

SOIL WATER FLOW PROCESSES:
A CRITICAL EVALUATION USING NUMERICAL
SIMULATIONS AND LYSIMETER DATA

by

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ABSTRACT

Physically-based soil water flow models generally use approaches based on Darcy's law and Richards' equation, and, although Darcy's law is itself an empirical approximation, such models have been well proven for ideal soils. Failures of Richards' equation to describe unsaturated water movement, however, are also reported. Anomalies have been attributed to the presence of a system of large, continuous, surface-connected pores in the soil, here referred to as macropores. Also, other phenomena, such as hysteresis of the soil hydraulic properties, can cause difficulties to adequately represent water flow.

A detailed data set for water movement in the unsaturated zone is available from Imperial College's experimental station at Silwood Park, where field lysimeters containing a sandy loam soil are being used to monitor the processes affecting radionuclide transport from a contaminated water table through the unsaturated zone and into a wheat crop. The main goal of this thesis is to study the data from this experimental facility, selecting relevant events and trying to understand and explain the physical phenomena involved, mainly those related to the problems of preferential pathways in soils. Mathematical modelling is applied to test the hypotheses proposed and to examine the weaknesses related to the use of Richards' equation, in order to identify its limitations and to develop ways to overcome them. Results from a dual porosity model are compared with the traditional single porosity approach and also with a model incorporating hysteresis in the relationship between moisture content and matric potential.

The data from the experimental station and the results of the simulations provided evidence of rapid, or preferential, flow mechanisms occurring in the lysimeters. The single porosity model showed weaknesses when trying to reproduce observed rapid flow events. This representation was improved by hysteretic simulations, but it was not possible to determine a unique set of parameters for all selected events. The results obtained by the application of a dual porosity model strongly suggest that tensiometer data can be represented by a combination of macro- and micropore effects. A physical interpretation of these results provides a theoretical basis for the future development of a model combining inputs from both macro- and micropores, which can allow a better understanding of soil water potential measurements.

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ERRATA

Page	Line and Paragraph	Corrected version	Instead of
29	2 nd line of penultimate paragraph	and, consequently, can be measured	and, consequently, can measured
39	8 th line of third paragraph	more than ten years old,	more then ten years old,
56	1 st line of first paragraph	the use of spectral analysis	the use spectral analysis
60	11 th line of second paragraph	period of 162 days in Tunisia	period of 162 in Tunisia
71	2 nd line of second paragraph	(3) constant pressure head	(3) constat pressure head
95	2 nd line of last paragraph	whether	wether
98	penultimate line of second paragraph	as an evidence of	as a evidence of
103	2 nd line of penultimate paragraph	did not intercept any macropore flow	did not intercept any macropore
103	6 th line of penultimate paragraph	while the other tensiometers reproduce	while the other tensiometer reproduce
143	16 th line of last paragraph	TDR estimates	TDR estimatives
165	7 th line of second paragraph	which is a good indication	which is a good indicative
192	last line of last paragraph	responses were obtained	responses were obtaining
233	1 st line of last paragraph	in such a model	in such model

CHAPTER 1 - INTRODUCTION

1.1 - Soil water flow processes: their importance and complexity

Soil and water resources are vital for mankind. These are the two fundamental resources of our agriculture, as well as of our natural environment. Phenomena of water movement and storage in the soil are of particular significance in relation to the hydrologic cycle, plant growth, crop production, and the movement of chemicals in the environment. In addition, these processes greatly influence overland flow, soil erosion and groundwater recharge. According to Hillel (1980) the necessity to manage soil and water resources efficiently on a sustained basis is one of the most vital tasks of our age.

The growing concern over the fate of chemicals released in the environment has resulted in an increasing interest in the role that water plays in the movement of solutes towards groundwater reserves and hence the water supply, or towards plant roots and, as a result, into the food chain. Water processes are the major influence behind the movement of solutes, while they are themselves, in general, not influenced by the solutes. These two facts imply that the modelling of solute movement has to be preceded by successful modelling of the hydrological processes taking place in the soil-plant system (Karavokyris, 1990).

Soil water flow involves complex processes, being controlled by many different factors: soil characteristics, agricultural practices, weather, etc. The solid phase frequently interacts with the water and air which permeate soil pores, and the whole system is seldom in a state of equilibrium. Besides that, soil hydraulic properties present enormous spatial variability. Consequently, to characterise the geometric and hydraulic features of the porous medium and, hence, to provide values for parameters of the models is a highly complicated task. The combinations of all these variables are numerous and intricate, bringing difficulties to the understanding, measurement, estimation and representation of their values. Mathematical modelling can be used to isolate the complex physical, chemical and biological phenomena entailed, in order to study them as simpler sub-systems and later rejoin them. In this way, several and diverse scenarios can be simulated.

Several models of soil water flow have been developed, using different approaches and different solution techniques. Any model, however complex, is always a simplification, an idealisation of reality and it has to be applied under the conditions and limitations for which it was developed. The results of a simulation have to be carefully analyzed, demanding good

knowledge of both the natural phenomena and the modelling concepts.

Some important soil water processes are related to the existence of preferential pathways, through which the water can bypass several layers of the soil. There is plenty of experimental evidence that preferential flow is common in field soils, so that water bypasses a portion of the soil matrix, going deeper and faster than it would take to seep through the soil matrix, and solutes travel from the surface to groundwater in shorter times than expected. The great majority of the experimental and theoretical works on preferential pathways deals with macropore flow, which includes water movement along desiccation cracks, animal burrows, root channels and similar soil voids that are surrounded by partially saturated soil matrix. Modelling water flow in macropores is a difficult task, entailing not only the representation of the flow processes inside the macropores, but also the problem of initiation of flow in the macropores and the interaction between the macropores and the soil matrix. A further complication is provided by the fact that macropores are very dynamic structures, being affected by the weather, by long-term ecological changes and by land use.

The models available for simulating preferential water flow help to understand some of the physical processes involved. However, the lack of experimental data on the nature of macropore flows, the structure of macropore systems and the interactions between the macropores and the matrix brings difficulties to define, calibrate and validate an adequate representation of a combined macropore/matrix system. There is the need to improve the quantification and understanding of macropore effects as well as their model representation in order to be able to better comprehend and represent water flow in unsaturated soils.

1.2 - Main objective and overview of the Thesis

A detailed data set for soil water movement in the unsaturated zone is available from Imperial College's experimental station at Silwood Park, where field lysimeters containing a sandy loam soil are being used to monitor the processes affecting radionuclide transport from a contaminated water table through the unsaturated zone and into a wheat crop. The main objective of this thesis is to perform a critical evaluation of the soil water flow processes in these lysimeters, with particular emphasis on preferential flow. This evaluation is obtained by a detailed study of the available data, that include continuously-monitored soil water states and fluxes, and also by performing numerical simulations of selected events using different competing theories. Specifically:

i) three representative models were selected in order to compare alternative modelling approaches and to get a better understanding of the processes responsible for water flow in the unsaturated zone: a physically-based, one dimensional model of saturated-unsaturated flow, SPW1 (Karavokyris et al., 1990); a dual porosity model, MACRO (Jarvis, 1991 and 1994); and a model of hysteresis considering air entrapment based on those presented by Kool and Parker (1987) and by Parker and Lenhard (1987);

ii) relevant events were identified in order to analyze the available data, assessing the performance of different modelling approaches and testing hypotheses to describe the physical processes governing the flux of water in the near surface environment: a set of 8 events where the evidence of rapid flow was significant and a set of 4 events where no evidence of preferential water flow can be assumed;

iii) soil hydraulic property values were estimated by the combined use of data from physical analysis of soil cores and by the adjustment of soil characteristic parametric relationships, through optimisation of objective functions applied to the available soil moisture characteristics and saturated conductivity data;

iv) the three models were applied in a comprehensive evaluation;

v) and the theoretical basis for a methodology that combines macro- and micropore effects in order to represent soil water potential measurements was introduced.

1.3 - Structure of the Thesis

In Chapter 2 a literature review is presented, synthesising the basic theories associated with water movement in unsaturated soils. Only the main concepts of major relevance to the understanding of the theories and models later adopted in this thesis are included.

Chapter 3 describes the models selected to be used in this thesis. It is composed of three main sections: models of unsaturated soil water flow, presenting the SPW1 model; models of preferential water flow, describing the MACRO model; and models of hysteresis, introducing the selected hysteresis model and the algorithm developed to estimate initial conditions in order to run this model in conjunction with SPW1. In each of these sections, a literature review precedes the description of the selected models, introducing and commenting on the most important approaches available to model the respective phenomena. The selected hysteresis

model and also the methodologies adopted by MACRO model to represent, in one flow domain, the soil water retention curve and the unsaturated hydraulic conductivity were included in a new version of SPW1 model, called SPW1hyst.

Chapter 4 introduces a description of the experimental facility and the available data. A description of the lysimeter equipment is presented, with special emphasis to the instrumentation related to soil moisture data. The identification and selection of events for posterior analysis and simulations is also included in this chapter.

Chapter 5 deals with the determination of soil properties for the lysimeters located at Imperial College's Field Research Station in Silwood Park. Values for the physical properties of the lysimeter soil were provided by physical analysis of soil cores. Estimates of parameter values and associated uncertainty of three different soil characteristic parametric relationships were obtained through the use of first-order error analysis applied to the available matric potential and soil moisture data.

Chapter 6 introduces the results of the SPW1hyst simulations applied to the events selected and described in chapter 4. This model was employed in order to test the strengths and limitations of traditional models of water flow in the unsaturated zone, based on Richards' equation. It was also applied to estimate the effects of hysteresis, and to assess the effect of vertical heterogeneity of saturated conductivity of the soil in the lysimeters.

Chapter 7 shows the results of MACRO model. The model was employed in both single and dual porosity modes, in order to assess the importance of macroporous flow. The effects of vertical heterogeneity in the saturated conductivity values were also investigated.

And finally, Chapter 8 summarises the main results and the most important conclusions obtained in this study, and presents suggestions for future work.

CHAPTER 2 - THE HYDROLOGY OF THE UNSATURATED ZONE

2.1 - Introduction

The majority of the processes involving soil water interactions in the field occur while the soil is in an unsaturated condition. For this reason, many aspects of hydrology are closely related to the behaviour of the unsaturated zone, such as infiltration, evaporation, groundwater recharge, soil moisture storage and soil erosion. Besides that, the liquid in the unsaturated zone is actually a solution of water and dissolved solid and gaseous constituents, so that soil water properties are intimately linked to the chemical and physical properties of the soil phase. The vadose zone represents the main conduit through which these liquid and gaseous constituents are attenuated and transformed as they move in both directions between the soil surface and the water table. The processes involved are in general complicated and difficult to describe quantitatively, usually including changes in the state and content of water, and involving complex relations among the variable soil wetness, suction and conductivity (Hillel, 1980; Nielsen et al., 1986).

All these processes are further complicated by the existence of preferential pathways, through which the water can bypass several layers of the soil. In this way, it may not only go deeper in a much shorter time than it would take to seep through the soil matrix, but it can also carry contaminants which would be expected to react with the surrounding soil, but, instead reach deep layers with almost unaltered concentrations.

Unsaturated flow has become one of the most important and active topics of research in soil physics in the last two decades, due both to its importance and complexity. Although significant theoretical and practical advances had been reached, the unsaturated zone remains a challenge to scientific understanding and technological management. According to Nielsen et al. (1986), the main problem in the investigations performed so far is that professionals with different backgrounds, such as biologists, groundwater hydrologists, geochemists and others, tend to concentrate on specific points of study, providing a segmented, disciplinary research. This situation is now changing as, in recent years, some researchers are starting to study the unsaturated zone in the context of a unified approach, that tries to include all pertinent physical, chemical and biological processes operative in the unsaturated zone.

The main objective of this chapter is to synthesise the basic theories associated with water movement in unsaturated soils. The main concepts regulating the water flow in saturated

and unsaturated soils are presented, including preferential flow, evaporation and water extraction by plant roots. We do not intend to present an exhaustive and complete description of all processes and concepts, as this is readily available in many textbooks (Childs, 1969; Hillel, 1980; Ward and Robinson, 1990). Important subjects, such as water transport in the plants, are not included in this review, as we aim to introduce only the main concepts of major relevance to the understanding of the theories and models later adopted in this thesis.

2.2 - Basic theory of soil water flow

Soil water flow is caused by a driving force resulting from a potential gradient. The soil water potential represents the work required to overcome the forces acting on the soil water in moving from a given datum to the point of interest, and the total potential is the sum of the gravitational, pressure and osmotic potential. Flow takes place in the direction of decreasing potential, and the rate of flow (flux) is proportional to the potential gradient. These principles apply in unsaturated, as well as saturated, soils.

The total water potential can be written as (Hillel, 1980; Ward and Robinson, 1990; Rawls et al., 1993):

$$\phi = \phi_g + \phi_p + \phi_o \quad (2.1)$$

where: ϕ = total soil water potential;

ϕ_g = gravitational potential;

ϕ_p = pressure potential;

ϕ_o = osmotic potential;

Potentials can be expressed on a mass, volume or weight basis. In hydrological studies, the use of potential on a weight basis is preferred. The potential then has the dimension of length and is referred to as "head" h , having the meaning of energy per unit weight. The pressure head of water is positive under a free-water surface (i.e., a water table) and negative above it. A negative hydraulic head signifies a pressure smaller than atmospheric, and it occurs whenever the soil becomes unsaturated.

The gravitational forces act in the direction of draining the water, causing a positive pressure. The main forces responsible for holding the water in the soil and, consequently,

causing negative tensions (suctions) are those of capillarity, adsorption and osmosis. Capillary forces result from surface tension at the interface between the soil air and soil water; adsorption is mainly caused by electrostatic forces in which the polar water molecules are attached to the charged faces of the solids; and osmotic pressure is due to the presence of solutes in the soil water, coming into play when there is a difference in solute concentration across a permeable membrane, as at a plant root surface (Ward and Robinson, 1990).

2.2.1 - Saturated flow and the Darcy's law

The actual geometry and flow pattern of water in the soil is too complicated to be described in microscopic detail. For this reason, flow through complex porous media is generally described in terms of a macroscopic flow velocity vector, which is the overall average of the microscopic velocities over the total volume of the soil (Hillel, 1980). The equation most commonly used to describe the flow of water in a saturated soil, Darcy's law, is based on this principle.

Darcy's law was derived in 1856 (Bear, 1972) as an analogy of laminar flow in pipes, empirically based on experiments on flow through saturated sand beds, by assuming that water moves proportionally to the forces acting on it. Considering multidimensional flow under anisotropic and nonuniform conditions, Darcy's law can be written as:

$$\vec{v} = -K \nabla \phi \quad (2.2)$$

where: $\vec{v}$ = flux vector;

K = hydraulic conductivity;

$\nabla \phi$ = gradient of soil water potential.

This law indicates that the flow of a liquid through a porous medium is proportional to the hydraulic gradient, which is the driving force acting on the liquid, and also proportional to the hydraulic conductivity, which is a property of the conducting medium. The hydraulic conductivity is relatively constant for a specific saturated soil. The negative sign in equation 2.2 indicates that water flows in the direction of a decreasing hydraulic potential.

According to Nielsen et al (1986), experimental evidence indicates that the equation may not

be valid for fine-textured soils at low flow rates, with some suggestion that a threshold potential gradient exists below which no flow occurs. Darcy's law is also thought to be invalid at high flow rates when flow ceases to be laminar (Childs, 1969; Bear, 1972).

It is important to note that Darcy's law does not attempt to describe the actual flow of water at any particular point in the soil. It is a macroscopic description of the flux of water through the soil and holds as a consequence of the overall effect of the microscopic behaviour of water (Karavokyris et al., 1990).

2.2.2 - Unsaturated flow and the Richards' equation

The moving forces in a saturated soil are the gradient of a positive pressure potential and the influence of gravity. In an unsaturated soil, the phenomena of adsorption and surface tension produce a subatmosphere pressure, or suction, known as matric suction, which is equivalent to a negative pressure potential. The gradient of this potential also constitutes a moving force, so that unsaturated flow is mainly controlled by a negative pressure distribution and the gravitational force (there is also the influence of osmosis, but it is generally neglected, in the presence of the other potentials, as it is only significant in the proximity of a semi-permeable membrane).

According to Hillel (1980), the most important difference between saturated and unsaturated flow is, perhaps, in the hydraulic conductivity. When the soil is saturated, all the pores are filled and conducting, so that continuity and conductivity are maximal. When the soil desaturates, some of the pores become air filled and the conductive portion of soil's cross sectional area decreases correspondingly. As suction develops, the first pores to empty are the largest ones, which are the most conductive, thus leaving water to flow only in the smaller pores. The empty pores must be circumvented, so that, with desaturation, tortuosity increases. In coarse-textured soils, water sometimes remains almost entirely in capillary wedges at the contact points of the particles, forming separate and discontinuous pockets of water. In aggregated soils, too, the large interaggregate spaces which confer high conductivity at saturation become (when empty) barriers to liquid flow from one aggregate to its neighbours. For these reasons, the transition from saturation to unsaturation generally entails a steep drop in hydraulic conductivity, which may decrease by several orders of magnitude.

According to Fredlund and Rahardjo (1993), Darcy's law also applies for the flow of water through an unsaturated soil, but the hydraulic conductivity cannot be assumed to be

constant. It has to be regarded as a variable which is predominantly a function of the water content or the matric suction of the unsaturated soil. This is basically the principle of Richards' equation.

The name of Richards is synonymous with the foundation of modern soil physics (Pullan, 1990). It was Richards who defined the total potential which was originally proposed for saturated porous media and, by physical reasoning, also obtained a generalised law describing unsaturated soil water flow. Richards applied the principle of conservation of mass to Darcy's law to obtain the partial differential equation of unsaturated flow. This equation is now recognised as the fundamental equation governing the flow of water in a partially saturated non-swelling porous medium and is consequently referred to as Richards' equation (Feddes et al., 1988; Pullan, 1990).

Richards extended Darcy's law for the flow of water through an isotropic saturated porous media, allowing its use for unsaturated flow, by admitting that the hydraulic conductivity was a function of moisture content of the medium. So, Darcy's law (equation 2.2) became, for unsaturated flow:

$$\vec{v} = -K(\theta) \nabla \phi \quad (2.3)$$

where θ is the moisture content.

The total potential ϕ is defined here relative to the reference state of water at atmospheric pressure and datum elevation $z = 0$. Here, z is the vertical space coordinate, taken positive downward. The energy state of the water is commonly expressed by the moisture potential ψ . Using the standard assumptions for unsaturated media we have

$$\phi(\theta) = \psi(\theta) - z \quad (2.4)$$

Continuity of mass, assuming incompressibility, results in

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot \vec{v} \quad (2.5)$$

which, combined to the differential soil water capacity, $C(\psi)=d\theta/d\psi$, and to equations 2.3 and 2.4, yields the Richards' equation:

$$C(\psi) \frac{\partial \psi}{\partial t} = \nabla \cdot (K \nabla \psi) - \frac{\partial K}{\partial z} \quad (2.6)$$

This equation holds quite generally in the sense that it describes the behaviour of saturated and unsaturated zones, it applies to both homogeneous and heterogeneous soils, and it does not depend on any requirement that relations between K , ψ and θ be single valued. The use of ψ instead of θ as the dependent variable has the advantage of being applicable in layered soils, where ψ remains continuous at the boundaries between layers (Vauclin et al., 1979; Feddes et al., 1988). If, however, K and ψ are single-valued functions of θ , it is often convenient to introduce the hydraulic diffusivity $D(\theta)$, defined by

$$D(\theta) = K(\theta) \frac{dK}{d\theta} \quad (2.7)$$

and rewrite equation 2.6 as

$$\frac{\partial \theta}{\partial t} = \nabla \cdot (D \nabla \theta) - \frac{dK}{d\theta} \frac{\partial \theta}{\partial z} \quad (2.8)$$

A major drawback of the formulation presented in equation 2.8 is that it can not be applied under saturated conditions, where all points are defined by $\theta=\theta_s$, θ_s being the saturated water content (Vauclin et al., 1979).

Richards' equation describes the soil water movement when subject to initial conditions in the soil profile, the input of water at the soil surface, and the conditions at the bottom of the soil profile. Initial conditions must be defined when transient soil water flow is modelled. In general, for one-dimensional representations, the initial conditions can be expressed as a profile of matric potential head varying with depth. When this data is not available, water content at

field capacity (defined as the amount of water remaining in the soil after the downward movement under gravity has largely ceased) or those in equilibrium with the groundwater table can be adopted. The boundary condition at the soil surface depends on the rate of water application: for intensities less than or equal to the saturated hydraulic conductivity, all the water infiltrates into the soil; for higher intensities, the water infiltrates into the soil until its surface becomes saturated, when the runoff begins. At the lower boundary, three different types of conditions can be defined: Dirilecht condition, when the pressure head is specified; Neumann condition, when the flux is specified; and Cauchy condition, when the flux is a function of a dependent variable. A special case of the Neumann condition is when unit gradient pressure differential is specified at the lower boundary, which is equivalent to free drainage case, so that the Darcian flux is equal to the hydraulic conductivity (Feddes et al., 1988; Rawls et al., 1993).

There are some simple analytical techniques that facilitate the application of the unsaturated flow equation to particular problems. One example is to employ the Boltzmann transformation to convert the diffusivity equation from its original form as a partial differential equation with two independent variables (space, x , and time, t) to the form of an ordinary differential equation, when gravity can be neglected and flow is monotonic. This technique is used to obtain solutions for soil water flow problems that involve horizontal, semi-infinite, homogeneous media of uniform initial wetness (Hillel, 1980). This and other analytical techniques, as pointed out by Nielsen et al. (1986), are only applicable to highly simplified systems and are not well suited for field applications. Consequently, numerical solutions are often employed. It is important to emphasise that the functions $K(\theta)$, $\psi(\theta)$ and $D(\theta)$ are highly nonlinear, and these nonlinearities cannot be ignored, so that, whatever the algorithm chosen to solve Richards' equation, it has to be able to cope with its nonlinearity.

2.2.3 - Moisture characteristic and hydraulic conductivity curves

The moisture characteristic curve, also known as the water retention characteristic, or capillary pressure-saturation curve, describes the soil's ability to store and release water. It is defined as the relationship between the soil water content and the matric potential. The hydraulic conductivity is a measure of the ability of the soil to transmit water and depends upon both the properties of the soil and the fluid. It is called saturated hydraulic conductivity for water contents at or above the saturation point ($\psi \geq 0$), and it is referred to as the unsaturated hydraulic conductivity for water contents below saturation ($\psi < 0$) (Rawls et al., 1993).

As commented in section 2.2.2, both the moisture characteristic curve, $\psi(\theta)$, and the

hydraulic conductivity as a function of volumetric soil water content, $K(\theta)$, are non-linear functions. Also, both vary with soil properties such as texture, porosity and bulk density.

Numerous attempts have been made to formulate mathematical relations capable of describing these curves. The two most popular models for the moisture characteristic curve are those proposed by Brooks and Corey (1964, 1966) and Van Genuchten (1980). According to Fayer and Simmons (1995), the main reasons for the dominance of these equations in current model applications is that they are simple, have a minimum number of parameters that allow for easy description, can be readily combined with conductivity models and easily fit water retention data in the wet region, where most flow occurs.

The Brooks-Corey equation can be written as

$$\begin{aligned} Se &= \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left(\frac{P_b}{\psi} \right)^\lambda & \text{if } \psi < P_b \\ Se &= 1 & \text{if } \psi \geq P_b \end{aligned} \quad (2.9)$$

where: Se = effective saturation;

θ = volumetric water content;

θ_r = residual volumetric water content, considered to be confined to small pores which do not form a continuous network;

θ_s = saturated volumetric water content, or maximum wetness;

ψ = matric potential;

P_b = air-entry pressure, or bubbling pressure: approximately the minimum suction in the drainage cycle at which a continuous nonwetting phase (air) exists in a porous medium;

λ = pore size distribution index.

The parameters θ_r , θ_s , P_b and λ have to be determined from available data. The saturated volumetric water content, θ_s , can be related to the porosity of the soil and, consequently, can be measured in laboratory, but the other three parameters have to be fitted to the data.

A major problem of the Brooks-Corey model is that it presents a discontinuity on its first derivative, at the air-entry pressure. This discontinuity can cause numerical instabilities during simulations of water movement in the soil using a numerical model, depending on the robustness

of the algorithm used to solve Richards' equation. Besides that, Milly (1987) found that the presence of the air-entry pressure is a source of discrepancies with field measured characteristics, and Michiels et al. (1989) state that the presence of a well-defined air-entry pressure is not always obvious in all soils.

The Van Genuchten equation is described by

$$Se = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[\frac{1}{1 + (\alpha|\psi|)^n} \right]^{(1-1/n)} \quad \text{if } \psi < 0 \quad (2.10)$$

$$Se = 1 \quad \text{if } \psi \geq 0$$

where: α = scaling parameter;
 n = curvature parameter.

As for the Brooks-Corey equation, the saturated volumetric water content, θ_s , can be measured in laboratory, but the other three parameters (θ_r , α and n) have to be fitted to the data. It has continuous derivatives for the whole of the water retention curve, avoiding the problems of numerical instabilities and discrepancies with measured data commented for Brooks-Corey equation.

Recently, new models were developed trying to get better representations for the soil water characteristic. Rossi and Nimmo (1994) proposed two models with continuous functions and continuous derivatives to represent the retention curve over the whole range of saturation, based on a power law function (analogous to Brooks-Corey equation) supplemented with a logarithmic function relating water content to suction in the high suction range. Kusogi (1994) presented a model which contains three parameters other than the saturated water content, θ_s , and the residual water content, θ_r , by applying a log-normal distribution to the pore radius distribution function, $f(r)=d\theta/dr$. Fayer and Simmons (1995) introduced a modification into Brooks-Corey and Van Genuchten equations in order to get better results in the dry range, by replacing the residual water content with an adsorption equation. Although all these equations seem to perform well, more applications are still necessary to address their applicability to real problems.

Various models were also developed to represent the hydraulic conductivity of

unsaturated soils. Alexander and Skaggs (1986) examined fourteen different methods to predict the unsaturated hydraulic conductivity from the soil water characteristics. Only the most important equations necessary to explain concepts and models presented in following sections are described next.

Burdine (1953) introduced a parallel tube model, by integrating the conductivity of water filled pores within each size interval over all pores present in the soil. According to Alexander and Skaggs (1986), this model forms the basis for many of the present methods for calculating K . It is expressed as:

$$K_r(S) = \frac{K}{K_s} = S e^2 \left[\left(\int_0^S dS/\psi^2 \right) / \left(\int_0^1 dS/\psi^2 \right) \right] \quad (2.11)$$

where: K_r = relative hydraulic conductivity;

K_s = saturated hydraulic conductivity;

S = saturation, the ratio of the volume of wetting fluid to the volume of interconnected pore space in a bulk element of the medium.

Brooks and Corey (1964) substituted their expression for the effective saturation (equation 2.9) into Burdine's equation to obtain

$$K_r = \left(\frac{P_b}{\psi} \right)^\eta; \quad \eta = 2 + 3\lambda \quad (2.12)$$

By putting the residual soil water content (θ_r) equal to zero, Campbell (1974) expressed the hydraulic conductivity as in equation 2.12, with $\eta = 2 + 2/b$ and $b = 1/\lambda$.

Mualem (1976a) introduced a modified form of Burdine's equation, including the effects of connecting pores, and obtained

$$K_r(S) = S e^\eta \left[\left(\int_0^S dS/\psi^2 \right) / \left(\int_0^1 dS/\psi^2 \right) \right]^2 \quad (2.13)$$

where n_m may be positive or negative. Analysing data for 45 different soils, he suggested the adoption of $n_m = 0.5$. Using Brooks-Corey's characteristic curve, he obtained an expression for the hydraulic conductivity of the type of equation 2.12, with $\eta = 2 + \lambda(2 + n_m)$.

Van Genuchten (1980) applied the Mualem integral form for the hydraulic conductivity (equation 2.13) to his characteristic curve (equation 2.10) to express the conductivity as

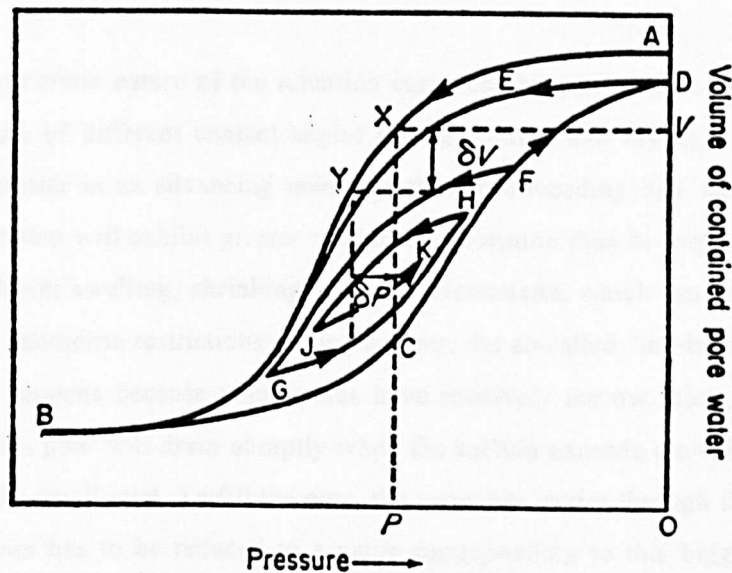
$$K_r = \frac{\{1 - (\alpha|\psi|)^{(n-1)} [1 + (\alpha|\psi|)^n]\}^2}{[1 + (\alpha|\psi|)^n]^{m/2}}; \quad m = 1 - 1/n \quad (2.14)$$

A great problem for all these equations is to determine the value of their parameters. One approach is to fit the equations to measured $K(\theta)$ or $\psi(\theta)$ data, by use of an optimisation algorithm. However, this data is not always available for a given soil, and can be quite expensive to measure. As soil textural data are more often available than $\psi(\theta)$ data, and more easily obtained than either $K(\theta)$ or $\psi(\theta)$ data, several authors have been trying to relate the moisture characteristic curve and the hydraulic conductivity to some of these soil properties. Some of the works (Arya and Paris, 1981; Rawls and Brakensiek, 1982; Haverkamp and Parlange, 1986; Saxton et al., 1986) use regression analysis to empirically fit the moisture characteristic or the hydraulic conductivity to soil textural data. Other researches (Rawls and Brakensiek, 1985; Alexander and Skaggs, 1987; Vereecken et al., 1989; Vereecken et al., 1990; Nachabe and Illangasekare, 1994) try to determine the parameters of some of the equations presented in the literature (specially for Campbell, Brooks-Corey and Van Genuchten equations) using easily measured soil properties. However, according to Ragab and Cooper (1993), predictions using these models are not always reliable, as many of them were obtained from regression analysis of data from soils of a limited region.

2.2.4 - Hysteresis and air entrapment

A function is said to exhibit hysteresis when the variation on the dependent variable is not only due to the present value of independent variables, but also to the previous state of them, so that the relationship is not unique. It has been observed that the wetting and drying curves of a soil differ: if a soil has its moisture content reduced according to a drying curve and the trend is reversed, the curve for the wetting soil will not follow the same path of the drying curve. This irreversibility in the relationship is called hysteresis. The hysteresis in the hydraulic conductivity curve, $K(\theta)$, is often small compared with that of the moisture characteristic, $\psi(\theta)$.

Typical moisture characteristic curves of a soil, as presented in figure 2.1, also show that the soil undergoing successive cycles of wetting and drying exhibits secondary and further order hysteretic loops. This nonuniqueness of the moisture characteristic causes considerable difficulty in modelling soil water movement, and, consequently hysteresis has been neglected in many numerical models (Childs, 1969; Nielsen et al., 1986; Rawls et al., 1993).



***AB*, drying from saturation**

BCD, rewetting with air entrapment

***FGHJK*, internal branches due to successive reversals**

Figure 2.1 - Typical moisture characteristics of a soil (after Childs, 1969)

According to Childs (1969), it is common that the first hysteresis cycle, starting from saturation, is not a closed one, because of air entrapment. Curve AB in figure 2.1 corresponds to the first withdrawal of water. When re-wetting from the minimum tension, point B, the air in some of the large pores will become isolated bubbles, as the smaller pores which surround them will fill first at relatively high suctions. If the suction is relaxed, there will be no entry of water to these pores, because the air cannot escape. Subsequent cycles, if carefully performed, are closed and reproducible. According to Poulovassilis (1970), this reproducibility suggests that air is always entrapped in the same pores, so that the first cycle imprisons all air possible of

entrapment. The difference between points A and D corresponds to the entrapped air.

A complete moisture characteristic between saturation as the initial state and the maximum possible suction, as curve DEB in figure 2.1, is called the main drying curve, or the boundary drying curve. In the reverse direction, curve BCD, from the minimum possible tension to zero suction is the main, or boundary, wetting curve. Other curves are called scanning curves: a characteristic beginning at an intermediate point on a boundary curve is a primary (drying or wetting) curve; a characteristic beginning at an intermediate point on a primary curve is a secondary (drying or wetting) curve.

The hysteretic nature of the retention curve can be attributed to different causes, such as: the presence of different contact angles during wetting and drying, so that the radius of curvature is greater in an advancing meniscus than in a receding one, and, consequently, the same water content will exhibit greater suction in desorption than in sorption; entrapped air, as commented above; swelling, shrinking or aging phenomena, which can cause changes in soil structure; and geometric restrictions of single pores, the so-called "ink-bottle" effect. The "ink-bottle" effect happens because many pores have relatively narrow inlets, so that, if initially saturated, such a pore will drain abruptly when the suction exceeds the value corresponding to the radius of the small inlet. To fill the pore, the water has to rise through the widest part of the pore and suction has to be reduced to a value corresponding to this bigger radius. Since the suction is inversely proportional to the radius of the pore, the same water content is achieved at a lower suction on re-wetting.

According to Víaene et al. (1994), there is no proof that these processes significantly control water movement in the field, but several works show that substantial errors in both water movement and solute transport can be caused by ignoring their effects. Russo et al. (1989) observed that flow models which neglect hysteresis can overestimate the effective vertical pore water velocity and also the solute velocity. Philip (1991) showed that there is a strong contrast between the relatively steep moisture profiles in the absorption region and the very gradual desorption profiles, and concluded that this difference is strengthened by capillary hysteresis. Parissopoulos and Wheeler (1992), based on simulations of groundwater recharge in southwest Saudi Arabia, observed that, although the effects were generally small, hysteresis can cause differences in water table rise of up to 50 %. Faybishenko (1995) observed important spatial and temporal variations in the hydraulic conductivity of soils due to entrapped air. All these works suggest that the hysteretic nature of the hydraulic properties of the soil has to be taken into account when studying unsaturated flow problems.

2.3 - Basic theory of preferential water flow

Different types of preferential flow mechanisms have been recognised. According to Flury et al. (1994), there is plenty of experimental evidence that preferential flow is common in field soils, being the rule rather than the exception. They identify preferential movement when water bypasses a portion of the soil matrix, and solutes travel from the surface to groundwater in shorter times than expected. This flow can be caused by processes as diverse as the movement of water along cracks or fissures in well structured, loamy to clayey soils; fingering caused by instability of the wetting front in structureless, sandy soils; or channelling of water through biopores, without penetrating the fine porous matrix. Their sprinkling experiments on 14 soils used for agricultural crop production in Switzerland showed that preferential flow was observed for most arable Swiss soils. Kung (1993) identifies three types of preferential flow: macropore, finger and funnel flow, with the latter two associated with layered soils. Using laboratory experiments with three different combinations of sands of different particle sizes, he observed that funnel flow, caused by abrupt textural discontinuity, can greatly accelerate contaminant transport. He also observed that funnel flow does not happen only in extremely dry sands, but it could occur even when the moisture content of the soil profile is at or above its field capacity. According to Babel et al. (1995), preferential flow has been recognised as responsible for faster responses of the solute in the vadose zone, and can take place either through macropores or by instability of the wetting front, which can lead to fingered flow. Their experiments with homogeneous coarse sands subject to continuous unsaturated infiltration showed strong evidence of fingering, suggesting that it may be much more common than generally recognised for solute transport in sandy soils.

The great majority of the experimental and theoretical works on preferential pathways deals with macropore flow. Beven and Germann (1982) mention the works of Schumacher, from 1864, Lawes et al., from 1882, Horton, from 1942, and Hursh, from 1944. More recently, using different experimental approaches, Anderson and Bouma (1973), Ehlers (1975), Pilgrim et al. (1978), Thomas and Philips (1979), Germann and Beven (1981), Hammermeister et al. (1982), Smettem and Collis-George (1985a), Germann (1986), Rice et al. (1991), Smettem et al. (1991), Smettem and Ross (1992), Ogden et al (1992), Leaney et al. (1993), Coulomb and Dever (1994), and Návar et al. (1995) also noted this significance.

According to Germann and Beven (1986), macropore flow - also referred to as short circuiting flow, bypassing flow, channelled flow, flow along preferred flow paths, preferential water flow - includes water movement along desiccation cracks, animal burrows, root channels

and similar soil voids that are surrounded by partially saturated soil matrix. Water in the macropore domain moves rapidly through relatively small pore volume fractions during short time periods. Water in the matrix domain, on the other hand, moves slowly through a much larger pore volume and has much longer residence times. Here it can seep in all directions due to capillary action while in the macropore domain gravity is the dominant driving force. The non-saturated soil matrix attracts water from the macropore domain due to capillarity, thus reducing flow rates in the macropore domain.

2.3.1 - The occurrence of macropore in soils

Macropores can be defined as large continuous openings in field soils, but it is not easy to determine when a pore is a macropore. Beven and Germann (1982) understand macropores as structures that permit nonequilibrium channelling flow, so that not all large voids are macropores, bringing difficulties to the classification of porosity. Various attempts to define a macropore have been made (Beven and Germann, 1982), classifying porosity with respect to pore size or hydraulic conductivity of the soil. But it must be stressed that pore structure is also of crucial importance (see discussions of Luxmoore, 1981, by Beven, 1981; Bouma, 1981; Skopp, 1981), and that other terms, such as preferential pathways or macrochannels, have been suggested to emphasise the importance of structure on flow dynamics.

According to Edwards et al. (1979), a system of large, surface-connected pores can be built by the activity of soil animals such as worms or ants, by the rooting of plants, and by physical processes such as shrinkage, freezing, and thawing. According to Beven and Germann (1982), macropores can be formed by the soil fauna, by plant roots, by cracks and fissures, or can be natural soil pipes.

It is also very important to notice the fact that macropores are a very dynamic structure. As noted by Beven and Germann (1982), the volume and structure of the macropore system will represent a dynamic balance between constructive and destructive processes. Any change in the soil-plant-animal community and in external conditions will affect this balance. Important effects on soil macropores are caused by the weather (through drought, soil freezing, frost, intense rainfalls, and also longer-term climatic changes), by long-term ecological changes and, perhaps more importantly, due to land use. Ploughing produces many cracks in the plough layer, but also cuts the natural macropores and may account for vertical discontinuities in the macropore network; the use of heavy machinery tends to increase the density of the upper soil layers and to destroy macropores, the same occurring with compaction by grazing animals. According to

Edwards et al. (1979), in arable soils, the large surface-connected pores are preserved only when tillage is reduced or omitted.

Macropore systems, again according to Beven and Germann (1982), under favourable conditions, can be produced within 1 to 2 years and may last for considerable periods of time. But the comments above show how quickly the effectiveness of a macropore system can be destroyed and help to explain some difficulties in understanding and modelling these systems.

2.3.2 - Macropores and water flow

Infiltration and subsurface stormflow can be highly influenced by the presence of macropores in the soil, mainly close to its surface. The experimental evidence of these phenomena are well presented by Beven and Germann (1982). This experimental evidence strongly suggests that theories of soil water that treat the soil as a relatively homogeneous porous medium, conforming to Darcian principles, may not adequately describe the infiltration and redistribution of water where the soil contains macropores.

According to Edwards et al. (1979), the large pore flow occurs only during or soon after heavy rainfall, and it seems to effectively bypass water held in the small pore soil matrix. Pores not connected with the surface are ineffective in transmitting water rapidly, but holes and cracks that are open at the surface can definitely move significant volumes of free surface water much deeper and faster than can be calculated by Darcy-type solutions alone. Hoogmoed and Bouma (1980) say that vertical infiltration of water occurs at the soil surface into the upper surface of the peds. Vertical flow of water into the cracks (or any other, relatively large, vertically continuous voids) occurs only when the application rate exceeds the vertical infiltration rate of the peds (direct flow of rain into the cracks is insignificant).

Based on experimental evidence, Beven and Germann (1982) present an interesting description of the process, which is summarised below.

In a simplified view, three stages of flow may be expected:

- First stage: overall input (precipitation, irrigation) is less than the infiltration into the matrix from the surface;
- Second stage: overall input is bigger than the infiltration into the matrix from the

surface, but this difference is less than the inflow to the macropores at the soil surface;

- Third stage: overall input is bigger than the sum of the infiltration into the matrix from the surface and the seepage into the macropores at the soil surface.

During the first stage, all water arriving at the surface is absorbed by micropores connected to the surface. Direct infiltration into the macropores can be neglected, since their contribution to total surface area is very small.

At the second stage, surface runoff on small scale may take place. Both macropores and micropores open to the soil surface take up water simultaneously. As soon as there is a significant flow into the macropores, flow down the walls will also start and lateral infiltration into the matrix will be initiated. These lateral losses will temporarily reduce the macropore flow and the depth of penetration of water along the walls of the macropore. The flow of water in the macropores can greatly increase the surface area available for infiltration into the matrix in this way.

During the third stage, significant amounts of water will begin to be stored at the soil surface, and overland flow will start on a large scale.

The second and third stages suggest a process that will not be adequately described by approaches to infiltration based on Darcy's law, since assumptions of homogeneity of hydraulic properties of the soil over some representative cross-sectional areas will no longer be valid. Water fluxes may vary several orders of magnitude over distances of few centimetres, and hydraulic gradients may no longer be properly defined for the soil as a whole. Any flow concept based on an "average" hydraulic gradient may be expected to fail.

It is important to realise that, according to these concepts, the same volume of water applied at a higher intensity may run deeper into the profile along the macropores. This would explain the heterogeneity of flow that has been observed in different experiments (DeVries and Chow, 1978; Bouma et al., 1980; Rice et al., 1991; Smettem and Ross, 1992).

Thomas and Phillips (1979) point out that it is not necessary that the macropores extend to the soil surface for flow down to them occur. In ploughed soils, deep flow through macropores is observed, even if they are disrupted in the top of the soil. They attribute the

initiation of water movement in the macropores to the low conductivity of the undisturbed soil, which would cause the water coming from the plough layer (of higher conductivity) to accumulate at the bottom of this layer. A process similar to that described as second stage of Beven and Germann conceptualisation would start, with water entering and moving down into the macropores.

Beven and Germann (1982) also discuss the role of macropores in subsurface stormflow. According to them, there is ample evidence that macropores may conduct water laterally downslope through otherwise unsaturated soils. Pilgrim et al. (1978) observed evidences of rapid subsurface throughflow on a large field plot. Leaney et al. (1993) considered flow through macropores as the major mechanism for throughflow in a gently sloping hillside podzolic soil. Návar et al. (1995), using data from an experimental forest plot, observed indications that macropore actively contributes to lateral drainage. For this to be an important mechanism in the supply of water to streams and consequently in the generation of subsurface stormflow, there must be a supply of water to the macropores in excess of lateral losses to the surrounding soil, as discussed above for the infiltration case. In addition, the macropore system must have a sufficient degree of connectivity to transmit water for some distance downslope or at least to a saturated zone that contributes to streamflow.

Beven and German's (1982) conceptualisation does not consider the fact that there is a gradual transition between macropores and capillary-sized pores, and also only explains the problem of water coming from the surface (precipitation, irrigation), neglecting the water that can come from the water table, due to contributions from neighbouring regions. On the other hand, it gives an overall view of the processes occurring in a soil with macropores and it also provides a clue for the problem of initiation of flow into the macropores. So, although simplified, that was the best description of the physical phenomena that could be found in the literature, and, even being more than ten years old, it is still the theoretic base for several models that will be discussed in following sections.

2.4 - Soil-plant-atmosphere interaction

Soil, plant and atmosphere form parts of a continuous flow path in which water moves at varying rates. Water moves in the soil profile according to a potential gradient, being absorbed by the root hairs and then translocated through the plant root and stem system to the leaves, where it is vaporised in the stomatal cavities and transferred to the atmosphere through the stomatal apertures.

Plant tissue is not a passive transmission medium, and the transport of water through the plant influences both root water uptake and transpiration. According to Feddes and Rijtema (1972), a common way of describing water flow through the entire soil-plant-atmosphere system is by electrical analogs. This approach is oversimplified, as resistances vary with transpiration rate, and a detailed description of the water movement through plants would require to represent plant tissue as a continuum. However, water flow is usually studied at either the leaf-air or the soil-root interface (Palmier, 1995).

