3	C:\ESM\SWAP\SwapSaOxa3\examples\Exercice\					

OUTPUT FILES

	INPUT FILES	Chemical Name	Soil Type	File name
		Chlorpyrifos	Sandy Loam	Result.bal
				Result.inc
Scenario1	C:\ESM\SWAP\SwapSaCh1\examples\Exercice\			Result.wba
Scenario2	C:\ESM\SWAP\SwapSaCh2\examples\Exercice\			Result.sba

Scenario3	C:\ESM\SWAP\SwapSaCh3\examples\Exercice\			Result.vap
		Dimethoate	Sandy Loam	Result.bal
				Result.inc
Scenario1	C:\ESM\SWAP\SwapSaDi1\examples\Exercice\			Result.wba
Scenario2	C:\ESM\SWAP\SwapSaDi2\examples\Exercice\			Result.sba
Scenario3	C:\ESM\SWAP\SwapSaDi3\examples\Exercice\			Result.vap
		Fenamiphos	Sandy Loam	Result.bal
				Result.inc
Scenario1	C:\ESM\SWAP\SwapSaFe1\examples\Exercice\			Result.wba
Scenario2	C:\ESM\SWAP\SwapSaFe2\examples\Exercice\			Result.sba
Scenario3	C:\ESM\SWAP\SwapSaFe3\examples\Exercice\			Result.vap
		Oxamyl	Sandy Loam	Result.bal
				Result.inc
Scenario1	C:\ESM\SWAP\SwapSaOxa1\examples\Exercice\			Result.wba
Scenario2	C:\ESM\SWAP\SwapSaOxa2\examples\Exercice\			Result.sba
Scenario3	C:\ESM\SWAP\SwapSaOxa3\examples\Exercice\			Result.vap

List of different Simulation files

SESOIL

	INPUT FILES	Chemical Name
Scenario1	C:\ESM\Sesoil\\CSOIL3307sCh1.INP	Chlorpyrifos
Scenario2	C:\ESM\Sesoil\\CSOIL3307sCh2.INP	
Scenario3	C:\ESM\Sesoil\\CSOIL3307sCh3.INP	
Scenario1	C:\ESM\Sesoil\\CSOIL3307sDi1.INP	Dimethoate
Scenario2	C:\ESM\Sesoil\\CSOIL3307sDi2.INP	
Scenario3	C:\ESM\Sesoil\\CSOIL3307sDi3.INP	
Scenario1	C:\ESM\Sesoil\\CSOIL3307sFe1.INP	Fenamiphos
Scenario2	C:\ESM\Sesoil\\CSOIL3307sFe2.INP	
Scenario3	C:\ESM\Sesoil\\CSOIL3307sFe3.INP	
Scenario1	C:\ESM\Sesoil\\CSOIL3307sOxa1.INP	Oxamyl
Scenario2	C:\ESM\Sesoil\\CSOIL3307sOxa2.INP	
Scenario3	C:\ESM\Sesoil\\CSOIL3307sOxa3.INP	

PRZM-2

Execution file : C:\ESM\PRZM2\exec\przm2

	INPUT FILES	Chemical Name	Soil Type	General File	Meteo File
		Chlorpyrifos	Sandy Loam	przmsC.INP	
Scenario1	c:\ESM\PRZM2\MscINP\przmsC1.INP				meteo
Scenario2	c:\ESM\PRZM2\MscINP\przmsC2.INP				meteo
Scenario3	c:\ESM\PRZM2\MscINP\przmsC2.INP				wet
		Dimethoate	Sandy Loam	przmsD.INP	meteo
Scenario1	c:\ESM\PRZM2\MscINP\przmsD1				meteo
Scenario2	c:\ESM\PRZM2\MscINP\przmsD2				wet
Scenario3	c:\ESM\PRZM2\MscINP\przmsD2				
		Fenamiphos	Sandy Loam	przmsF.INP	
Scenario1	c:\ESM\PRZM2\MscINP\przmsF1				
Scenario2	c:\ESM\PRZM2\MscINP\przmsF2				
Scenario3	c:\ESM\PRZM2\MscINP\przmsF2				
		Oxamyl	Sandy Loam	przmsO.INP	
Scenario1	c:\ESM\PRZM2\MscINP\przmsO1.INP				
Scenario2	c:\ESM\PRZM2\MscINP\przmsO2.INP				
Scenario3	c:\ESM\PRZM2\MscINP\przmsO2.INP				
	OUTPUT FILES				
		Chlorpyrifos	Sandy Loam		
Scenario1	c:\ESM\PRZM2\testOUsC1\			przm.OUT	
Scenario2	c:\ESM\PRZM2\testOUsC2\				
Scenario3	c:\ESM\PRZM2\testOUsC3\				
		Dimethoate	Sandy Loam		
Scenario1	c:\ESM\PRZM2\testOUsD1\			przm.OUT	
Scenario2	c:\ESM\PRZM2\testOUsD2\				
Scenario3	c:\ESM\PRZM2\testOUsD3\				
		Fenamiphos	Sandy Loam		
Scenario1	c:\ESM\PRZM2\testOUsF1\			przm.OUT	
Scenario2	c:\ESM\PRZM2\testOUsF2\				
Scenario3	c:\ESM\PRZM2\testOUsF3\				
		Oxamyl	Sandy Loam		
Scenario1	c:\ESM\PRZM2\testOUsO1\			przm.OUT	
Scenario2	c:\ESM\PRZM2\testOUsO2\				
Scenario3	c:\ESM\PRZM2\testOUsO3\				