In the next sections, an introductory review of the main concepts related to the representation of the processes of water uptake by plant roots and evapotranspiration is presented. The water transport through the plant tissue is not included in the review because these concepts are not fundamental for the simulations performed with the models later adopted in this thesis. Detailed descriptions of all these processes can be found in Monteith (1975), Russell (1977), Molz (1981), Feddes et al. (1988) and Burman and Pochop (1994).

2.4.1 - Evaporation and evapotranspiration

Evaporation is the process of conversion of the water at the earth's surface into vapour and its transference to the atmosphere. Its most important forms are evaporation from open water surfaces and bare soil, evaporation of intercepted moisture from vegetation surfaces, and transpiration, when water vapour escapes from within plants. The combined processes of evaporation and transpiration constitute the evapotranspiration, which is controlled both by meteorological and soil moisture conditions. The main meteorological factors are solar energy which set the broad limits and govern the main variations in the rate of evaporation; humidity, with the rate of evaporation being proportional to the difference between the actual and the saturated humidities; and diffusion processes, which are necessary to transfer the water vapour to the atmosphere (Ward and Robinson, 1990; Palmier, 1995).

As previously commented, transpiration is dependent on a sequence of water-moving processes, and soil, plant and atmosphere form parts of a continuous flow path of varying resistances. The complexity of the physical and chemical processes involved leads to the use of simplified concepts in order to evaluate evapotranspiration. One of the most important of these concepts is that of potential evapotranspiration, defined by Penman (1956) as "the evaporation from an extended surface of short green crop, actively growing, completely shading the ground, of uniform height and not short of water". According to this concept, the potential evapotranspiration is the maximum possible evaporative loss from a vegetation-covered surface,

all restrictive conditions fulfilled (Ward and Robinson, 1990).

There are several techniques to measure the rate of evaporation. Ward and Robinson (1990) refers to approaches using atmometers, evaporimeters, evaporation pans, percolating gauges, lysimeters, soil moisture status, whole-plant evaporation chambers, macroscale measurements of the catchment water balance, and modern compact portable instruments. According to Palmier (1995), many of these techniques are expensive and very demanding in terms of maintenance, while others can have large errors associated to the estimated evaporation rate, so that numerous empirical and semi-empirical models, using readily available, routine meteorological measurements to estimate evaporation were developed. From these models, the Thornthwaite formula and the Penman equation (especially the modified Penman-Monteith formula) are probably the most widely used.

Thornthwaite's formula computes the monthly potential evapotranspiration as a function of mean air temperature and hours of daylight. Although highly empirical, and despite the fact that it does not always provide accurate estimates of monthly or short-term potential evapotranspiration, this model has been adopted more widely than any other, mainly because of its convenience and easiness of application (Ward and Robinson, 1990).

The Penman combination equation is based on fundamental physical principles, as it computes potential evapotranspiration combining the aerodynamic and the energy balance methods. The aerodynamic method is based on the turbulent diffusion of water vapour, by assuming that the aerodynamic resistance, which associates the flow of water vapour to the difference in vapour pressure at two different levels above ground, is related to a momentum flux between the same two levels. The energy balance method is based on the assumption that the transfer resistances of heat and water vapour are equal, so that the ratio of the sensible heat, used for heating the air, and the latent heat of evaporation, used for evaporation (Bowen ratio) is directly proportional to the ratio of the differences in temperature and vapour pressure measured between any two heights. Defining the available energy (sum of the sensible heat and latent heat) as the net radiation minus the soil heat flux, the inputs necessary to apply the method are measurements of the net radiation, soil heat flux, and temperature and vapour pressure at two or more different heights. Both aerodynamic and energy balance methods provide accurate estimates of evaporation rates, but their use is limited by the need for sensitive meteorological instruments at several heights. For this reason, Penman (1948) incorporated some empirical concepts to his combination equation, in order to allow the use of commonly measured meteorological variables, such as average daily speed, saturated vapour pressure at the

temperature of the air and the vapour pressure of the air (all at a height of 2 m). Monteith (1965) explicitly incorporated the effects of aerodynamic resistance and surface resistance to account for variations of evaporation between vegetation covers that differ in terms of wetness, structure and physiology (Ward and Robinson, 1990; Shuttleworth, 1993; Burman and Pochop, 1994; Palmier, 1995). The resultant Penman-Monteith combination equation is described as:

$$\lambda_v E = \frac{\Delta H + \frac{\rho c}{r_a} [e_s(T) - e]}{\Delta + \gamma(1 + r_s/r_a)} \quad (2.15)$$

where: E = evapotranspiration rate;
 λ_v = latent heat of vaporisation;
H = sensible heat: $H = R_n - G$ (R_n is the net radiation and G is the soil heat flux);
 Δ = rate of change of saturated vapour pressure with temperature;
 ρ = density of the air;
c = specific heat of the air;
 $e_s(T)$ = saturated vapour pressure at temperature T;
e = absolute vapour pressure of water at dew point temperature;
 r_a = aerodynamic resistance;
 r_s = surface resistance;
 γ = psychrometer constant.

This equation can be used to estimate the value of the potential evapotranspiration. To estimate the actual evapotranspiration for a specified crop, the values of r_a and r_s appropriate to this particular crop are required. A more frequent alternative is to estimate first the potential evapotranspiration rate and then multiply this rate by K_e , the crop coefficient. This crop coefficient is not a constant, but, in fact, it is a function of the soil volumetric moisture content, called the moisture extraction function (Shuttleworth, 1993; Burman and Pochop, 1994).

According to Shuttleworth (1993), the overall behaviour of the moisture extraction function during a drying cycle follows the pattern shown in figure 2.2, where θ_f is the field capacity, θ_w is the wilting point, and θ_d is typically 50 to 80 % of θ_f . The field capacity was defined in section 2.2.2. The wilting point is defined as the minimum water content of the soil at which a plant can extract water. According to Feddes et al. (1976), the wilting point varies

with the osmotic pressure of plant tissues, so that there is no single value for this parameter. The pressure head for wilting points varies from -10,000 cm to -20,000 cm, but, for practical purposes, a value of about -15,000 cm can be adopted. In the process described by figure 2.2, it is supposed that a saturated soil first drains up to the field capacity, and then the drying process proceeds with little soil moisture restriction, until the soil moisture falls to θ_w , when the hydraulic conductivity and the transpiration rate start to fall. They fall until the wilting point is reached, when the conductivity is supposed null. Shuttleworth (1993) assumes that this behaviour is similar for both crops and soils and also that, under prolonged drought, the crop begins to die and the evapotranspiration rate is no longer controlled by meteorological conditions, but by soil characteristics, especially by hydraulic conductivity.

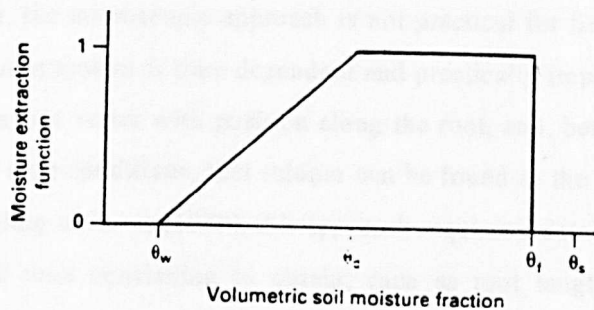


Figure 2.2 - General pattern of the moisture extraction function (after Shuttleworth, 1993)

2.4.2 - Water extraction by plant roots

According to Jarvis (1989), root water uptake is perhaps one of the most difficult components of the soil water balance to model. Spatial and temporal variations in the pattern of root water uptake are common. For example, in a uniformly wet soil profile, almost all water is extracted from close to the soil surface, where root densities are largest. If the top layers are dry, the water necessary for the transpiration process has to be provided by sparsely rooted, moist, soil horizons deeper in the profile.

The aim of studies at the soil-root interface is to estimate the rate of water uptake by plant roots from a given volume of soil. Two main approaches can be identified for the description of water uptake by plant roots: the microscopic approach, which considers the radial soil-water flow to a single root; and the macroscopic approach, that takes the integrated properties of the entire root system, in which a volumetric sink term, representing water extraction by plant roots, is added to the continuity equation for flow of water in the soil and, consequently, included as a term in the Richards' equation.

A classical example of the microscopic approach is the model proposed by Gardner (1960), which is based on assumptions that a typical root is represented by an infinitely long and narrow cylinder of constant radius and water-absorbing properties, with the steady state soil water flow equation solved analytically by assuming radial flow. According to Molz (1981), this model and others, such as Hillel et al. (1976), based on an analogy to Ohm's law, were very influential and stimulated much research.

However, the microscopic approach is not practical for field applications. The detailed geometry of the root system is time dependent and practically impossible to measure, the water permeability of a root varies with position along the root, and, besides that, this representation considers steady state conditions, that seldom can be found in the field (Molz, 1981; Feddes et al., 1988). According to Jarvis (1989), this approach requires a detailed knowledge of data which is expensive and time consuming to obtain, such as root length densities and the relative magnitude of resistances to the flow of water in the soil-plant atmosphere continuum.

An alternative solution is to use the simpler macroscopic approach, which represents the root uptake by a volumetric sink term included in the Richards' equation. The resultant equation can be given by

$$\frac{\partial \theta}{\partial t} = \nabla (K \nabla \phi) - U_r \quad (2.16)$$

where U_r is the water extraction function, which can depend on space, time, water potential, water content, hydraulic conductivity of the soil, difference in pressure head between the soil and the root interior, or a combination of these variables (Feddes et al., 1976; Molz, 1981).

Several different empirical and semi empirical forms for the sink term can be found in

the literature. Many of these functions (Whisler et al., 1968; Molz and Remson, 1970; Feddes et al., 1974; Jarvis, 1989) assume that the soil surrounding the root presents the dominant resistance to water flow, compared to that in root tissue. However, there is experimental and theoretical evidence that the resistance of the root system usually dominates the resistance of the soil close to the roots (Molz, 1981). This evidence suggests that models based on the resistance of the soil are conceptually wrong. On the other hand, the determination of parameters for a function based on root characteristics can be expensive and time consuming, as root conditions change with time and depth. For this reason, Feddes et al. (1976) justify the definition of the water uptake by roots as a function of the water content in the soil in order to facilitate its implementation in field scale models.

According to Palmier (1995), many authors have been applying dynamic models based on the combination of Richards' equation with sink terms for the root water uptake with promising results. Jarvis (1989) mentions that these models frequently show a general agreement with measured data. However, the success or failure of most of the water extraction functions proposed is not clearly defined, as many models have been called successful simply because they can be made to fit data (Molz, 1981). Although these results can help to justify the use of such methodologies, they do not ensure that a better understanding of the processes associated with root water uptake is obtained. According to Jarvis (1989), it is difficult to formulate a simple function which can adequately represent the temporal and spatial variations in root water uptake and, consequently, unrealistic patterns are common (particularly for the drying process and for idealised initial and boundary conditions, such as uniform initial soil water content, zero recharge, or constant evaporation). The development of a better knowledge of soil-root interface properties and also of water transport in the plant tissue is necessary in order to improve the ability to properly represent water extraction by plant roots.

CHAPTER 3 - MODELLING WATER FLOW IN THE UNSATURATED ZONE

3.1 - Introduction

A model is a representation, a simplification of reality. Models can differ from each other due to their purposes, structure, or the precision of representation of the different processes, being constrained by the quantity and quality of the available data, the difficulty of mathematically representing the physical phenomena, and the simplification of the spatial distribution of some variables, such as precipitation and infiltration capacity.

According to the techniques used in modelling, different criteria can be adopted to classify the mathematical models. Based on definitions and discussions by Clarke (1973), Tucci (1986), Chevallier (1988), Kauark Leite (1990) and Wheater et al. (1993), models can be classified as: (1) linear or non-linear, if the principle of superposition is valid or not (i.e., if y_1 and y_2 are system outputs, corresponding to the inputs x_1 and x_2 , respectively, the response of a linear model to the input x_1+x_2 will be y_1+y_2); (2) stochastic or deterministic, if any input, output or error variable is regarded as random variable, having a probability distribution or not; (3) continuous or event-based, if it continuously simulates a hydrological time-series or performs the simulations event by event; (4) dynamic or static, according to whether some variables change with time or not (if all variables and parameters are independent of time, the model is static); (5) distributed or lumped, if the values of its input variables and parameters change in space or not; (6) empirical, conceptual or physically based, according to the way they seek to characterise the system response. The empirical models do not take into consideration the physical processes internal to the system, merely establishing direct relations between input and output variables; the conceptual models use physical concepts to represent the system, but these representations are simplified and it is not possible to physically identify the parameters; the physically based models try to describe, in a detailed and realistic form, all physical, chemical and biological processes in the system, taking into account their spatial and temporal variation, based on continuum mechanics, usually through numerical solutions of the relevant equations of motion.

It is important to emphasise that the limits between the conceptual and physically based models are not absolutely clear and defined. In principle, the physically based models need no fitting, as all their parameters can be determined from physical characteristics of the system, while the conceptual models require calibration, because some of the parameters can not be measured. Actually, the present knowledge is still far from a complete and appropriate causal

theory of all processes involved. Even in the most advanced physically based models, some parameters or coefficients cannot be properly measured. Besides that, it is possible to find several apparent contradictions in the model classifications, such as: the continuous models actually use fixed timesteps; the distributed models simulate the system as a collection of small lumped sub-systems; physically based models frequently use empirical equations to represent certain processes. These contradictions could lead to the conclusion that these classifications have only academic use, but, according to Kauark Leite (1990), they are useful to help the model user to better understand the choices made by the modellers and also to give guidance to the data gathering and to the understanding of the results of the simulations.

Several models have been developed to simulate the water flow in the unsaturated zone. Mangold and Tsang (1991) present a review of 56 subsurface hydrological and hydrochemical models. Anderson et al. (1993) report a number of over 40 different computer models for subsurface flow. Each model presents distinct features and objectives, according to the modellers knowledge of the available algorithms and also depending on the problem to be solved. This problem could be consequence of different questions to be solved, such as lack of data or the need to test different ways of simulating a process which is not well represented in the available models.

Due to the great number of available models, it is increasingly justifiable to select an existing model and, if necessary, to modify it, in order to satisfy the specific needs of the user, instead of developing new codes.

In this chapter, some of the most important approaches available in the literature to model water flow in unsaturated soils are described and commented on. A general view of the present situation is provided, assessing the main issues that have already been addressed and those remaining to be investigated, and introducing the models selected to be used in this thesis. The chapter is divided according to the objectives of this thesis, i.e., to compare alternative modelling approaches in order to get a better understanding of the processes responsible for water flow in the unsaturated zone. For this reason, it is composed of three main sections: models of unsaturated soil water flow, models of preferential water flow and models of hysteresis.

3.2 - Modelling unsaturated soil water flow

According to Ross (1990), Richards' equation, presented in section 2.2.2, is the commonly accepted basis for detailed studies of soil water movement. The majority of the conceptual and physically based models of flow in the unsaturated zone nowadays employs Richards' equation. A great number of analytical and semianalytical solutions of the Richards' equation can be found in the literature (Pullan, 1990; Warrick et al., 1991; Srivastava and Yeh, 1991). However, as already commented in section 2.2.2, these analytical solutions are of limited use, and, consequently, numerical methods are commonly employed. There is a great variety of numerical solutions, adopting different forms of the nonlinear Richards' equation, and different ways of discretization, according to the objectives of each modeller. These models can be considered quite satisfactory in view of the limited precision of the soil data, but a lot of computational effort and field data is required to effectively represent the actual variability of the medium. Alternative ways to deal with these problems, such as the use of transfer functions or stochastic techniques are frequently used.

3.2.1 - Unsaturated soil water flow models

The main numerical approaches for the solution of partial differential equations, such as Richards', are the finite difference method and the finite element method. The finite difference method represents normal gradients by differences, but can not account for tangential gradients. It is simpler to implement, but requires a regular grid even for highly irregularly shaped regions. In the finite element method the domain is discretised into a series of rigid elements and in each of these a simple polynomial approximation to the exact solution is taken using variational techniques or weighted residuals principles, such as Galerkin's method. The finite element method can handle irregular geometry and tangential as well as normal gradients, but it is a most complex scheme for computation. Many other techniques are being tried for both analytical and numerical solutions, such as the integral finite difference method, the boundary element method, analytic elements, or the use of stochastic or transfer function models (Feddes et al., 1988; Mangold and Tsang, 1991; Anderson et al., 1993).

Huyakorn and Pinder (1983) report that the use of finite differences in subsurface simulation began in the late fifties, with the interest of the oil industry in the forecast of reservoir performance. Applications to groundwater flow appeared later on, during the sixties, when the ability to accommodate spatially variable material properties made the numerical approach attractive, and the finite difference method, being the only well-established

methodology available at the time, was the obvious choice. According to Nielsen et al. (1986), the first finite difference methods were developed to predict unsaturated flow only (Hanks and Bowers, 1962; Rubin and Steinhardt, 1963), but one and multidimensional models were subsequently developed considering both saturated and unsaturated zones. Freeze (1969) was probably the first to describe the transient saturated-unsaturated flow in a single equation. The first three-dimensional finite difference model of saturated-unsaturated transient flow was proposed in a classical work by Freeze (1971).

The time integration by finite difference is commonly performed using the Picard or the Newton-Raphson iterative schemes (for details, see Huyakorn and Pinder, 1983). Although the Picard method is simpler to code and faster on a per-iteration basis, comparative studies (Huyakorn et al., 1984; Kaluarachchi and Parker, 1989; Paniconi et al., 1991) show that it converges slowly, requiring a greater number of iterations, so that its global computational cost is similar to the application of the Newton-Raphson method.

Several finite difference methods to solve variably saturated problems have been proposed in the last decades, in the majority of the cases based on one-dimensional solution. Haverkamp et al. (1977) compared six of the most frequently used numerical schemes, obtaining good agreement with measured water content profiles for all models, but they reported significant differences in computational efficiency. Considering computer time and stability problems, the implicit schemes showed a widest range of applicability for simulating saturated-unsaturated water movement in the soil.

Ross (1990) introduced two finite difference methods for solving Richards' equation in one dimension: an advancing front method, where spatial grid points were added as the infiltration/redistribution front advance, and a fixed grid method. He used a mass-conserving form of Richards' equation with implicit iterative methods, which allowed large time steps to be taken. He observed that the advancing front method was more efficient than the fixed grid solution, and that large spatial increments could be adopted by the use of a hyperbolic sine transform for the matric potential. However, the Newton-Raphson iterations occasionally failed to converge, for both methods advancing front and fixed grid, requiring the user to alter limits on the step size and implying that an algorithm to control the solution is needed if these methods were coupled into larger programs.

Parissopoulos and Wheeler (1988) refer to the development of a great number of implicit solution schemes, using the Gauss elimination, the Iterative Alternating Direction Implicit

(IADI), The Line Successive Over-Relaxation (LSOR), the Strongly Implicit Procedure (SIP), and the Newton-Raphson method. They analyzed the performance of a two-dimensional finite difference model using the IADI method and observed that important errors can occur due to the geometry of the finite difference grid, the convergence criterion and the iteration parameter.

Various other models are available in the literature (see reviews by Mangold and Tsang, 1991 and Anderson et al., 1993). According to Clement et al. (1994), finite difference methods have been widely used for one-dimensional problems, but fewer researchers applied this methodology in higher dimensions. Generally these applications have limitations, due to numerical instabilities and convergence difficulties, caused by inefficiencies in the schemes used to solve the two-dimensional, non-linear equations. Successful and efficient finite difference solutions to two-dimensional, variably saturated flow are presented by Kirkland et al. (1992), who introduced two methods: one defining a new variable for the transformed Richards' equation, which has the characteristics of water content when soil is unsaturated and of pressure when it is at or near saturation; and a pressure-based method which uses flux updating. The transformed Richards' equation presented computational advantages, because it is mass conserving, noniterative and more stable at a flux boundary during the initial time steps for infiltration into dry soils. However, Clement et al. (1994) observe that, as this model was developed to solve infiltration problems in dry soils, it does not account for the effects of specific storage, and consequently it can not accurately represent transient drainage and seepage phenomena in large domains. In order to overcome this problem, Clement et al. (1994) developed a two-dimensional finite difference algorithm, based upon central differences in space, implicit formulation in time, and a modified Picard iteration to handle the nonlinearity of the governing equation. A computationally efficient algorithm, the preconditioned conjugate gradient method, is used to solve the difference equations, which performed well for infiltration fronts, transient water tables, and also transient seepage fronts. Also, the solutions obtained are mass conserving within the unsaturated zone.

According to Huyakorn and Pinder (1983), the method of finite differences is very popular mainly because it is conceptually straightforward, with its fundamental concepts readily understood. It also presents a firm theoretical foundation, due to its extensive history, so that several algorithms have been developed for its solution. Feddes et al. (1988) state that the advantage of this method is its simplicity and efficiency in treating the time derivatives. Its main drawbacks are its incapacity to deal with complex geometries, a slow convergence, and difficulties in treating moving boundary conditions.

Karavokyris et al. (1990) say that two drawbacks of finite-difference schemes are their low flexibility with respect to the coupling of the soil water model to models of related processes and the lack of a variable time-step. They developed a coupled soil-plant-water model (SPW1 model), that combines a soil water and a plant water model. For the solution of this model, they introduced the use of the numerical method of lines, that relies on the discretization of a parabolic or hyperbolic partial differential equation with respect to the independent variables of space, reducing the equation to a system of ordinary differential equations with time as the only independent variable. Several efficient algorithms are available for the solution of such systems of ordinary differential equations. According to Karavokyris et al. (1990), the advantages of the method of lines compared to finite difference schemes are increased computational efficiency, enhanced error growth control, the ability to add or delete equations from the overall system, and increased modularity of the model program. The limitations of the method are its relatively high requirements in terms of computer storage, and the condition that the original partial difference equation has to be of a form that can be discretised into a system of ordinary differential equations. These characteristics make this method particularly attractive for the coupling of the soil water model to models of related processes, such as a plant water model.

Finite element methods are another alternative for the problems presented by finite difference techniques, as they are capable of solving complex flow geometries, nonlinear and time-dependent boundary conditions, and possess a high flexibility in following rapid soil water movement.

Finite element solution techniques became available in the late sixties, initially applied only to saturated flow (Nielsen et al., 1986). Neuman (1973) presented a model to simulate saturated-unsaturated flow through porous media using finite elements. This work opened a path followed by numerous researchers, leading the development of several two- (Kaluarachchi and Parker, 1987b and 1989) and three-dimensional models (Frind and Verge, 1978; Huyakorn et al., 1986; Binley et al., 1989 and Paniconi and Wood, 1993).

Frind and Verge (1978) introduced a Galerkin finite element model based on the general saturated-unsaturated continuity equation. The authors obtained costs of computation which they considered not unreasonable, but they observed a lack of compatibility in the optimum size of saturated and unsaturated elements: in the saturated case, elements sizes of the order of meters or tens of meters can be used, but the unsaturated condition demands elements sizes of the order of centimetres or tens of centimetres. This lack of compatibility did not allow a whole basin

three-dimensional modelling. Huyakorn et al. (1986) presented a three-dimensional finite element model where soil function terms inside the element are determined by an influence coefficient technique, with the values of the soil parameters at the element centroidal adopted for the element as a whole, avoiding numerical integration and saving computational costs. The model showed great flexibility in representing complex geometry with irregular boundary conditions, layering and lateral discontinuities. The influence coefficient technique was also used by Kaluarachchi and Parker (1987b) in a two-dimensional finite element model using a fourth-order Runge-Kutta time integration method, obtaining good rates of convergence and solution accuracy for heterogeneous soil profiles with highly non-linear soil properties. Binley et al. (1989) employed another approach to evaluate the soil functions in the element, by the use of numerical integration. In this work, they examined the effect of heterogeneity in the three-dimensional simulation of hypothetical hillslopes and concluded that both peak discharges and volumes of runoff are affected by the variability of soil characteristics. More recently, Paniconi and Wood (1993) developed a three-dimensional catchment scale numerical model for fluid flow in variably saturated porous media, designed to take advantage of digital elevation data bases. They observed that spatial information for the saturated conductivity may be necessary to match both low and high discharge events. Nowadays, finite element techniques are very commonly used to simulate water flow and chemical transport in variably saturated porous media, as, for example, in Yeh et al (1993).

According to Nielsen et al. (1986), the most important advantage of finite element techniques over standard finite difference methods is probably its ability to more accurately describe irregular system boundaries in multidimensional simulations, as well as to more easily include nonhomogeneous medium properties. However, they also state that finite difference methods seem not to be better or worse than finite element schemes (at least for one-dimensional simulations).

Another modelling approach is the use of transfer function models. Himmelblau (1970) defines the transfer function as the ratio of the Laplace transform of the output divided by the Laplace transform of the input of models represented by n th-order linear ordinary differential equations with constant coefficients and zero initial conditions. The transformation of an arbitrary input signal into an output signal for a linear system is achieved by means of the impulse response function, which defines the response of the system to a narrow pulse input at the inlet end. The impulse response function is also known as a weighting function, as the response is equivalent to weighting the input values at various times from zero to the final time (a convolution process). According to Box and Jenkins (1970), transfer functions are dynamic

input-output models that can show the effect of any given series of inputs on the output of a system subject to inertia (i.e. a system in which a change in the input will have no immediate effect on the output but instead will produce a delayed response, with the output eventually coming to equilibrium at a new level). Jury (1982) defines a transfer function model as a device commonly used by electrical engineers and hydrologists to characterise systems whose internal mechanisms are unknown or unknowable. Generally, transfer functions are used to model complex systems in a simple way by characterising the output flux as a function of the input flux.

The transfer function approach has been used to model solute transport through unsaturated soil. Jury (1982) developed a transfer function model using a distribution function of solute travel times from the soil surface to a reference depth. With this model he simulates the average solute concentrations at any depth and time for arbitrary solute inputs or water application variability, through highly variable field systems. Jury et al. (1986), using the solute lifetime pdf (probability density function), generalised this model to describe the movement of a solute that may undergo physical, chemical, or biological transformations as it moves in a soil through which the water flow can vary in both space and time. White and Magesan (1991) developed a transfer function model based on the pdf of travel times for nitrate or a surface-applied tracer such as chloride or tritiated water.

Transfer functions provide an alternative approach to problems concerning uncertainty about the exact description of the transport or reaction process, and also to applications where data is difficult to obtain. However, experimental determination of an approximate transfer function for a process of unknown dynamics is complicated by noise and nonlinearities in the process. Besides that, difficulties lie in accurately identifying the transport volume and the average soil solution concentration due to the spatial variability inherent in field soils.

According to Gelhar (1986), heterogeneity of aquifer materials seems to be omnipresent, due to the variable processes involved in the genesis of permeable earth materials. One approach to deal with this complex structure of aquifer materials and extreme variability of flow properties would be to construct a detailed deterministic model which represents the actual heterogeneity of the aquifer. However, for realistic field problems, the degree of spatial resolution would require enormous computational resources and would be impractical in terms of the amount of data required. Alternatively, and in contrast to the deterministic solutions, another way to treat the problem of flow in soils with macropores is through stochastic modelling, where the hydraulic variables and soil properties are treated as random variables.

According to Benjamin and Cornell (1970), a random variable is a numerical variable whose specific value cannot be predicted with certainty before an experiment. The behaviour of a random variable is described by its probability law, which may be characterised through its probability distribution. For continuous random variables, the probability density function (pdf) and the cumulative density function (cdf) are alternative forms by which to describe its probability distribution.

A random variable whose properties depend on an argument can be interpreted as a random (stochastic) process. Box and Jenkins (1970) define a stochastic process as a statistical phenomenon that evolves in time according to probabilistic laws. If its properties are unaffected by a change of time origin, this process is in statistic equilibrium, and is called a stationary stochastic process. A data set constitutes a possible realization of the random process, while the infinite set of possible realizations is the ensemble of the process. The probabilistic definition of the ensemble defines the random process, which is fully described by defining the joint probability density function of the random process at all possible values of the argument.

According to El-Kadi (1987), stochastic models, when compared to deterministic models, are more realistic representations of field situations and also better predictive tools, if their data requirements are satisfied. These models can examine errors that arise from neglecting variability and they can also test the sensitivity of the model output to changes in parameter statistics. However, Yevjevich (1974) states that only an integration of both deterministic and stochastic approaches can lead to reliable understanding and description of water resources systems. An example of a model of that type is presented by Kiefer (1993).

Monte Carlo is one of the most commonly used stochastic techniques. Monte Carlo techniques, according to Protopapas and Bras (1990), use generators for random fields to obtain a large number of possible responses of the system. Then the sample output is statistically analyzed to compute its first and second moments. The number of replicates should be sufficiently large to guarantee insensitive results.

Monte Carlo techniques were utilised by Freeze (1980) and Hopmans et al. (1988). Freeze (1980) presents a stochastic-conceptual model, where a mathematical model uses a set of physically based equations to route rainfall events through a hillslope, with these events and the hillslope parameters being defined by a set of stochastic processes. He introduced a general model by considering the effects of different elements of the rainfall-runoff problem (rainfall patterns, hydraulic conductivity and aquifer topography) on the runoff variability. The

autocorrelation structure of different elements was also considered. His work suggests that the distributions of hydraulic conductivities over a watershed should not be neglected. Hopmans et al. (1988) used a Monte Carlo technique to examine the stochastic nature of soil-water pressure head and vertical and horizontal flux density under two-dimensional unsaturated steady flow conditions. Random autocorrelated scale factors were generated to describe a stationary random field of hydraulic conductivity functions and the water flow equation was numerically solved for steady state infiltration and evaporation in a two-dimensional domain. Their results seem to show that lateral flow in a predominantly vertical flow situation may have a considerable magnitude in layered soil systems.

Monte Carlo techniques can simulate the actual field conditions provided that the statistical properties of the soil hydraulic properties are a reflection of the actual field variability. However, according to Yeh (1992), a large number of realizations is necessary to obtain meaningful statistics from the output, implying that their simulations are time consuming. Also, they do not give direct insight in how output variables are controlled by the spatial variability of soil parameters, as no clear relationship between the statistics of input and output parameters can be easily derived.

Similarly to Monte Carlo techniques, Cordova and Bras (1981), Dagan and Bresler (1983), and Mishra et al. (1990), developed approaches where input variables for conceptual models are stochastically generated and then applied to these models. Cordova and Bras (1981) developed the pdf of infiltrated water volumes as a function of climatic and soil parameters to be used as input for a physical-conceptual model of the soil moisture depletion process. Dagan and Bresler (1983) derived models of water flow in the upper soil layer of spatially variable fields, assuming field variability only in the horizontal plane. They considered the saturated hydraulic conductivity as a random variable of lognormal distribution, with head suction and moisture content related to it by simple analytical relationships. A simplified solution of vertical flow in a homogeneous column, based on the concept of moving front, was developed with the aim of deriving the expectations and variances of the moisture content, suction heads, hydraulic conductivity, and water flux as functions of depth and time for infiltration and redistribution. Mishra et al. (1990) developed an algorithm for generating spatially autocorrelated unsaturated flow properties using particle size distribution data, with the soil hydraulic properties described locally by the parametric model of Van Genuchten (1980). Their approaches are more economical, in terms of computing time, than a Monte Carlo simulation, but the results are restrained due to the simplifications in both the methodology for generating the stochastic inputs and the conceptual models adopted.

Another very common stochastic methodology is the use spectral analysis associated with perturbation techniques. Spectral analysis is based on the assumption that any stationary stochastic process can be represented by a combination of harmonic series, where the frequency can vary continuously in the range 0-0.5 cycles (Box and Jenkins, 1970). According to Jenkins and Watts (1968), a stationary stochastic process is simply described by its autocovariance function. An equivalent description is provided by its power spectrum, which is the Fourier transform of the autocovariance function. According to Bakr et al. (1978), by using the Fourier representation, perturbed forms of the flow equation can be solved for the spectrum of the head or flow in terms of the spectrum of the hydraulic conductivity field. Thus, given the covariance of the input hydraulic conductivity, the resulting head variance can be determined.

Spectral analysis in combination with perturbation technique was utilised by Bakr et al. (1978), Gelhar et al. (1979), and Yeh et al. (1985a, b, c). Bakr et al. (1978) represented the variation of the hydraulic conductivity as a spatial stochastic process which is characterised by a covariance function. They used the theory of spectral analysis to solve perturbed forms of the stochastic differential equation of flow through porous media. The results of the analysis demonstrate the importance of spatial correlation structure and multidimensional flow. Gelhar et al. (1979) analyzed the longitudinal dispersion produced as a result of vertical variations of hydraulic conductivity in a stratified aquifer by treating the variability of conductivity and concentration as homogeneous stochastic processes. They solved the stochastic differential equation for the concentration field through the use of spectral representations. Their results show that for large time the longitudinal dispersivity approaches a constant value which is dependent on statistical properties of the medium. Yeh et al. (1985a, b, c), using the spectral analysis approach, solved the equation for stochastic steady infiltration into a three-dimensional heterogeneous aquifer. Their analysis is based upon spectral solutions of a perturbation approximation of the stochastic flow equation. Analytical expressions were derived to describe the variance of soil water pressure head, flux, and the effective hydraulic conductivity as a function of the soil medium and the mean flow characteristics. Their study showed the importance of considering both the correlation structure of hydraulic conductivity and the three-dimensional effects.

The discretization of the random conductivity field and of the flow equation can result in potential errors, especially when large discontinuities in conductivity occur between blocks. These errors can be circumvented by solving the flow equation analytically with a continuum representation of the random conductivity field. Spectral theory is a suitable tool which may be used to describe this continuous behaviour where the random field is statistically homogeneous

(Bakr et al., 1978). The spectral method in combination to perturbation solutions has the added advantage that it applies to multidimensional systems and temporal variability and it yields analytical expressions for the variance of output variables. However, according to Hopmans et al. (1988), it is based on simplifying assumptions which may not hold true in an actual field situation. For example, the perturbation technique is only applicable to unbounded domains. Also, it assumes stationarity, and some variables, such as the hydraulic conductivity, are likely to be non-stationary, because of changes in depositional environments which may contain heterogeneity (Yeh, 1992).

Also combinations of these techniques are utilised. Zhu et al. (1990) used a hybrid perturbation-Monte Carlo approach to derive general expressions for effective medium properties to be used as an "equivalent" homogeneous medium. Random fields of unsaturated flow parameters were generated from the statistics of grain size data and expressions for effective properties were derived from perturbation approximations of the governing equations of unsaturated flow. As pointed out by the authors, the practical utility of the method depends on the feasibility of developing procedures for estimating effective properties from information on local property statistics without general recourse to Monte Carlo simulations.

It is important to highlight that no approach or method has proved to be better than all others, as different methods have worked well in different applications (Mangold and Tsang, 1991). For these reasons, choosing the method depends on the problem to be solved and on the preference of the user (Anderson et al., 1993).

3.2.2 - The numerical model SPW1

A combined experimental and modelling study into the processes affecting radionuclide transport from a contaminated water table through the unsaturated zone and into a wheat crop is being undertaken by Imperial College on behalf of UK Nirex Ltd. The physically-based soil-plant-water model, SPW1 (Karavokyris et al., 1990), was developed as part of this study and was selected for this thesis, in order to test the use of Richards' equation to represent the available experimental data.

The SPW1 model combines a plant water and a soil water sub-models in a single model. It can be run under three different combinations of these two sub-models: (1) only soil water simulations; (2) soil water model simulations involving root uptake in response to evapotranspiration rates; and (3) simulations using the fully coupled soil-water-plant model. In

this thesis, the model was applied using the second option. For this reason, only the features related to the soil-water model and to the root uptake are presented here. A detailed description of the complete model can be found in Karavokyris et al. (1990) and in Butler (1991a).

The soil water flow model uses the Darcy-Richards' equation to model one-dimensional unsaturated flow. It equates the changes in soil pore volume storage for a representative elementary volume with the divergence of the vertical water flux across the boundaries of the same volume and any volumetric losses due to root uptake occurring within that volume. The numerical method of lines is applied to solve this parabolic partial differential equation.

The model allows the selection of a soil moisture characteristic and an unsaturated hydraulic conductivity relationships. For the soil moisture characteristic, the available options are the use of the equations presented by Van Genuchten (1980), Philip (1957)/Haverkamp et al. (1977), or Saxton et al. (1986). The unsaturated hydraulic conductivity can be obtained by the use of the relations introduced by Mualem (1976a), Philip (1957)/Haverkamp et al. (1977), Saxton et al. (1986) or Nwabuzor (1984).

Three types of boundary conditions are possible: specified pressure (Dirilecht condition), specified flux (Neumann condition), or unit gradient pressure differential (Neumann condition). These boundary conditions are allowed to vary with time when necessary, according to information supplied by the user.

Under the adopted option for running SPW1 (soil water model simulations involving root uptake in response to evapotranspiration rates), the time-varying total soil evapotranspiration rate is provided by the user and it is apportioned by the model into two components: soil surface evaporation and plant transpiration. This division is made according to the following relationships:

$$\begin{aligned} ES &= \mathcal{F} ET \\ U_r &= (1 - \mathcal{F}) ET \\ \mathcal{F} &= \max[(-0.3 LAI + 1.0); (0.1)] \end{aligned} \tag{3.1}$$

where: ES = soil surface evaporation rate;
 ET = total evapotranspiration rate;
 U_r = total root uptake rate;

LAI = leaf area index.

The model adopts a layering of the root system. The rate of water uptake U_i from each layer i is calculated independently so that the total overall rate, U_r , is given by the sum of all layers. Provided the root zone layers of the plant model coincide with soil layers of the soil water model, the uptake U_i is introduced in the soil water model as a sink term for layer i . The rate of water uptake from layer i is given by

$$\begin{aligned} U_i &= \frac{\Psi_n - \Psi_c}{R_n + R_{xi}} \\ R_{xi} &= r_x X \\ R_n &= \frac{r_r}{(l_n)_{ef}} \end{aligned} \quad (3.2)$$

where: Ψ_n = root surface water pressure in layer i ;
 Ψ_c = canopy water pressure;
 R_n = radial resistance to water entry into the root;
 R_{xi} = total axial resistance
 r_x = axial resistance per unit length of root;
 r_r = radial resistance per unit length of root;
 X = equivalent stem length;
 $(l_n)_{ef}$ = effective root length of layer i

The effective root length accounts for the effect of the soil-root interface and anaerobiosis. The effects of anaerobiosis, which are due to a marked increase in root resistance that occurs in saturated or nearly saturated soils as a result of oxygen deficiency, are represented by decreasing the effective root length by a factor of 100, when the gas filled porosity is below 0.01. Over this value, only the effect of the soil-root interface is considered. Hence,

$$\begin{aligned} (l_n)_{ef} &= \frac{\theta_i}{\theta_{si}} l_n & \text{if } (\theta_{si} - \theta_i) > 0.01 \\ (l_n)_{ef} &= \frac{\theta_i}{100} & \text{if } (\theta_{si} - \theta_i) \leq 0.01 \end{aligned} \quad (3.3)$$

where θ_i and θ_{si} are the actual and saturated moisture contents of layer i and l_i is the total length of roots in layer i .

Karavokyris et al. (1990) performed a validation of the soil water model using three sets of published results: two data sets of infiltration of water in homogeneous sand and clay columns under restricted initial and boundary conditions, from Haverkamp et al. (1977); and a set of measurements in a layered soil in the field, from Vachaud et al. (1981) and Vauclin and Vachaud (1981). They used the Haverkamp et al. (1977) data to compare the results of a quasianalytical solution, as proposed by Philip (1957), against SPW1 model simulations under three different conditions: infiltration of water into Yolo light clay; infiltration of water in fine sand, keeping constant pressure at the surface; and infiltration of water in fine sand, maintaining a constant flux at the surface. The data from Vachaud et al. (1981) and Vauclin and Vachaud (1981) refer to a series of detailed measurements of tension and water content carried over a period of 162 in Tunisia, in a cylindrical section of layered natural soil. Simulations of SPW1 were compared with the data and also with an implicit finite-difference model that Vauclin and Vachaud (1981) applied to the same experiment. Besides these validations using experimental and field data, a comparative test of the soil water model against an alternative model employing an entirely different solution technique was also undertaken, in order to test the model's capabilities in handling multiple soil layers and extreme boundary conditions. The model selected for the comparison, the Saturated-Unsaturated Mass Transport model (SUMATRA) (Van Genuchten, 1978), employs a fundamental soil water flow equation identical to that of SPW1 model, but has a completely different solution technique, involving Hermitian finite element representation. The authors concluded that their model seems well capable of handling the types of problems which occur in the field and has been shown to perform in a superior manner against an internationally recognised unsaturated flow model.

3.3 - Modelling preferential water flow in soils

Macropores may occupy only a marginal proportion of the entire porosity and they may contribute to flow only over a short time period. Their flow capacity, however, may exceed the volume flux density of the soil matrix by orders of magnitude. Water transported constituents, which are prone to adsorption by the soil matrix during seepage, are likely to break through a soil layer via macropores with almost unaltered concentrations. In addition, macropores are considered one of the most dynamic soil structure elements with respect to land use practice and soil formation processes (Germann and Beven, 1985).

It is not surprising, thus, that Grant et al. (1991) dare to say that few problems in soil physics present more difficult practical problems than do water and solute flow through macropores. According to Jarvis et al. (1991), to date only a few models have been developed that can account for macropore flow processes. Actually, several models of water flow in macropores have been developed (Edwards et al., 1979; Hoogmoed and Bouma, 1980; Beven and Germann, 1981; Germann and Beven, 1985; Germann and Beven, 1986; Beven and Clarke, 1986; Corwin et al., 1991; Grant et al., 1991; Jarvis, 1991), but, according to Grant et al. (1991), few include realistically the effects of soil hydraulic property variability and rainfall runoff dynamics, factors these authors believe should be included to predict macropore soil-water flow in soils subjected to natural rainfall.

3.3.1 - Preferential water flow models

The great majority of the available deterministic models for water flow in a soil with macropores use a domain concept to model combined macropore/matrix systems. The micropores are treated as one domain that conforms to hydraulic principles based on Darcy's law, and the macropores are a second domain, with the description of interactions between the domains completing the model. According to Beven and Germann (1981), the use of a domain concept in modelling a combined system was introduced because approaches based on Darcy's law and the Richards equation had been well proven in the past, and, so, any model of a combined micropore/macropore system should reduce to a Darcy-type model when there are no macropores.

Beven and Germann (1982) identify five components that should be specified in this kind of model: the nature of flows in the matrix domain (generally modelled by Richards' equation, with the boundary conditions specified based on simplifications of the geometry of the aggregate), the nature of flows in the macropore system (which may often be laminar, but, as the macropores are not generally smooth sided, it will hasten the transition of quasi-turbulent or turbulent flow), the spatial and temporal characteristics of the macropore network (with its inherent variability), the interaction between the domains (which depends on the supply of water within the macropores and the hydraulic conditions within the matrix), and the initiation of flow in the macropores. None of the available models are entirely satisfactory on all five criteria listed above.

Beven and Germann (1981) noted the use of a domain concept to model water flow in a combined micropore/macropore system by Muskat, in 1946, in a study of saturated flow

through fissured limestone. Later, Edwards et al. (1979), Hoogmoed and Bouma (1980), and Jarvis et al. (1991) also used this approach, generally based on the conceptualization of flow in soils with macropores similar to that presented by Beven and Germann (1982) and described in section 2.3.2.

The model of Edwards et al. (1979) tries to simulate the flow in a cylindrical column having a central, surface-connected, noncapillary-sized hole extending partway into the column. It is assumed that the soil and the initial water content are uniform with depth, and that the soil column receives heavy precipitation of constant intensity. Also, air can freely escape from the lower end of the column. Flow in the micropores is treated in two dimensions (vertically and radially away from the macropore) using a solution of the Richards' equation. Flow in the macropore is modelled using a simple accounting procedure for given depth increments with input at the surface and infiltration losses to the micropores at the side of the macropore. It is assumed that, during heavy rainfall, excess rain that does not infiltrate through the soil surface flows into the hole. After the hole fills with water, excess surface water is allowed to runoff. So, the sequence of simulation is: vertical infiltration through the soil surface; water ponding in the hole; lateral (radial) infiltration from the hole; and runoff. Numerical experiments were performed with this model in order to evaluate the effect of a surface-connected hole upon infiltration, by comparing the results with and without a hole. Also, the effect of hole diameter, hole depth, and number of holes per unit area were studied.

The model uses a very simplified characterization of the progress of wetting in the macropore. It does not consider possible effects either of air entrapment or movement in the column, or of hydraulic resistance to flow of surface water into the hole. It simulates only the effect of a single pore and, so, it does not account for the interconnection of the macropores, rather treating the system as a collection of regularly spaced surface-connected vertical holes in a field. Even so, it was able to demonstrate the importance of macropores on infiltration and runoff, at least under conditions of heavy rainfall, and the effects of the geometry of the hole (depth and diameter) and the number of holes per unit surface area.

Hoogmoed and Bouma (1980) developed a model to simulate infiltration, including preferential flow into clay soils with shrinkage cracks. The model combines vertical infiltration into the upper surface of the soil, downward flow into the cracks, and horizontal absorption from the cracks into the soil. Vertical infiltration into the upper surface of the soil was simulated with an one-dimensional solution of the Darcy equation. Depth of ponding at any given time is determined by the difference between rain intensity and infiltration rate. Flow of the water into

the cracks from the surface starts when the ponding depth reaches a preset threshold value, and the excess water (rainfall minus vertical infiltration into the soil) flows into the cracks. Water flowing into the cracks is absorbed horizontally into the soil, according to Richards' equation. The model was applied to a 20 cm thick soil, with a threshold value of ponding depth of 0.2 cm.

The authors tried to develop a quasi three-dimensional model, including vertical infiltration into the surface, depth of penetration of the wetting front and moisture content of the wetted zone. According to Beven and Germann (1982), this model includes an important innovation in the way in which the wetted surface area in the macropores changes over time is accounted for and uses relationships for surface wetting based on the detailed experimental work of Bouma and Decker (1978). However, as the previous model, it still uses a simplified accounting procedure for the calculation of flow within the macropores.

The model of Beven and Germann (1981) also combines flow in the micropore system, flow in the macropore system and the interaction between these two domains. The flow in the micropores is simulated through Richards' equation for a one-dimensional vertical system, assuming single valued (non-hysteretic) functions for the diffusivity, $D(\theta)$, and for the hydraulic conductivity, $K(\theta)$. The macropore flow model uses laminar film flow assumptions to derive a relationship between moisture content and flow. It assumes a separation into saturated and unsaturated zones and also supposes that an approximate size distribution can be made up of a collection of N class sizes of circular pores and M class sizes of cracks. Fully saturated laminar flow is obtained through the relations developed by Childs (1969). A similar development for partially saturated flow leads to a kinematic wave equation, which is solved by an implicit finite difference scheme. The interaction between the domains is controlled within the micropore system, with the form of a Darcy-type flow in a horizontal direction. Rainfall in excess of infiltration into both macropores and micropores is assumed to be removed instantaneously as surface runoff. At the lower boundary a condition of constant water content is assumed.

This model is an important step through a more general model to simulate the effect of a realistic distribution of pores at given depths in the profile of a field soil. However, according to Beven and Germann (1982), it still uses a very simple description of the interaction between macropores and matrix. Besides that, the authors discussed the problems of scale associated with using such a macroscopic representation of flow in the channels. The previous approach, adopted by Edwards et al. (1979), is to restrict the scale of interest to that corresponding to the representative elementary volume (REV) for the micropore system, with single macropores, then imposing special boundary conditions for a micropore solution. In the model of Beven and

Germann (1981), the predictions are made at the scale of the REV for the macropores, which is very much larger than the REV for the soil matrix and also significantly larger than many measurement techniques. Consequently, it brings difficulty to validate its predictions by measurements in the field.

The use of kinematic wave approaches to macropore flow was also presented by Germann (1985), applied to water flow in a saturated soil matrix; by Germann and Beven (1985), who expanded this approach to include water uptake into the matrix of the top soil and that surrounding the macropores; and by Germann and Beven (1986), who used kinematic wave theory to assess the distribution of a macropore conductance parameter, through the use of a distribution function approach. Also, a boundary layer infiltration model, which was extended to lateral flow in a sloping soil, was developed by Germann (1990). In all these works, there is the aim of trying to move from the two-domain in the direction of more unified theories, which could better represent the gradual transition between macropores and capillary-sized pores. This aim is sought through the representation of the macropore system as a collection of independent pathways. Also trying to avoid the representation of soil water as divided in two phases, Steenhuis et al. (1990) proposed a model in which several pore water velocities are defined. The flow paths are essentially in the vertical direction with gravity being the main driving force, and the interconnection of different flow paths in the soil results in a mixing between the pore groupings. The multiple domains were obtained by grouping pore sizes through piecewise linear approximations of the unsaturated conductivity function. They assumed the hydraulic gradient remaining relatively constant near unity, implying that the forces associated with the matric potential gradient are negligible compared with the gravitational forces. This assumption can be applicable to preferential downward water movement, but it will fail to represent capillary rise of water.

More recent examples of the two-domain approach include various simplifications, trying to facilitate their application to practical field problems. The model MACRO (Jarvis, 1991; Jarvis et al., 1991) assumes gravity flow of water and a simple power law function to represent the conductivity in the macropore region and uses a numerical solution to Richards' equation for transient water flow for the micropores. The exchange between domains is null if the micropores are saturated, otherwise being computed by an empirical source/sink term. This model employs a very simple empirical description of the interaction between macropores and matrix and uses an empirical relation to describe the value of the conductivity in the macropore region. Chen and Wagenet (1992), on the other hand, used the Chezy-Manning equation to describe the flow in the macropores, while adopting the classic approach of the Richards' equation for the flow in

the matrix domain, and Philip's infiltration equation to represent mass exchange between the two regions. Their representation considers only horizontal movement between the macropore and matrix domains and assumes turbulent flow in the macropores. Gerke and Van Genuchten (1993) proposed a conceptualization which assumes that the Richards' equation can be applied to both pore systems, trying to produce a model with all parameters related to physical properties of the medium. Although their representation simplifies the description of water flow in a structured porous medium and is able to simulate various degrees of nonequilibrium, it may not be strictly valid for the macropore region when, for high velocities, the flow regime changes from laminar to turbulent. Besides that, some of the parameters are not easily measured experimentally.

It is important to emphasise that there have been no significant theoretical advances in field-scale models. Usually, these models adopt simplified assumptions to compute macropore flow, as reported by Thomas and Beasley (1986), who adapted the ANSWERS model to run in forested catchments through the inclusion of simplified seepage and pipe flow components. Actually, the multiplicity of flow paths that water can take downhill could make specification of interactions between macropore and matrix very complex, so that constructing such a model is not a trivial task (Beven and Germann, 1982).

The statistical and stochastic models presented in section 3.2.1 can be useful alternatives to represent the spatial variability of soil properties. However, they do not specifically simulate preferential flow, although they implicitly consider its consequences. Examples of statistical and stochastic techniques used specifically to simulate the macropore flow are presented and discussed below.

Smettem and Collis-George (1985b) used a Monte Carlo simulation to predict the distribution of steady state infiltration rate values for different infiltrometer ring sizes in a soil with vertical macropores, assuming that macropores greater than 0.5 mm diameter are randomly distributed with a density distribution described by the Poisson series. Arithmetic mean numbers of macropores for four pore radius classes were determined. The computations were done by determining the average pore radius in each radius class and assigning a steady state volume flux by an empirical equation. Next, the Poisson parameter, λ_p , was estimated from the mean number of macropores in a size class for a specified ring size. The Poisson equation was approximated by generating 1000 λ_p random integers in the range 0-1000 for each class and counting the repetition frequency. Finally, 1000 values of the macropore volume flux density were obtained by integrating the volume flux through the number of classes and the number of pores in each class. The results indicate that, in a soil with well-vented macropores, hydraulic properties are

influenced by the number, size, areal and temporal patterns of the macropores.

The model was useful to indicate the importance of the presence and physical characteristics of macropores in the preferential flow. It provided a useful method of determining the distribution of steady state infiltrometer rate at different sampling scales. However, it considered only vertical infiltration through an infiltrometer ring, neglecting the effects of horizontal interactions. Besides that, increasing difficulties occur for actual field conditions, because it would be necessary to have a large representative sample area to integrate the effects of macropores, as small areas would produce skewed parameter distributions. And finally, the consideration of steady state flow can reduce its utility for simulation of practical conditions.

Beven and Clarke (1986) used a statistical approach to tackle the scale problem. They formulated their model for the case of a single channel, using the assumptions of the Green and Ampt (1911) model of vertical infiltration to describe infiltration from the walls and base of a cylindrical channel. After the infiltration capacity of the soil matrix alone is exceeded, there is a time to ponding, after which the soil surface becomes saturated and the water flows into the channel, under the assumptions of laminar flow. After the channel is filled, the infiltration capacity of the soil depends both on the vertical infiltration at the surface and infiltration at depth through the walls and sides of the channel. The radial infiltration from the channel wall occurs still under the Green-Ampt assumptions, now adapted for horizontal infiltration with radial symmetry. The infiltration from the channel base is also estimated under these assumptions, now considering an effective hydrostatic pressure head equal to the depth of the macropore. This model was then generalised to a statistical population of channels with radii and depths following probability distributions $p(r)dr$ and $p(z)dz$, respectively, and with the vertical axes of the channels intersecting the horizontal soil surface at points which have a Poisson distribution. In this way, it was possible to incorporate the sampling problem for spatially extensive channel populations directly into the calculation of variances of moisture contents at a given depth.

This model has presented an interesting statistical framework for evaluating the effect of channelling flow on infiltration into soil blocks of a given area. It presupposes minimal information about a channel network in a soil, namely a distribution of sizes, a distribution of depths, and a distribution of numbers per unit area. In addition, a more realistic, although simple, treatment of the interactions between channels and soil matrix than those used in the previous methods was developed. On the other hand, as noted by the authors themselves, the case of a network of channels involving junctions between channels is not analyzed, nor the case

where the supply of water to the channels is limited by the application rate, so that only part of the channel walls are wetted. And also, the variability of the spatial and temporal characteristics of the macropore network is neglected.

Grant et al. (1991) hypothesise that a useful model of macropore soil-water flow may be derived from well-documented variability in soil hydraulic properties. They developed a simple stochastic model of infiltration where probability density functions (pdf) for cumulative infiltration, infiltration rate, and infiltrating-water flux are proposed. The pdfs for cumulative infiltration and infiltration rate are derived by assuming that the saturated hydraulic conductivity is a lognormal-distributed random variable. For a flat and smooth soil surface the pdf for infiltrating-water flux is derived from the pdf for infiltration rate, by assuming that water failing to infiltrate into portions of the soil with lower infiltration rates will flow over the soil surface, eventually being accepted by areas with higher infiltration rates. Macropore soil water flow is predicted by the pdf for infiltrating-water flux in a more pronounced way as the rainfall rate approaches the mean infiltration rate.

This approach is quite simplified, neglecting important factors that could have a strong influence on infiltration, such as slope and surface roughness. It also uses empirical relations to derive its pdfs, not being concerned with the explanation of the real physical phenomena involved. However, it can provide a useful tool for the simulation of the flow, since it uses simple stochastic relations instead of trying to fully represent the geometry of the aggregate, as in the domain concept. Also, its results clearly show the necessity to include infiltration rate variability and runoff contributions to infiltrating-water flux in models of macropore soil-water flow.

3.3.2 - The numerical model MACRO

MACRO is a deterministic model of non-steady state water and solute transport in macroporous field soils which includes a comprehensive treatment of the field water balance, dealing with vertical unsaturated soil-water flow, rainfall interception, root water uptake, saturated fluxes to tile drains and irrigation. It does not provide any new physically based concept for modelling water flow in soils with macropores; instead, it tries to put together simple formulations and well known concepts in order to provide a conceptual framework that can be easily applied to field soils, with or without macropore flow. It was selected for this thesis, in order to test the effects of preferential movement in unsaturated soil water flow.

Processes related to solute transport were not simulated in this thesis. For this reason, the features related to these processes are not presented here. A detailed description of the complete model can be found in Jarvis (1994).

The model may be run in either one or two flow domains with no change in the hydraulic properties assumed to characterise the soil. In two domains, macropores and micropores operate as separate, though interacting, flow regions, each characterised by a degree of saturation, a conductivity and a flux. In the one-domain case, the model reduces to the standard Richards' equation. The total porosity in a soil layer is partitioned into micropores and macropores at a given boundary water content (θ_b) and boundary potential (ψ_b), corresponding to a boundary hydraulic conductivity (K_b). When MACRO is run in one flow domain and θ is in the macropore region ($\theta > \theta_b$), ψ is computed by a linear $\psi(\theta)$ function and a simple power law function is used to represent $K(\theta)$. In the micropore region ($\theta < \theta_b$), Brooks and Corey (1964) moisture retention and Mualem's (1976a) hydraulic conductivity functions are adopted. These relations are defined by:

$$\begin{aligned} \psi &= \psi_b \left[\frac{\theta_s - \theta}{\theta_s - \theta_b} \right] \quad ; \quad K = K_b + (K_s - K_b) \left[\frac{\theta - \theta_b}{\theta_s - \theta_b} \right]^{n^*} \quad \text{if } \theta_b < \theta \leq \theta_s \\ \psi &= \psi_b \left[\frac{\theta - \theta_r}{\theta_b - \theta_r} \right]^{-\frac{1}{\lambda}} \quad ; \quad K = K_b \left[\frac{\theta - \theta_r}{\theta_b - \theta_r} \right]^{n^* + 2 + \frac{2}{\lambda}} \quad \text{if } \theta_r \leq \theta \leq \theta_b \end{aligned} \quad (3.4)$$

where n^* is an empirical exponent accounting for pore size distribution in the macropores.

In the two-domain case, water flow in the macropores is calculated using Darcy's equation assuming a unit hydraulic gradient (i.e. laminar flow under gravity: ψ is not required), while equivalent expressions to those in equation 3.4 are used to characterise the soil hydraulic properties:

$$\begin{aligned} \psi_{mi} &= \psi_b (Se_{mi})^{-\frac{1}{\lambda}} \\ K_{mi} &= K_b (Se_{mi})^{n^* + 2 + \frac{2}{\lambda}} \quad ; \quad K_{ma} = K_{s_{ma}} (Se_{ma})^{n^*} \\ Se_{mi} &= \frac{\theta_{mi} - \theta_r}{\theta_b - \theta_r} \quad ; \quad Se_{ma} = \frac{\theta_{ma}}{e_{ma}} \end{aligned} \quad (3.5)$$

where the subscripts $_{mi}$ and $_{ma}$ refer to micro- and macropores respectively and e_{ma} is the macroporosity. In order to account for swelling and shrinkage, e_{ma} and Ks_{ma} are represented by

$$\begin{aligned} e_{ma} &= e_s + p(\theta_b - \theta_{mi}) \\ Ks_{ma} &= (Ks_{min} - Kb) \left[\frac{e_{ma}}{e_s} \right]^{m^*} \end{aligned} \quad (3.6)$$

where p is the slope of the shrinkage characteristic, e_s is the minimum value of macroporosity, given by $(\theta_s - \theta_b)$, Ks_{min} is the minimum saturated hydraulic conductivity of a swelling soil attained when $e_{ma} = e_s$, and m^* is an empirical exponent.

Empirical functions are also used to describe the leaf area index (LAI), root depth and root water uptake. The leaf area index is a function of the day number in the year and two empirical exponents (x_1 and x_2), so that LAI is zero before crop emergence, rises up to a maximum value at the day of maximum leaf area, and then decreases to its value at harvest. Root depth is constant for a perennial crop, while for an annual crop it increases linearly from a minimum value at crop emergence to attain a maximum value when the crop has a maximum leaf area. The calculated LAI is used to partition the total evapotranspiration, provided by the user, into soil evaporation and transpiration, using an empirical relation. Root water uptake (U_r) is calculated from evaporative demand, root distribution and soil water content. The potential root water uptake is obtained as a function of the amount of water stored in the canopy and the transpiration, by using an empirical correction factor to account for enhanced evaporation loss from a wet canopy. Root length is assumed to be distributed logarithmically with depth, according to an empirical root distribution parameter (ζ). All these empirical relations are described by Jarvis (1994).

Richards' equation is used to calculate vertical water fluxes in unsaturated soil, including a sink term accounting for root water uptake (U_r) and a sink/source term for the exchange of water between macro- and micropore domains (U_w):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] - U_r \pm U_w \quad (3.7)$$

Water exchange is treated as an approximate first-order process, neglecting the effect of gravity and assuming a rectangular-slab geometry for the aggregates:

$$U_w = \frac{3 D_w \gamma_w}{d^2} (\theta_b - \theta_{mi}) \quad (3.8)$$

$$D_w = \frac{D_{\theta b} + D_{\theta mi}}{2} Se_{ma}$$

where: D_w = effective water diffusivity;

γ_w = scaling factor, assumed equal to 0.8;

d = effective diffusion pathlength, equal to half the aggregate width;

$D_{\theta b}$ = water diffusivity at the boundary water content;

$D_{\theta mi}$ = water diffusivity at the current micropore water content

For the Mualem/Brooks-Corey model, $D_{\theta mi}$ is given as:

$$D_{\theta mi} = \frac{Kb \psi_b (Se_{mi})^{n+1+\frac{1}{\lambda}}}{\lambda(\theta_b - \theta_r)} \quad (3.9)$$

while $D_{\theta b}$ is obtained by setting Se_{mi} in equation 3.9 to unity.

The boundary condition at the soil surface controls the partitioning of net precipitation between micro- and macropores. The surface boundary condition is chosen in order to avoid over-saturation in the micropores in the top soil layer:

$$\begin{aligned} I_{mi} &= R & ; & & I_{ma} &= 0 & & \text{if } R \leq I_{max} \\ I_{mi} &= I_{max} & ; & & I_{ma} &= R - I_{max} & & \text{if } R > I_{max} \end{aligned} \quad (3.10)$$

where: R = net rainfall;

I_{mi} = input to micropores;

I_{ma} = input to macropores;

I_{max} = infiltration capacity of the micropores

The infiltration capacity of the micropores is approximated by

$$I_{\max} = \Delta z_{sl} (\theta_{b,sl} - \theta_{sl}) + \Delta t q_{\text{out}(sl)} \quad (3.11)$$

where the subscript *sl* refers to the surface soil layer and $q_{\text{out}(sl)}$ is the amount of water flowing out of this layer.

Five different bottom boundary conditions are available: (1) constant hydraulic gradient; (2) zero flux; (3) constant pressure head; (4) a water table located in the profile; and (5) a lysimeter with free drainage. The first two options are classical Neumann-type boundary conditions and the third option is a standard Dirichlet-type boundary condition. For the remaining two options, the calculated flux rate depends on the direction of the hydraulic gradient at the base of the profile: if a lysimeter boundary condition is adopted, the flux out of the soil profile is equal to $K(d\phi/dz)$ when the hydraulic gradient is positive, and zero otherwise; for the bottom boundary condition of a water table located in the soil profile, the flux out of the soil profile is zero when the hydraulic gradient is positive, and is equal to $K(d\phi/dz)$ otherwise.

The numerical solution for this model was obtained by decoupling calculations with respect to the flow domains. Vertical water fluxes are first calculated in the micropore domain. When there is excess of water, they are routed to the macropores. Also, several different techniques are employed: Richards' equation is solved by explicit finite difference procedures; stability criteria for water flux is used to automatically choose a time step for maximum speed of execution, while ensuring numerical stability of the explicit solution; average soil hydraulic properties are determined at the boundaries between adjacent soil layers, tending to smooth out differences in hydraulic properties; an implicit, unconditionally stable, numerical procedure is used for the macropores.

A sensitivity analysis and also indication on appropriate methods for input parameter estimation for the MACRO model are presented by Jarvis (1991). These indications are used as general rules when determining the parameter values in this thesis.

3.4 - Modelling hysteresis and air entrapment

Successive cycles of wetting and drainage are present in most applications related to unsaturated flow, and, consequently, the hysteretic nature of the hydraulic properties of the soil plays a role in these processes. However, unanimity does not exist concerning the significance of hysteresis on field scale flow and transport predictions. According to Kaluarachchi and Parker

(1987a), while a number of studies have demonstrated that substantial errors may be incurred by ignoring hysteresis, others have found effects to be rather small. Although various attempts have been made to describe hysteresis mathematically, Mualem (1984b) says that it is frequently ignored in numerical models, mainly due to the complexity of the hysteresis theories and of the numerical solution of unsaturated flow problems, which is greatly increased with alternating boundary conditions if hysteresis is included, and also due to the need of a large amount of data for model calibration.

3.4.1 - Mathematical models of hysteresis and air entrapment

A number of empirical or theoretically based models for describing hysteresis in the soil water retention function have been developed. The theoretical models are based on the domain theory of capillary hysteresis, while the empirical techniques rely on the analysis of observed moisture retention characteristics shape and properties, generally by assuming that scanning curves can be scaled from the main hysteresis loop (Kool and Parker, 1987; Viaene et al., 1994). According to Kaluarachchi and Parker (1987a), $\theta(\psi)$ exhibits closure at $\psi=0$ for most of these models, indicating residual air entrapment to be either nonexistent or independent of saturation history. This can be a constraint to field applications, where variations in air entrapment can substantially affect water flow.

The domain theory describes a porous medium as a collection of elementary pore domains, whose properties are independent of the states of adjacent pores. The pore domain has only two stable states, either empty or full. In a wetting process, the pore is empty until the wetting capillary head (ψ_w) is reached, when it flips over to a filled state. In drainage, the pore remains water filled until the drying capillary head (ψ_d) is achieved. At this moment the pore is totally drained. Each pore is characterised by two length scales which can be interpreted as the radius of the pore and the radius of its constricted connection with other pores. These radii can be uniquely related to the wetting and drying capillary heads, ψ_w and ψ_d . Knowledge of a pore-water density distribution function, $f(\psi_d, \psi_w)$, allows determination of the moisture content by integrating over the domains that are filled after any series of wetting or drying. The independent domain model based in this theory is calibrated on the basis of a family of primary scanning curves (Mualem and Morel-Seytoux, 1979a; Kool and Parker, 1987; Viaene et al., 1994).

Poulovassilis (1962) observed good agreement between theoretical predictions by the independent domain model and measured scanning curves for glass beads. Poulovassilis and

Childs (1971), however, did not find as good agreement when using sand. Mualem and Morel-Seytoux (1979a) report that other investigators reported considerable discrepancies between the theory and observations, for materials such as glass beads, sand and various loam soils.

Topp (1971) observed that pore interaction effects can be significant, and suggested a dependent-domain theory, which accounts for pore blockage against air entry near saturation and air blockage against water entry at low water content. Although improvements were obtained with this model, a large amount of measured data is necessary, including sets of both drying and wetting families of scanning curves.

Mualem (1973) suggested a variant of the independent domain theory, called Model I. This model uses a similarity hypothesis, according to which $f(\psi_d, \psi_w)$ is represented as a product of two independent distribution functions, allowing its calibration solely from the measured main hysteretic loop, with the scanning curves expressed analytically. A more flexible independent domain model, Model II, was suggested by Mualem (1974). This model accounts for a reversible contribution of the pore domains to the wetting and drying processes, besides including effects of entrapped air and allowing calibration based only on the measured main loop. For soils having a narrow pore size distribution and a major portion of the hysteretic loop in the range of the air entry, Mualem and Dagan (1975) propose the use of Model III, a dependent domain model which takes into account the effect of pore blockage against air entry in drying processes. A generalised version of this model, Model IV, was proposed by Mualem (1976b), accounting also for pore blockage against water entry. A higher degree of accuracy is achieved, but these dependent models require data of primary scanning curves in addition to the two main branches. Simplifications of these models were developed by Parlange (1976), Mualem (1977), Mualem and Miller (1979) and Mualem (1984a). These simplifications require reduced amounts of experimental data, but result in a cruder representation of the data.

Several empirical models for describing hysteretic flow were also developed (Hanks et al., 1969; Dane and Wierenga, 1975; Kool and Parker, 1987; Parker and Lenhard, 1987). Some of these algorithms fail to provide closure of the scanning loops, so that the predicted water content tends to decrease when the tension is varied cyclically, creating a "pumping effect", as described by Klute and Heermann (1974). Jaynes (1984) used experimental data to compare the performance of Model II (Mualem, 1974) with three of these empirical models: the Point method (Dane and Wierenga, 1975), the Linear method (Hanks et al., 1969) and his own Slope method. The Point method calculates the value of θ at the new tension from the θ values of the main wetting and drying curves. The Linear method approximates the scanning curves by a straight

line of arbitrary slope spanning the main wetting and drying curves. The Slope method uses the slopes of the main wetting and drying curves to compute the differential soil water capacity, $C=d\theta/d\psi$. While closure of the scanning curves is ensured for Model II and for the Linear method, the Slope and Point methods take no special precaution to create scanning curves that close, resulting in pronounced pumping effect, which could significantly affect their performance when simulating numerous successive wetting-drying cycles in soils. None of these models considers air entrapment. The four methods yielded similar results for a simple unsaturated hysteretic flow problem, and Jaynes favoured the Linear method because of its simplicity.

Kool and Parker (1987) combined Van Genuchten's equation with an empirical model which scales scanning drying curves from the main drying curve and wetting scanning curves from the main wetting curves. Drying scanning curves are obtained by replacing θ_s by θ_s^* , which scales the main drying curve to pass through the reversal point and the residual moisture content. Wetting scanning curves are obtained by replacing θ_r by θ_r^* , which scales the main wetting curve to pass through the reversal point and the saturated moisture content. Effects of air entrapment are also included in the model, using an empirical relation developed by Land (1968). The model compared well with Mualem's Model II for two flow problems in which pumping was not important. Its main advantages are its small number of parameters, which minimise data requirements for calibration, and the fact that it involves little additional computational effort compared to a nonhysteretic simulation. One main disadvantage is that the scanning loop is not closed, so that pumping effects are present for cyclic variations of the pressure head, as commented above.

Parker and Lenhard (1987) employed an empirical procedure to rescale main branches functions to pass through appropriate reversal points, enforcing closure of scanning loops. This is achieved through an interpolation between the two previous reversal points for each chord in a scanning loop. The method performed quite well against experimental data by Parker and Lenhard (1987) and also by Lenhard et al. (1991). This model presents the advantages of the algorithm of Kool and Parker (1987), i.e., small number of parameters and little additional computational effort, and, besides that, it also prevents pumping effects. However, it needs the knowledge of two previous reversal points which can bring the necessity of large storage requirements. Also, when the simulation starts in a scanning curve, these two reversal points have to be known in order to set the initial conditions for simulation, which can be a problem for field applications.

Hysteretic phenomena are observed also in the $K(\theta)$ and the $K(\psi)$ relationships. The

domain theory can be used to predict the hysteresis of $K(\theta)$ and the $K(\psi)$, as proposed by Mualem (1976b). Some of the empirical models also consider the hysteresis in the hydraulic conductivity (Kool and Parker, 1987; Lenhard and Parker, 1987). However, the magnitude of the $K(\theta)$ hysteresis is very limited, being almost a unique function (Mualem and Morel-Seytoux, 1979b; Kool and Parker, 1987) and, consequently, many practical applications use the unique function $K(\theta)$ instead of a $K(\psi)$ function.

3.4.2 - The adopted hysteresis algorithm

A model of hysteresis considering air entrapment on water flow in the unsaturated zone based on those presented by Kool and Parker (1987) and by Parker and Lenhard (1987) was adapted and tested in order to run in conjunction with the SPW1 model. One of the main advantages of this model is its parametric simplicity, which facilitates its implementation with minimal effort, as it does not require any parameter that was not previously included in model SPW1. On the other hand, it had the disadvantage that it is necessary to know two previous reversal points, bringing difficulties to its utilization with field data, when the whole previous history of the experiment is unknown. In order to allow the use of the hysteresis model when the previous reversal points are unknown, an algorithm to estimate these reversal points was developed, providing the initial conditions for simulation. A new version of SPW1 model, called SPW1hyst, incorporates the hysteresis model and the initial conditions algorithm (and also includes the methodologies adopted by MACRO model to represent, in one flow domain, the soil water retention curve and the unsaturated hydraulic conductivity). In the following sections, the model for hysteresis simulation and the algorithm for setting the initial conditions are presented.

3.4.2.1 - Model for hysteresis simulation

It is assumed that the main drying and wetting curves can be described by Brook-Corey's (1964), Van Genuchten's (1980), or MACRO's one flow domain relationships, as presented in equations 2.9, 2.10 and 3.4, respectively. The main drying curve is denoted by $\theta^d(\psi)$ and the main wetting curve by $\theta^w(\psi)$. To obtain the most general description, all parameters of the characteristic curve are considered as variables. So, adopting Van Genuchten's equation, the main hysteretic loop is described by the parameter vector $(\theta_s^w, \theta_r^w, \alpha^w, n^w)$ for the main wetting curve and $(\theta_s^d, \theta_r^d, \alpha^d, n^d)$ for the main drying curve, yielding a total of eight unknown parameters. For the case of Brook-Corey's or MACRO's one flow domain relationships, the parameter vectors are $(\theta_s^p, \theta_r^p, \lambda^p, P_b^p)$ and $(\theta_s^p, \theta_r^p, \lambda^p, \psi_b^p)$, respectively, where p is an index

denoting whether a drying ($p=d$) or wetting ($p=w$) curve is considered. A simplification may be obtained by setting $\theta_r^d = \theta_r^w = \theta_r$.

To describe the scanning curves, it employs an empirical procedure which rescales main branch functions to pass through appropriate reversal points. In the present method, closure of scanning loops is enforced, preventing the pumping effect that would occur when pressure head undergoes cyclic variations, as commented by Klute and Heermann (1974) and by Jaynes (1984). Rescaling the main curves is achieved via

$$\theta(\psi) = [\theta^p(\psi) - \theta^p(\psi_{l-1}^A)] \frac{[\theta_l^A - \theta_{l-1}^A]}{[\theta^p(\psi_l^A) - \theta^p(\psi_{l-1}^A)]} + \theta_{l-1}^A \quad (3.12)$$

where (ψ_l^A, θ_l^A) and $(\psi_{l-1}^A, \theta_{l-1}^A)$ represent the most recent and preceding reversal points, respectively, regardless of path direction and $l-1$ is the order of the scanning curve. If we designate $l=0$ at $(\psi, \theta) = (-\infty, \theta_r)$ and $l=1$ at $(\psi, \theta) = (0, \theta_r^d)$, then any path will be described by equation 3.11 with $p=d$ (drainage) for odd l and $p=w$ (wetting) for even l .

When the closure of a scanning curve occurs, l must be decremented, as $\theta(\psi)$ resumes its previous path. That is, when $\theta > \theta_{l-1}^A$ for even l (wetting) or when $\theta < \theta_{l-1}^A$ for odd l (drainage), then l is decremented by 2 and the reversal point potentials and moisture contents of the closed loop may be purged from memory. Since potentials and moisture contents for $l+1$ reversal points will need to be stored for all spatial locations in a numerical simulation, storage requirements may become large when high-order scanning curves occur. In practice it is necessary to impose a limit to the scanning curve of order $l-1$. When this limit is reached, $\theta(\psi)$ may be regarded as nonhysteretic until closure brings l back into the allowed range. In most circumstances, hysteretic effects will become small beyond second- or third-order scanning curves ($l=3,4$) and the empirical nature of the interpolation scheme presented here probably does not justify refinement beyond this level (Parker and Lenhard, 1987).

The effects of air entrapment are incorporated in the model using relationships given by Aziz and Setari (1979). These relationships were actually developed by Land (1968), after analysing data from several previous papers and finding from these data that the difference in the reciprocals of the initial and final gas saturation (S_{gi}^* and S_{gr}^* , respectively) are approximately constant for a given sand. Observing that residual saturation increases with the

initial gas saturation, and that, when the initial gas saturation is unity, the residual gas saturation is the maximum gas saturation (S_{gr}^*), Land empirically stated that

$$\frac{1}{S_{gr}^*} - \frac{1}{S_{gi}^*} = \frac{1}{S_{gr}^*_{\max}} - 1 \quad (3.13)$$

Defining the residual saturations for air-water as functions of the water content leads to

$$S_{gr}^* = \frac{\theta_s^d - \theta_s^w}{\theta_s^d - \theta_r} \quad (3.14)$$

$$S_{gi}^* = \frac{\theta_s^d - \theta_s^A}{\theta_s^d - \theta_r} \quad (3.15)$$

$$S_{gr}^*_{\max} = \frac{\theta_s^d - \theta_s^w}{\theta_s^d - \theta_r} \quad (3.16)$$

where θ_s^w is the water content at saturation upon wetting along an arbitrary primary scanning curve beginning at a reversal point (ψ_2^A, θ_2^A) . Substituting equations 3.14, 3.15 and 3.16 into equation 3.13 we obtain

$$\theta_s^w = \theta_s^d - \theta_{ar} \quad (3.17)$$

with

$$\theta_{ar} = \frac{1}{[(\theta_s^d - \theta_2^A)^{-1} + (\theta_s^d - \theta_s^w)^{-1} - (\theta_s^d - \theta_r)^{-1}]} \quad (3.18)$$

where θ_{ar} is the residual air entrapment.

According to Kool and Parker (1987), the relationships obtained are empirical in nature and are not expected to describe the process of air entrapment very accurately, but, lacking more rigorous procedures, they provide a useful approximation. Their advantage is that they introduce no additional parameters and can be incorporated directly into the available model. Parker and Lenhard (1987) assume that equation 3.18 holds for higher order scanning curves associated with a specified primary wetting path. Figure 3.1 graphically describes all the features presented so far.

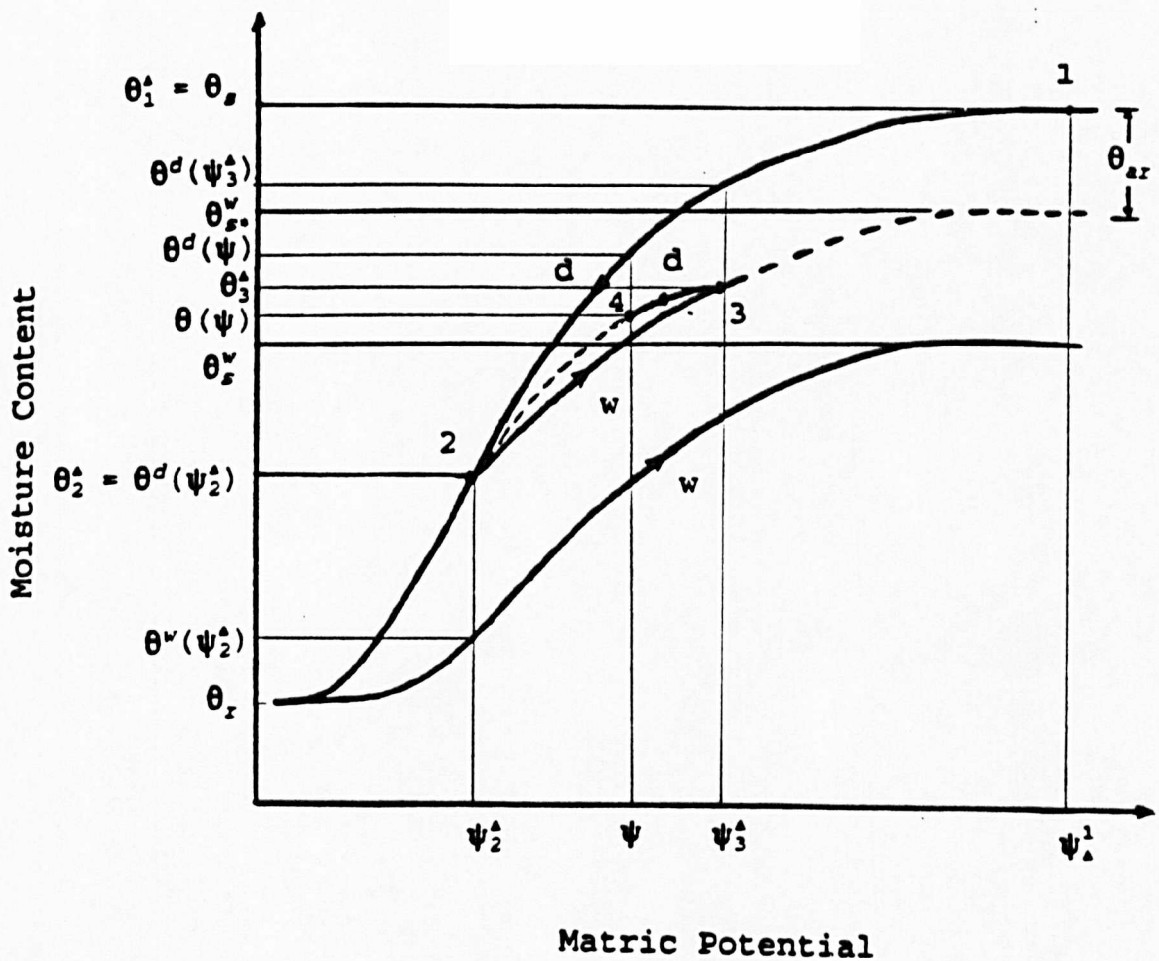


Figure 3.1 - Hypothetical moisture content path as described by the hysteresis model

3.4.2.2 - Algorithm for setting the initial conditions

As previously mentioned, the selected model has the disadvantage that it is necessary to know two previous reversal points to simulate any scanning curve, which brings difficulties to its utilization with field data. The following algorithm was developed in order to estimate these reversal points and provide the necessary initial conditions for simulation.

Examining equation 3.12, it is possible to realise that, for each main or scanning curve in the simulation path, the two previous reversal points are constants. So, equation 3.12 can be represented for a specified chord as

$$\theta(\psi) = [\theta^p(\psi) - C1^{\text{chord}}]C2^{\text{chord}} + C3^{\text{chord}} = \theta^p(\psi) C2^{\text{chord}} + C4^{\text{chord}} \quad (3.19)$$

where $C1^{\text{chord}}$, $C2^{\text{chord}}$, $C3^{\text{chord}}$ and $C4^{\text{chord}}$ are constants for each chord in the simulation path, as represented in figure 3.1. If any two points are known in a chord, it is possible to compute the values of $C2^{\text{chord}}$, and $C4^{\text{chord}}$ for this chord and, with them, the previous reversal points can be obtained.

If any two points are known in a scanning first-order (primary) wetting curve, such as in chord 2-3 in figure 3.1, it is possible to compute $C2^{2-3}$ and $C4^{2-3}$. Applying equation 3.19 at point 2 in figure 3.1:

$$\theta_2^{\Delta} = \theta^d(\psi_2^{\Delta}) = \theta^w(\psi_2^{\Delta}) C2^{2-3} + C4^{2-3} \quad (3.20)$$

The values of ψ_2^{Δ} and θ_2^{Δ} are obtained by solving equation 3.20.

If any two points are known in a scanning second-order (secondary) wetting curve, such as in chord 3-4 in figure 3.1, it is possible to compute $C2^{3-4}$ and $C4^{3-4}$ and, when the closure of this scanning curve occurs (point 2)

$$\theta_2^{\Delta} = \theta^d(\psi_2^{\Delta}) = \theta^d(\psi_2^{\Delta}) C2^{3-4} + C4^{3-4} \quad (3.21)$$

Solving equation 3.21, we obtain ψ_2^Δ and θ_2^Δ . With these values, it is possible to compute θ_{*}^w , using equations 3.17 and 3.18. $C2^{2-3}$ and $C4^{2-3}$ are calculated as

$$C2^{2-3} = \frac{\theta_2^\Delta - \theta_{*}^w}{\theta^w(\psi_2^\Delta) - \theta_{*}^w} \quad (3.22)$$

and

$$C4^{2-3} = \theta_{*}^w (1 - C2^{2-3}) \quad (3.23)$$

Then, at point 3:

$$\theta^d(\psi_3^\Delta) C2^{3-4} + C4^{3-4} = \theta^w(\psi_3^\Delta) C2^{2-3} + C4^{2-3} \quad (3.24)$$

Solving equation 3.24, the values of ψ_3^Δ and θ_3^Δ are determined.

Equations 3.20, 3.21 and 3.24 can be generalised by:

$$\theta^w(\psi_l^\Delta) C2^{2-3} - \theta^d(\psi_l^\Delta) C2^{3-4} + C4^{2-3} - C4^{3-4} = 0 \quad (3.25)$$

Admitting scanning curves of up to second-order (maximum $l=3$), equations 3.22, 3.23 and 3.25 can be used to estimate the values of ψ and θ at the previous reversal points, given any two known points in the chord. In the algorithm developed, the logical sequence followed can be summarised as follows:

- 1 - identify whether drying or wetting curve by examining the two known points in the chord;
- 2 - identify whether main or scanning curve by comparing the two known points in the

chord with the main drying and wetting curves;

- 3 - if in a scanning curve, compute the previous reversal points using equations 3.22, 3.23 and 3.25. Equation 3.25 is solved through the application of Newton-Raphson procedure.

3.4.2.3 - Validation of the numerical algorithm

The hysteresis simulation program described above was tested using data and parameter values from Parker and Lenhard (1987): experimental main drainage and primary imbibition curves for air-water movement in a sandy porous medium, and the parameters obtained through a non-linear least-squares regression analysis of this data. Considering the presence of experimental and parameter error, the hysteresis simulation program performed quite well in reproducing the experimental results obtained by Parker and Lenhard (1987), as shown in table 3.1, where replicates 1, 2 and 3 refer to three different samples from the same soil.

Table 3.1 - Hysteresis simulation model against data from Parker and Lenhard (1987)

Capillary Head (cm)	Saturation			Capillary Head (cm)	Saturation	
	Replicate 1	Replicate 2	Computed		Replicate 3	Computed
10.3	0.78	0.84	0.88	10.3	0.82	0.88
22.5	0.58	0.64	0.66	19.4	0.67	0.71
49.7	0.34	0.39	0.38	46.8	0.39	0.40
78.6	0.16	0.28	0.26	74.2	0.25	0.27
97.4	0.13	0.25	0.22	98.9	0.21	0.21
149.6	0.10	0.23	0.15	148.2	0.18	0.15
99.4	0.11	0.24	0.19	99.0	0.20	0.20
63.5	0.15	0.28	0.27	61.0	0.24	0.28
41.3	0.24	0.34	0.37	41.7	0.31	0.37
28.9	0.34	0.43	0.48	27.4	0.42	0.49
13.0	0.51	0.61	0.75	13.7	0.57	0.73

In order to test the algorithm for setting the initial conditions, data from Parker and Lenhard (1987) and also synthetic data were used. The synthetic data were generated using Van Genuchten's characteristic curve, allowing scanning curves of up to second-order and adopting the following parameter vectors:

- main drying curve: $\theta_s^d = 47.55\%$
 $\theta_r^d = 5.00 \%$
 $\alpha^d = 0.17 \text{ cm}^{-1}$
 $n^d = 1.40$

- main wetting curve: $\theta_s^w = 46.49\%$
 $\theta_r^w = 5.00 \%$
 $\alpha^w = 0.10 \text{ cm}^{-1}$
 $n^w = 1.44$

The results, presented in table 3.2, show that the model was able to preview the reversal point values with good accuracy. For primary wetting curves, only one previous reversal point is presented in table 3.2, as the other reversal point is, by definition, $(\psi, \theta) = (0, \theta_s^d)$.

Table 3.2 - Results of the initial conditions algorithm

Values provided as known points		Order of scanning curve	Reversal points		Source of data
1st point	2nd point		Actual	Computed	
$\psi = 0.00 \text{ cm}$ $\theta = 41.71\%$	$\psi = -4.00 \text{ cm}$ $\theta = 39.91\%$	secondary	$\psi = -7.00 \text{ cm}$ $\theta = 38.64\%$	$\psi = -6.99 \text{ cm}$ $\theta = 38.65\%$	Synthetic
			$\psi = 3.00 \text{ cm}$ $\theta = 41.71\%$	$\psi = 2.94 \text{ cm}$ $\theta = 41.71\%$	
$\psi = -4.00 \text{ cm}$ $\theta = 39.41\%$	$\psi = 0.00 \text{ cm}$ $\theta = 40.62\%$	primary	$\psi = 3.00 \text{ cm}$ $\theta = 41.71\%$	$\psi = 2.94 \text{ cm}$ $\theta = 41.71\%$	Synthetic
$\psi = -10.00 \text{ cm}$ $\theta = 33.02 \%$	$\psi = -5.00 \text{ cm}$ $\theta = 34.86\%$	primary	$\psi = -18.00 \text{ cm}$ $\theta = 30.77\%$	$\psi = -17.98 \text{ cm}$ $\theta = 30.78\%$	Synthetic
$\psi = -99.40 \text{ cm}$ $S = 0.11$	$\psi = -63.50 \text{ cm}$ $S = 0.15$	primary	$\psi = -149.60 \text{ cm}$ $S = 0.10$	$\psi = -150.13 \text{ cm}$ $S = 0.12$	Parker and Lenhard
$\psi = -63.50 \text{ cm}$ $S = 0.15$	$\psi = -41.30 \text{ cm}$ $S = 0.24$	primary	$\psi = -149.60 \text{ cm}$ $S = 0.10$	$\psi = -150.00 \text{ cm}$ $S = 0.12$	Parker and Lenhard
$\psi = -28.90 \text{ cm}$ $S = 0.34$	$\psi = -13.00 \text{ cm}$ $S = 0.51$	primary	$\psi = -149.60$ $S = 0.10$	$\psi = -148.30 \text{ cm}$ $S = 0.13$	Parker and Lenhard

ψ = soil water tension
 θ = moisture content
 S = saturation

3.5 - Conclusions

Several models of water flow in unsaturated soils with or without macropores have been developed, using different approaches and different solution techniques. However, there is great difficulty to mathematically represent the physical phenomena entailed. According to Brusseau and Rao (1990), one of the major limitations to predicting flow and transport in structured soils is perhaps not our inability to develop mathematical models, but rather an inability to characterise the geometric and hydraulic features of the porous medium and, hence, to provide values for parameters of the models.

Few models realistically include the effects of soil hydraulic property variability and rainfall runoff dynamics. Also, stability and convergence problems, caused by inefficiencies in the numerical schemes used to solve the highly non-linear equations, are present in many methodologies. Besides that, among the two domain models, none of them are entirely satisfactory on all five criteria that should be specified in this kind of model. In addition, the scale of the REV for the macropores, which is very much larger than the REV for the soil matrix and also significantly larger than many measurement techniques, brings difficulty for validation of model predictions by measurements in the field.

The models available for representing preferential water flow are important in suggesting that macropores play an important role in the hydrology of some field soils. These models help to understand some of the physical processes entailed, but, as noted by Beven and Germann (1982), it is still necessary to add a further level of complexity to ideas and models of the movement of water through field soils, as a number of problems remain to be solved in defining, calibrating, and validating an adequate model of a combined macropore/matrix system. Attempts at modelling made so far have served to highlight the lack of experimental data on the nature of macropore flows, the structure of macropore systems and the interactions between macropores and the matrix. Until such data become available, both for single macropores and for complete networks, such models cannot be considered as more than exploratory hypotheses or, more important, cannot be validated.

Several empirical or theoretically based methodologies for describing hysteresis in the soil water hydraulic properties have been developed. However, this phenomenon is frequently ignored in field scale flow and transport numerical models, mainly due to the complexity of the hysteresis theories and to the need of a large amount of data for model calibration. Some of the available empirical models do not ensure closure of the scanning loops, so that pumping effects

are expected for cyclic variations of the pressure head. Also, many methodologies do not consider air entrapment, which can be a constraint to field applications.

Different modelling techniques have worked well in different applications, and choosing a model depends on the problem to be solved and on the preference of the user. Given the present state of knowledge, it is necessary to identify which are the best modelling approaches that could be adopted for a specific goal and then select the most applicable method. Under some circumstances, instead of starting the development of a new model, it can be more advisable to adapt an available model so that it can be able to include the representation of new phenomena.

Three models were selected to be used in this thesis, in order to compare alternative modelling approaches and to get a better understanding of the processes responsible for water flow in the unsaturated zone: SPW1 (Karavokyris et al., 1990), MACRO (Jarvis, 1991 and 1994), and a model of hysteresis considering air entrapment based on those presented by Kool and Parker (1987) and by Parker and Lenhard (1987).

The SPW1 model was selected to test the strengths and limitations in the use of Richards' equation. It is a physically-based soil-plant-water model, developed as part of a combined experimental and modelling study into the processes affecting radionuclide transport from a contaminated water table through the unsaturated zone and into a wheat crop, which is being undertaken by Imperial College on behalf of UK Nirex Ltd. The data from this experiment is used in this thesis. SPW1 does not include the representation of preferential water flow or hysteresis in the hydraulic properties of the soil, but it has been shown to be capable of handling the types of problems which occur in the field and to perform in a superior manner against an internationally recognised unsaturated flow model.

The MACRO model was selected in order to test the effects of preferential movement in unsaturated soil water flow. It is a deterministic model of non-steady state water and solute transport in macroporous field soils that can be run in either one or two flow domains. It includes a comprehensive treatment of most of the processes involved, using simple formulations in order to provide a modelling device that can be easily applied to field soils. Its major disadvantage is its empirical nature, but actually few other models of preferential soil water flow can be said to have a real physical base.

A model of hysteresis considering air entrapment on water flow in the unsaturated zone

based on those presented by Kool and Parker (1987) and by Parker and Lenhard (1987) was adapted and tested in order to run in conjunction with the SPW1 model. An algorithm to estimate previous reversal points was developed, in order to provide the initial conditions for simulation with this hysteresis model. One of the main advantages of the selected model is its parametric simplicity, which facilitates its implementation with minimal effort, as it does not require any parameter that was not previously included in model SPW1. The hysteresis model and the initial conditions algorithm have been shown to perform well when tested against experimental and synthetic data.

The hysteresis model and the initial conditions algorithm and also the methodologies adopted by MACRO model to represent, in one flow domain, the soil water retention curve and the unsaturated hydraulic conductivity were included in a new version of SPW1 model. This new version, called SPW1hyst, is used in this thesis for hysteretic and non-hysteretic simulations of one domain models based on the solution of the Richards' equation.

CHAPTER 4 - THE EXPERIMENTAL STATION AND AVAILABLE DATA

4.1 - Introduction

The direct measurement of percolation through the unsaturated soil zone to the water table is a difficult task, which can hardly be done reliably in the field. According to Haverkamp et al. (1977), the description of infiltration in the field is very complicated, since the initial and boundary conditions are usually not constant, while the soil characteristic may vary with time and space. Different processes occur simultaneously, and a complete control, measurement and understanding of the phenomena involved is difficult, even with the use of extensive instrumentation. A widely used alternative is to employ lysimeters for this purpose (Marshall and Holmes, 1988). According to Sharma (1985), lysimeters isolate a soil-vegetation sample hydrologically, being able to keep its representativeness and that of its enclosure, without modifying the microclimate. They allow the control and measurement of most of the processes associated with the movement of water through the soil, providing conditions for a better understanding of the different phenomena.

A detailed data set for water movement in the unsaturated zone is available from the experimental study which Imperial College is undertaking on behalf of UK Nirex Ltd, at the College's Field Research Station at Silwood Park, near Ascot, England. In this experiment, eight field lysimeters of cross sectional area 182cm by 91cm, containing a sandy loam soil to a depth of either 40 or 70cm and a crop of wheat are being used to monitor the processes affecting radionuclide transport from a contaminated water table through the unsaturated zone and into a wheat crop. The lysimeters have controlled water tables at 5cm above the base of the soil and are instrumented with tensiometers, thermistor probes, time domain reflectometers (TDR), and access tubes for neutron probes, borescopes and redox probes.

The data collected from these lysimeters show several events where strong evidence of rapid water flow can be identified. A detailed analysis of the soil moisture data set was necessary in order to better understand and simulate the processes involved in these events.

A description of this experimental facility and the available data is presented in this chapter. The identification and selection of events with evidence of rapid water flow, for posterior analysis and simulations, is also described in this chapter. Some events where slow water flow can be assumed are also selected, in order to assess the performance of different modelling conceptualisations under this condition, in addition to the situation described above.

4.2 - Imperial College's lysimeter experiment at Silwood Park

The experimental station at Silwood Park was designed as part of a contract undertaken by Imperial College under the Nirex Safety Assessment Research Program (NSARP). NSARP was established primarily to develop methods to evaluate the risks of possible migration of radionuclides from a proposed repository in the UK for low and intermediate level radioactive wastes. The envisaged pathways for the movement of radionuclides included transport by groundwater to the near-surface, unsaturated, soil water zone and consequent uptake by vegetation. The nature and quantification of the involved mechanisms required specific experimental investigation in order to provide a basis on which to construct and to parametrise mathematical models able to describe the physical and chemical processes present in this context. The main objective of the work is to investigate the behaviour of radionuclides in the near-surface environment, particularly with regard to soil water transport and vegetation uptake, using both experimental and theoretical modelling work (Burne, 1991; Burne et al., 1994).

This experimental facility has a particular design characteristic: a controlled water table, which allows the measurement of the flow through the base of the lysimeter, providing the full knowledge of the lower boundary condition and allowing better understanding of the processes involved, as one of the major unknowns is now regulated and quantified. The soil moisture data (soil water contents and suctions) obtained from this station showed evidence of rapid water flow, suggesting the necessity of a detailed study into the processes involved in preferential water flow in the unsaturated zone.

4.2.1 - General layout

The experimental facility comprises an automatic weather station and eight concrete lysimeters. These lysimeters were originally constructed in 1960, to the imperial measurements of 6' x 3' (plan) x 3' (depth) or, in metric units, 182cm x 91cm x 91cm, and were refurbished to be used in this experiment. In order to maintain fixed water table depths in each lysimeter, and to allow the introduction of radionuclide contamination from below the water table, the lysimeters were designed with the following features: a substrate of polyethylene beads in all lysimeters; a PVC manifold within the substrate; a total depth of 70cm for four of the lysimeters (deep lysimeters: A, B, E and F); a total depth of 40cm for the other four lysimeters (shallow lysimeters: C, D, G and H); water table located at 5cm above the bead/soil interface (i.e., 35cm depth for shallow lysimeters and 65cm depth for deep lysimeters); a geotextile filter at the bead/soil interface; and a false bottom in the shallow lysimeters; a horizontal datum 5cm above

the soil surface. A crop of wheat was grown in the lysimeters. These features are illustrated in figures 4.1, 4.2 and 4.3 (Burne, 1991; Burne et al., 1994).

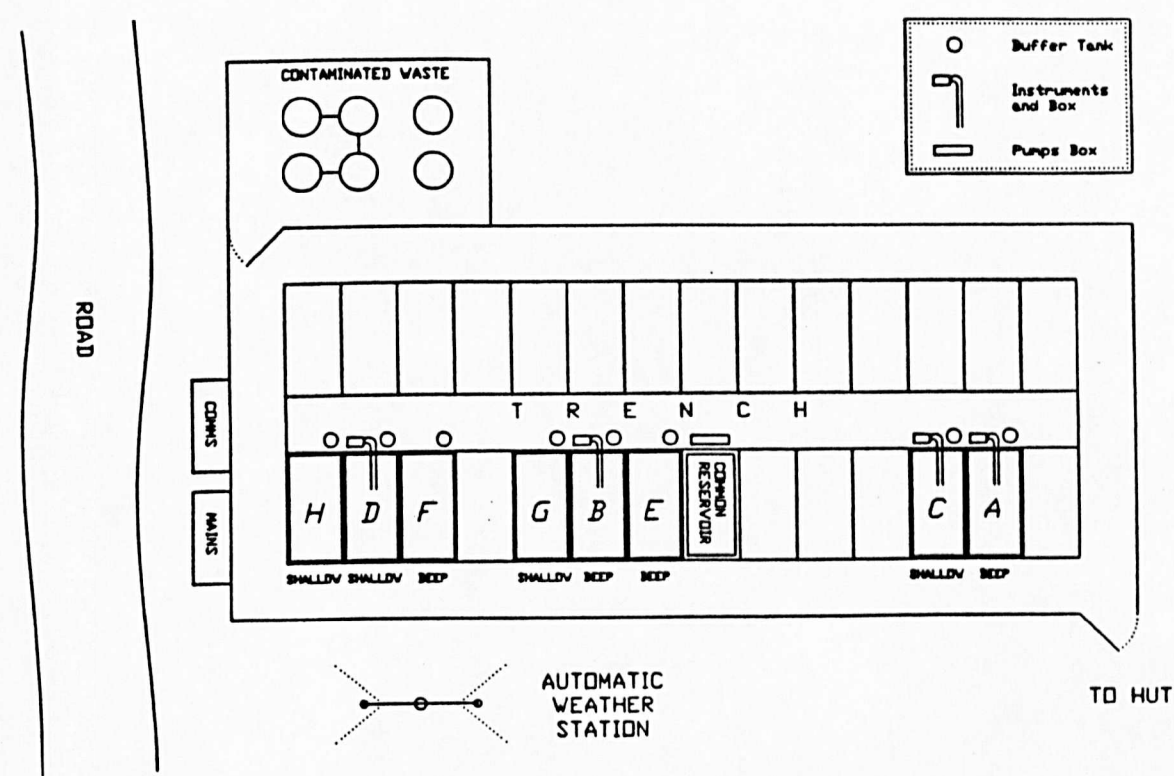


Figure 4.1 - Layout of the lysimeters (after Burne et al., 1994)

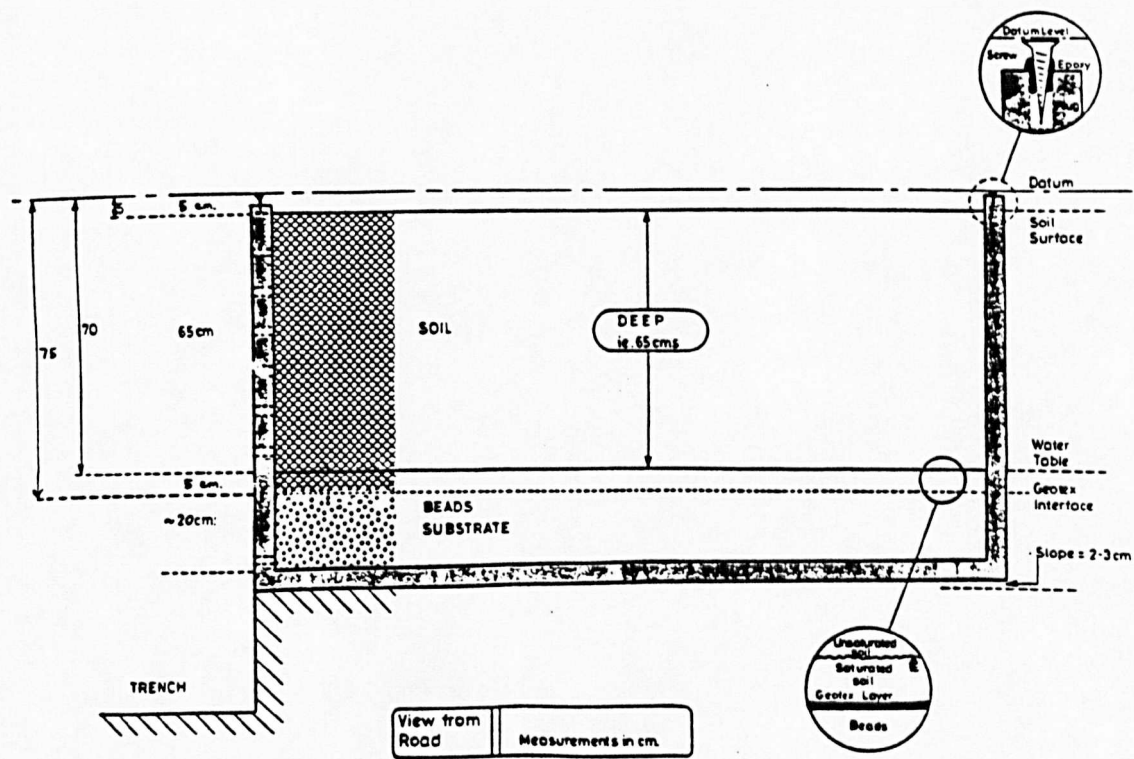


Figure 4.2 - Longitudinal section of a deep lysimeter (after Burne et al., 1994)

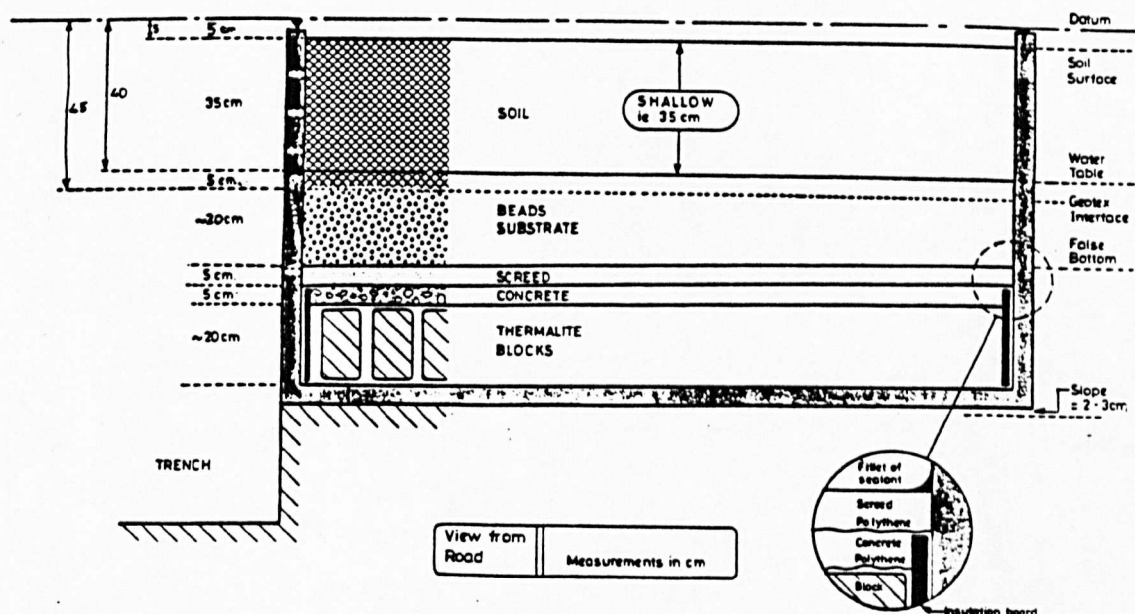


Figure 4.3 - Longitudinal section of a shallow lysimeter (after Burne, 1991)

The lysimeters were filled with sieved, mixed and homogenised Silwood soil. The properties of this sandy loam soil are presented and discussed in chapter 5.

4.2.2 - Lysimeter instrumentation

Each of the lysimeters was instrumented with equipment for measuring soil moisture properties, root distribution and redox potential. Measurements of crop height, leaf area index and pH were also taken. All eight lysimeters were chemically analyzed, but only four (namely, deep lysimeters A and B, and shallow lysimeters C and D) were monitored intensively with respect to soil dynamic response at every timestep (equivalent to a 100th of a day interval, or 14min 24s). The other four (namely, deep lysimeters E and F, and shallow lysimeters G and H) were replicates, designed to act as a cross-check.

In the following sections a description of the lysimeter equipment is presented, with special emphasis to the instrumentation related to soil moisture data. For these instruments, an explanation of their main principles is given, together with their expected accuracy and possible sources of error in measuring the soil water properties. The procedures taken in the experimental station in order to minimise these errors are also described.

4.2.2.1 - Tensiometers and pressure transducers

Childs (1969) defines a tensiometer as a combination of manometer and porous membrane for measuring soil water suction. According to Stannard (1992), a tensiometer is comprised of a porous surface (usually a ceramic cup) connected to a pressure sensor by a water-filled conduit. The porous cup, buried in a soil, transmits the soil water pressure to a manometer, a vacuum gage, or an electronic-pressure transducer (here referred to as a pressure transducer). During normal operation, the saturated pores of the cup prevent bulk movement of soil gas into the cup.

Standard tensiometers are used to measure matric potentials between the values of 0 and approximately -870cm of water (corresponding to about 0.8bar) in the unsaturated zone by creating a saturated hydraulic link between the soil water and a pressure sensor. The use of multiple installations allows matric potential and elevation data to be employed to determine direction and, in some cases, quantity of water flux (Stannard, 1992). According to Hillel (1980), the use of several tensiometers at different depths can allow calculation of the hydraulic gradients in the soil profile. Measurement of the hydraulic gradient is particularly important in the region below the root zone, where the direction and magnitude of water movement cannot be easily established. Matric potential data can also be used to determine the approximate water content in the soil, knowing the moisture-characteristic curve.

Under some circumstances, the rate of transfer of water between tensiometer and soil may not be fast enough to allow an accurate measurement of the changing matric potential in the soil. Furthermore, the volume of the exchange may itself upset the matric potential of the soil at the site of measurement. This is a particular problem when using manometers to quantify the soil water pressure. To overcome this, pressure transducers can be employed (as in the present experimental facility) to allow equilibrium to be maintained with negligible interchange of water between soil and tensiometer cup (Marshall and Holmes, 1988).

Pressure transducers convert pressure, or pressure difference, into a voltage (or current signal). A calibration equation supplied by the manufacturer is used to convert the measured signal into pressure or tension at the pressure-transducer port. Tensiometers equipped with pressure transducers are well suited to collect large quantities of data. Measurements can be made often and recorded automatically by a data logger or a strip-chart recorder. The extreme sensitivity of the pressure transducer results in the shortest possible time response, making this type of tensiometer ideal for tracking wetting fronts. However, the extreme sensitivity also

causes pressure-transducer tensiometers to be particularly susceptible to transient temperature effects caused by thermal expansion and contraction of water in the tensiometer. Pressure transducers (and above-ground connecting tubing) can be enclosed in an insulated (and, if need be, heated) shelter or surface pit to minimise temperature fluctuations. The shelter or pit needs to be placed so that it does not disturb the natural flow field at the location of the porous cup (Stannard, 1992).

The sensing elements of a typical pressure transducer are semiconductive resistors, embedded in a diaphragm that moves from applied pressure. As the resistors shorten or lengthen, there is a change in their resistances, which can be translated into a nearly linear function of pressure that is almost independent of temperature. A large degree of accuracy can be achieved, with errors of the tensiometer-transducer system ranging from 1cm H₂O to 2cm H₂O. This accuracy is degraded further by drift, so that the pressure transducer requires recalibration at regular intervals (Stannard, 1992).

According to Hoelscher et al. (1993), pressure transducers are widely used in soil hydrology investigations and are generally accepted as the most effective and efficient means of measuring soil water potentials, with highly accurate readings achievable in transducer/tensiometer applications. According to Silver (1980), transducers with accuracies on the order of 0.02% are commonly available at moderate prices.

It is commonly found that air bubbles form in the tensiometer cup after a time (Childs, 1969). These do not cause the complete breakdown of the method, as it is the case when air penetrates the porous membrane from outside and is continuous with the external atmosphere, but nevertheless they are a source of error.

Each one of the monitored lysimeters in the experimental facility at Silwood Park was supplied with an array of tensiometers and pressure transducers: six for the deep lysimeters (A and B), at depths of 10, 20, 30, 40, 50 and 60cm below the soil surface, and three for the shallow lysimeters (C and D), at depths of 10, 20 and 30cm below the soil surface. No consideration of horizontal variability in the measurements was taken into account, as only one array of tensiometers was installed in each lysimeter. This implies homogeneous horizontal behaviour, which can be a source of error, particularly in the presence of macroporous flow. The tensiometers were inserted through holes in the trench wall slightly downwards into the lysimeters, at a slope of 2cm depth in 50 cm length (an angle of about 2 degrees with the datum). The open end of the tensiometers was provided with an elbow which stood vertically

upwards, to facilitate the purging of air. For the same reason, the holes for the thin-bore tube to the transducers were on the underside of the tensiometers (Burne et al., 1994). The pressure transducers were installed in boxes fixed to the trench wall, in order to be protected from the elements and thus reducing transient temperature effects. They were arranged so that the sensing element in each transducer was in line with the centre of the porous cup, avoiding the need for head correction terms. Also, as a regular task at the lysimeter site, any transducer drift was reset on a monthly basis, and the tensiometers were bled whenever necessary, to eliminate air bubbles (Burne, 1991).

The precision of measurement of this system can be checked by comparing the measured tensions at equilibrium conditions with calculated tensions from the equilibrium profile. The values obtained for these tensiometers were between 1cm and 2cm, in accordance with accuracies found in the literature.

4.2.2.2 - Neutron probe

The neutron moisture meter, or neutron probe, consists of two main components: a probe, which is lowered into an access tube inserted vertically into the soil, and which contains a source of fast neutrons mounted next to, but well shielded from, a detector of slow neutrons; and a scaler or ratemeter to monitor the flux of slow neutrons scattered by the soil. A neutron has approximately the same mass as a hydrogen atom, but is light compared with almost all other elements occurring in soils. Consequently, in accordance with the laws of conservation of energy and momentum, fast neutrons will bounce off, without much loss of speed, when colliding elastically with other particles of much greater mass, but will share their energy and become slowed down when the collision is with hydrogen atoms. Hence, the effectiveness of a soil in slowing down fast neutrons is a measure of the amount of hydrogen present. Since by far the greater proportion of all the hydrogen present is in form of water, it is also a measure of the amount of water in the soil (Childs, 1969; Hillel, 1980).

Although attempts have been made to predict the relation between slow neutrons count rate and soil wetness from theoretical considerations, such are the anomalies and variability among different soils that it is best to calibrate the neutron probe specifically for each soil type and set of circumstances in which it is to be used (Hillel, 1980). According to Marshall and Holmes (1988), there is no universal calibration curve, and the slopes of different calibrations may vary up to 25 per cent.

It has become general practice to calibrate the neutron probe in term of R/R_s against moisture content, where R is the count rate in the soil, for a given time interval, and R_s is the count rate in a laboratory standard. This procedure has the disadvantage that there is a small increase in overall error caused by the additional random counting error inherent in the term R_s . This error can be minimised by taking a very long count or the mean of many short standard counts. The use of a 64s count compared with a 16s count can reduce the random error by nearly 50%. On the other hand, the use of a counter rate ratio ensures continuity of records and removes any bias due to slow ageing of components, use of more than one probe, or a change of sensitivity of the probe. Laboratory standards can be made of any moderating material (i.e., one containing a high hydrogen density). Water is the ideal liquid moderator, because it is cheap, available anywhere, has no unpleasant characteristics, contains as much hydrogen per unit volume as any possible alternative, and its count rate seems to be substantially independent of temperature (Bell, 1987).

Another problem of the neutron probe is the so-called surface effect. With the commonly used radium-beryllium or americium-beryllium sources, the sphere of influence, or effective volume of measurement, varies with a radius of less than 10cm in a wet soil to 25cm or more in a dry soil. Consequently, measurements close to the surface (say, within 20cm of the surface, depending on soil wetness) are precluded because of the escape of fast neutrons through the surface (Hillel, 1980).

The main advantage of the method is the fact that it is non-destructive and can be used for long term monitoring. According to Bell (1987), the neutron probe is best used in situations where non-destructive measurements of moisture change are required in the same profile on many occasions.

The neutron probe has gained wide acceptance as a tool for measuring soil water content in situ, being able to give accurate measurements (Silvestri et al., 1991). According to Marshall and Holmes (1988) the precision in water content determination can be as good as 2mm standard deviation in a total water content of 450mm in the soil profile to a depth of 1.5m. However, several authors (Haverkamp et al., 1984; Carneiro and De Jong, 1985; Ruygrock, 1988) alert for the possible errors caused by poor calibration.

In the experimental station at Silwood Park, aluminium tubes measuring 4cm diameter and 75cm length were vertically inserted into the deep lysimeters (A,B, E and F) to allow access for the neutron probe used in this experiment. Measurements were taken weekly, at the depths

of 20cm, 30cm, 40cm, 50cm and 57cm. As for the tensiometers, homogeneous horizontal behaviour was implied, and only one access tube was installed in each lysimeter. The soil moisture values were computed using the calibration curve provided by Bell (1987) for the Wallingford Probe applied to a loamy soil. This curve assumes soil moisture as a linear function of the quotient R_c/R_w , where R_c is the measured rate count given by the ratescaler for the interval of 64s, and R_w is the standardised rate count in water. R_w was obtained each day the neutron probe was used, as the average of 10 readings of the ratescaler for 64s, with the probe lowered in the centre of sensitivity of a mass of clean water. These procedures ensure a reduction of the random counting error in the term R_w .

It is important to emphasise that the use of a calibration curve which is not derived specifically for the mixed and homogenised Silwood soil in the lysimeters is a source of error that cannot be neglected. Nwabuzor (1984) performed a neutron probe calibration for the original Silwood soil. The curve obtained in that study was not adopted for the lysimeter experiment because the soils were not exactly the same. The soil in the lysimeters was obtained from the Silwood soil, but it was sieved, mixed, homogenised and recompact, so that some of the properties could have been altered. This is of special importance when considering that stones were removed during the sieving process, and this procedure can change the values of the moisture volume fraction. Besides that, when confidence intervals of 95% for the calibration curve obtained by Nwabuzor are considered, the curve provided by Bell for loamy soils falls in the accepted range, providing some justification for its use.

4.2.2.3 - Time-domain reflectometer

Time-domain reflectometry (TDR) is a technique operating over a range of radio frequencies, which can be used to measure the high-frequency electrical properties of materials, such as the dielectric constant of the soil. As water has a dielectric constant much higher than that of soil particles (80 for water, against 2 to 5 for soils), it governs the dielectric constant of the soil. Consequently, a measure of the dielectric constant of soil is a good measure of its water constant (Topp and Davis, 1985a). According to Topp et al. (1980), the dielectric constant is strongly dependent on the water content of the soil but almost independent of soil type, density, texture and salt content, and with no significant temperature dependence.

In the TDR technique for measuring soil water contents, a step voltage pulse or signal is propagated along parallel pair transmission lines. The parallel rods or wires serve as conductors and the soil, in which the rods are installed, serves as the dielectric medium. The

signal propagates as a plane wave in the soil, guided by the pair of rods, and is reflected from the end of the transmission line, returning back to the TDR receiver. The time interval between sending and receiving the reflected signal relates directly to the propagation velocity of the signal in the soil, which is indicative of the volumetric water content, being smaller as the water content increases (Topp and Davis, 1985a).

The soil moisture to a depth of soil can be computed according to an empirical relation developed by Topp et al. (1980). This relation is a third degree polynomial equation fit to data from four mineral soils, determined from measurements of the dielectric constant with an accuracy of $\pm 0.02 \text{ m}^3/\text{m}^3$ and a precision of repeatability of $\pm 0.01 \text{ m}^3/\text{m}^3$.

According to Topp and Davis (1985a, 1985b), the accuracy of the TDR technique is comparable to that of gravimetric samples, being able to give a precise and immediate determination of soil water content in the field with an accuracy of 2% .

Pairs of stainless steel rods for a TDR were inserted into each one of the monitored lysimeters. The depths for TDR readings in the deep lysimeters (A and B), were at 15, 25, 35, 45, 55 and 65cm below the soil surface; for the shallow lysimeters (C and D), at depths of 15, 25 and 35cm below the soil surface. A TDR calibration was performed for the Silwood soil, and a third degree polynomial equation was fit to the data and compared with the one provided by Topp et al (1980), presenting very similar shapes (Burne, 1993). This curve was adopted to determine the soil moisture to a depth of soil.

4.2.2.4 - Water table level control

During the whole duration of the experiment, the water table was meant to be maintained at a fixed level, 5cm above the base of the soil, in each lysimeter. This was achieved via a system of buffer tanks, opto-electronic water level switches, peristaltic pumps and a common reservoir.

A buffer tank was connected to each lysimeter substrate. Inside the buffer tank, an opto-electronic device acted as an on/off switch depending whether it was covered by water or not. The buffer tank was connected via a peristaltic pump to a large reservoir, common to all lysimeters. When the sensor detected a falling water level, the pump moved water from the reservoir to the buffer tank; and, when the level raised, from the buffer tank to the reservoir. In this way, the level in the buffer tank was held constant, stabilising the level in the lysimeter. The

water balance was measured by counting the revolutions in both directions of the pump, and by measuring the storage in the buffer tank with a float and potentiometer water level gauge (Burne et al., 1994).

The opto-electronic device has a hysteresis of 1mm if correctly orientated and can therefore resolve the water level to within this level of precision. There is an error in assuming that the water table will be always at the same depth as that of the buffer tank, as some delay should occur until both heights are equalised. However, alternative methods to control the lysimeter water level directly, through a header tank or peristaltic pumps directly connected to the lysimeter substrate (Channon, 1988), showed that the lysimeters were prone to develop air locks or air bubbles in the substrate or in the soil if water was forced in or out too vigorously. In the chosen water table level control system it is the buffer tank level which is regulated by the peristaltic pump, preventing the air entrapment caused otherwise.

4.2.2.5 - Summary table of sensors and measurands

As already mentioned, a number of instruments, probes and access tubes were placed in the lysimeters. In addition to the tensiometers, access tubes for the neutron probe, stainless steel rods for the TDR, and the system of buffer tanks, opto-electronic water level switches and peristaltic pumps for water level control already described in the previous sections, each lysimeter had the following devices: a stilling-well, made from perforated PVC, as a backup for manually measuring the water table elevation; three Perspex tubes to allow observation and quantification of root development using a borescope; thermistors buried at the same depth as the tensiometers, in the four instrumented lysimeters, to measure temperature values; platinum electrodes at 5cm to 10cm depth intervals, in lysimeters B and C, for quantifying redox potential.

Measurements of leaf area index (using the inclined point quadrat method) and crop height (based on a sample of 21 plants per lysimeter) were also performed.

Some of the measurements were recorded 100 times a day, by automatic dataloggers, while others were taken manually, every week or fortnight, or every quarter. A summary of all instruments, sensors and measurands in the lysimeters, categorised according to frequency of measurement, is presented in table 4.1.

Table 4.1 - Lysimeter instrumentation

Frequency of measurement	Measuring device	Measurand
Every Timestep (100/day)	Tensiometer + Transducer	Soil moisture suction
	Thermistor probe	Soil temperature
	Peristaltic pump	Pumping revolutions
	Float + potentiometer	Water level in buffer tank
Every Week or Fortnight	Time domain reflectometer	Soil moisture content
	Neutron probe	Soil moisture content
	Borescope	Root distribution
	Inclined point quadrat	Leaf area index
	Ruler	Crop height
Every Quarter	pH meter	pH
	Platinum electrodes	Redox potential

4.2.3 - Automatic weather station

An automatic weather station was established, consisting of the sensors presented in table 4.2.

Table 4.2 - Automatic weather station instrumentation

Sensor	Measurand
Solarimeter	Direct solar radiation
Net radiometer	Earth/sky radiation balance
Platinum resistance probe	Air temperature
Dielectric hygrometer	Relative humidity
Anemometer / wind vane	Wind speed magnitude
	Wind vector magnitude
	Wind vector direction
	Wind vector direction Standard Deviation
	Rainfall
Tipping bucket A	Rainfall
Tipping bucket B	

All sensors presented in table 4.2 had measurement taken at each timestep, in a total of 100/day. Tipping buckets A and B are identical standard raingauges measuring a volume equivalent to 0.5mm height, and they were installed at a distance of 20m within each other, to allow quality control and backup information.

4.3 - Selected events: analysis of the soil moisture data

An investigation of the soil moisture data set shows that nearly 70% of all rainfall events caused sharp response in soil moisture suction along the whole depth profile, providing strong evidence of rapid water flow. These fast responses were characterised by an abrupt increase of the soil moisture suctions measured in all tensiometers, reaching a peak value in intervals of time under 12 hours (and sometimes much faster) after the rainfall, with an also quick (although less rapid) recession, when the tensions fall back to, or nearly to, the original values. Such a fast response can hardly be reproduced using a traditional model of water flow in the unsaturated zone, based on Richards' equation, as this theory implies a much slower movement of water, especially for the recession curve. A detailed analysis of the soil moisture data set was necessary in order to identify the processes present in these rapid flow events so that they can be better understood and simulated. The matric potential data provided by the tensiometers and the influx through the base of the lysimeters are the only soil moisture information continuously recorded. For this reason, the following analysis is restricted to these data.

The matric potential data was used to identify the pattern of response of the system to rainfall input, with special emphasis to recognising evidences of rapid, or preferential, water flow. A response to rainfall in the tensiometers located at 50cm and 60cm depth reaching a peak value under 12 hours, and also presenting a quick recession can not be well explained by models which suppose a slow flow of water through the soil matrix, as predicted by capillary theory (or Darcian principles). Under unsaturated conditions, as not all of the soil pores are filled and conducting, continuity and conductivity are not maximal, and, as the soil gets dryer, the hydraulic conductivity is expected to decrease by several orders of magnitude (Hillel, 1980). For this reason, a steep recession curve is not expected to be achieved under these models, even if a sharp rise in matric potentials can be obtained. Other mechanisms, such as macropore flow, have to be considered to reproduce the observations. Consequently, this sort of response at lower depths can be considered as a evidence of preferential flow, and the data from the deep lysimeters (A and B) is the more appropriate to identify rapid flow events.

Another continuously recorded source of data for the identification of rapid flow events is the influx/outflux of water through the base of the lysimeters. As described in section 4.2.2.4, these volumes were measured by counting the revolutions of the peristaltic pumps connecting the buffer tanks of each lysimeter to the common reservoir and also by the storage in the buffer tank, determined with a float and potentiometer water level gauge. As the system envisages to maintain the water table at a fixed level, a movement of water from the lysimeter to the

common reservoir, initiating immediately after the rapid increase of water tensions in the deeper tensiometers, would mean that a volume of water was transmitted very quickly to the bottom of the lysimeter, reinforcing the hypothesis of rapid flow.

It is important to notice that the possibility of water flowing down close to the walls of the lysimeter and causing a rapid response in the water table level can not be wholly excluded, although any obvious gaps were filled in routine maintenance. This volume of water would not be registered by the tensiometers, as their porous cups are located in the middle of the lysimeters and accessed by side-entry. However, the water table level control system would indicate this influx of water, by the activation of the peristaltic pumps. By the combined analysis of the bottom influx and the tensiometer response it is possible to identify both the hypothesis of water bypass through macropores and the possibility of water running down close to the walls.

The whole matric potential data set for lysimeters A and B is graphically reproduced in the figures of Appendix I. The system was fully operational from 23/04/90 (Julian date 90113) to 12/04/94 (Julian date 94102). Defining an event as a rise in the matric potential record against time as a result of rainfall input and the following recession, when the tensions go back to, or nearly to, the initial conditions, a total of more than 160 events was identified during these four years. From this total, more than 110 events present quick responses from the tensiometers located at the bottom of the lysimeters. A detailed study of each one of these events was performed, in order to identify any experimental procedure, error or operation (such as zeroing or purging air from the tensiometers, a pump failure due to blockage, etc.) that could be the cause for the record indication. After this examination, a set of 8 events representative of the different situations observed in the whole data set for which evidences of rapid flow were present was selected and designated for detailed analysis and later application of the different modelling approaches discussed in chapter 3. A set of 4 events where no evidence of preferential water flow can be assumed was also selected. All these events are presented and discussed in the following sections.

4.3.1 - Analysis of the selected rapid flow events

The selected events with evidence of rapid flow are summarised in table 4.3 and presented in more detail in figures 4.4 to 4.11. The responses of matric potential for three different depths along the soil profile are shown in these figures, together with the cumulative influx of water through the bottom of the lysimeters. Whenever appropriate, a zero reference line is also plotted, in order to emphasise the closeness to saturation suggested by the tensiometer

data. These events will be denominated 'selected rapid flow events'. When referred to, each event will be identified by its julian starting date. As mentioned above, they exemplify the most important features and different patterns of response observed in the whole data set, for the 110 events identified among the whole data set as showing quick responses from the tensiometers located at the bottom of the lysimeters. Table 4.3 also shows the total rainfall and the maximum intensity observed in an one hour period, as registered by the tipping buckets of the automatic weather station, and the total evapotranspiration, estimated using the Penman model.

Table 4.3 - Selected rapid flow events

Starting date		Ending date		Total Rainfall (mm)	Max. Intensity (mm/h)	Total ET by Penman (mm)
Julian	Gregorian	Julian	Gregorian			
90158	07/06/90	90162	11/06/90	14.0	6.0	10.5
90230	18/08/90	90242	30/08/90	21.5	3.5	31.0
90291	18/10/90	90297	24/10/90	16.0	6.5	3.8
91017	17/01/91	91030	30/01/90	9.5	2.0	3.0
91119	29/04/91	91124	04/05/91	33.0	3.0	6.6
91136	16/05/91	91138	18/05/91	3.0	0.5	3.2
91198	17/07/91	91204	23/07/91	19.0	6.5	16.1
91211	30/07/91	91218	06/08/91	25.0	5.5	18.3

The initial conditions of event 90158 (figure 4.4) are of a very dry soil, with values of matric potentials approximately at -4.5m and -6m for the top tensiometers of lysimeters A and B, respectively. There are two main rainfall inputs to this event: the first in the evening of day 90158 (07/06/90), with a registered peak of 3.5mm; and the second in the evening of day 90159 (08/06/90), when rainfall reached 1.5mm. The total precipitation for the whole event was of 14mm, and the estimated total evapotranspiration of 10.5mm. The tensiometers at lysimeter B registered an immediate response to the first rainfall along the whole depth profile. The top tensiometer reached near-saturation conditions in an interval of less than 6 hours, starting from a very dry soil (matric potential of approximately -6m). The second rainfall stimulated a quick rise of the registered tensions of the tensiometers in the top and middle of the profile, but no response can be observed at 50cm depth. The top tensiometer again registered near-saturation conditions, with a rise in the matric potential from an initial value under -3m to nearly zero in less than 8 hours. The tensiometers of lysimeter A, however, showed sensitivity only to the second rainfall input, with tensions rising from around -4m to nearly zero, but the response was not transmitted down along the soil profile.

A possible explanation for the different pattern of responses is that the tensiometers of

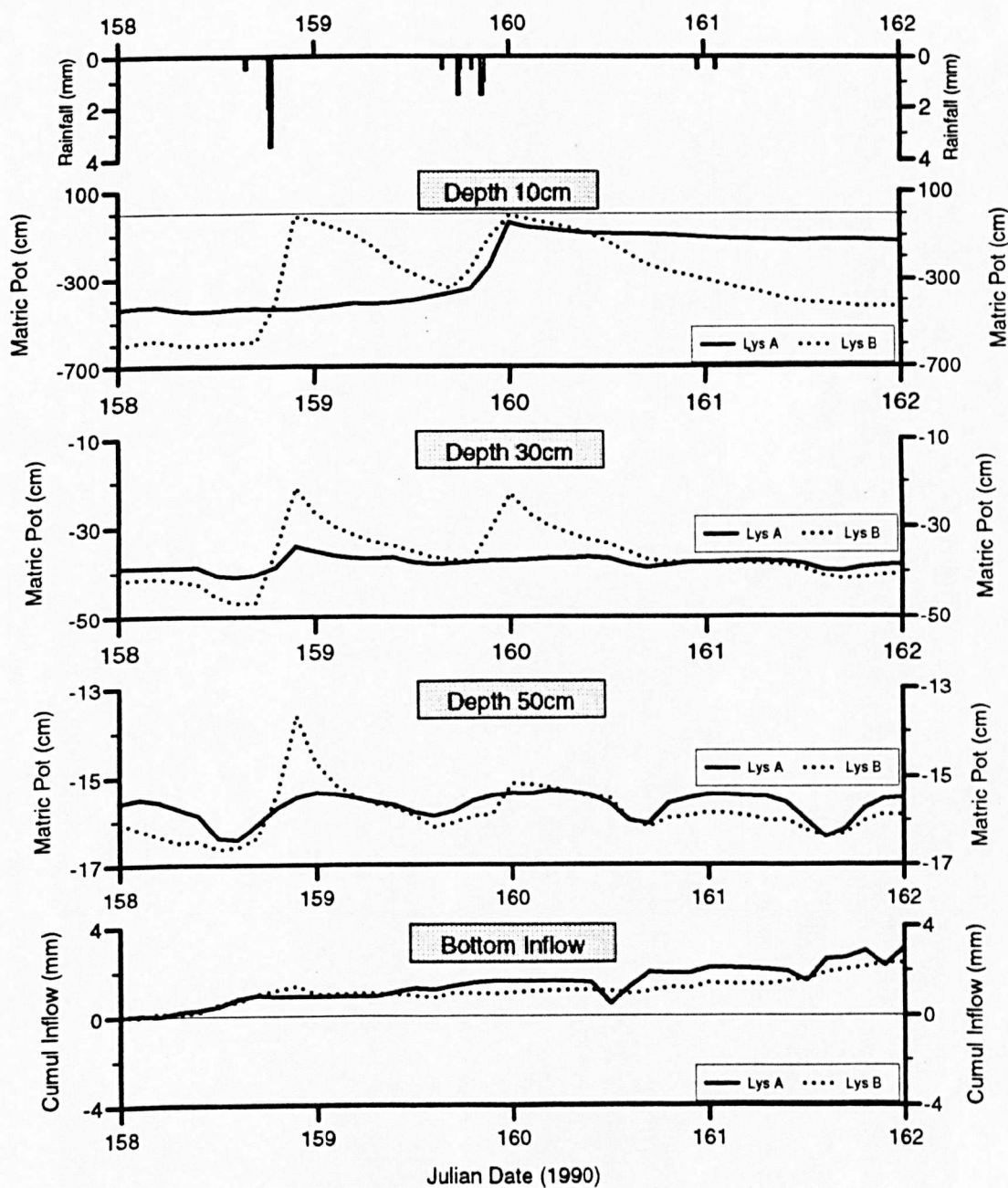


Figure 4.4 - Selected rapid flow event 90158

lysimeter B were intercepting a preferential path flow, but the same did not happen in lysimeter A. Assuming the water flow conceptualisation presented in chapter 2, as described by Beven and Germann (1982), the first rainfall would have been enough for lysimeter B to reach the second stage of the process, when the input is bigger than the infiltration into the matrix from the surface, and macropores open to the soil take up water, which flows down. The volume of water was enough to compensate for lateral losses into the matrix from the walls of the macropores, and the flow reached the deeper layers of the lysimeter. For the second rainfall input, as the intensity was smaller, the lateral losses were big enough to reduce the macropore flow and allow penetration of the water along the walls of the macropore only until the middle of the profile. The tensiometers in lysimeter A did not intercept any macropore and, consequently, the water flow followed the slow patterns of infiltration predicted by capillary theory.

The difference in the recession curves of both lysimeters reinforce these hypothesis. The recession was very fast in lysimeter B, which is consistent with macropore flow: as soon as water stopped to be transmitted by the macropores, the water content in the macropores quickly dropped due to lateral infiltration into the matrix, what was reflected by the tensiometer response. In lysimeter A, the only process registered is infiltration into the matrix and a slow redistribution, consistent with the principles of capillary flow.

It is also important to observe that, for both lysimeters, there is a clear diurnal effect observed in the deep tensiometers, with the matric potentials varying cyclically along a 24 hours period, presenting a minimum value in the beginning of the afternoon and a maximum in the middle of the night. This behaviour was probably caused by evapotranspiration effects, which are maximum during the day and minimum during the night. The rapid flows occurring at the top and middle of the profile do not allow a clear confirmation of this same behaviour at these depths, although some indication is identifiable at 30cm.

In both lysimeters the bottom inflow shows a nearly constant flow of water from the common reservoir to the lysimeters, with a total equivalent to nearly 3.5mm. This happened to keep the water table level fixed at 5cm above the base of the lysimeters, compensating effects of evapotranspiration and rain. The total added value of precipitation and bottom inflow is equivalent to a mean water input of less than 4.5mm per day. Considering the time of the year (beginning of June) and the extremely dry initial conditions of the soil, it is not unrealistic to infer that part of this water was absorbed into the soil, reducing its dryness (as the values of matric potential in the end of the event were higher than in the beginning), and taken out by evapotranspiration processes. An estimated evapotranspiration of 10.5mm indicates that

approximately 7mm of water were absorbed into the soil.

In event 90230 (figure 4.5), similar initial conditions and pattern of response are observed. The soil is initially very dry, with the top tensiometers presenting matric suctions of about 6.5m and 7m for lysimeters A and B, respectively. The total precipitation along the whole event was of 21.5mm, with a peak of 1.5mm in the morning of day 90231 (19/08/90), and the estimated total evapotranspiration is 31.0mm. The tensiometers in lysimeter B registered a rapid response to the rainfall input, transmitted along all the soil profile, for both the rise and the recession of the observed tensions. The top tensiometer showed a rise in matric potentials from almost -7m to near-saturation conditions in less than 10 hours. In lysimeter A, the matric potential near the surface rises very slowly as response to the rainfall. Its top tensiometer took more than 5 days to reach its maximum value of matric potential. There is, however, a registered response of deeper tensiometers in lysimeter A, but not as intense as in lysimeter B. The diurnal effects caused by evapotranspiration can be observed for the whole depth profile of both lysimeters during this event.

The same explanation applied to event 90158 can be applied again to lysimeter B: its tensiometers were intercepting a preferential path flow and the rainfall input was big enough to initiate flow down into the macropores, so that it reached the deeper layers of the lysimeter.

The response of the top tensiometer in lysimeter A indicates that it did not intercept any macropore and, consequently, the only process registered is slow infiltration into the matrix. But the data from the deeper tensiometers in lysimeter A seem to show that some rapid flow is occurring. An interpretation of these data is that there is preferential flow in lysimeter A, even if the top tensiometer is not intercepting a preferential path flow. In this case, the data from this tensiometer would reflect matrix water flow, while the other tensiometer reproduce the influence of macropores. The fact that in the previous event none of the tensiometers of lysimeter A presented evidence of intercepting a macropore does not mean that this situation could not change during the 60 days between both events: as commented in chapter 2, macropores are a very dynamic soil structure, being affected both by natural causes, such as weather, and, mainly, due to land use. The winter wheat was harvested on the 26/07/90 (Julian date: 90207), and this activity could have caused new preferential paths to be formed, either by directly affecting the soil structure, or due to new macropores resulting from dead roots.

As in event 90158, lysimeter B shows a nearly constant inflow of water from the common reservoir to the lysimeters, with a total equivalent to nearly 17mm. The total water

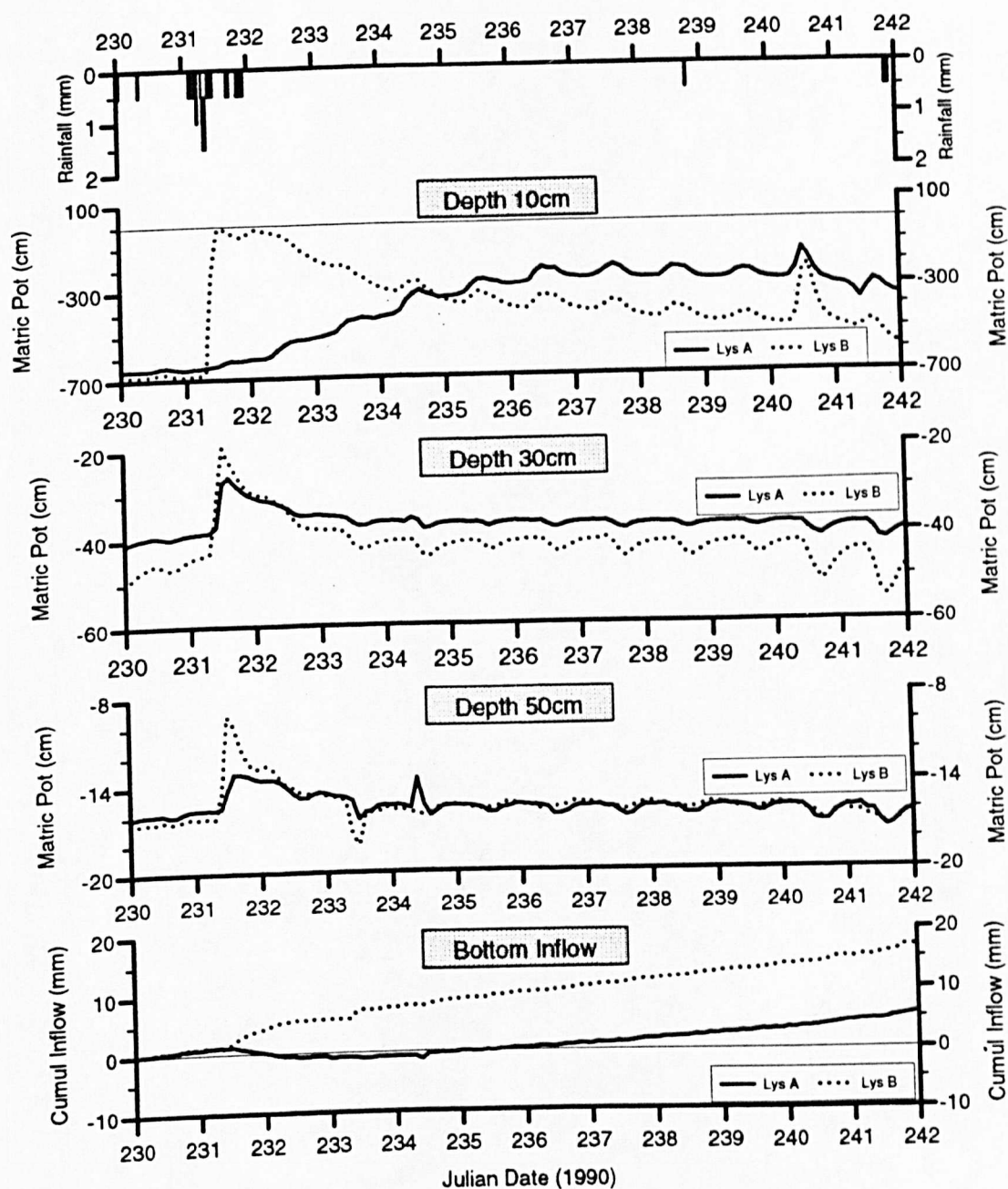


Figure 4.5 - Selected rapid flow event 90230

input (rainfall and bottom inflow) is approximately 38.5mm, equivalent to less than 3.5mm per day. This value is not unlikely to be compensated by absorption into the soil and evapotranspiration processes, especially due to the extremely dry initial conditions of the soil and the time of the year (second half of August). An estimated evapotranspiration of 31.0mm indicates that approximately 7.5mm of water were absorbed into the soil. Lysimeter A, however, shows a movement of water from the lysimeter to the common reservoir initiating just after the beginning of the rapid increase of water tensions in the middle and deep tensiometers. This behaviour gives further support to the hypothesis of rapid flow in lysimeter A, as it indicates that a volume of water was transmitted very quickly directly to the bottom of the lysimeter. If only capillary flow were present, the rainfall water would be expected to be partially absorbed by the very dry soil matrix, seeping slowly downwards.

Initial conditions for event 90291 (figure 4.6) are not as dry as in the previous events. The top tensiometers of lysimeters A and B register matric potentials of about -0.7m and -1.7m, respectively. The total precipitation along the whole event was of 14mm, with a peak of 3.5mm in the evening of day 90291 (18/10/90), and the total estimated evapotranspiration is 3.8mm. The tensiometers from both lysimeters show fast response of matric potential as result of the rainfall input, but a slow recession curve in the top layer. The main difference between the tension records of lysimeters A and B is in the initial conditions, as lysimeter B shows a dryer top layer in the beginning of the event. After the rain, both lysimeters show very similar records for the 10cm deep tensiometer. For the deeper tensiometers there is a lag in the responses, with lysimeter B presenting slightly faster responses: in lysimeter B, all tensiometers react immediately after the beginning of the rainfall; in lysimeter A, the deeper tensiometers start to register a rise in the matric potentials only after the tensions from the top tensiometer reach their maximum value. Both lysimeters present fast matric potential recession curves at 30cm and 50cm depths. The diurnal effects caused by evapotranspiration can only be identified at the 50cm tensiometer.

It seems that the deeper tensiometers from lysimeter B are intercepting macropores directly connected to soil surface, while in lysimeter A the water has to seep through the top layer before reaching the preferential flow paths. The slow recession curve of the top tensiometer in lysimeter A seems to confirm this hypothesis. Lysimeter B presents a recession curve very similar to the one registered in A. A rapid rise of the matric potential followed by a slow recession can be reproduced by a Darcian conceptualisation. This fact could mean that, during this event, the 10cm deep tensiometers in lysimeters A and B are not intercepting a macropore.

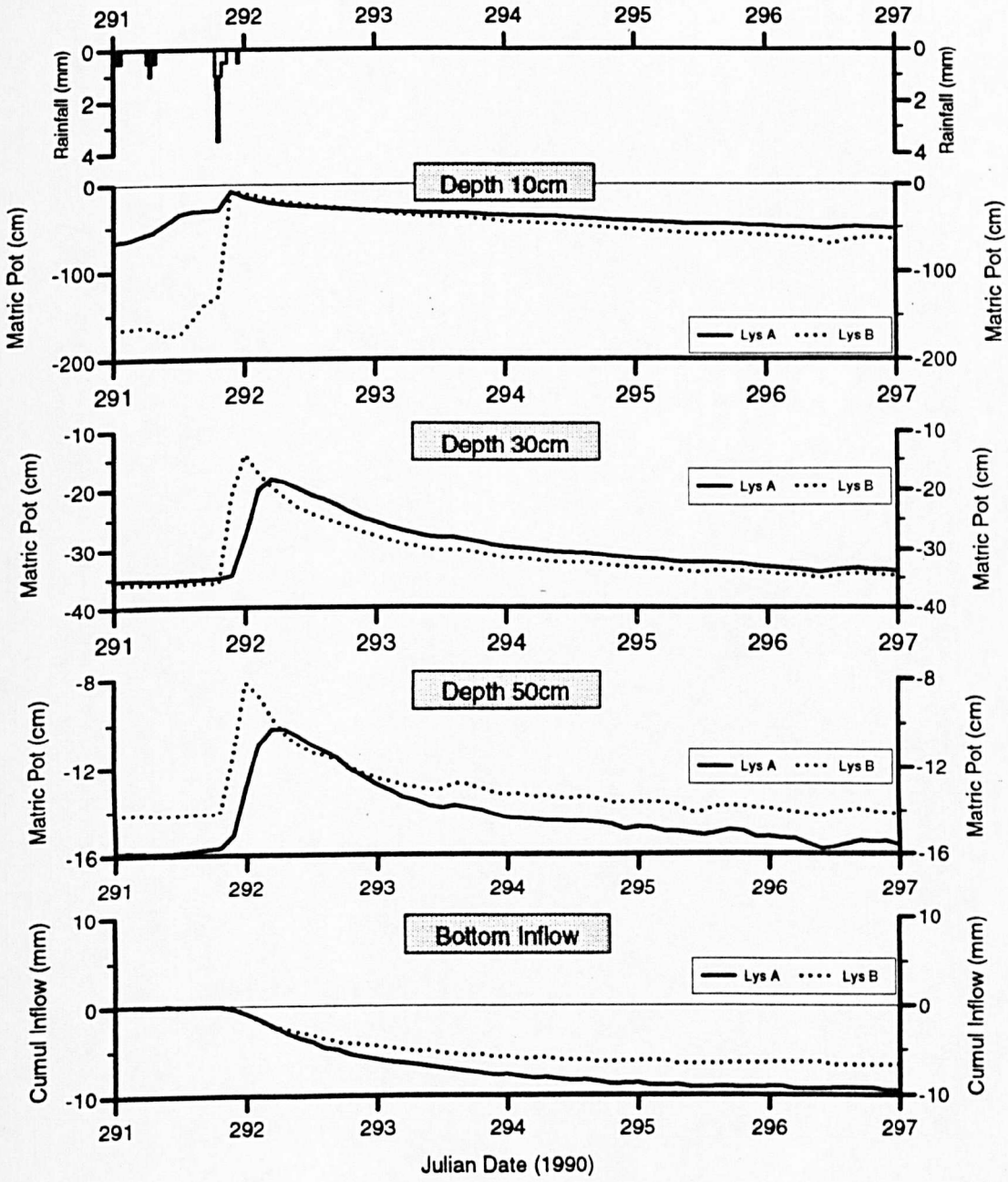


Figure 4.6 - Selected rapid flow event 90291

For both lysimeters there is movement of water from the lysimeter to the common reservoir initiating just after the beginning of the rapid increase of water tensions in the middle and deep tensiometers. As commented for event 90230, it shows that a volume of water was transmitted very quickly directly to the bottom of the lysimeter, reinforcing the hypothesis of rapid flow.

In events 91017, 91119, 91198, and 91211 (respectively, figures 4.7, 4.8, 4.9 and 4.10), the records from the tensiometers of lysimeters A and B are very similar. In all these events there are strong evidences of rapid flow, as the matric potentials respond very quickly to the rainfall inputs, along the whole soil profile. The data from tensiometers at the bottom and middle of the soil depth profile show that the tensions not only rise quickly, but also the recession curves are steep. In the top layer the behaviour is similar to that described for lysimeter B in event 90291: a quick rise, but a slow recession curve. This pattern is observed in most of the identified rapid flow events. Also, for all these events, the bottom inflow presents evidence of rapid flow, as there is always flow of water out of the lysimeter and into the common reservoir, coincident with the rapid increase of water tensions.

Event 91136 (figure 4.11) is different from the other events, because the change in matric potential was due to water added through the base of the lysimeters, rather than a response to rainfall input. As reported by Butler (1991b), a progressive dilution of the radiochemical concentrations in the lysimeters hydraulic system occurs during the winter months, as a result of rainfall excess over evaporation. A re-dosing of the radiochemical concentrations is therefore necessary in order to establish a uniform radiochemical concentration throughout the whole of the hydrological control system at the start of the main crop growth season in Spring. The re-dosing of the lysimeter substrate is achieved by re-circulating the substrate solution via a feed line from a dosing bottle. The procedures for radiochemical re-dosing have been described by Wadey (1991).

A sharp rise in the lower tensiometers on all four instrumented lysimeters had occurred during the first re-dosing (16-17 May 1991 - Julian date: 91136-91137), in response to 3 litres added through the base of the lysimeter. This was followed by a less rapid fall back to the original values (Butler, 1991b). The very sensitive responses of the water tables in all lysimeters, with a rise of up to 21.8cm for lysimeter B, were far greater than those which could be explained by treating the soil as a uniform porous medium, strongly suggesting by-pass or preferential flow mechanisms.

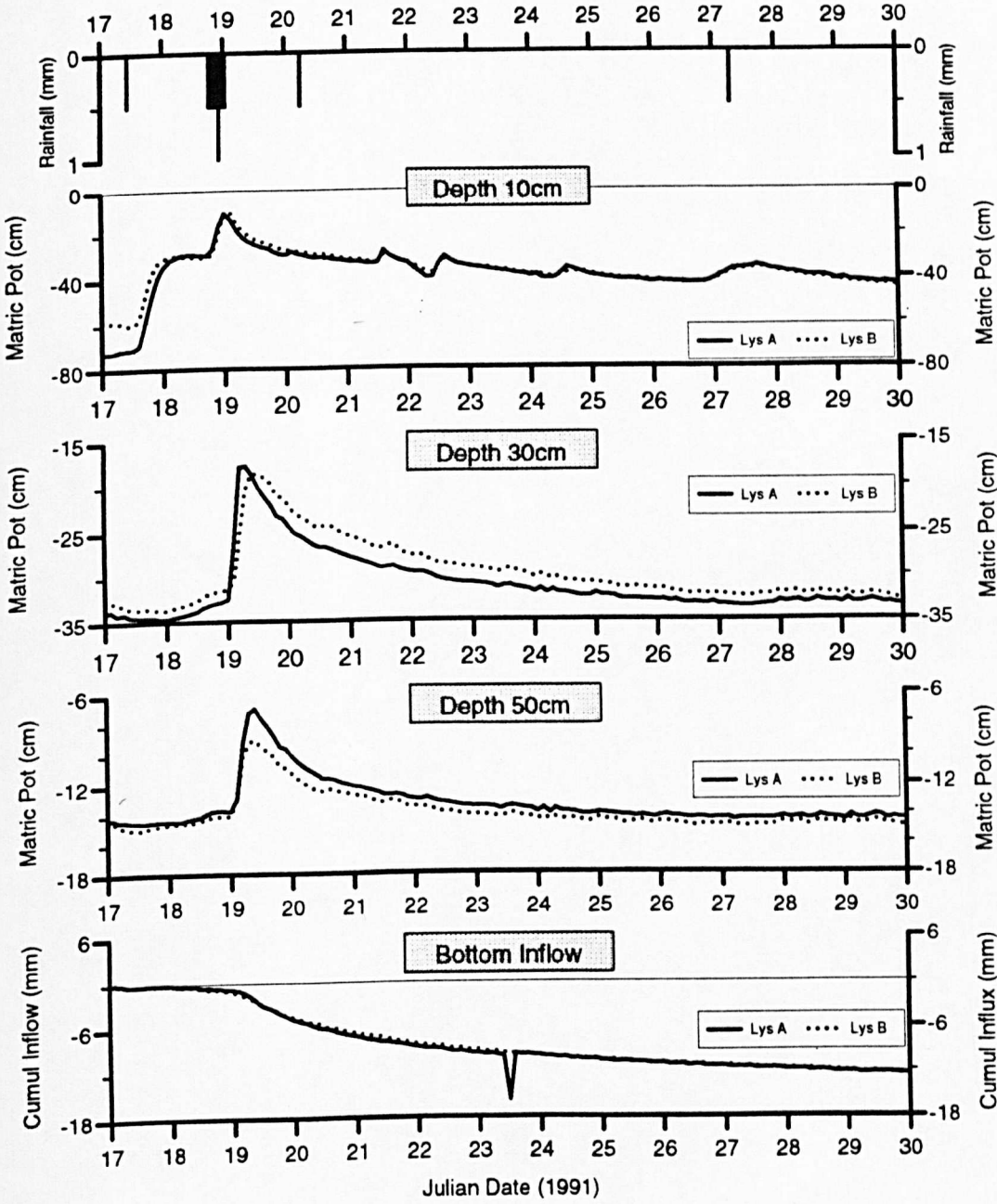


Figure 4.7 - Selected rapid flow event 91017

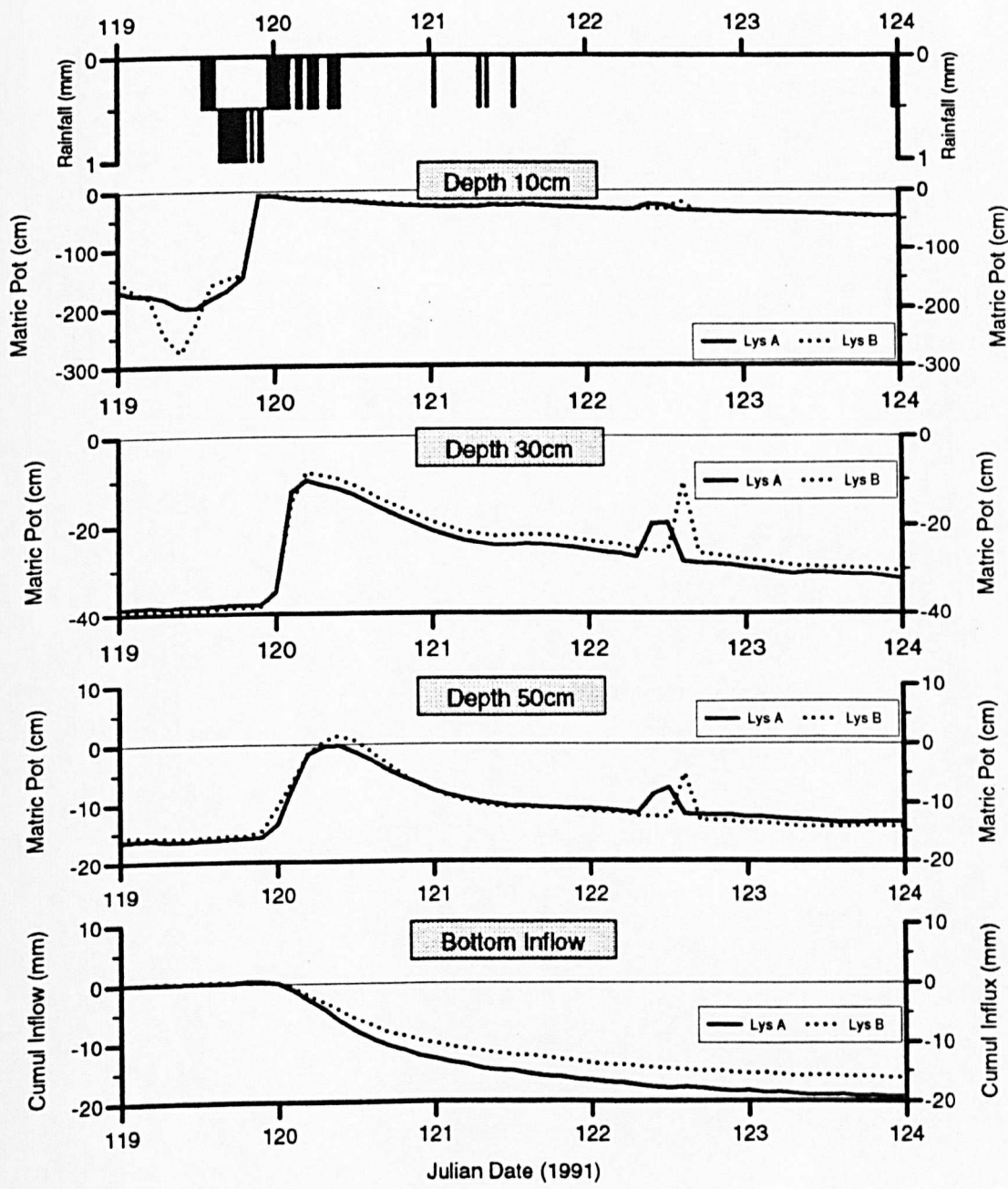


Figure 4.8 - Selected rapid flow event 91119

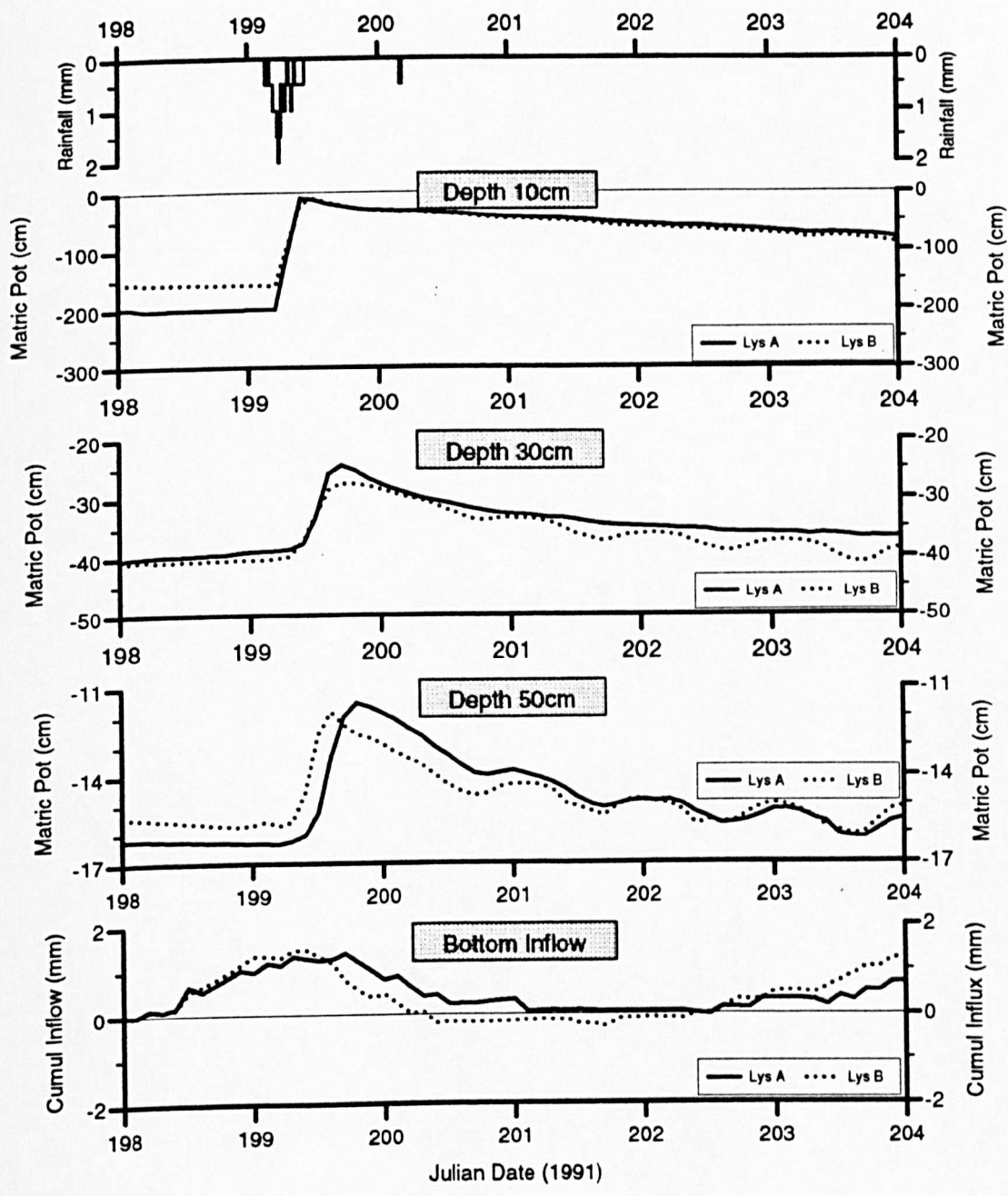


Figure 4.9 - Selected rapid flow event 91198

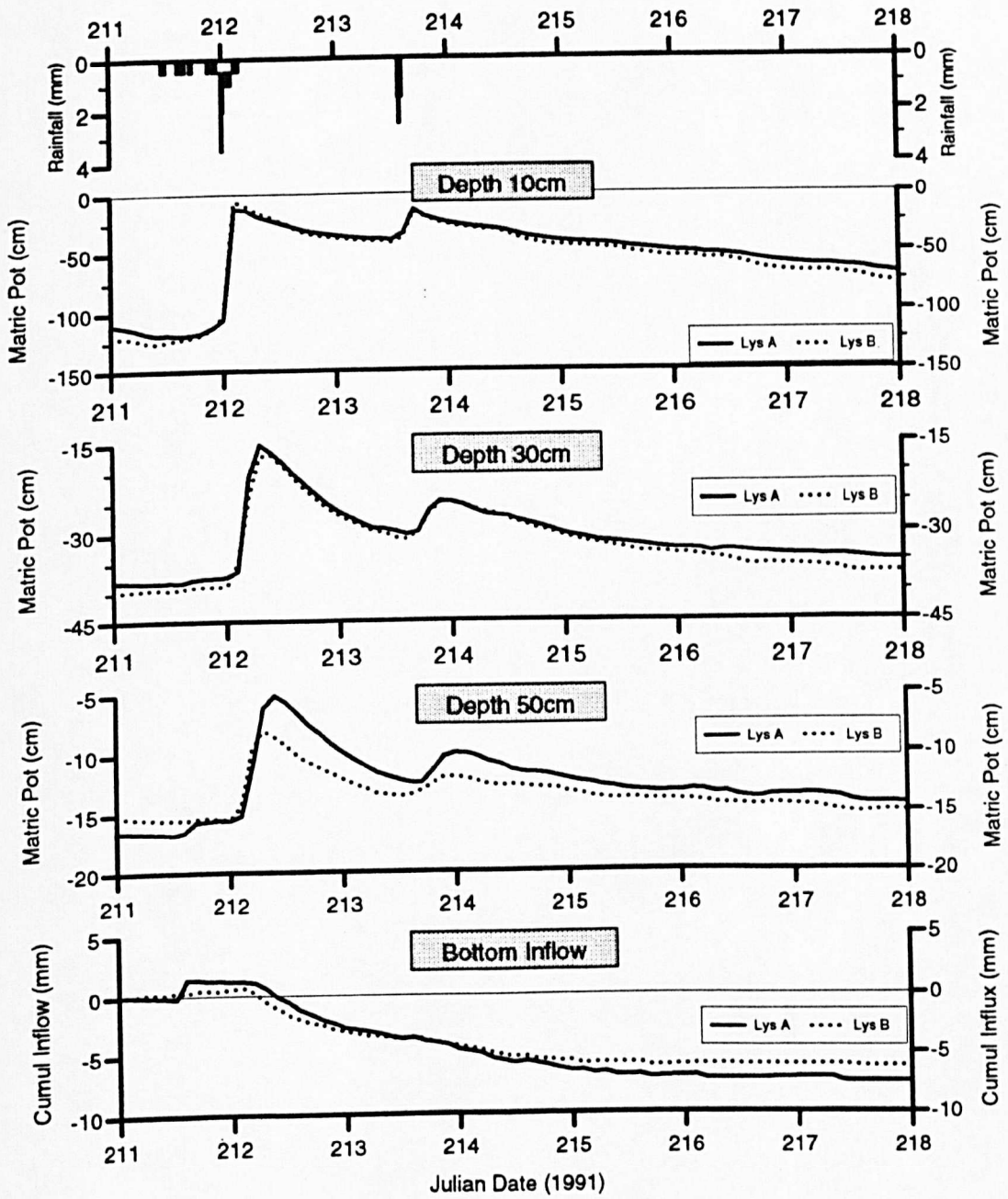


Figure 4.10 - Selected rapid flow event 91211

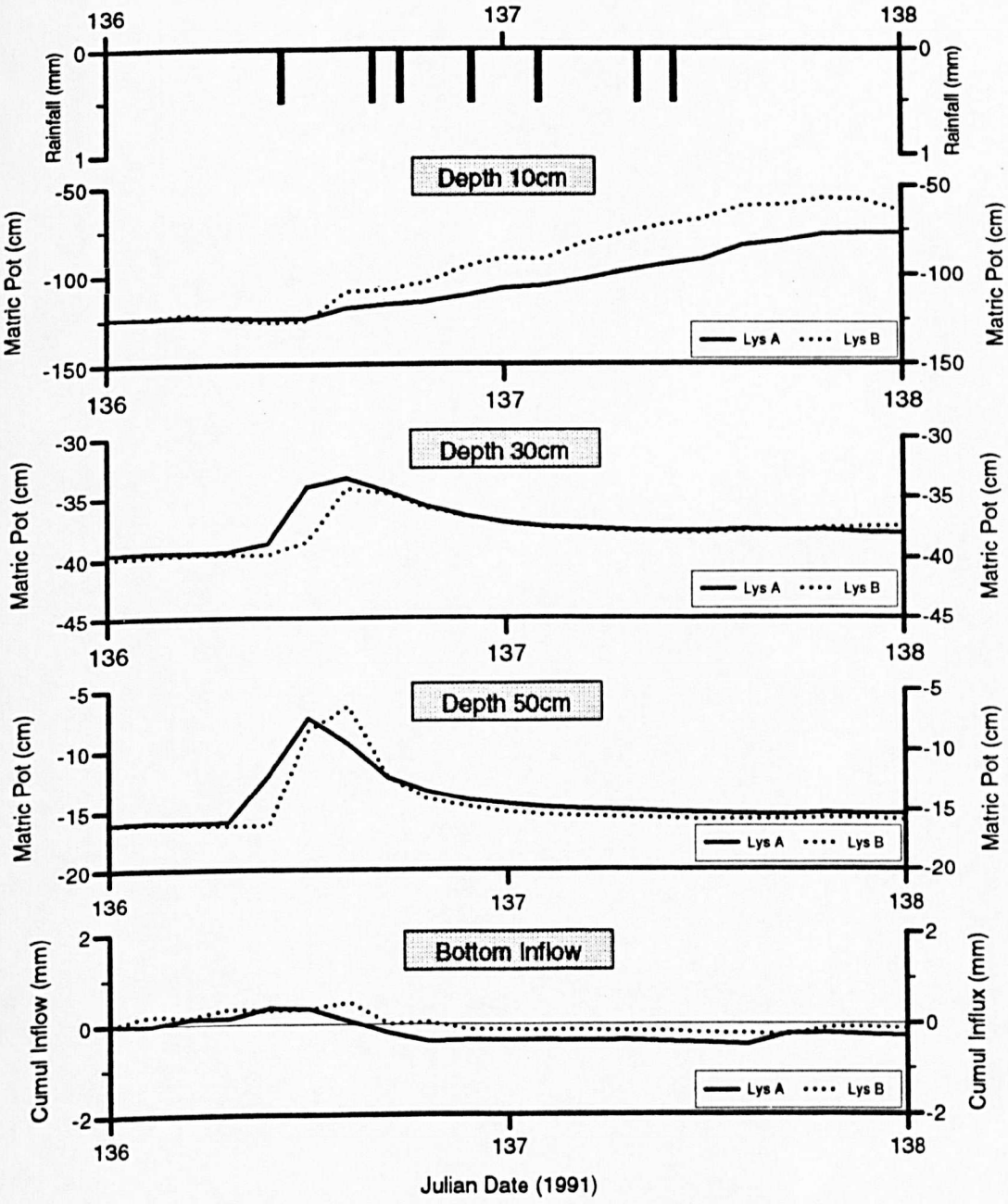


Figure 4.11 - Selected rapid flow event 91136

These eight events cover all observed main features in the identified rapid flow events, as the great majority of the events present very similar patterns. Due to this repeatability of the main characteristics of the events, even though this small sample consists of less than 10% of the total number of events identified, it represents the main processes observed in the rapid flow events, and enable us to test the technical viability of the different modelling approaches described in chapter 3.

4.3.2 - Analysis of the selected slow flow events

The selected events with no evidence of rapid flow are presented in table 4.4 and figures 4.12 to 4.15. These events will be denominated 'selected slow flow events'. As for the selected rapid flow events, the responses of matric potential for three different depths along the soil profile and the cumulative influx of water through the bottom of the lysimeters are shown in these figures, and a zero reference line is plotted whenever appropriate. Also, as the selected rapid flow events, each of the selected slow flow events will be identified by its julian starting date.

Table 4.4 - Selected slow flow events

Starting Date		Ending Date		Total Rainfall (mm)	Max. Intensity (mm/h)	Total ET by Penman (mm)
Julian	Gregorian	Julian	Gregorian			
90129	09/05/90	90135	15/05/90	7.0	2.5	10.7
91108	18/04/91	91118	28/04/91	10.5	2.0	14.9
91165	14/06/91	91174	23/06/91	11.5	1.5	20.8
91204	23/07/91	91211	30/07/91	9.0	1.0	20.2

All selected slow flow events present similar characteristics: even when the 10cm deep tensiometers register sensitivity to the rainfall input, this response is not quickly transmitted down into the soil, and is not noticeable in the tensiometers in the middle and bottom of the profile. The rainfall intensities are low, which could explain why in these events there is no evidence of rapid flow: perhaps the input was not enough to exceed infiltration capacity into the matrix in the top of the soil, and, consequently, the contribution of macropore flow is irrelevant. Also, the total rainfall is always smaller than the estimated total evapotranspiration. Therefore, the bottom inflow consistently shows a nearly constant flow of water from the common reservoir to the lysimeters, in order to keep the water table level fixed at 5cm above the base of the lysimeters, compensating effects of evapotranspiration. It is important to emphasise that these selected slow flow events are those where biggest values of rainfall were observed without

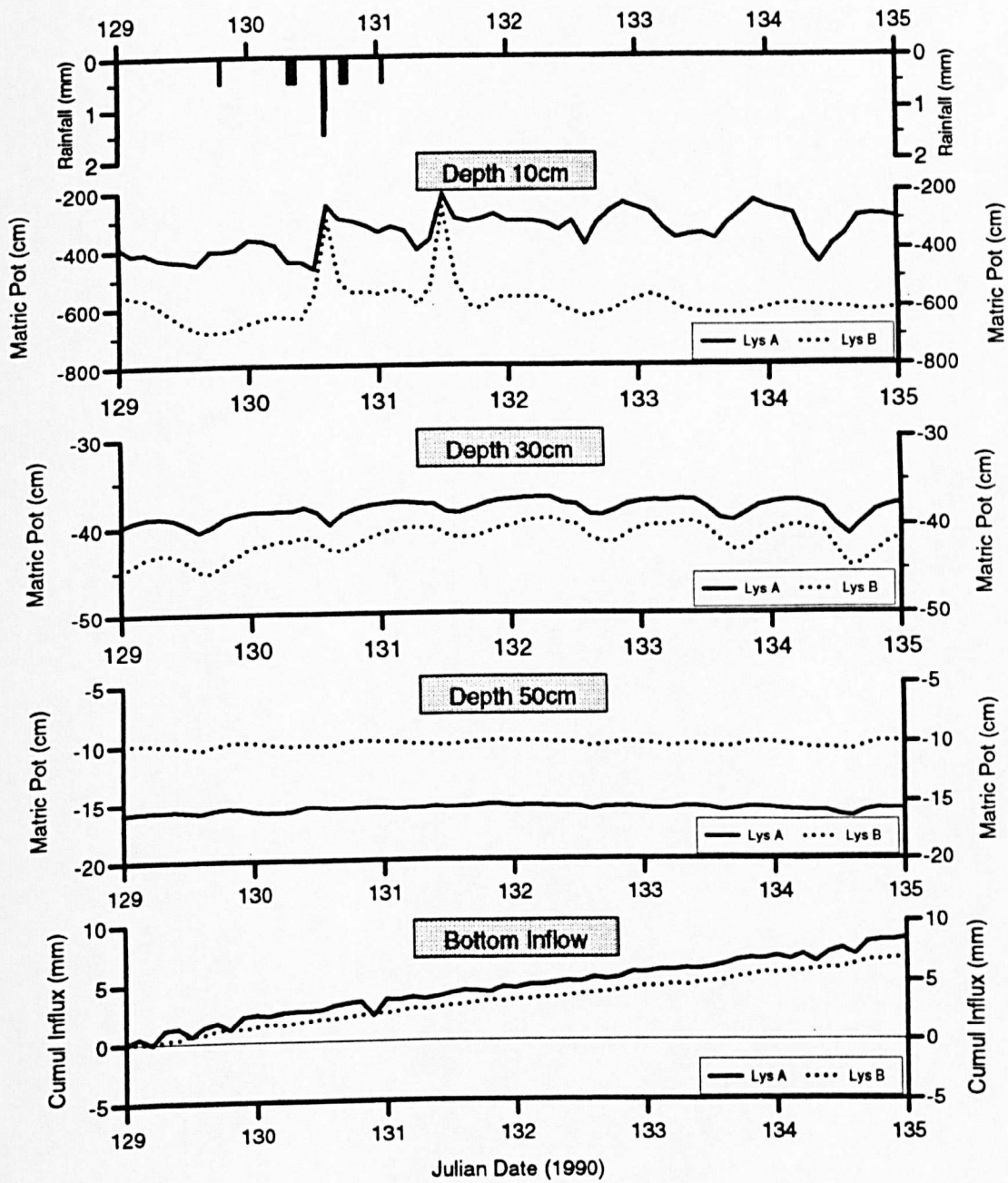


Figure 4.12 - Selected slow flow event 90129

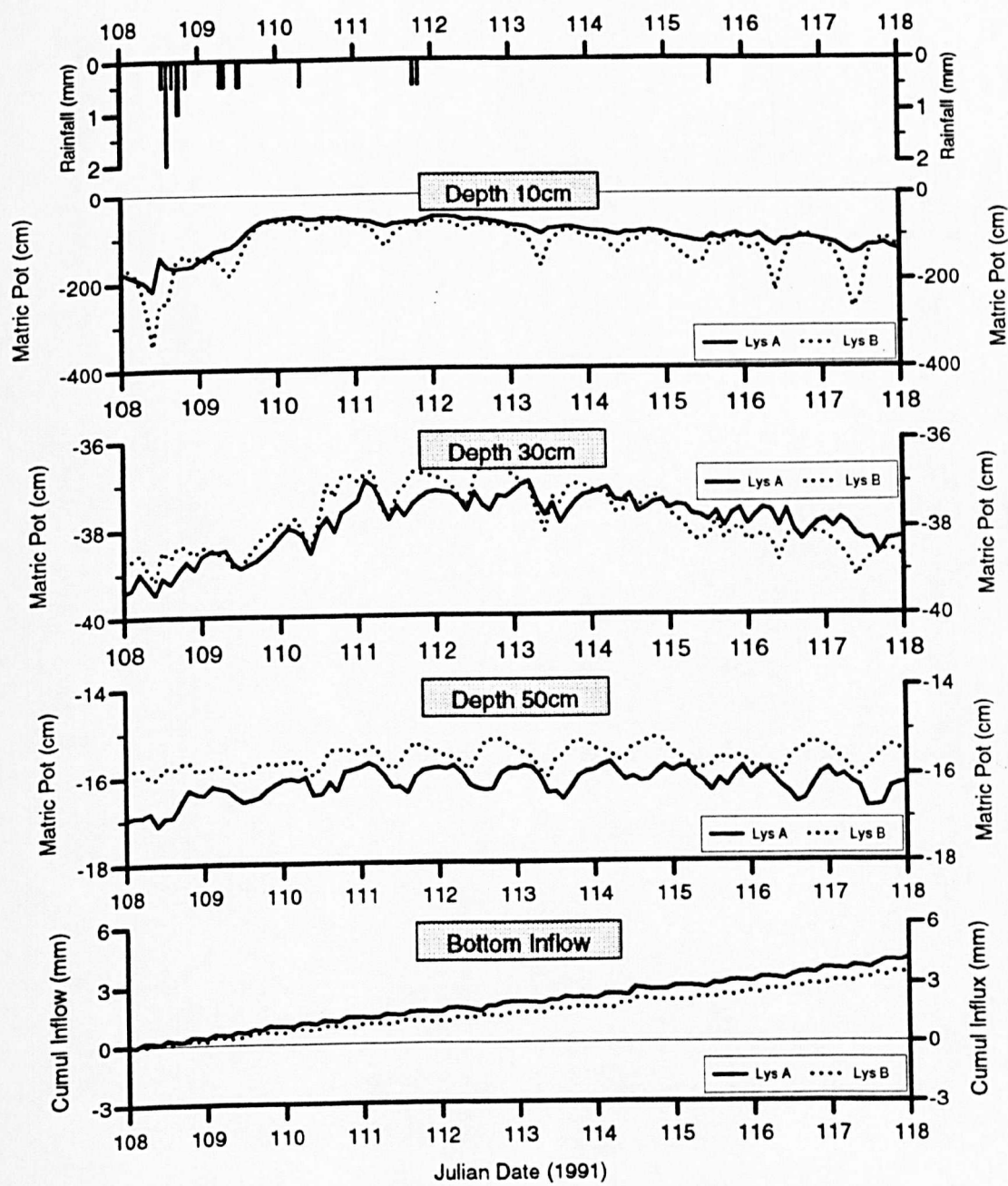


Figure 4.13 - Selected slow flow event 91108

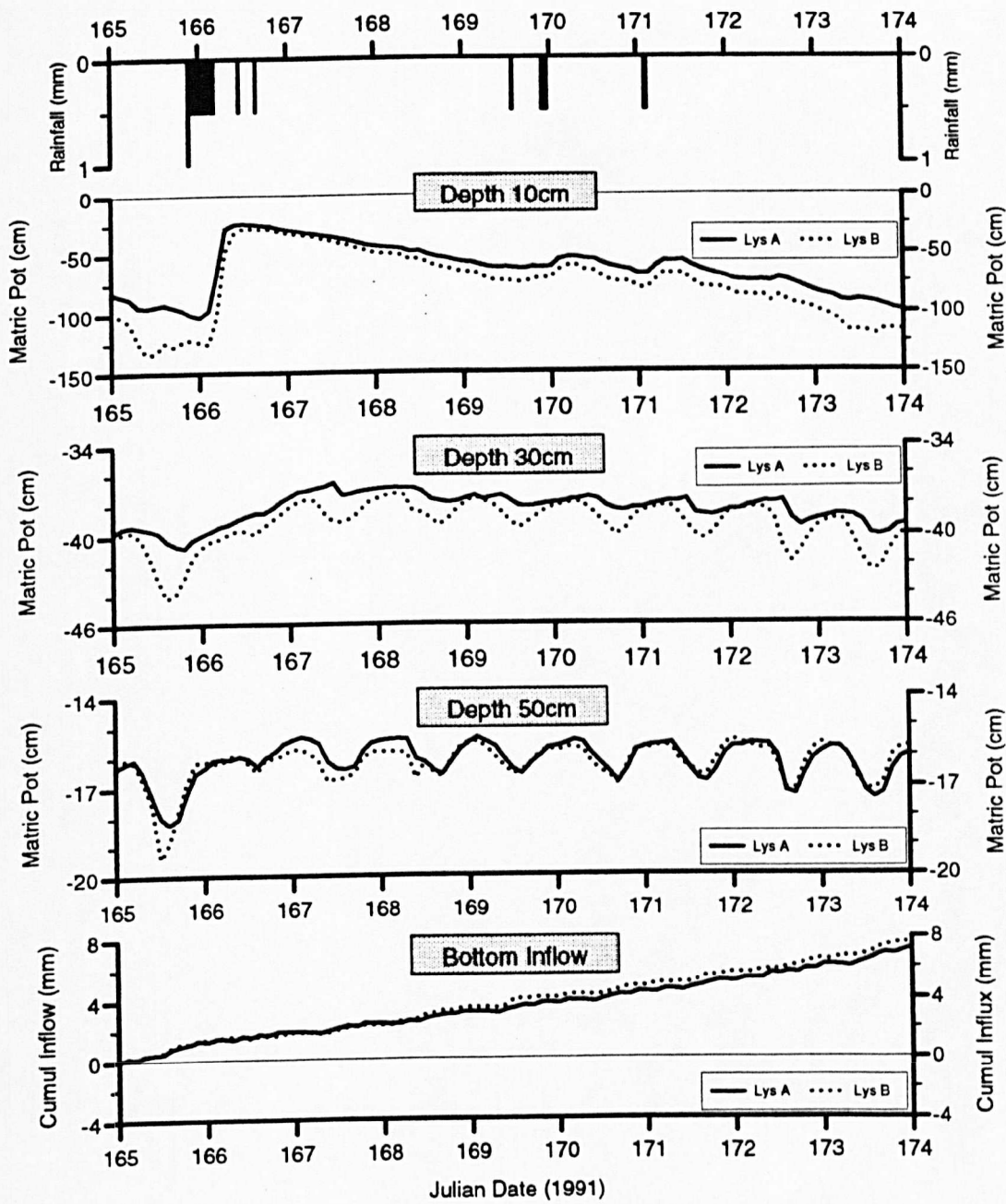


Figure 4.14 - Selected slow flow event 91165

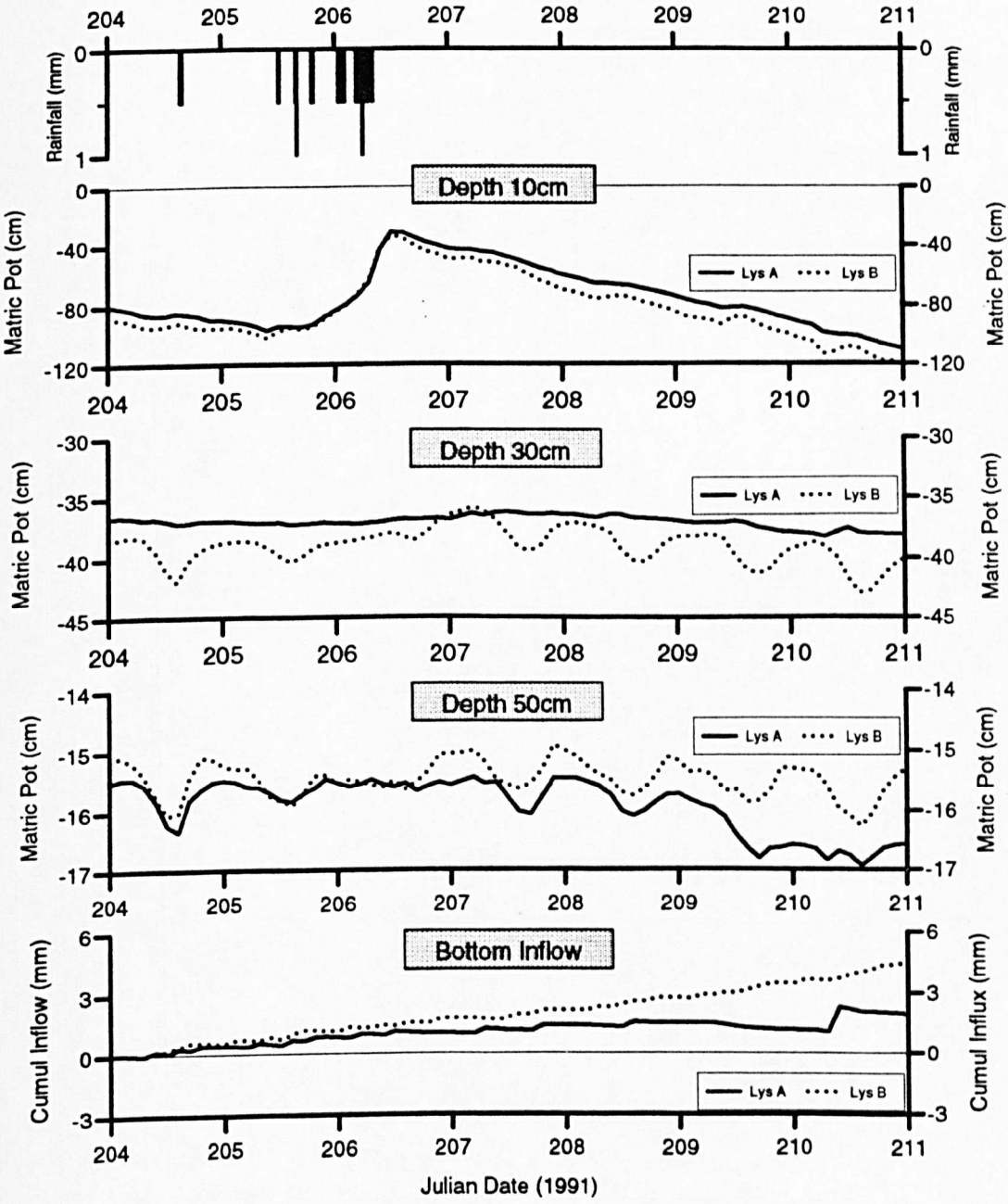


Figure 4.15 - Selected slow flow event 91204

evidence of rapid flow; in the other slow flow events the rainfall input is generally smaller and, in some cases, of similar magnitude. Also, in all selected slow flow events the diurnal effects caused by evapotranspiration can be observed for the whole depth profile.

The slow flow events were selected in order to test both single and dual porosity modelling approaches. Applying single porosity modelling approaches to these slow flow events helps to verify if their conceptualisation and parametrisation is appropriate to represent the experimental set, at least when there is no preferential flow. The simulations of the selected slow flow events with the use of a dual porosity modelling approach verify their performance to simulate this situation and help to test the hypothesis that the rainfall input was not enough to cause rapid flow.

4.4 - Conclusions

As part of a combined experimental and modelling study of radionuclide transport in vegetated soils, detailed lysimeter experiments were undertaken at Silwood Park, near Ascot, England, based on controlled water table conditions. The experimental station, consisted of an automatic weather station and eight concrete lysimeters, was designed as part of a contract undertaken by Imperial College under the Nirex Safety Assessment Research Program (NSARP).

Each of the lysimeters was provided with equipment for measuring root distribution, redox potential, crop height, leaf area index, pH and soil moisture properties (access tubes for neutron probe, TDR, pressure-transducers + tensiometers systems), and procedures were taken in the experimental station in order to minimise data error. Of the eight lysimeters, four were monitored intensively at each timestep, in a total of 100 measurement/day. The other four were replicates and were measured weekly to act as a cross-check. The system designed to control the water table level allows the measurement of the flow through the base of the lysimeter, providing full knowledge of the lower boundary condition. A combined analysis of the bottom influx and the tensiometer response can help to identify water flowing down the walls of the lysimeters, and also can provide evidence of rapid flow.

The data collected from these lysimeters show several events where evidence of rapid water flow can be identified, determining the necessity of a detailed analysis of the soil moisture data set in order to better understand and simulate the processes involved in these events.

A total of more than 160 events is noticeable during the four years the experimental

station was fully operational. From this total, more than 110 events present immediate response from the tensiometers located at the bottom of the lysimeters, providing evidence of preferential or rapid water flow. After a detailed study of these events, a set of 8 events, where the evidence of rapid flow was significant and representative of the different situations observed in the whole data set, was selected and designated for detailed analysis and later mathematical simulations. This set of eight events covers all observed main features in the identified rapid flow events, as the great majority of them present very similar patterns. A set of 4 events where no evidence of preferential water flow can be assumed is also identified. Both sets of events were selected in order to assess the performance of different modelling approaches and to test hypothesis describing the physical processes governing the flux of water in the near surface environment.

CHAPTER 5 - MEASUREMENT AND ESTIMATION OF SOIL PROPERTIES

5.1 - Introduction

The use of numerical models for simulating and understanding subsurface water flow is receiving increasing attention, and more detailed and sophisticated models are being developed. Greater model sophistication implies greater data needs, both in terms of quality and quantity. Due to the multiphase characteristic of flow in the unsaturated zone, the determination of flow properties is especially complex and, consequently, difficulties in model calibration are strongly present for models dealing with flow in this part of the soil.

According to Kool et al. (1987), hydraulic and transport properties of the unsaturated zone are commonly determined by imposing rather restrictive initial and boundary conditions, so that the governing equations can be inverted by analytical or semi-analytical methods. Experimental analyses based on direct measurements are generally time-consuming and expensive due to the need to meet conditions requisite for the explicit calculation of model coefficients. Often the governing equations themselves need to be linearised or otherwise approximated to allow their (semi-)analytical inversion. Another limitation results from the need to impose relatively simple initial and boundary conditions, which can be problematic for field experiments. Also, information concerning parameter uncertainty is not readily obtained from direct inversion techniques.

An alternative to the experimental approach is the prediction of hydrologic properties from routinely measured textural and structural soil properties (Arya and Paris, 1981). According to Mishra et al. (1989), since soil textural information is more easily obtained than static or dynamic hydraulic data, an appealing alternative for estimating soil properties is from a particle size distribution (PSD). Methods have been proposed for computing soil water retention relations from PSD data using regression equations (Rawls and Brakensiek, 1982 and 1985; Saxton et al., 1986) or via models with quasiphysical bases (Arya and Paris, 1981). Although the estimation of soil hydraulic properties from PSD data may offer substantial savings in experimental effort over more direct calibration methods, accuracy will generally be reduced. As commented in section 2.2.3, as many of these models were obtained using data from soils of a limited region, predictions using such models can incur in errors, as they are not necessarily valid for other areas.

An alternative and more flexible approach is to employ parameter estimation techniques

to solve the inverse problem. Parametric relationships are supposed to be applicable to the system, and the coefficients are determined by means of an optimisation algorithm that extremises some objective function. A major advantage is that experimental conditions can be selected on the basis of convenience and expediency, rather than by a need to simplify the mathematics of the direct inversion process. Also, if information concerning parameter uncertainty and effects on model accuracy is desired, it can be easily obtained from the parameter estimation analysis. However, the ability to determine the specific form of the constitutive properties of the system is sacrificed, and some model formulation which is presumed to hold to a sufficient degree of approximation must be assumed. Consequently, the problem of parameter identification arises, which involves performing the estimation analyses for many possible models, and selecting from those models the most accurate or precise one in terms of some objective criterion (Kool et al. , 1987).

This chapter deals with the determination of soil properties for the lysimeters located at Imperial College's Field Research Station in Silwood Park. Values for the particle size distribution, saturated conductivity, porosity, dry bulk density and void ratio were provided by physical analysis of soil cores taken from the lysimeters. Estimates of parameter values and associated uncertainty of three different soil characteristic parametric relationships were obtained through the use of first-order error analysis applied to the available matric potential and soil moisture data.

5.2 - Physical analysis of soil cores from the lysimeters

Soil particle size analysis was available from the experimental study which Imperial College is undertaking on behalf of UK Nirex Ltd. This data was obtained from two cores taken from the deep lysimeter B, during the course of the experiment. The results of this particle size analysis are presented in following sections.

At the end of the period when the system of eight lysimeters was fully operational (from 23/04/90, or Julian date 90113, to 12/04/94, or Julian date 94102), two lysimeters were selected for destructive sampling: F, a deep lysimeter (70cm depth), and G, a shallow lysimeter (40cm depth). In following sections the results of the physical analysis of the soil cores taken from these lysimeters are described, comprising tests of saturated conductivity, porosity, dry bulk density and void ratio.

5.2.1 - Materials and methods

The available data for particle size distribution (PSD) is presented and discussed in section 5.2.2. It was acquired through soil particle size analysis, using a hydrometer method, of two cores from deep lysimeter B, dated 06/08/90 (Julian date 90218) and 28/07/92 (Julian date 92210). The methodology employed for these tests, as described in a personal communication by Chacksfield (1994), is presented in Appendix II (Soil particle size analysis using hydrometer method).

A falling head permeameter apparatus was assembled in the Hydrology Laboratory, at Ascot, to perform tests of saturated conductivity, porosity, dry bulk density and void ratio on cores taken from the destructive sampling of lysimeters F and G. It consists of a permeability cell, a set of core cutters, a standpipe panel, a soaking tank, a funnel and silicone tubing. A detailed description of the apparatus is presented in Appendix III (Instructions for using the falling head permeameter), together with the procedure for its use and the equations necessary for the calculations

The cores used with the permeameter apparatus were taken at different depths in each lysimeter, in order to obtain a better representation of the vertical variability of the physical properties of the soil. Lysimeter G (which presents a total depth of 40cm) had cores extracted from two layers, the first at 0cm depth (top at the soil surface), called layer G0, and the second at 20cm depth, called layer G20. The cores from lysimeter F (with total depth of 70cm) were obtained from three different layers: at 0cm depth (layer F0), at 25cm depth (layer F25) and at 50cm depth (layer F50). All these depths refer to the top of the cores and the core samplers are 13cm long.

Due to the dimensions of the cores for this test (10cm diameter and 13cm length), they were extracted always after all other destructive sampling were performed, in order to avoid excessive disturbance of the soil in the lysimeters before other analysis. The number of cores for permeability tests extracted per layer was determined by the availability of core samplers on the day of sampling. For this reason, four cores were taken from layer G0 and seven cores from each of the other layers, a total of 32. Tests for the saturated conductivity were performed for each of these cores, as well as the determination of the porosity, dry bulk density and void ratio.

5.2.2 - Summary of the soil particle size analysis

A summary of the results of the soil particle size analysis using hydrometer method of the 2 cores taken from the deep lysimeter B is presented in table 5.1. These results seem to show a small variation of the soil particle distribution with depth. The small size of the sample (only two cores) does not allow further statistical analysis, but it gives sufficient information in order to identify a sandy loam soil.

Table 5.1 - Particle Size Analysis - Summary of the Results

Core Identification	Sample Depth (cm)	% Silt	% Clay	% Sand
Lysimeter B 06/08/90 Julian date 90218	0 - 10	7.2	2.6	90.2
	10 - 20	7.6	4.8	87.6
	20 - 30	9.5	3.6	86.9
	30 - 40	9.6	4.4	86.0
	40 - 50	9.6	3.8	86.6
	50 - 60	8.8	4.0	87.2
	60 - 70	7.4	1.8	90.8
Lysimeter B 28/07/92 Julian date 92210	0 - 10	9.6	2.6	87.8
	10 - 20	6.8	3.8	89.4
	20 - 30	10.1	1.5	88.4
	30 - 40	6.5	6.0	87.5
	40 - 50	10.9	1.0	88.1
	50 - 60	13.8	0.6	85.6
	60 - 70	6.7	0.6	92.7

Clay: 0 - 2 μm
 Silt: 2 - 50 μm
 Sand: > 50 μm

5.2.3 - Summary of the permeameter test results

A summary of the results of the physical analysis of the 32 cores taken from the destructive sampling of lysimeters F and G is presented in table 5.2. In this table, the column "No. of Tests" refers to the number of single tests performed on one core for the determination of the saturated conductivity. The recommended minimum number of single tests per core is 3. However, for values of conductivity near to or smaller than 0.05cm/h, this number could be reduced (as the time taken for each single test would be long; near or more than 1 hour), under the condition of internal consistency of the test, i.e., when the conductivity calculated at

intermediate levels keeps a constant value until the end of the single test. The columns "Mean Ks" and "Std Dev" refer to the computed values of mean and standard deviation of the single tests, for each core.

Table 5.2 - Physical Analysis of the Cores - Summary of the Results

LYSIM NAME	DEPTH (cm)	CORE No	POROS (%)	DRY BLK DENSITY (g/cm ³)	VOID RATIO (-)	SAT CONDUCT			OBS
						No.OF TESTS	MEAN Ks (cm/h)	STD DEV (cm/h)	
G	0	G0-1	52.9	1.18	1.13	5	0.88	0.03	-
G	0	G0-2	44.9	1.24	0.81	3	26.57	1.41	-
G	0	G0-3	50.4	1.17	1.02	3	162.10	2.62	-
G	0	G0-4	47.9	1.18	0.92	6	100.48	8.99	-
G	20	G20-1	-	-	-	-	-	-	HOLE
G	20	G20-2	42.2	1.67	0.73	3	0.68	0.01	-
G	20	G20-3	37.9	1.61	0.61	6	0.75	0.32	N STB
G	20	G20-4	37.4	1.59	0.60	11	22.56	20.53	N STB
G	20	G20-5	35.7	1.58	0.55	2	0.066	0.003	-
G	20	G20-6	46.7	1.51	0.87	3	0.17	0.006	-
G	20	G20-7	42.4	1.48	0.74	3	0.09	0	3*.09
F	0	F0-1	44.9	1.20	0.82	6	36.00	21.29	N STB
F	0	F0-2	45.8	1.21	0.85	3	323.01	5.22	-
F	0	F0-3	45.4	1.29	0.83	6	6.26	0.18	-
F	0	F0-4	43.0	1.19	0.75	6	15.37	1.22	-
F	0	F0-5	47.8	1.18	0.92	6	30.24	3.17	-
F	0	F0-6	49.1	1.22	0.97	7	30.35	3.13	-
F	0	F0-7	47.8	1.20	0.92	4	93.39	7.94	-
F	25	F25-1	34.0	1.55	0.52	3	0.26	0.01	-
F	25	F25-2	31.0	1.18	0.45	3	308.02	20.75	-
F	25	F25-3	29.9	1.40	0.43	4	0.18	0.05	3*.16
F	25	F25-4	37.1	1.50	0.59	4	0.93	0.04	-
F	25	F25-5	37.1	1.70	0.59	3	0.17	0.006	-
F	25	F25-6	36.1	1.54	0.56	3	8.24	0.12	-
F	25	F25-7	38.5	1.61	0.63	3	0.52	0.05	-
F	50	F50-1	34.1	1.68	0.52	6	9.42	6.46	N STB
F	50	F50-2	33.0	1.71	0.49	1	0.017	-	96min
F	50	F50-3	35.5	1.67	0.55	1	0.030	-	52min
F	50	F50-4	35.5	1.64	0.55	1	0.031	-	54min
F	50	F50-5	34.4	1.67	0.52	1	0.027	-	45min
F	50	F50-6	32.3	1.68	0.48	1	0.026	-	64min
F	50	F50-7	36.7	1.64	0.58	3	244.95	4.41	-

N STB = Not stabilised - Core rejected for Ks analysis

HOLE = Hole in the centre of the core - Core rejected

3*.09 = Three cores with K=0.09cm/h

96min = Time taken for a single test

Results obtained from 5 different cores were rejected due to problems during the tests. Core G20-1 (lysimeter G, extracted from depth 20cm) presented a hole in the centre of the core at the end of the test and had to be excluded. Cores G20-3, G20-4, F0-1 and F50-1 did not stabilise during the permeability tests, as the saturated conductivity computed for repeated single tests for each one of these cores did not converge, presenting a smaller value after each repetition of the procedure. The results of saturated conductivity obtained with these cores were rejected, but their values of porosity, dry bulk density and void ratio were accepted for statistical analysis.

The small number of valid results for each layer brings difficulty for the selection of the statistical distributions to be used in the analysis. As commented by Benjamin and Cornell (1970), with small samples, two distributions of quite dissimilar density functions may both seem to fit the data. The selection of a convenient distribution in these cases is dictated by professional reasons, such as previous knowledge of a suitable distribution, the relative importance of computational tractability, accuracy of representation and failure of a model to reproduce certain aspects displayed in data (limits, skew, etc.). These considerations lead to the selection of distributions that present computational tractability and are known to be likely to represent the variables analyzed.

The main statistics computed for porosity, dry bulk density and saturated conductivity results are presented in the next sections. Void ratio results were not analyzed because they do not provide any information that can not be obtained from porosity values. The equations and definitions for the statistics tests are presented in Appendix IV, based on Benjamin and Cornell (1970) and on Green and Margerison (1978). Student's t-test statistics were used due to the small size of the samples.

5.2.4 - Statistical analysis of porosity results

An analysis of the moments and of the coefficients of skewness and kurtosis presented in table 5.3 shows the inadequacy of distributions such as Gamma and Exponential to represent the porosity data, specially due to the small value of the skewness (see Appendix IV). A normal distribution, which presents computational tractability and is known to be likely to represent this variable, is consistent with the statistics presented in table 5.3. Also a log-normal distribution is consistent with the statistics presented in table 5.4. For these reasons, the statistical analysis were performed under the hypothesis of two different distributions: normal or log-normal.

Table 5.3 - Porosity - Moments about the mean

LYSIM NAME	DEPTH (cm)	n	POROSITY (%)						
			$\bar{x}$	s	$ s/\bar{x} $	m_3	g_1	m_4	g_2
G	0	4	49.0	3.4	0.07	- 2.0	-0.05	129.8	0.97
G	20	6	40.4	4.1	0.10	19.6	0.28	368.3	1.30
G	ALL	10	43.8	5.8	0.13	13.0	0.07	1631.4	1.44
F	0	7	46.3	2.1	0.05	- 1.5	-0.17	27.8	1.43
F	25	7	34.8	3.3	0.09	-13.7	-0.38	147.4	1.24
F	50	7	34.5	1.5	0.04	- 0.2	-0.06	7.7	1.52
F	ALL	21	38.5	6.1	0.16	99.2	0.44	2242.3	1.62

n = sample size

 $\bar{x}$ = sample mean

s = sample standard deviation

 m_n = sample n^{th} moment about the mean g_1 = sample coefficient of skewness g_2 = sample coefficient of kurtosis

Table 5.4 - Logarithm of Porosity - Moments about the mean

LYSIM NAME	DEPTH (cm)	n	ln of POROSITY (%)						
			$\bar{y}$	s_y	$ s_y/\bar{y} $	my_3	g_1	my_4	g_2
G	0	4	3.890	0.070	0.018	$-3 \cdot 10^{-3}$	-0.09	$2 \cdot 10^{-3}$	0.96
G	20	6	3.694	0.100	0.027	$2 \cdot 10^{-4}$	0.23	$1 \cdot 10^{-4}$	1.26
G	ALL	10	3.773	0.132	0.035	$-2 \cdot 10^{-4}$	-0.09	$5 \cdot 10^{-4}$	1.47
F	0	7	3.833	0.045	0.012	$-1 \cdot 10^{-3}$	-0.15	$6 \cdot 10^{-4}$	1.52
F	25	7	3.546	0.097	0.027	$-4 \cdot 10^{-4}$	-0.44	$1 \cdot 10^{-4}$	1.30
F	50	7	3.540	0.045	0.013	$-8 \cdot 10^{-4}$	-0.09	$6 \cdot 10^{-4}$	1.34
F	ALL	21	3.640	0.154	0.042	$1 \cdot 10^{-3}$	0.29	$9 \cdot 10^{-4}$	1.64

n = sample size

 $\bar{y}$ = mean value of the logarithms of the sample s_y = standard deviation of the logarithms of the sample my_n = n^{th} moment about the mean of the logarithms of the sample g_1 = coefficient of skewness of the logarithms of the sample g_2 = coefficient of kurtosis of the logarithms of the sample

The samples were analyzed in order to verify if there is a significant difference between the mean values of porosity observed in the different layers of a lysimeter. A level of significance of 1% was adopted, and the comparisons were made between the means of layer G0 against G20, F25 against F50, and F0 against F25. In all of these comparisons, the null hypothesis is that both means are the same; the alternative hypothesis is that the means are different. The statistics are computed using the equations presented in Appendix IV (Equations and definitions for the statistics tests), for test between means drawn from two samples, assuming normal distributions with unequal unknown variances (Benjamin and Cornell, 1970; Green and Margerison, 1978).

For the comparison between the means of layer G0 against G20, the realisation of the statistic T is 3.605, and $f=7.440$. For a significance level of 1%, the Student's distribution gives us $t_{(0.5\%,7)}=3.499$. So, the null hypothesis is rejected and there is a significant difference between the mean values of porosity for layers G0 and G20, at a significance level of 1%, assuming a normal distribution.

For the comparison between the means of layer F25 against F50, the realisation of the statistic T is 0.219, and $f=8.378$. For a significance level of 1%, the Student's distribution gives us $t_{(0.5\%,8)}=3.355$. So, the null hypothesis is accepted and there is no significant difference between the mean values of porosity for layers F25 and F50, at a significance level of 1%, assuming a normal distribution.

For the comparison between the means of layer F0 against F25, the realisation of the statistic T is 7.779, and $f=10.175$. For a significance level of 1%, the Student's distribution gives us $t_{(0.5\%,10)}=3.169$. So, the null hypothesis is rejected and there is a significant difference between the mean values of porosity for layers F0 and F25, at a significance level of 1%, assuming a normal distribution. As a direct consequence, there is also a significant difference between the mean values of porosity for layers F0 and F50, as F25 and F50 do not present significant difference, and the observed mean for F50 is slightly smaller than that of F25.

Assuming a log-normal distribution, the results are:

Layer G0 against G20: $T=3.645$; $f=7.920$; $t_{(0.5\%,7)}=3.499$
 H_0 rejected at 1% of significance

Layer F25 against F50: $T=0.148$; $f=8.468$; $t_{(0.5\%,8)}=3.355$
 H_0 accepted at 1% of significance

Layer F0 against F25: $T=7.101$; $f=8.468$; $t_{(0.5\%,8)}=3.355$
 H_0 rejected at 1% of significance

The conclusions drawn from the hypothesis of log-normal distribution are exactly the same as those obtained from the hypothesis of normal distribution: there is a significant difference between the mean values of porosity for layers G0 and G20, for layers F0 and F25 and also for layers F0 and F50; there is no significant difference between the mean values of porosity for layers F25 and F50 (always at a level of significance of 1%).

These results show that the porosity of the top layer can be accepted as higher than those of the deeper layers. This behaviour can be explained by the higher biological activity in the top layer, due to the bigger number of roots and small animals, such as worms.

5.2.5 - Statistical analysis of dry bulk density results

The moments and the coefficients of skewness and kurtosis for the dry bulk density data are presented in tables 5.5 and 5.6.

Table 5.5 - Dry Bulk Density - Moments about the mean

LYSIM NAME	DEPTH (cm)	n	DRY BULK DENSITY (g/cm ³)						
			$\bar{x}$	s	$ s/\bar{x} $	m_2	g_1	m_4	g_2
G	0	4	1.19	0.03	0.03	$3 \cdot 10^{-3}$	1.06	$2 \cdot 10^{-4}$	1.98
G	20	6	1.57	0.07	0.04	$2 \cdot 10^{-3}$	0.06	$3 \cdot 10^{-3}$	1.26
G	ALL	10	1.42	0.20	0.14	$-2 \cdot 10^{-3}$	-0.21	$2 \cdot 10^{-3}$	1.15
F	0	7	1.21	0.04	0.03	$7 \cdot 10^{-3}$	1.06	$6 \cdot 10^{-4}$	2.34
F	25	7	1.50	0.17	0.11	$-4 \cdot 10^{-3}$	-0.71	$2 \cdot 10^{-3}$	2.11
F	50	7	1.67	0.02	0.01	$2 \cdot 10^{-4}$	0.21	$6 \cdot 10^{-7}$	3.75
F	ALL	21	1.46	0.22	0.15	$-2 \cdot 10^{-3}$	-0.21	$3 \cdot 10^{-3}$	1.08

n = sample size

$\bar{x}$ = sample mean

s = sample standard deviation

m_n = sample n^{th} moment about the mean

g_1 = sample coefficient of skewness

g_2 = sample coefficient of kurtosis

Table 5.6 - Logarithm of Dry Bulk Density - Moments about the mean

LYSIM NAME	DEPTH (cm)	n	ln of DRY BULK DENSITY (g/cm ³)						
			$\bar{y}$	s_y	$ s_y/\bar{y} $	my_2	g_1	my_4	g_2
G	0	4	0.176	0.027	0.153	$1 \cdot 10^{-3}$	0.64	$6 \cdot 10^{-7}$	1.17
G	20	6	0.452	0.044	0.097	$-6 \cdot 10^{-4}$	-0.07	$5 \cdot 10^{-4}$	1.31
G	ALL	10	0.342	0.147	0.430	$-8 \cdot 10^{-4}$	-0.26	$5 \cdot 10^{-4}$	1.07
F	0	7	0.193	0.029	0.150	$3 \cdot 10^{-3}$	1.20	$2 \cdot 10^{-4}$	3.06
F	25	7	0.398	0.119	0.299	$-1 \cdot 10^{-3}$	-0.84	$5 \cdot 10^{-4}$	2.34
F	50	7	0.513	0.015	0.029	$2 \cdot 10^{-7}$	0.05	$8 \cdot 10^{-8}$	1.50
F	ALL	21	0.368	0.151	0.410	$-1 \cdot 10^{-3}$	-0.29	$6 \cdot 10^{-4}$	1.21

n = sample size

$\bar{y}$ = mean value of the logarithms of the sample

s_y = standard deviation of the logarithms of the sample

my_n = n^{th} moment about the mean of the logarithms of the sample

g_1 = coefficient of skewness of the logarithms of the sample

g_2 = coefficient of kurtosis of the logarithms of the sample

As for the porosity data, the normal and log-normal distributions were selected for the statistical analysis of the dry bulk density data. Also as with the porosity data, the samples were analyzed in order to verify if there is a significant difference between the mean values of dry bulk density observed in the different layers of a lysimeter, at a level of significance of 1%.

Assuming a normal distribution, the results are:

Layer G0 against G20: $T=11.774$; $f=7.221$; $t_{(0.5\%,7)}=3.499$
 H_0 rejected at 1% of significance

Layer F25 against F50: $T=2.628$; $f=6.166$; $t_{(0.5\%,6)}=3.707$
 H_0 accepted at 1% of significance

Layer F0 against F25: $T=4.393$; $f=6.662$; $t_{(0.5\%,6)}=3.707$
 H_0 rejected at 1% of significance

Assuming a log-normal distribution, the results are:

Layer G0 against G20: $T=12.283$; $f=7.993$; $t_{(0.5\%,7)}=3.499$
 H_0 rejected at 1% of significance

Layer F25 against F50: $T=2.537$; $f=6.191$; $t_{(0.5\%,6)}=3.707$
 H_0 accepted at 1% of significance

Layer F0 against F25: $T=4.428$; $f=6.710$; $t_{(0.5\%,6)}=3.707$
 H_0 rejected at 1% of significance

As with the porosity data, the conclusions drawn from the hypothesis of log-normal distribution for the dry bulk density are exactly the same as those obtained from the hypothesis of normal distribution: there is a significant difference between the mean values of dry bulk density for layers G0 and G20, for layers F0 and F25 and also for layers F0 and F50; there is no significant difference between the mean values of dry bulk density for layers F25 and F50 (always at a level of significance of 1%). Again, the higher biological activity in the top layer can explain these results of lower density in the top layer when compared with deeper ones.

5.2.6 - Statistical analysis of saturated conductivity results

The moments and the coefficients of skewness and kurtosis for the saturated conductivity data are presented in table 5.7. The statistics presented in this table are computed considering the mean value of saturated conductivity of a core as one single observed value, avoiding the bias that could be caused by the different number of repetitions of single tests for each core.

The high value of the sample coefficient of variation ($s/\bar{x}$) in table 5.7 and the results of the tests, presented on table 5.2, show that the saturated conductivity obtained with cores F0-2, F0-7, F25-2, F25-6 and F50-7 appear to be significantly higher than the other values of the respective layers, seeming to arise from different distributions and justifying a study to identify if they are outliers in these samples. The small number of valid results for lysimeter G (only 4 values for each layer) does not allow the identification of possible outliers.

Table 5.7 - Saturated Conductivity - Moments about the mean

LYSIM NAME	DEPTH (cm)	n	SATURATED CONDUCTIVITY (cm/h)						
			$\bar{x}$	s	$ s/\bar{x} $	m_2	g_1	m_4	g_2
G	0	4	72.51	73.14	1.01	$7 \cdot 10^{-4}$	0.18	$2 \cdot 10^{-7}$	0.84
G	20	4	0.25	0.29	1.16	$2 \cdot 10^{-2}$	0.70	$9 \cdot 10^{-3}$	1.27
G	ALL	8	36.38	61.52	1.69	$3 \cdot 10^{-3}$	1.08	$3 \cdot 10^{-7}$	2.40
F	0	6	83.10	121.43	1.46	$2 \cdot 10^{-4}$	1.19	$6 \cdot 10^{-8}$	2.59
F	25	7	45.47	115.81	2.55	$3 \cdot 10^{-4}$	1.62	$7 \cdot 10^{-8}$	3.79
F	50	6	36.36	92.05	2.53	$1 \cdot 10^{-4}$	1.89	$3 \cdot 10^{-8}$	4.41
F	ALL	19	53.57	105.83	1.98	$2 \cdot 10^{-4}$	1.83	$5 \cdot 10^{-8}$	4.57

n = sample size

$\bar{x}$ = sample mean

s = sample standard deviation

m_n = sample n^{th} moment about the mean

g_1 = sample coefficient of skewness

g_2 = sample coefficient of kurtosis

The single tests performed for these five cores are internally consistent, and the results of the repetitions of the test for each of these cores resulted in values of saturated conductivity similar to those already obtained for a same core. This behaviour is reflected in table 5.2 by the small value of the standard deviation when compared with the mean K. However, these cores presented evidence of soil structure, with visible macropores, suggesting that there was a preferential pathway through the core. In this case, the results obtained for these cores would not represent the same physical phenomena observed on the other cores: in these cores the water flow would be mainly gravity-driven, not being able to be explained by capillary theory. The

concept of saturated conductivity could not be applied to these results, and the data relative to these cores would have to be rejected.

Discordancy tests were applied to verify if there is enough statistical evidence to reject the data from these cores. The discordancy tests for outliers adopted in this report are described by Barnett and Lewis (1984) and are presented in Appendix V (Discordancy tests for outliers in univariate normal samples - equations, definitions and tables) as tests N_1 and N_4 , for a single upper outlier and for several upper outliers, respectively. The working hypothesis (null hypothesis) for the tests is that all cores in the sample come from a same normal distribution, $N(\mu, \sigma^2)$; the alternative hypothesis is that there are outliers, which arise from separate normal distributions, each with the same variance of the original distribution (σ^2), but with distinct means, all exceeding μ . The results, summarised in table 5.8, show that there is statistical evidence to identify all five cores as outliers, at a significance level of 1%, assuming univariate normal samples.

Table 5.8 - Discordancy tests for the saturated conductivity

Level of significance = 1%

LAYER NAME	TEST FOR A SINGLE OUTLIER				TEST FOR TWO OUTLIERS		
	T_{N1}	$SP(T_{N1})$	TAB.VAL	H0:ACC/REJ	T_{N4}	TAB.VAL	H0:ACC/REJ
F0	1.976	0.5%	1.94	H0rejected	0.006	0.019	H0rejected
F25	2.267	$< 10^{-3}\%$	2.10	H0rejected	$5 \cdot 10^{-4}$	0.044	H0rejected
F50	2.266	$< 10^{-3}\%$	1.94	H0rejected	-	-	-

T_{N1}, T_{N4} = tests statistics

$SP(t)$ = significance probability

TAB.VAL = tabulated significance value

H0:ACC/REJ = null hypothesis: accepted or rejected

The saturated conductivity data was also tested for a log-normal distribution. The moments and the coefficients of skewness and kurtosis for the logarithms of the saturated conductivity data are presented in table 5.9, and the results for the discordancy tests are summarised in table 5.10.

The results of table 5.10 show that there is statistical evidence to identify cores F25-2, F25-6 and F50-7 as outliers, at a significance level of 5%, assuming univariate log-normal samples, but not for cores F0-2 and F0-7. Also, for a significance level of 1%, still under the assumption of univariate log-normal samples, only core F50-7 can be identified as a outlier, as can be observed comparing the values of T_{N1} and T_{N4} from table 5.10 with the tabulated values at a significance level of 1%, presented in table 5.8.

Table 5.9 - Logarithm of Sat. Conductivity - Moments about the mean

LYSIM NAME	DEPTH (cm)	n	ln of SATURATED CONDUCTIVITY (cm/h)						
			$\bar{y}$	s_y	$b_y/\bar{y}$	my_3	g_1	my_4	g_2
G	0	4	3.21	2.355	0.733	-7.0	-0.54	35.2	1.14
G	20	4	-1.82	1.035	0.568	0.5	0.46	1.3	1.09
G	ALL	8	0.69	3.174	4.560	9.4	0.29	114.9	1.13
F	0	6	3.62	1.383	0.382	0.7	0.28	5.5	1.51
F	25	7	0.33	2.735	8.390	20.0	0.98	129.8	2.32
F	50	6	-2.14	3.748	1.755	71.1	1.35	572.1	2.90
F	ALL	19	0.59	3.533	6.009	5.0	0.11	218.0	1.40

n = size of the sample

$\bar{y}$ = mean value of the logarithms of the sample

s_y = standard deviation of the logarithms of the sample

my_n = n^{th} moment about the mean of the logarithms of the sample

g_1 = coefficient of skewness of the logarithms of the sample

g_2 = coefficient of kurtosis of the logarithms of the sample

Table 5.10 - Discordancy tests for ln of saturated conductivity

Level of significance = 5%

LAYER NAME	TEST FOR A SINGLE OUTLIER				TEST FOR TWO OUTLIERS		
	T_{N1}	$SP(T_{N1})$	TAB.VAL	H0:ACC/REJ	T_{N2}	TAB.VAL	H0:ACC/REJ
F0	1.564	24%	1.82	H0accepted	0.175	0.056	H0accepted
F25	1.976	3.85%	1.94	H0rejected	0.048	0.102	H0rejected
F50	2.038	$< 10^{-3}\%$	1.82	H0rejected	-	-	-

T_{N1}, T_{N2} = tests statistics

$SP(t)$ = significance probability

TAB.VAL = tabulated significance value

H0:ACC/REJ = null hypothesis: accepted or rejected

The hypothesis of a log-normal distribution does not give evidence for the identification of all five cores as outliers. However, the results of the discordancy tests under the hypothesis of a normal distribution and also the physical evidence of preferential water flow due to the presence of visible macropores lead us to classify all five cores as outliers and consequently reject them. Table 5.11 presents the moments and the coefficients of skewness and kurtosis for the saturated conductivity data from lysimeter F after rejecting the outliers.

Table 5.11 - Saturated Conductivity
Moments about the mean after rejection of the outliers

LYSIM NAME	DEPTH (cm)	n	SATURATED CONDUCTIVITY (cm/h) after rejection of outliers						
			$\bar{x}$	s	$ s/\bar{x} $	m_3	g_1	m_4	g_2
F	0	4	20.555	11.846	0.576	-303.1	-0.18	$2 \cdot 10^{-4}$	0.77
F	25	5	0.412	0.322	0.782	$2 \cdot 10^{-2}$	0.66	$2 \cdot 10^{-3}$	1.47
F	50	5	0.026	0.006	0.231	$-1 \cdot 10^{-7}$	-0.50	$2 \cdot 10^{-3}$	1.15
F	ALL	14	6.029	11.106	1.842	$2 \cdot 10^{-3}$	1.43	$5 \cdot 10^{-4}$	3.35

n = sample size
 $\bar{x}$ = sample mean
s = sample standard deviation
 m_n = sample n^{th} moment about the mean
 g_1 = sample coefficient of skewness
 g_2 = sample coefficient of kurtosis

The samples obtained after the rejection of the outliers were analyzed in order to verify if there is a significant difference between the mean values of saturated conductivity observed in the different layers of lysimeter F, at a level of significance of 1%, assuming a normal distribution. The null hypothesis is that both means are the same; the alternative hypothesis is that the means are different. The results are:

Layer F25 against F50: $T=2.680$; $f=4.003$; $t_{(0.5\%,4)}=4.604$
 H_0 accepted at 1% of significance

Layer F0 against F25: $T=3.400$; $f=3.004$; $t_{(0.5\%,3)}=5.841$
 H_0 accepted at 1% of significance

Layer F0 against F50: $T=3.466$; $f=3.000$; $t_{(0.5\%,3)}=5.841$
 H_0 accepted at 1% of significance

These results show that, assuming a normal distribution and at 1% of significance, there is no evidence to assume significant difference among the saturated conductivities of the three layers of lysimeter F. This happens due to the high spatial variation of the saturated conductivity, not only vertically, but also horizontally. Because of this variation, the saturated conductivity can present strongly different values not only at different layers, but even at the same depth.

However, it is clear from the data that there is a difference of one or even two orders

of magnitude between the results for different layers. According to El-Kadi (1987), some flow parameters, such as the saturated hydraulic conductivity, are highly variable in space even within the same geologic formation, and its value may range over several orders of magnitude. Gelhar (1986) shows data which indicate a 4 order of magnitude variation of permeability within a relatively homogeneous sandstone unit. For this reason, even without statistical evidence to assume significant difference among the saturated conductivities of the three layers of lysimeter F, the mean values of saturated conductivity presented for the different depths in table 5.11 are selected to simulate vertical heterogeneity in the soil.

5.3 - Adjustment of soil characteristic parametric relationships

As commented in section 5.1, an alternative to direct experimental determination of material properties is to apply parameter estimation techniques to solve the inverse problem using a full numerical model. The constitutive relationships supposed to be applicable to the system are defined a priori and the values for their parameters are estimated by optimisation of the numerical model with respect to an objective function, using a calibration data set. Particular attention has to be devoted to the problem of ill-posedness of an inverse problem. According to Carrera and Neuman (1986) a problem is ill-posed when it fails to satisfy one or more of the following requirements: (1) a solution exists; (2) the solution is unique for any given response of the system; and (3) the solution is stable. Ill-posedness in the inverse problem can be caused by nonuniqueness, nonidentifiability, or by instability. According to Russo et al. (1991), a problem is nonunique when it has local minima or global minimum at more than one point in the parameter space; the parameters are nonidentifiable if more than one parameter set leads to a given response; and instability means that small errors in the response data can result in large changes in the estimated parameters. In order to diminish the problems brought by nonuniqueness, Abeliuk and Wheeler (1990) suggest the reduction of the dimensionality of the problem by the use of ancillary data. The degree of ill-posedness brought by nonidentifiability can be decreased by the inclusion of prior information about the model parameters in the estimation criterion, as shown by Russo et al. (1991).

Several methods have been described in the literature for estimating parameters in soil hydraulic property models. According to Mishra et al. (1989), one common approach is to take static $\theta(\psi)$ measurements and fit them to the desired soil water retention model. Frequently used expressions are those developed by Brooks and Corey (1964, 1966) and Van Genuchten (1980). Once the retention function is estimated, the conductivity relation, $K(\theta)$, can be evaluated from the respective parametric equations if the saturated conductivity, K_s , is known. Another approach

to model calibration is to conduct a dynamic flow experiment (i.e., infiltration, redistribution and/or drainage event), and use the observed water content, pressure head and/or boundary flux data to invert the governing initial-boundary value problem.

Whatever the approach used, the issue of uncertainty can not be omitted. Uncertainty in model predictions results from three primary sources: (1) uncertainty in the model itself, because of an incomplete understanding of the underlying physical process(es), leading to incorrect and/or oversimplified representation of reality; (2) uncertainty in the model parameters, because of error in estimating parameters; and (3) error in the data, due to measurement error and/or spatial variability in properties of the medium. According to Mishra and Parker (1989), model formulations are usually assumed to be sufficiently accurate. In this work, the model error is assessed by testing different formulations and comparing the results among themselves and also with the data. The error in the data is reflected in the estimated parameters, so that the parameter uncertainty is due to errors in the methodology for parameter estimation and also to inaccuracy in the observations; thus the uncertainty analysis in this chapter will be focused on parameter uncertainty.

According to Mishra and Parker (1989), two common methods for evaluating the uncertainty associated with a process resulting from error in its parameters are Monte Carlo simulation and first-order error analysis (e.g., Benjamin and Cornell, 1970). Monte Carlo simulation involves forming random vectors of input parameters from prescribed probability distributions, repeatedly simulating the process, and computing summary statistics (i.e., mean and variance) of process performance. First-order error analysis is based on a first-order Taylor expansion around the mean values of parameters, assuming small parameter perturbations and negligible higher-order terms. Summary statistics can be estimated if mean, variance and/or covariance of the input parameters are known. The first-order error analysis procedure is more popular than Monte Carlo simulation as it entails considerably less computational effort for problems with small number of parameters whereas, for relatively simple flow problems, it provides results of comparable accuracy.

In order to evaluate the parameter values and their associated uncertainty, an estimator has to be used. Beck (1987) identifies four types of estimator: ordinary least squares (OLS) estimator, weighted least squares (WLS) estimator, maximum likelihood (ML) estimator, and Bayesian estimator. No a priori knowledge of the statistical properties of any of the sources of uncertainty is required for OLS estimation; the estimates of the parameters are derived by minimising the sum of the squared errors between the observed and estimated behaviour of the

system. A WLS estimator yields estimates which minimise a weighted sum of squared errors, where the weighting matrix is chosen according to engineering judgement. An ML estimator requires the a priori knowledge of the probability density function for the population of observations as a function of the unknown, and constant, parameter vector. For the Bayesian estimator, the parameter vector is considered to be a random variable, so that a priori knowledge of the probability density functions of the observed values, the estimated parameter vector and also the conditional probability density function of the observations and the parameter vector are required.

According to Kool et al. (1987), the OLS formulation has probably been the most popular one, due to its simplicity and because it requires a minimum amount of information. When observation errors are normally distributed, are uncorrelated and have a constant variance, the OLS estimates possess optimal properties; when the normality assumption alone is violated, OLS can still be used with good results (Beck and Arnold, 1977; Bard, 1974).

In the next sections a methodology for estimating the parameter values and associated uncertainty, based on first-order error analysis is presented. As commented in section 4.2.2.5, and shown in table 4.1, soil moisture content measurements in the experiment were taken manually, every week or fortnight. This resolution does not allow the use of a simulation optimisation method, and only static $\theta(\psi)$ measurements are taken for the parameter estimation. The methodology is utilised for estimating the parameters of three different parametric relationships: Van Genuchten's equation, Brooks-Corey's equation and the MACRO model methodology, already described in chapters 2 and 3. The results of the adjustment of the available data to these relationships are compared, and a set of parameters for each relationship is selected to be applied in the simulations described in chapter 6.

5.3.1 - Methodology for estimation of parameter values and associated uncertainty

According to Kool et al. (1987), many parameter estimation problems can be formulated as a weighted least-squares minimisation problem:

$$\min_p O(p) = \frac{1}{2} [o - \hat{o}(p)]^T W [o - \hat{o}(p)] + \frac{1}{2} (p - \hat{p})^T V (p - \hat{p}) \quad (5.1)$$

where the objective function $O(p)$ is a function of the model parameters p , $p = \{p_1, \dots, p_m\}^T$;

$\mathbf{o} = \{o_1, \dots, o_n\}^T$ is the observation vector; $\delta(\mathbf{p}) = \{\delta_1(\mathbf{p}), \dots, \delta_n(\mathbf{p})\}^T$ represents the predicted response for a given parameter vector $\mathbf{p}$; $\hat{\mathbf{p}}$ represents direct estimates or measurements of the parameters $\mathbf{p}$; and $\mathbf{W}$ and $\mathbf{V}$ are symmetric weighting matrices. The objective is to find the parameter vector $\tilde{\mathbf{p}}$ that minimises equation 5.1, resulting in a best fit between the model and available data.

If we set $\mathbf{W}$ equal to the identity matrix and $\mathbf{V}$ to zero, equation 5.1 reduces to the ordinary least-squares (OLS) estimator:

$$\min_{\mathbf{p}} O(\mathbf{p}) = \frac{1}{2} [\mathbf{o} - \delta(\mathbf{p})]^T [\mathbf{o} - \delta(\mathbf{p})] = \frac{1}{2} \sum_{i=1}^n [o_i - \delta_i(\mathbf{p})]^2 \quad (5.2)$$

Information concerning uncertainty in the parameter estimates obtained by solving equation 5.2, i.e., in fitting the selected parametric model to $\theta(\psi)$ data, is contained in the parameter covariance matrix, defined by:

$$\mathbf{C} = E[(\mathbf{p} - \hat{\mathbf{p}})(\mathbf{p} - \hat{\mathbf{p}})^T] \quad (5.3)$$

The elements of $\mathbf{C}$ are the individual parameter variances, $\text{Var}[p_i]$, and the covariances, $\text{Cov}[p_i, p_j]$, which are computed during the non-linear estimation of $\tilde{\mathbf{p}}$ from $\theta(\psi)$ data. For non-linear regression problems, a first-order approximation to the covariance matrix, $\mathbf{C}$, is given by (Beck and Arnold, 1977):

$$\mathbf{C} = \mathbf{S}^2 \mathbf{H}^{-1} \quad (5.4)$$

where $\mathbf{S}^2$ is the estimated variance of the residual at the solution ($O(\tilde{\mathbf{p}})$), given by

$$\mathbf{S}^2 = \frac{O(\tilde{\mathbf{p}})}{n-m} \quad (5.5)$$

with n being the number of observations, and m the number of unknown parameters, and $\mathbf{H}$ is the Hessian, or matrix of second derivatives of the objective function with respect to the parameters, estimated as $\mathbf{H} = \mathbf{J}^T \mathbf{J}$, where $\mathbf{J}$ is the parameter sensitivity matrix (Jacobian matrix).

The Hessian must be positive semi-definite at any unconstrained minimum of O , given that $O(p)$ has continuous second derivatives and it has its components defined by

$$H_{ij} = \frac{\partial^2 O}{\partial p_i \partial p_j} \quad (5.6)$$

Using first-order error analysis and assuming small perturbations around the mean values, parameter uncertainties due to input parameter error for a quantity, f , which depends on the parameter vector, p , can be estimated based on (Mishra et al., 1989; Mishra and Parker, 1989):

$$E[f] = f(\hat{p}) \quad (5.7)$$

and

$$\text{Var}[f] = \sum_i \sum_j \frac{\partial f}{\partial p_i} \frac{\partial f}{\partial p_j} \text{Cov}[p_i, p_j] \quad (5.8)$$

Thus, the expected value (first moment) is the same as that obtained with the estimated parameters, whereas the variance (second moment) depends on the variance-covariance relation of the input parameters as well as the sensitivity of the process to these parameters.

The covariance of two random variables, Y_1 and Y_2 , where both are functions of the parameter vector, p , can be obtained in a similar manner as:

$$\text{Cov}[Y_1, Y_2] = \sum_i \sum_j \frac{\partial Y_1}{\partial p_i} \frac{\partial Y_2}{\partial p_j} \text{Cov}[p_i, p_j] \quad (5.9)$$

These expressions, i.e., equation 5.8 for the variance and equation 5.9 for the covariance, are used to estimate parameter uncertainties due to input parameter error. Defining the standard deviation (s) as the square root of $\text{Var}[f]$, a confidence interval for the quantity f can be obtained as:

$$P[f(\hat{p}) - t_{(\alpha/2, n)} \cdot s \leq f(p) \leq f(\hat{p}) + t_{(\alpha/2, n)} \cdot s] = 1 - \alpha \quad (5.10)$$

where P denotes probability, $t_{(\alpha/2, n)}$ is given by the Student's distribution, α is the significance level, m is the number of parameters and n is the number of observed values.

An appropriate algorithm is necessary to minimise the objective function $O(p)$. According to Finsterle and Pruess (1995), Newton-type minimisation algorithms are appropriate when using the least squares formulation. In Newton's method, the objective function is locally approximated by a quadratic form which allows iterative computation of an improved parameter vector from a previous estimate, using the Hessian matrix and a gradient vector. As the Hessian matrix is expensive to calculate and may also become negative-definite if the model is strongly non-linear, the use of approximations to its value is frequently adopted.

The parameter estimation and uncertainty analysis described above were implemented in a FORTRAN code. The minimum of the objective function $O(p)$ is obtained either through the use of NAG (Numerical Algorithms Group, 1987) routine E04CCF or E04FDF. Routine E04CCF minimises a general function $F(x)$ of m independent variables by the Simplex method. The Simplex method uses a geometrical figure of $N+1$ points, where N is the number of variables, computing the function value only at these points. At each iteration, the vertex of the simplex is reflected in the centre of gravity of the remaining vertices and the function value at this new point is compared with the remaining function values. Depending on the outcome of this test the new point is accepted or rejected, a further expansion move may be made, or a contraction may be carried out (Nelder and Mead, 1965). The method is slow, but it is robust and can be applied to any objective function. Routine E04FDF uses a quasi-Newton method for finding an unconstrained minimum of a sum of squares. Quasi-Newton methods approximate the Hessian by a matrix which is modified at each iteration to include information about the curvature of O along the latest search direction. Although not as robust as Newton-type methods (which use the Hessian matrix to define the search direction in the iterative solution by actually computing its value), quasi-Newton methods can be more efficient because H is not computed (or approximated by finite-differences) at each iteration. Both Newton and quasi-Newton methods can only be applied to objective functions defined as a sum of squares. When a Newton or a quasi-Newton method is used, the Hessian is obtained during the parameter estimation and, consequently, the uncertainty associated with the selected parameters can be easily assessed with little additional effort, what does not happen for the Simplex solution. Thus, when routine E04FDF is used in the program developed for the parameter estimation, the associated

uncertainty is obtained by the use of NAG routine E04YCF, which returns estimates of elements of the variance-covariance matrix of the computed regression coefficients for a nonlinear least-squares problem. These estimates are derived from the Jacobian of the function $O(p)$ at the solution.

The program developed for parameter estimation and uncertainty analysis processes tension and moisture data in order to adjust the parameters of the selected characteristic curve relationship, for any combination of soil layers. After adjusting the parameters, a simulation is performed, using the fitted values to estimate the moisture contents and compute the errors and coefficient of determination, again for any combination of soil layers (not necessarily the same used for fitting). The available $\theta(\psi)$ measurements taken at depths of 10, 20, 30, 40, 50, and 60cm below the soil surface of the deep lysimeters A and B during the whole operational period of the lysimeters were used as input data.

Estimation of the parameter values is obtained as follows. The saturated moisture content is obtained as the mean value of the moisture contents for matric potentials greater than an offset (zero for Van Genuchten's equation, air entry pressure for Brooks-Corey's equation, and boundary water potential for MACRO's methodology). The remaining parameters are determined by the Simplex or quasi-Newton routine, in order to minimise the objective function. When the quasi-Newton routine is used, the uncertainty associated with the determination of these parameters is also estimated. Initial values have to be provided for all parameters. Finally, the program also allows the selection of parameters that should not be optimised, keeping the initial values provided and reducing the dimensionality of the problem. This feature is specially useful for fixing the values of the saturated and residual moisture contents (θ_s and θ_r , respectively).

5.3.2 - Van Genuchten's equation

The methodology described in the previous section was applied in order to optimise the parameters of Van Genuchten's equation, already described in chapter 2 (section 2.2.3) as:

$$Se = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[\frac{1}{1 + (\alpha|\psi|)^n} \right]^{(1-1/n)} \quad \text{if } \psi < 0 \quad (5.11)$$

$$Se = 1 \quad \text{if } \psi \geq 0$$

where S_e is the effective saturation, α is the scaling parameter, and n is the curvature parameter.

In some optimisations, particularly for the bottom soil layers (data from depths of 30, 40, 50 and 60cm), there is insufficient information for calculating θ_r . Consequently, values of little or even no physical meaning could be obtained (either θ_r bigger than 20% or negative values). In order to avoid this problem, a physically meaningful value of θ_r was chosen, for all parametric relationships, based on results of previous optimisations. Values between 1 and 10% were tested, and $\theta_r=5\%$ was adopted, while the other parameters (θ_s , α and n) were determined by the optimisation program. With this value, the coefficient of determination was usually equal or very close to the one obtained by allowing θ_r to be fitted by the optimisation algorithm. Fixed values of θ_r were also tested. In the following sections, results of optimisations using the mean values of porosity (obtained from the physical analysis of the cores described in section 5.2.4: 46% for the top layer and 35% for the bottom layers of a deep lysimeter) as fixed values of θ_r are compared among themselves and also with θ_r computed by the program. The simulations were performed using both Simplex or quasi-Newton routines, for different initial values of the optimised variables, in order to reduce the possibility of obtaining an optimised parameter vector which actually represents a local minimum. As the results with the different routines and initial values provided coincident results up to the third decimal place, they were adopted as global minima. This procedure does not ensure that uniqueness in the parameter determination is guaranteed, but is a good indication that the obtained values can be the best possible solution for the optimisation problem. The uncertainty due to input parameter error is obtained from the results of the optimisations using the quasi-Newton routine. Table 5.12 summarises the most important results.

When data from all layers was used to fit the parameters (equivalent to considering a homogeneous soil), a value of $\theta_s=42\%$ was obtained by the model. This value was also used as a fixed value in optimisations of other combinations of soil layers, in order to compare the results with those using the saturated conductivities suggested by the results obtained by porosity determined from the physical analysis of the cores. The results of the optimisations using $\theta_s=42\%$ always provided higher values of the coefficient of determination (R^2) than those using the mean porosity values, as shown in table 5.12. It is important to emphasise that the values of R^2 for the top soil (layers 1 and 2) are very low; only when the other layers were included in the optimisation it was possible to obtain R^2 values close to 0.90.

Table 5.12 - Adjustment of Van Genuchten's equation

Noteworthy results

Lysimeter	Fit to layers	Simul. layers	α (1/cm)	n (-)	θ_r (%)	θ_s (%)	simul. mean relat. error	simulated R ²
A	1+2+3+4+5+6	1+2+3+4+5+6	0.06	1.70	5.00	42.0	0.09	0.87
	1+2+3+4+5+6	1+2+3+4+5+6	0.09	1.56	5.00	46.0	0.09	0.86
	1+2+3+4+5+6	1+2+3+4+5+6	0.03	2.00	5.00	35.0	0.12	0.71
	1	1	0.19	1.34	5.00	42.0	0.16	0.61
	1	1	0.28	1.33	5.00	46.0	0.16	0.60
	2	2	0.11	1.47	5.00	42.0	0.08	0.61
	2	2	0.17	1.43	5.00	46.0	0.09	0.60
	1+2	1+2	0.17	1.36	5.00	42.0	0.12	0.60
	1+2	1+2	0.25	1.35	5.00	46.0	0.12	0.60
	3+4+5+6	3+4+5+6	0.04	2.04	5.00	42.0	0.05	0.88
	3+4+5+6	3+4+5+6	0.03	3.32	5.00	35.0	0.10	0.57
	1+2+3+4+5+6	1	0.06	1.70	5.00	42.0	0.18	0.36
	1+2+3+4+5+6	2	0.06	1.70	5.00	42.0	0.10	0.42
	1+2+3+4+5+6	1+2	0.06	1.70	5.00	42.0	0.14	0.39
	1+2+3+4+5+6	3+4+5+6	0.06	1.70	5.00	42.0	0.06	0.86
B	1+2+3+4+5+6	1+2+3+4+5+6	0.07	1.48	5.00	42.0	0.09	0.80
	1+2+3+4+5+6	1+2+3+4+5+6	0.13	1.39	5.00	46.0	0.10	0.77
	1+2+3+4+5+6	1+2+3+4+5+6	0.03	1.69	5.00	35.0	0.12	0.65
	1	1	0.11	1.32	5.00	42.0	0.23	0.39
	1	1	0.20	1.29	5.00	46.0	0.24	0.36
	2	2	0.14	1.34	5.00	42.0	0.08	0.73
	2	2	0.23	1.31	5.00	46.0	0.08	0.72
	1+2	1+2	0.15	1.31	5.00	42.0	0.16	0.46
	1+2	1+2	0.26	1.28	5.00	46.0	0.16	0.44
	3+4+5+6	3+4+5+6	0.05	1.91	5.00	42.0	0.05	0.88
	3+4+5+6	3+4+5+6	0.03	3.11	5.00	35.0	0.09	0.62
	1+2+3+4+5+6	1	0.07	1.48	5.00	42.0	0.23	0.31
	1+2+3+4+5+6	2	0.07	1.48	5.00	42.0	0.08	0.63
	1+2+3+4+5+6	1+2	0.07	1.48	5.00	42.0	0.15	0.40
	1+2+3+4+5+6	3+4+5+6	0.07	1.48	5.00	42.0	0.07	0.83

Layer 1: 0 - 15 cm (data from instruments at 10cm depth)

Layer 2: 15 - 25 cm (data from instruments at 20cm depth)

Layer 3: 25 - 35 cm (data from instruments at 30cm depth)

Layer 4: 35 - 45 cm (data from instruments at 40cm depth)

Layer 5: 45 - 55 cm (data from instruments at 50cm depth)

Layer 6: 55 - 70 cm (data from instruments at 60cm depth)

The set of parameters fitted considering the soil as homogeneous, with $\theta_s=42\%$, was also applied to estimate the moisture contents and compute the errors and coefficient of determination for other combinations of soil layers, as shown in table 5.12. The coefficients of determination obtained for the top soil (layers 1 and 2) were sensibly smaller than those obtained

when only data from these layers was used in the fitting. The mean relative errors (mean value of the quotient: simulated error / observed value), however, present small increase. The results of table 5.12 are graphically displayed in figures 5.1, 5.2, and 5.3. As lysimeters A and B show similar behaviours, only the curves for lysimeter A are presented.

Figure 5.1 shows the characteristic curves obtained for lysimeter A using Van Genuchten's equation under the hypothesis of homogeneous soil, for values of saturated conductivity of 35%, 42% and 46%.

The 10cm data presents big scatter when compared with data from other layers. Data from 10cm depth, even presenting this big variability, can not be neglected, because it is the only layer which shows matric potentials lower than -100cm. It is, consequently, very important in the representation of the dry end of the soil profile, being the best source for the determination of the value of the residual water content (θ_r). This big scatter is probably due to variations in time and space: as the measurements of water content and matric potential were taken at different locations and not exactly at the same time, the correspondence between them is not ensured. These errors affect the whole profile, but they are expected to be bigger in the top layer because it presents a more dynamic response when compared to other depths. This is the first layer to receive the rainfall input, it reacts quickly to it and acts as a buffer, transmitting the water response downwards only when it exceeds the matrix capacity, so that the other layers receive a faded input. It is also the layer with higher biological activity, which can result in increased heterogeneity. This effect is enhanced by the difference in the source of data for the moisture content: for the top layer, the soil moisture was obtained from TDR measurements at 15 cm depth, while neutron probe estimatives at 20, 30, 40, 50 and 57 cm depth were adopted for the other layers. TDR estimatives were used for the top layer because, as commented in section 4.2.2.2, neutron probe measurements close to the surface of the soil are prone to error, due to the escape of fast neutrons to the atmosphere. As the matric potentials were given by tensiometer data at 10, 20, 30, 40, 50 and 60 cm below the soil surface, measurements of ψ coincide in depth with θ estimatives for all layers but the top one. Consequently, both horizontal and vertical errors affect the data adopted for the 10 cm depth, while measurements for the other layers are influenced by horizontal heterogeneities only. Besides that, neutron probe measurements are integrated over an effective volume of a sphere of influence with radius of 10 to 25 cm, so that it is an average of this volume, while TDR measures the propagation of a plane wave in the soil, guided by parallel rods spaced by around 10 cm. Consequently, the neutron probe measurement has a bigger representative elementary volume (REV), neglecting heterogeneity at smaller scales, which could be detected by the TDR.

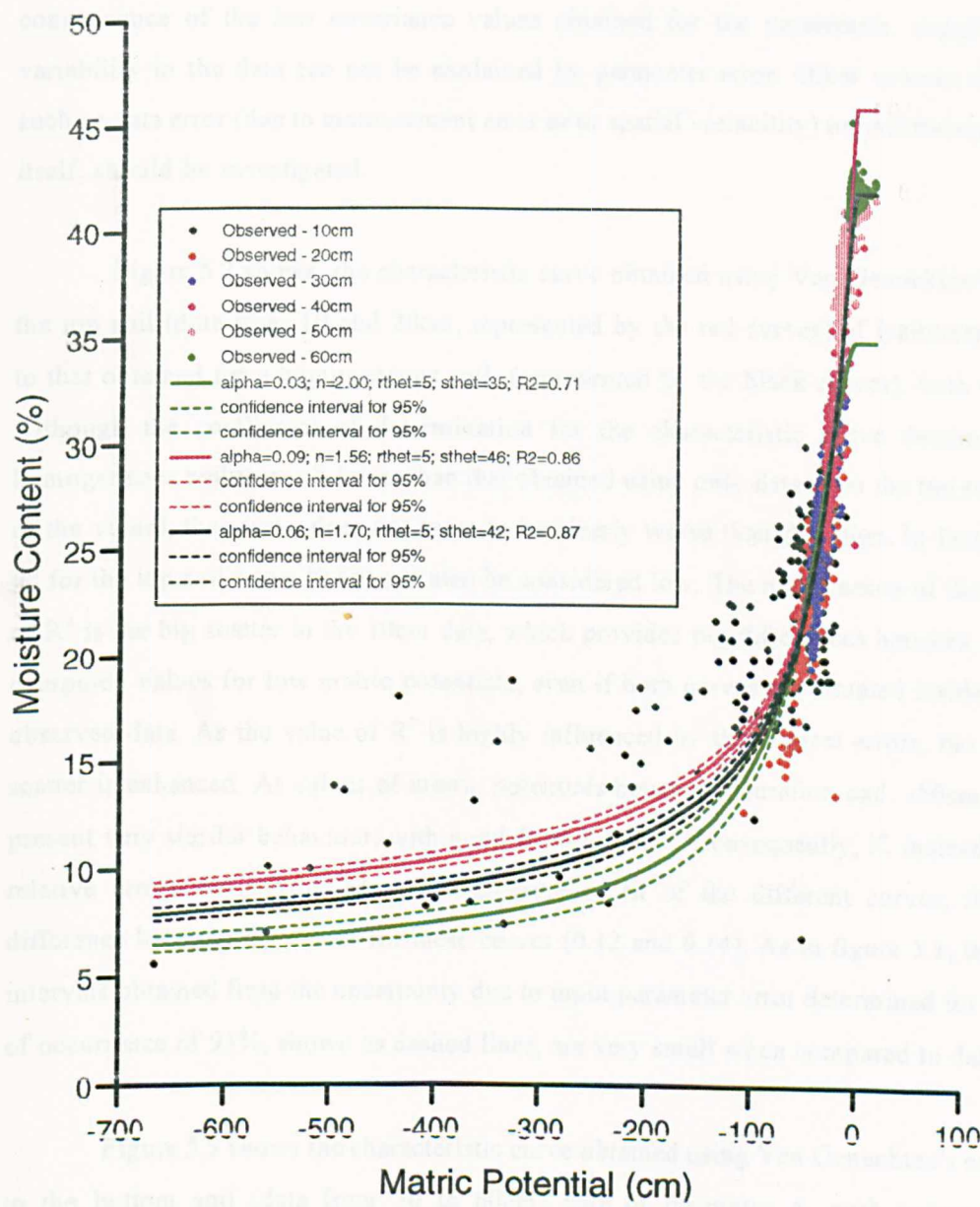


Figure 5.1 - Van Genuchten's eq. fitted to Lys A data (all layers)

The big scatter in data from 10cm depth does not allow the identification of what curve presents a better fit for the dry range of the profile. In the range of matric potentials between -50cm and saturation all curves present very similar behaviour. At saturation, however, only the curve fitted with $\theta_s=42\%$ seems to properly represent the data. The value of 35%, suggested by the porosity data for the bottom layers, is clearly underestimating the observed $\theta(\psi)$ data, while $\theta_s=46\%$ seems to be an overestimate. This fact suggests that the value of saturated conductivity of 42% is the more adequate for this data set. The confidence intervals obtained from the uncertainty due to input parameter error determined for a probability of occurrence of 95% (i.e., significance level $\alpha=0.05$) are shown as dashed lines. The small range of these intervals is a consequence of the low covariance values obtained for the parameters, suggesting that the variability in the data can not be explained by parameter error. Other sources of uncertainty, such as data error (due to measurement error or to spatial variability) or uncertainty in the model itself, should be investigated.

Figure 5.2 shows the characteristic curve obtained using Van Genuchten's equation for the top soil (data from 10 and 20cm, represented by the red curves) of lysimeter A compared to that obtained for a homogeneous soil (represented by the black curves), both with $\theta_s=42\%$. Although the coefficient of determination for the characteristic curve determined using a homogeneous soil is much lower than that obtained using only data from the top soil (nearly 2/3 of the value), that curve does not seem to be clearly worse than the other. In fact, the value of R^2 for the top soil curve (0.60) can also be considered low. The main reason of these low values of R^2 is the big scatter in the 10cm data, which provides big differences between observed and computed values for low matric potentials, even if both curves are situated inside the range of observed data. As the value of R^2 is highly influenced by the biggest errors, the effect of this scatter is enhanced. At values of matric potentials between saturation and -50cm, both curves present very similar behaviour, with good fit to the data. Consequently, if, instead of R^2 , mean relative errors are considered as the measure of fit of the different curves, there is small difference between the values for these curves (0.12 and 0.14). As in figure 5.1, the confidence intervals obtained from the uncertainty due to input parameter error determined for a probability of occurrence of 95%, shown as dashed lines, are very small when compared to data variability.

Figure 5.3 shows the characteristic curve obtained using Van Genuchten's equation fitted to the bottom soil (data from 30 to 60cm) data of lysimeter A, with values of saturated conductivity of 35% (represented by the green curves) and 42% (represented by the red curves), compared to that obtained for a homogeneous soil with $\theta_s=42\%$ (represented by the black curves). All curves present similar behaviour for matric potentials between -50cm and saturation.

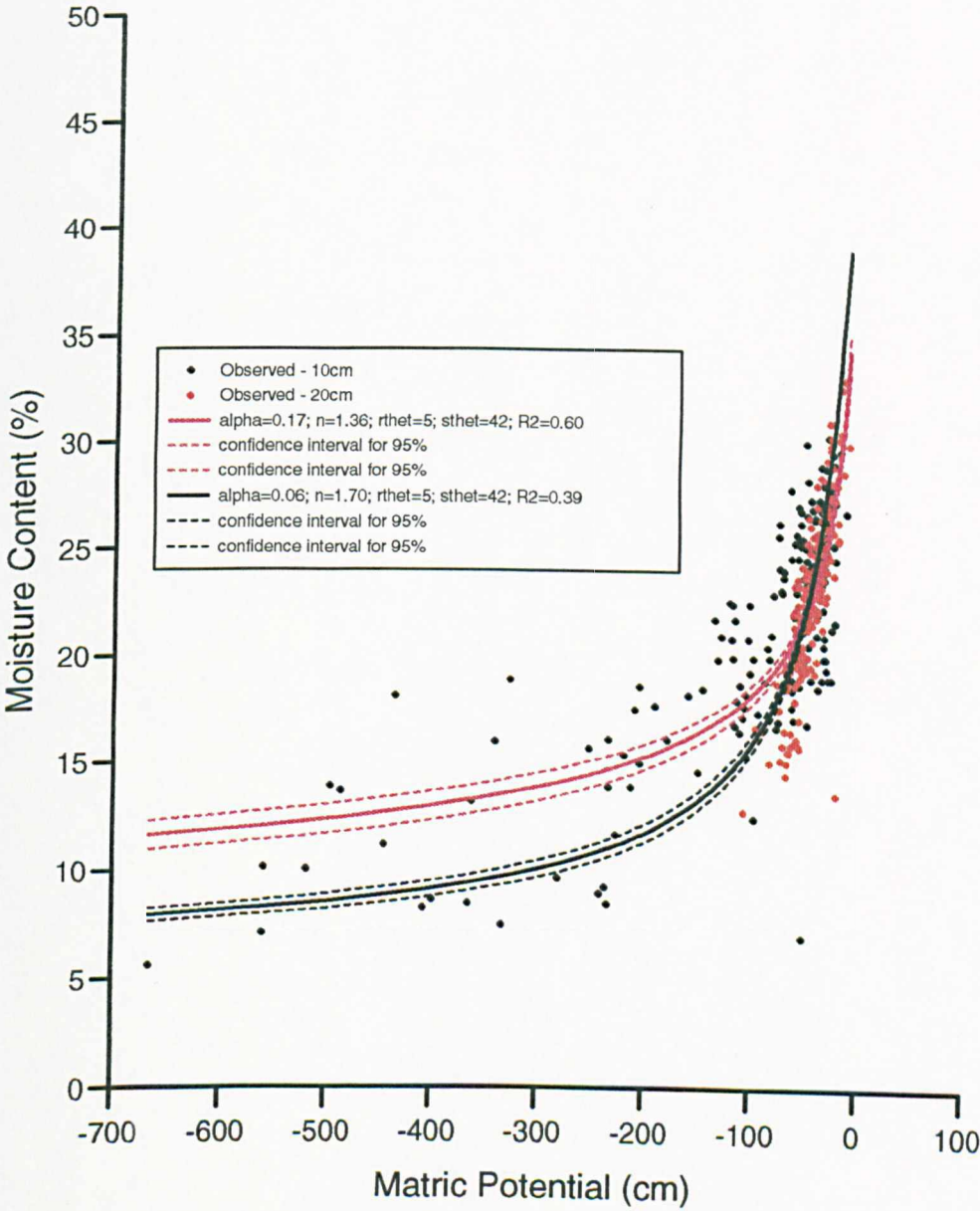


Figure 5.2 - Van Genuchten's eq. fitted to Lys A data (top layers)

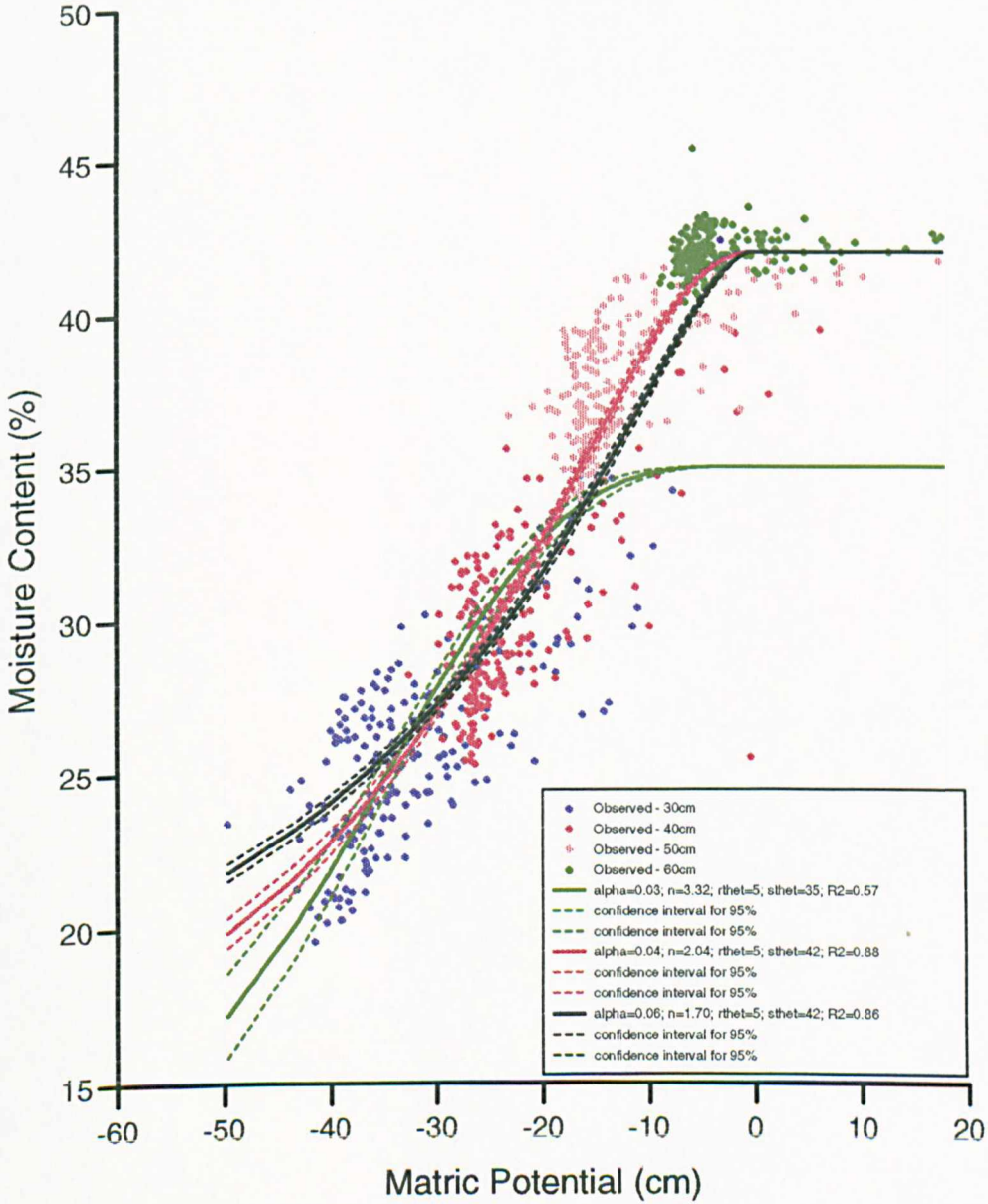


Figure 5.3 - Van Genuchten's eq. fitted to Lys A data (bottom layers)

However, the value of 35%, suggested by the porosity data for the bottom layers, is clearly underestimating the observed $\theta(\psi)$ data at saturation, while the other two curves show a very good fit at this range. Even with the variation in data for these layers being much lower than in top soil, again the confidence intervals obtained from the uncertainty due to input parameter error determined for a probability of occurrence of 95%, are very small when compared to data variability, suggesting that other sources of error can be of great importance.

These results seem to show that the use of the hypothesis of homogeneous soil for the determination of Van Genuchten's soil moisture characteristic curve is a valid assumption. The curves for homogeneous soils lead to smaller values of R^2 , compared to those obtained using only data from the respective layers (with $\theta_s=42\%$), but similar errors to assuming different sets of parameters along the soil profile are obtained, justifying its use.

5.3.3 - Brooks-Corey's equation

Brooks-Corey's equation was already described in chapter 2 (section 2.2.3) as:

$$\begin{aligned} Se &= \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left(\frac{P_b}{\psi} \right)^\lambda & \text{if } \psi < P_b \\ Se &= 1 & \text{if } \psi \geq P_b \end{aligned} \quad (5.12)$$

where Se is the effective saturation, P_b is the air-entry pressure and λ is the pore size distribution index.

The parameters of the Brooks-Corey soil moisture characteristic may be determined by either graphical or automatic numerical procedures. A popular log-log procedure for automatic estimation leads to a linear least squares optimisation problem (Milly, 1987). According to Brooks and Corey (1964 and 1966), to determine the pore-size distribution index, λ , it is necessary to plot the logarithm of the effective saturation against the logarithm of the suctions. As the effective saturation is a function of the residual moisture content (θ_r) and the saturated moisture content (θ_s), these values have to be determined so that the data form two straight line segments, a horizontal one corresponding to saturation and a sloping one whose slope and intercept define P_b and λ .

Figure 5.4 shows the data and characteristic curve obtained for lysimeter A, under the

hypothesis of a homogeneous soil, plotted as effective saturation against matric suction, in a log-log scale. The choice of residual and saturated moisture contents shows to be adequate, as the data clearly form two straight line segments, and the air-entry pressure can be easily identified. The results obtained with this methodology applied to data from lysimeters A and B are presented in table 5.13, for $\theta_r=5\%$ and $\theta_s=42\%$.

Table 5.13 - Adjustment of Brooks-Corey's equation (Log-Log method)

Noteworthy results

Lysimeter	Fit to layers	Simul. layers	λ	θ_r (%)	θ_s (%)	P_b (cm)	simulated R^2
A	1+2+3+4+5+6	1+2+3+4+5+6	0.35	5.00	42.0	-5.73	0.84
	1	1	0.45	5.00	42.0	-8.48	0.51
	2	2	0.43	5.00	46.0	-6.90	0.56
	1+2	1+2	0.43	5.00	42.0	-7.37	0.54
	3+4+5+6	3+4+5+6	0.23	5.00	35.0	-4.14	0.76
	1+2+3+4+5+6	1	0.35	5.00	42.0	-5.73	0.59
	1+2+3+4+5+6	2	0.35	5.00	42.0	-5.73	0.49
	1+2+3+4+5+6	1+2	0.35	5.00	42.0	-5.73	0.56
	1+2+3+4+5+6	3+4+5+6	0.35	5.00	42.0	-5.73	0.75
	1+2+3+4+5+6	1+2+3+4+5+6	0.30	5.00	42.0	-5.45	0.77
B	1	1	0.39	5.00	46.0	-9.75	0.29
	2	2	0.32	5.00	46.0	-5.65	0.70
	1+2	1+2	0.36	5.00	46.0	-7.70	0.38
	3+4+5+6	3+4+5+6	0.25	5.00	35.0	-4.58	0.76
	1+2+3+4+5+6	1	0.30	5.00	42.0	-5.45	0.31
	1+2+3+4+5+6	2	0.30	5.00	42.0	-5.45	0.69
	1+2+3+4+5+6	1+2	0.30	5.00	42.0	-5.45	0.42
	1+2+3+4+5+6	3+4+5+6	0.30	5.00	42.0	-5.45	0.77
	1+2+3+4+5+6	1+2+3+4+5+6	0.30	5.00	42.0	-5.45	0.77
	1+2+3+4+5+6	1+2+3+4+5+6	0.30	5.00	42.0	-5.45	0.77

Layer 1: 0 - 15 cm (data from instruments at 10cm depth)

Layer 2: 15 - 25 cm (data from instruments at 20cm depth)

Layer 3: 25 - 35 cm (data from instruments at 30cm depth)

Layer 4: 35 - 45 cm (data from instruments at 40cm depth)

Layer 5: 45 - 55 cm (data from instruments at 50cm depth)

Layer 6: 55 - 70 cm (data from instruments at 60cm depth)

The values obtained with the log-log method were used as initial estimates for the optimisation methodology described in section 5.3.1. The value of θ_r and θ_s were fixed as 5% and 42%, respectively, and the other parameters (λ and P_b) were determined by the optimisation program. Simulations were also performed with fixed value of $P_b=-10$ cm.

Table 5.14 summarises the most important results obtained with the optimisation program.

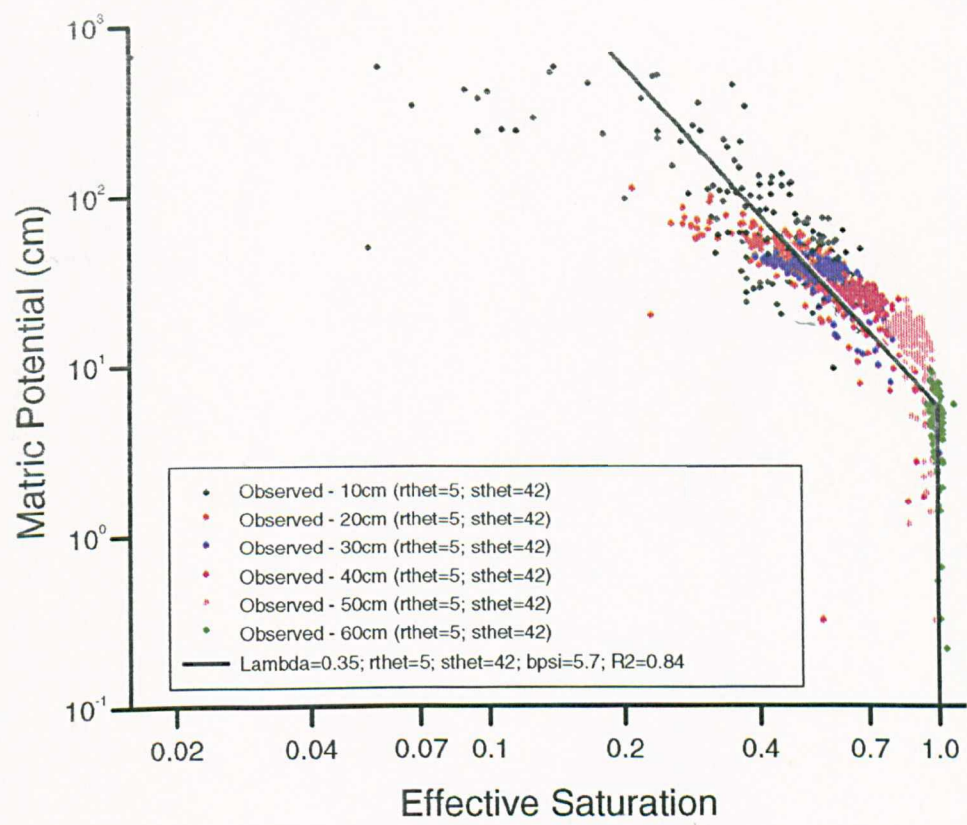


Figure 5.4 - Brooks-Corey's eq. fitted to Lys A data (Log-Log Method)

Table 5.14 - Adjustment of Brooks-Corey's equation (optimisation method)

Noteworthy results

Lysimeter	Fit to layers	Simul. layers	λ (-)	θ_r (%)	θ_s (%)	P_h (cm)	simul. mean relat. error	simulated R^2
A	1+2+3+4+5+6	1+2+3+4+5+6	0.46	5.00	42.0	-9.27	0.08	0.88
	1+2+3+4+5+6	1+2+3+4+5+6	0.49	5.00	42.0	-10.00	0.08	0.88
	1	1	0.31	5.00	42.0	-4.16	0.16	0.60
	1	1	0.47	5.00	42.0	-10.00	0.17	0.46
	2	2	0.37	5.00	42.0	-5.25	0.09	0.58
	2	2	0.54	5.00	42.0	-10.00	0.09	0.46
	1+2	1+2	0.33	5.00	42.0	-4.34	0.12	0.59
	1+2	1+2	0.51	5.00	42.0	-10.00	0.13	0.45
	3+4+5+6	3+4+5+6	0.48	5.00	42.0	-10.08	0.06	0.87
	3+4+5+6	3+4+5+6	0.47	5.00	42.0	-10.00	0.06	0.87
	1+2+3+4+5+6	1	0.46	5.00	42.0	-9.27	0.16	0.49
	1+2+3+4+5+6	2	0.46	5.00	42.0	-9.27	0.11	0.39
	1+2+3+4+5+6	1+2	0.46	5.00	42.0	-9.27	0.14	0.47
	1+2+3+4+5+6	3+4+5+6	0.46	5.00	42.0	-9.27	0.06	0.86
	1+2+3+4+5+6	1	0.49	5.00	42.0	-10.00	0.16	0.45
	1+2+3+4+5+6	2	0.49	5.00	42.0	-10.00	0.11	0.38
	1+2+3+4+5+6	1+2	0.49	5.00	42.0	-10.00	0.13	0.44
	1+2+3+4+5+6	3+4+5+6	0.49	5.00	42.0	-10.00	0.06	0.87
B	1+2+3+4+5+6	1+2+3+4+5+6	0.36	5.00	42.0	-8.16	0.09	0.80
	1+2+3+4+5+6	1+2+3+4+5+6	0.42	5.00	42.0	-10.00	0.09	0.78
	1	1	0.29	5.00	42.0	-6.89	0.24	0.35
	1	1	0.35	5.00	42.0	-10.00	0.23	0.33
	2	2	0.28	5.00	42.0	-4.37	0.08	0.71
	2	2	0.43	5.00	42.0	-10.00	0.09	0.57
	1+2	1+2	0.24	5.00	42.0	-3.76	0.16	0.43
	1+2	1+2	0.39	5.00	42.0	-10.00	0.16	0.36
	3+4+5+6	3+4+5+6	0.44	5.00	42.0	-9.62	0.06	0.84
	3+4+5+6	3+4+5+6	0.45	5.00	42.0	-10.00	0.06	0.84
	1+2+3+4+5+6	1	0.36	5.00	42.0	-8.16	0.23	0.31
	1+2+3+4+5+6	2	0.36	5.00	42.0	-8.16	0.08	0.61
	1+2+3+4+5+6	1+2	0.36	5.00	42.0	-8.16	0.16	0.39
	1+2+3+4+5+6	3+4+5+6	0.36	5.00	42.0	-8.16	0.06	0.83
	1+2+3+4+5+6	1	0.42	5.00	42.0	-10.00	0.23	0.25
	1+2+3+4+5+6	2	0.42	5.00	42.0	-10.00	0.09	0.56
	1+2+3+4+5+6	1+2	0.42	5.00	42.0	-10.00	0.16	0.34
	1+2+3+4+5+6	3+4+5+6	0.42	5.00	42.0	-10.00	0.06	0.83

Layer 1: 0 - 15 cm (data from instruments at 10cm depth)
 Layer 2: 15 - 25 cm (data from instruments at 20cm depth)
 Layer 3: 25 - 35 cm (data from instruments at 30cm depth)

Layer 4: 35 - 45 cm (data from instruments at 40cm depth)
 Layer 5: 45 - 55 cm (data from instruments at 50cm depth)
 Layer 6: 55 - 70 cm (data from instruments at 60cm depth)

The values of coefficient of determination with λ and P_e optimised by the program were always bigger than those of the log-log method (table 5.13), for the same combination of layers. This can be explained by the fact that the log-log method was applied using all measurements for parameter estimation. According to Milly (1987), its proper application generally requires the solution of more than one linear problem for each data set, with elimination of data that clearly do not fall on either the horizontal or sloping segment.

As for the fitting of parameters of Van Genuchten's equation, the values of R^2 for the top soil (layers 1 and 2) are very low; only when the other layers were included in the optimisation it was possible to obtain R^2 values close to 0.90. The sets of parameters fitted considering the soil as homogeneous were also applied to estimate the moisture contents and compute the errors and coefficient of determination for other combinations of soil layers, as shown in table 5.14. Again, the coefficients of determination obtained for the top soil (layers 1 and 2) were sensibly smaller than those obtained when data from these layers was used in the fitting, but the mean relative errors were very similar, and very close results were obtained for the bottom layers (layers 3, 4, 5, and 6) either considering homogeneous soil or fitting the parameters with data from the proper layers.

The results of table 5.14 are graphically displayed in figures 5.5, 5.6, and 5.7. As lysimeters A and B show similar behaviours, only the curves for lysimeter A are presented.

Figure 5.5 shows the characteristic curves obtained for lysimeter A using Brooks-Corey's equation under the hypothesis of homogeneous soil, for a saturated conductivity of 42% and air-entry pressure either optimised by the model (represented in red) or with a fixed value of 10cm (represented in black). Both curves are very similar and present a good fit to the data. As for Van Genuchten's equation, the confidence intervals obtained from the uncertainty due to input parameter error determined for a probability of occurrence of 95%, shown as dashed lines, are very small when compared to data variability.

Figure 5.6 shows the characteristic curves obtained using Brooks-Corey's equation for the top soil (10 and 20cm) of lysimeter A with air-entry pressure either optimised by the model (represented in blue) or with a fixed value of 10cm (represented in green), compared to those obtained for a homogeneous soil, also with air-entry pressure optimised by the model (represented in red) or with a fixed value of 10cm (represented in black). All four curves present similar behaviour. The coefficients of determination are low, but this is mainly due to the big scatter in the 10cm data, as commented for Van Genuchten's curves. All curves are well

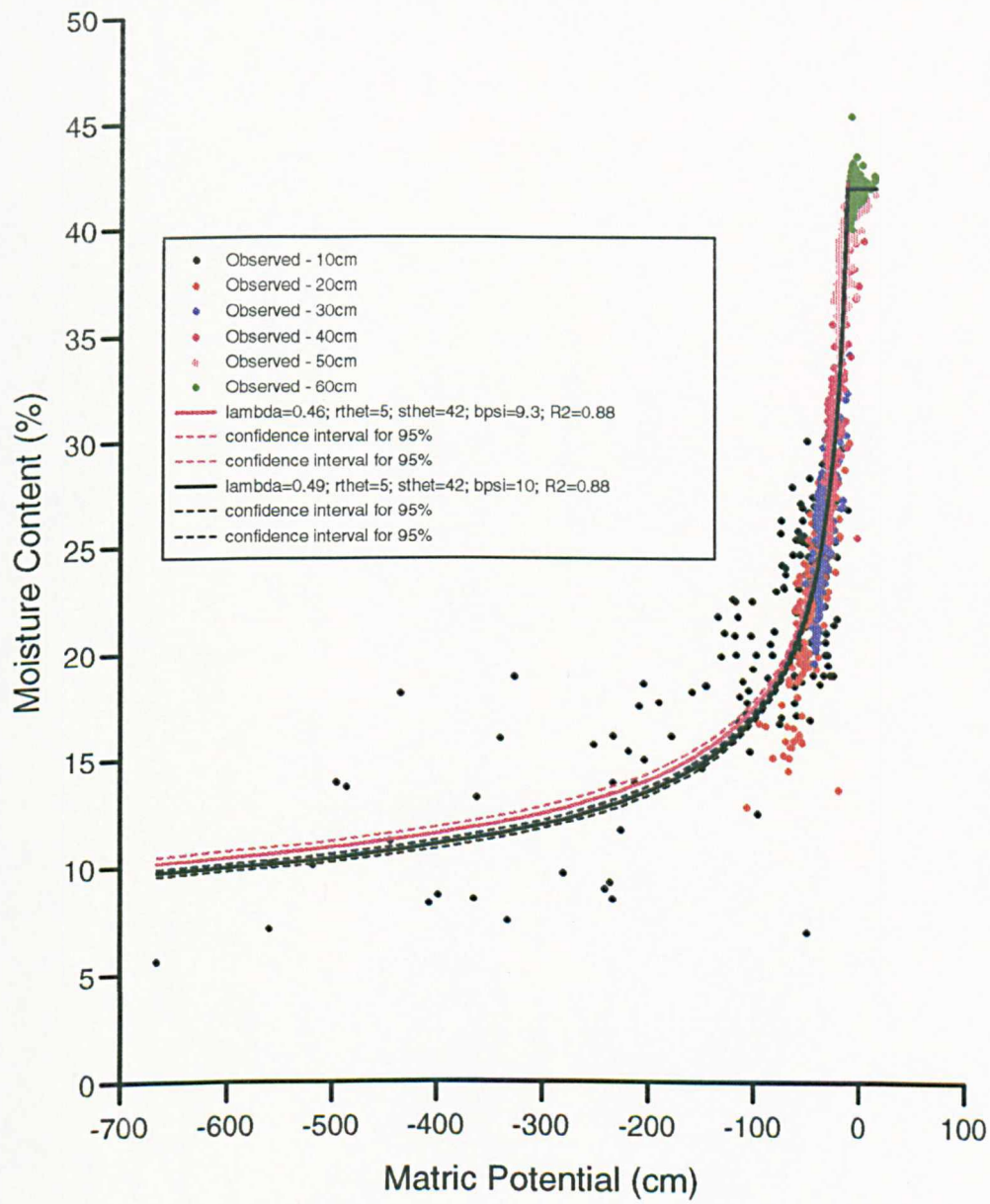


Figure 5.5 - Brooks-Corey's eq. fitted to Lys A data (all layers)

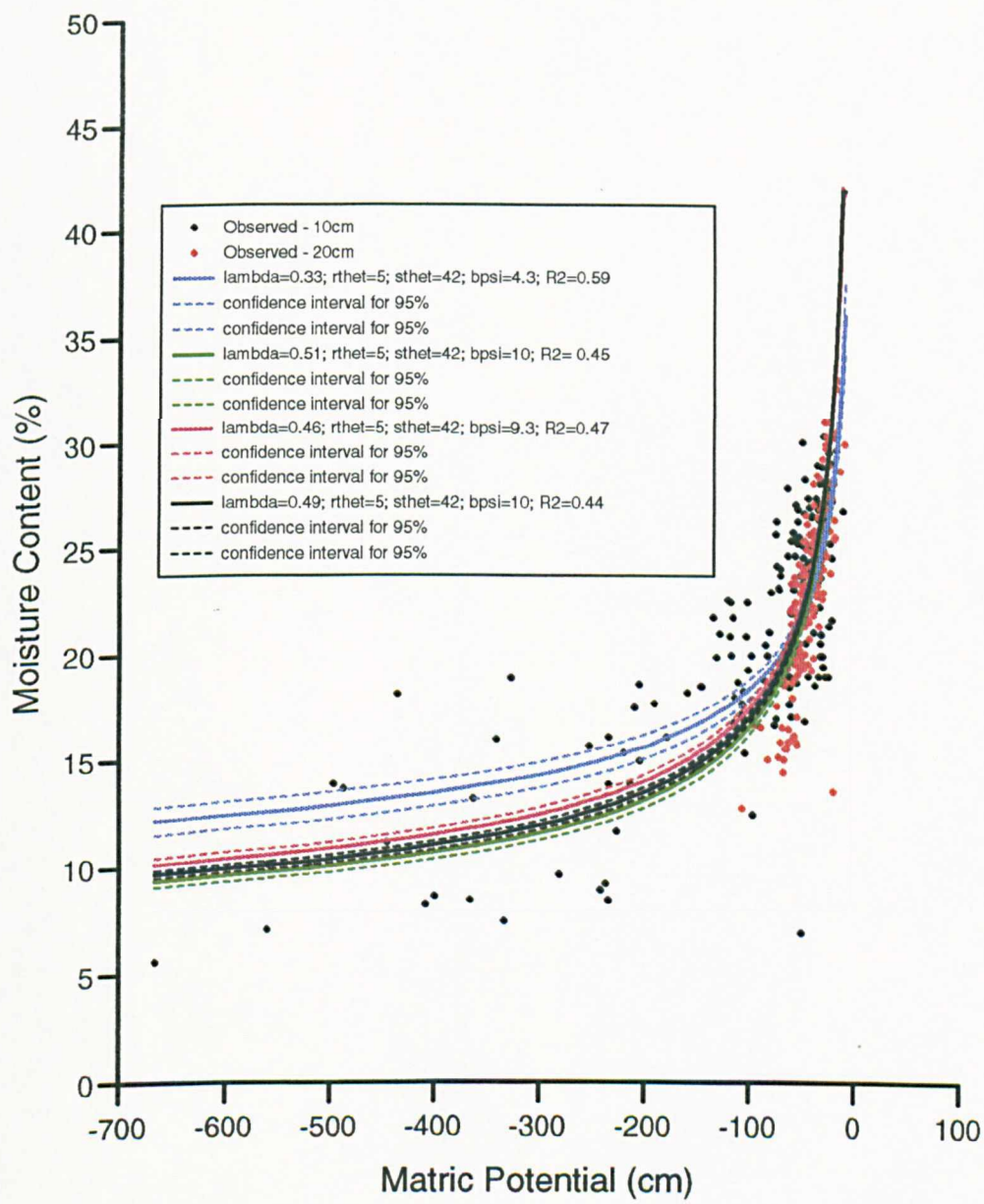


Figure 5.6 - Brooks-Corey's eq. fitted to Lys A data (top layers)

inside the range of observed data and show a good fit to the data, especially for values of matric potentials between -50cm and saturation. As for the other figures, the confidence intervals obtained from the uncertainty due to input parameter error determined for a probability of occurrence of 95% are very small when compared to data variability.

Figure 5.7 shows the characteristic curve obtained using Brooks-Corey's equation fitted to the bottom soil (data from 30 to 60cm) data of lysimeter A, with values of air-entry pressure either optimised by the model (represented in blue) or fixed at 10cm (represented in green), compared to those obtained for a homogeneous soil, also with values of air-entry pressure optimised by the model (represented in red) or fixed at 10cm (represented in black). All four curves present very similar behaviour, with very good fit to the data.

As in the analysis of Van Genuchten's equation, it seems that the hypothesis of homogeneous soil for the determination soil moisture characteristic does not imply bigger errors than assuming different sets of parameters along the soil profile. This fact suggests the adoption of the set of parameters determined for a homogeneous soil to be applied for the whole soil profile.

Lenhard et al. (1989) present a methodology for converting parameters of Van Genuchten's retention function to equivalent parameters of Brooks-Corey's relationship, by equating the differential fluid capacities, $\partial S_e / \partial \psi$, at $S_e = 0.5$, leading to:

$$\begin{aligned}\lambda &= \frac{m_n}{1 - m_n} (1 - 0.5^{1/m_n}) \\ P_b &= \frac{\overline{S_x}^{-1/\lambda}}{\alpha} (\overline{S_x}^{1/m_n} - 1)^{(1 - \eta)} \\ \overline{S_x} &= 0.72 - 0.35e^{-\eta}\end{aligned}\tag{5.13}$$

where m_n is related to the Van Genuchten parameter, n , by $m_n = 1 - 1/n$.

Applying this set of relationships to Van Genuchten's parameters obtained for a homogeneous soil for lysimeter A (i.e., $\alpha = 0.06$ and $n = 1.70$), we obtain $\lambda = 0.57$ and $P_b = 10.5$. Using the data from lysimeter B ($\alpha = 0.07$ and $n = 1.48$), the values for Brooks-Corey's parameters are $\lambda = 0.42$ and $P_b = 9.64$. These values are similar to those obtained from the optimisations.

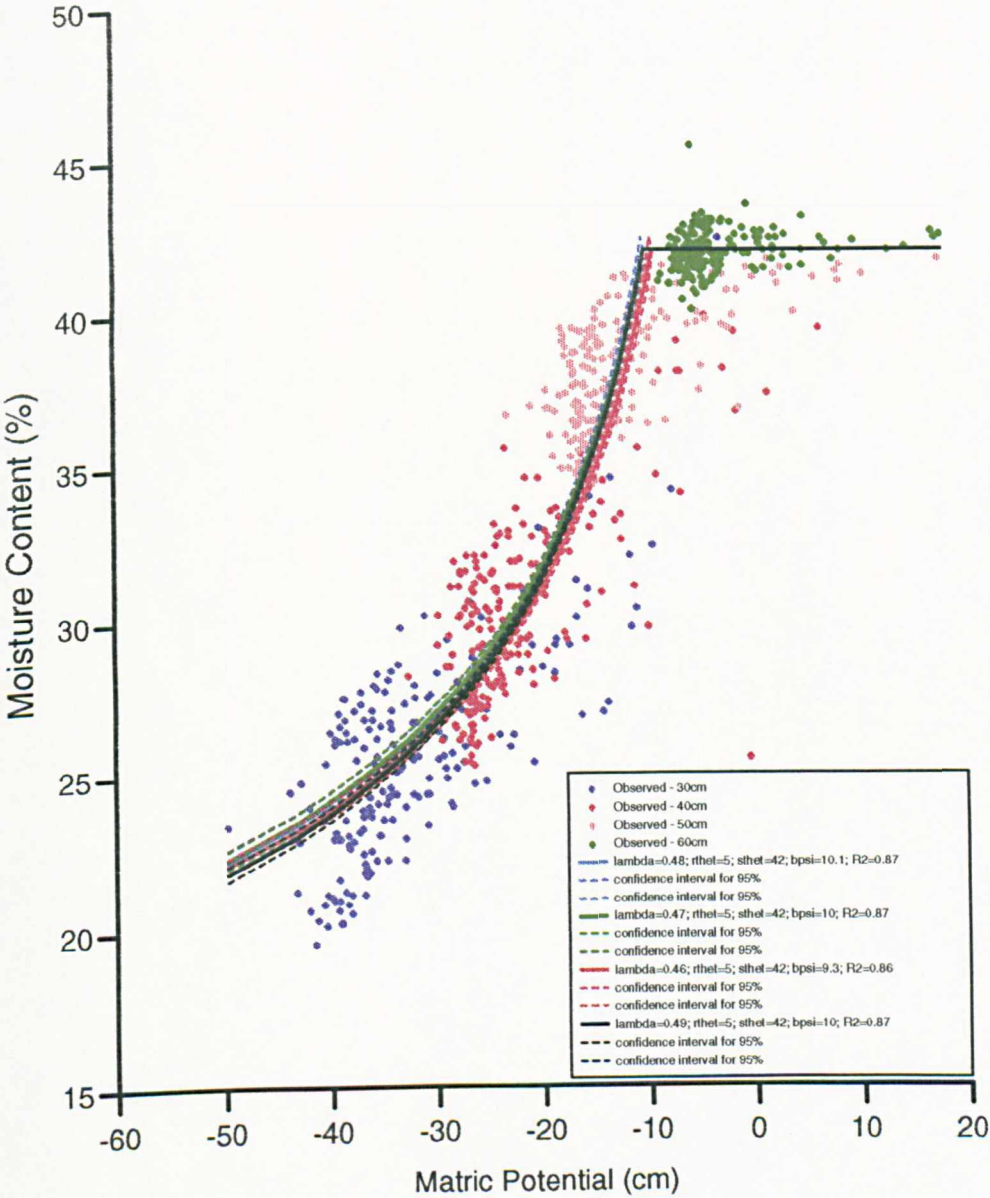


Figure 5.7 - Brooks-Corey's eq. fitted to Lys A data (bottom layers)

5.3.4 - Modified Brooks-Corey's equation - MACRO methodology

The MACRO model was already described in chapter 3 (section 3.3.2). It uses a modified Brooks-Corey's water characteristic curve, so that, in the two-domain case, the total soil porosity is partitioned into two components, micropores and macropores, with specified boundary water content (θ_b) and potential (ψ_b). In one flow domain, an approximate value of water content is calculated assuming a linear $\theta(\psi)$ in the macropore region, so that the soil moisture characteristic is given by:

$$\begin{aligned} Se &= \frac{\theta - \theta_r}{\theta_b - \theta_r} = \left(\frac{\psi_b}{\psi}\right)^\lambda & \text{if } \psi < \psi_b \\ Se &= \frac{\theta_s - \theta}{\theta_s - \theta_b} = \left(\frac{\psi_b}{\psi}\right) & \text{if } \psi_b \leq \psi < 0 \\ Se &= 1 & \text{if } \psi \geq 0 \end{aligned} \quad (5.14)$$

The optimisation methodology was applied in order to fit the parameters of MACRO in one flow domain. The values of θ_r and θ_s were fixed as 5% and 42%, respectively, while λ and θ_b were determined by the optimisation program, for different values of ψ_b . Table 5.15 summarises the most important results.

As for the Van Genuchten and Brooks-Corey equations, the values of R^2 for the top soil (layers 1 and 2) are very low; only when the other layers were included in the optimisation it was possible to obtain R^2 values close to 0.90. Again, the coefficients of determination obtained for the top soil (layers 1 and 2) when using the curves fitted to homogeneous soil were sensibly smaller than those obtained when data from these layers was used in the fitting, but the mean relative errors were very similar, and very close results were obtained for the bottom layers (layers 3, 4, 5, and 6). The results of table 5.15 are graphically displayed in figures 5.8, 5.9, and 5.10.

Figure 5.8 shows the characteristic curves obtained for lysimeter A using MACRO's methodology under the hypothesis of homogeneous soil, for a saturated conductivity of 42% and boundary pressure either optimised by the model (represented in red) or with a fixed value of 10cm (represented in black). Both curves are very similar and present a good fit to the data.

Figure 5.9 shows the characteristic curves obtained using MACRO's methodology for

the top soil (data from 10 and 20cm - represented in red) of lysimeter A compared to those obtained for a homogeneous soil (represented in black), both with boundary pressure value fixed as 10cm. The coefficients of determination are low, but both curves are well inside the range of observed data and show a good fit to the data, especially for values of matric potentials between -50cm and saturation.

Figure 5.10 shows the characteristic curve obtained using MACRO's methodology fitted to the bottom soil (data from 30 to 60cm - represented in red) data of lysimeter A compared to those obtained for a homogeneous soil (represented in black). The curves present very similar behaviour, with very good fit to the data.

Table 5.15 - Adjustment of MACRO's characteristic curve

Noteworthy results

Lysimeter	Fit to layers	Simul. layers	λ (-)	θ_r (%)	θ_s (%)	θ_b (%)	Ψ_b (cm)	simul. mean relat. error	simulated R^2
A	1+2+3+4+5+6	1+2+3+4+5+6	0.46	5.00	45.0	37.97	-12.0	0.08	0.88
	1+2+3+4+5+6	1+2+3+4+5+6	0.46	5.00	42.0	40.70	-10.0	0.08	0.88
	1	1	0.31	5.00	42.0	33.24	-10.0	0.16	0.60
	2	2	0.38	5.00	42.0	34.89	-10.0	0.09	0.59
	1+2	1+2	0.33	5.00	42.0	33.41	-10.0	0.12	0.59
	3+4+5+6	3+4+5+6	0.45	5.00	42.0	41.13	-10.0	0.06	0.87
	1+2+3+4+5+6	1	0.46	5.00	42.0	40.70	-10.0	0.16	0.49
	1+2+3+4+5+6	2	0.46	5.00	42.0	40.70	-10.0	0.11	0.39
	1+2+3+4+5+6	1+2	0.46	5.00	42.0	40.70	-10.0	0.13	0.47
	1+2+3+4+5+6	3+4+5+6	0.46	5.00	42.0	40.70	-10.0	0.06	0.87
B	1+2+3+4+5+6	1+2+3+4+5+6	0.35	5.00	45.0	36.93	-12.0	0.09	0.79
	1+2+3+4+5+6	1+2+3+4+5+6	0.35	5.00	42.0	39.18	-10.0	0.09	0.81
	1	1	0.27	5.00	42.0	36.89	-10.0	0.24	0.37
	2	2	0.29	5.00	42.0	35.11	-10.0	0.08	0.71
	1+2	1+2	0.27	5.00	42.0	35.37	-10.0	0.16	0.44
	3+4+5+6	3+4+5+6	0.40	5.00	42.0	40.30	-10.0	0.05	0.85
	1+2+3+4+5+6	1	0.35	5.00	42.0	39.18	-10.0	0.23	0.32
	1+2+3+4+5+6	2	0.35	5.00	42.0	39.18	-10.0	0.08	0.63
	1+2+3+4+5+6	1+2	0.35	5.00	42.0	39.18	-10.0	0.15	0.41
	1+2+3+4+5+6	3+4+5+6	0.35	5.00	42.0	39.18	-10.0	0.06	0.85

Layer 1: 0 - 15 cm (data from instruments at 10cm depth)
 Layer 2: 15 - 25 cm (data from instruments at 20cm depth)
 Layer 3: 25 - 35 cm (data from instruments at 30cm depth)

Layer 4: 35 - 45 cm (data from instruments at 40cm depth)
 Layer 5: 45 - 55 cm (data from instruments at 50cm depth)
 Layer 6: 55 - 70 cm (data from instruments at 60cm depth)

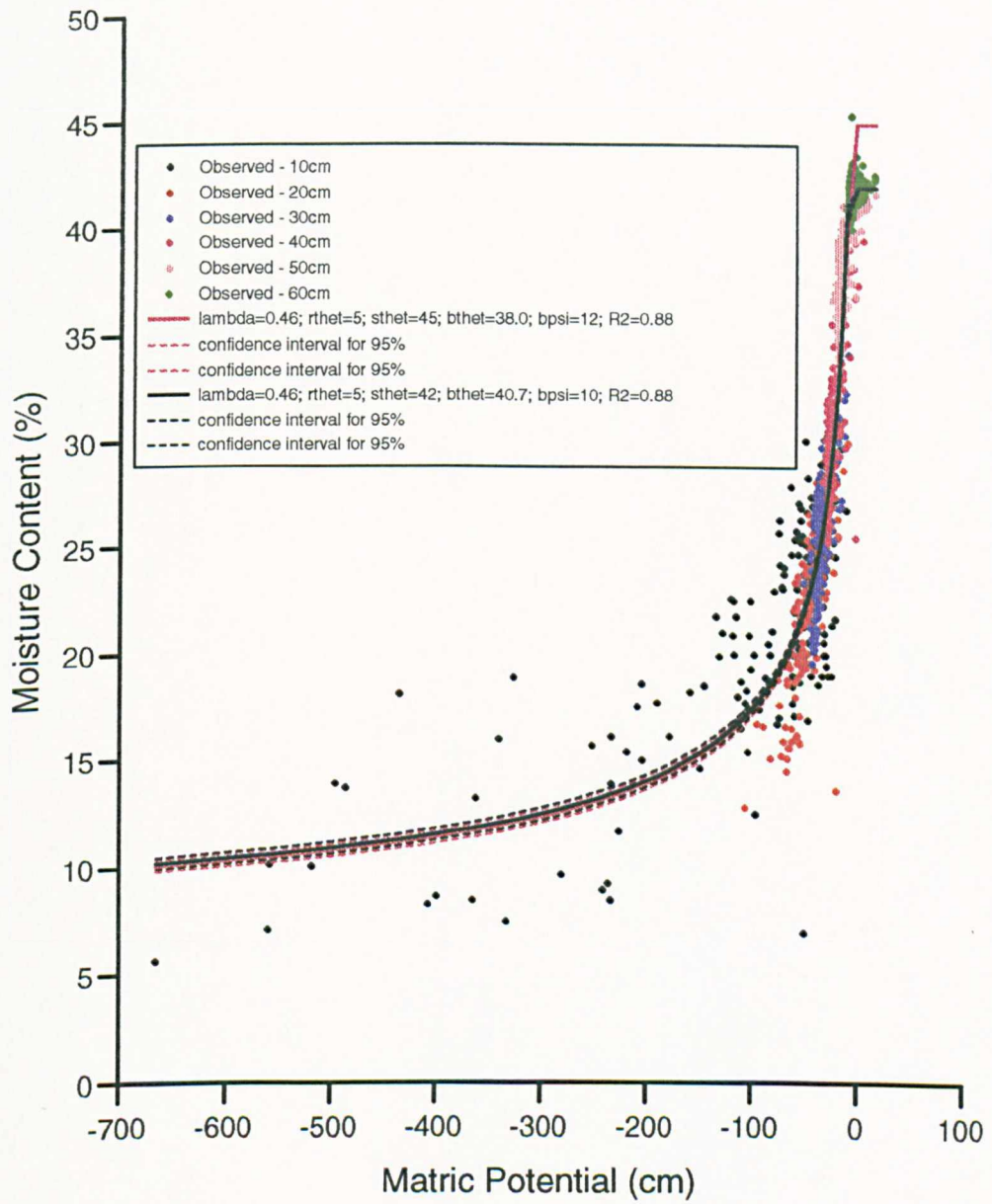


Figure 5.8 - MACRO's curve fitted to Lys A data (all layers)

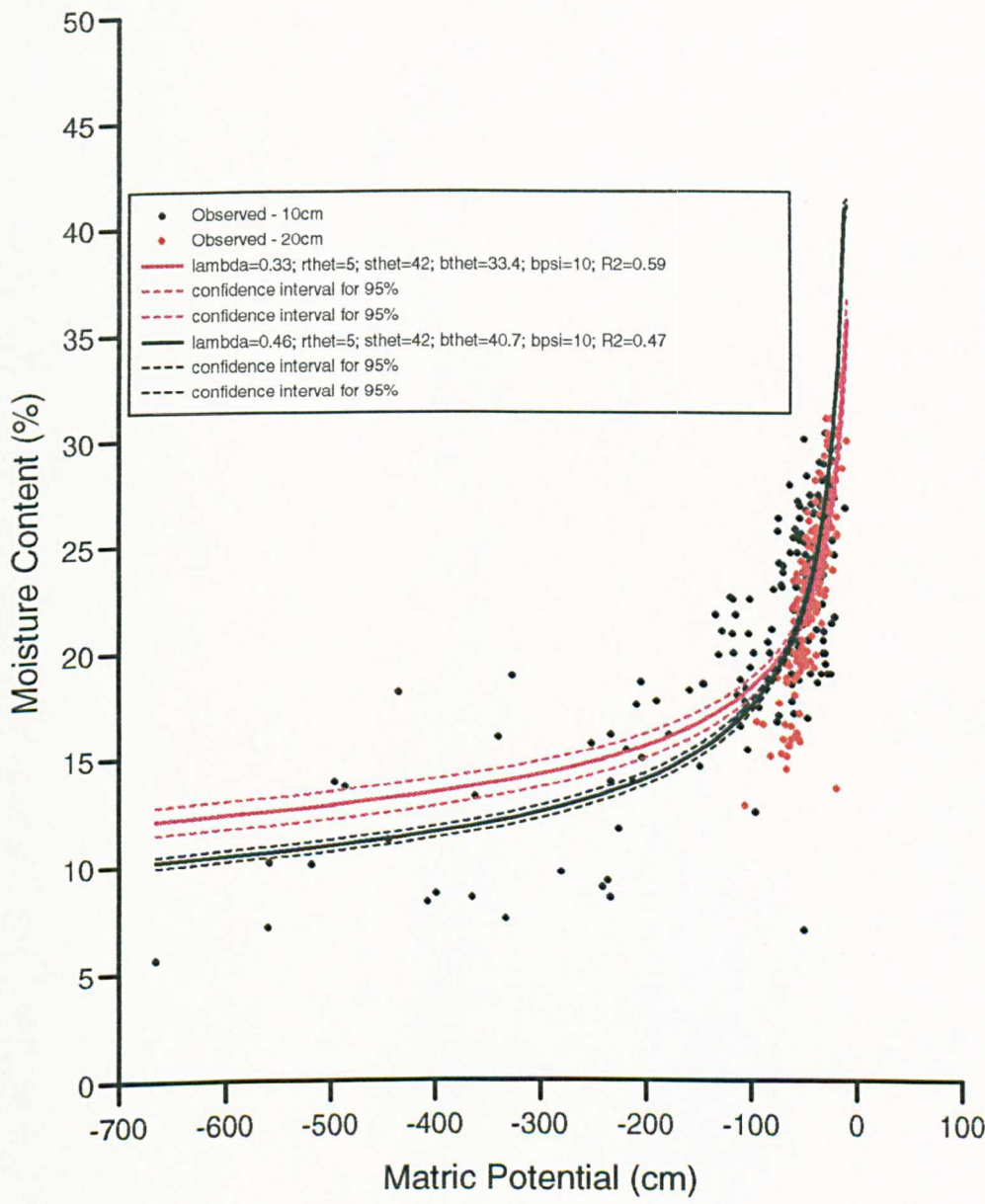


Figure 5.9 - MACRO's curve fitted to Lys A data (top layers)

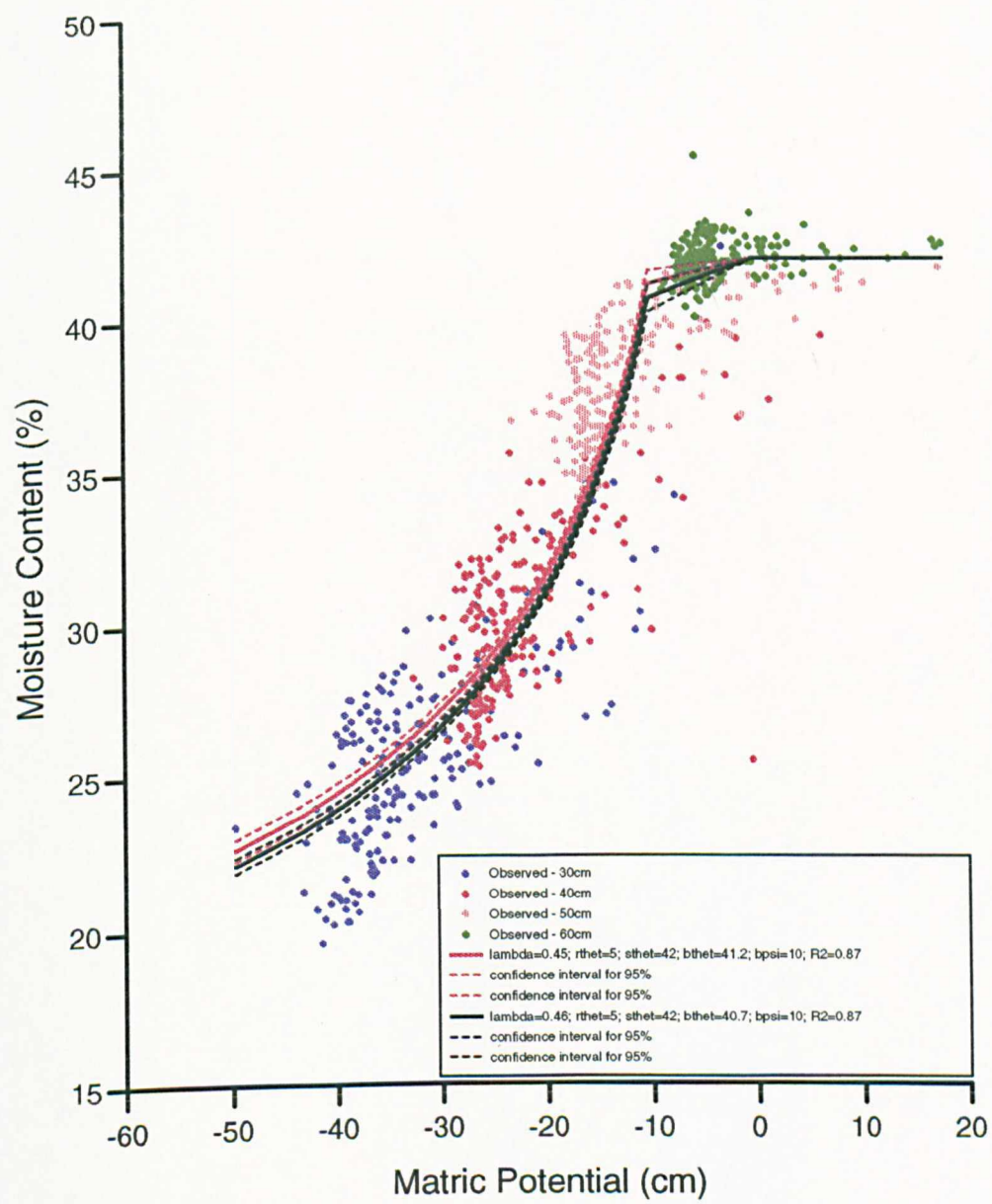


Figure 5.10 - MACRO's curve fitted to Lys A data (bottom layers)

As for Van Genuchten's and Brooks-Corey's equation, fitting the soil moisture characteristic curve under the assumption of homogeneous soil does not imply bigger errors than assuming different sets of parameters along the soil profile. It is suggested the selection of the set of parameters determined for a homogeneous soil to be applied to the whole soil profile.

5.3.5 - Comparison of the results for the different relationships

As shown in previous sections, fitting the soil moisture characteristic curve under the assumption of homogeneous soil does not imply bigger errors than assuming different sets of parameters along the soil profile, for any of the three relationships analyzed (Van Genuchten, Brooks-Corey and MACRO). For this reason, the sets of parameters obtained under the hypothesis of homogeneous soil are selected to represent the whole soil profile, and the curves fitted to lysimeter A are compared in figure 5.11.

Brooks-Corey's and MACRO's curves are very similar along the whole profile. This is an expected result, as MACRO is actually a modified Brooks-Corey's relationship. The values of coefficient of determination (0.87 for Van Genuchten and 0.88 for Brooks-Corey and MACRO) and of mean relative error (0.09 for Van Genuchten and 0.08 for Brooks-Corey and MACRO) are very close for the three curves. The adopted Van Genuchten curve produces lower estimates of moisture contents than the others for matric potentials smaller than -50cm, but the differences are not big (under 3%). For matric potentials higher than -50cm all three curves produce very similar results, with good fit to the data.

None of the three curves can be identified as having a clear better fit to the data. Brooks-Corey and MACRO relationships have the disadvantage of presenting discontinuity in its derivatives at the air-entry pressure, which can cause numerical instabilities during simulations, as already discussed in section 2.2.3. However, it seems that they present a negligibly better fit to the dry range of the data set than the Van Genuchten's equation, although the big scatter for these values complicates its analysis. A comparison of figures 5.3, 5.7 and 5.10 shows that, close to saturation, Van Genuchten's curve does not quite coincide with the clusters of data observed for depths 50cm and 60cm, while Brooks-Corey and MACRO relationships seem, again, to fit the data slightly more adequately.

Figure 5.12 presents a comparison of the adopted curves for lysimeters A and B. It is noticeable that the curves fitted to lysimeter B data produce higher estimates of moisture contents than those of lysimeter A, for almost the whole range of matric potential values. This

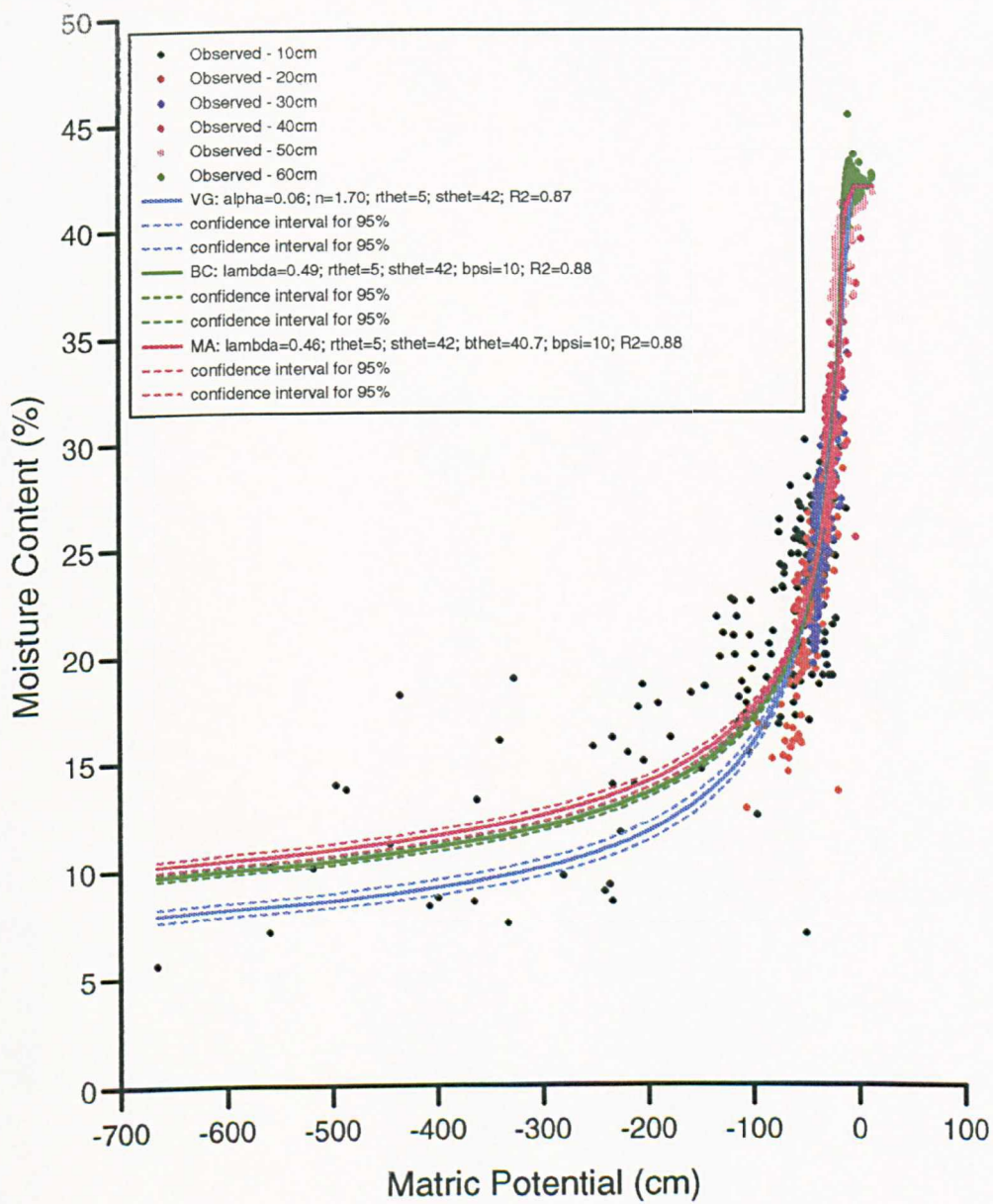


Figure 5.11 - Comparison of fitted eq. to Lys A data (all layers)

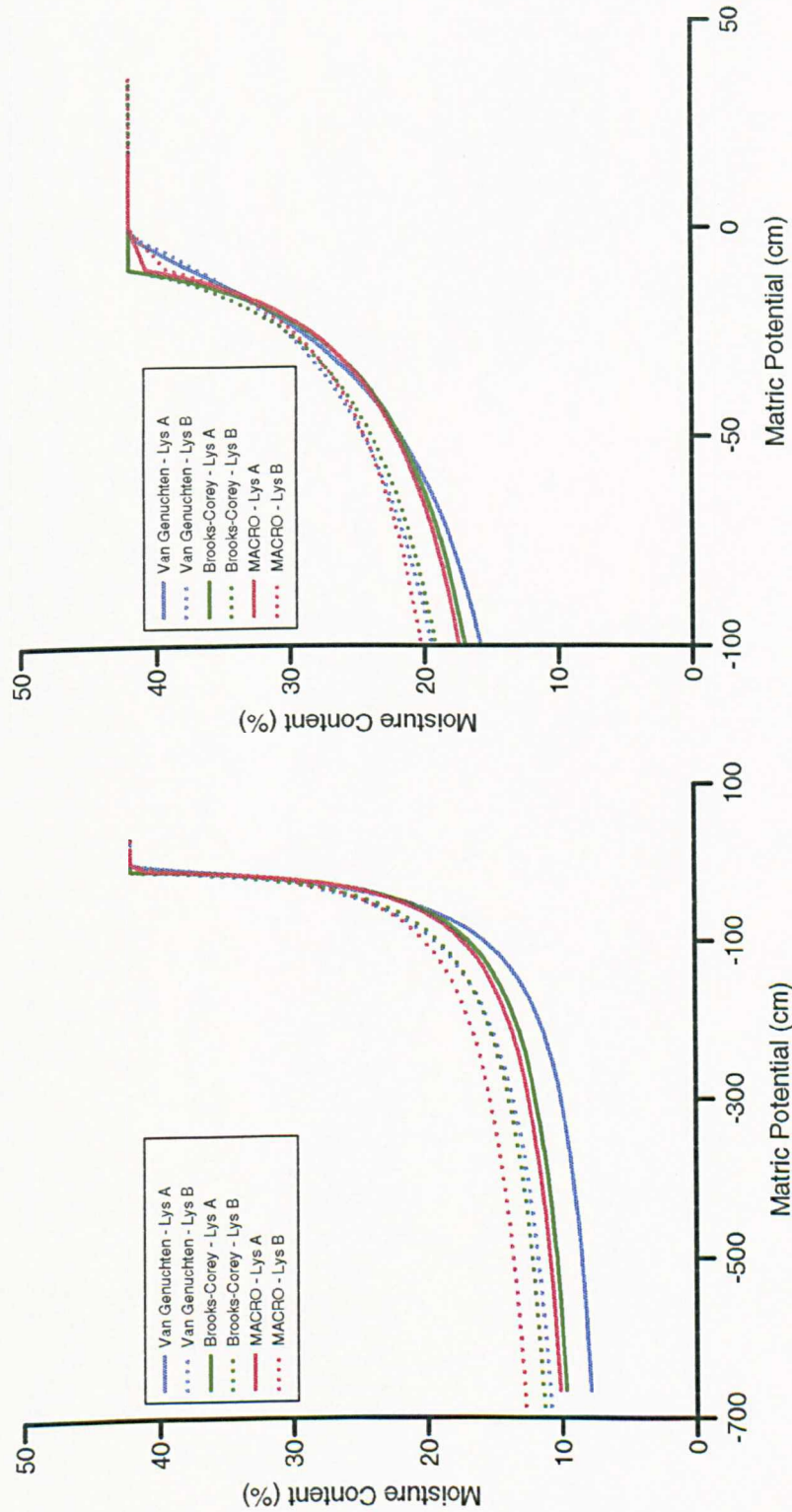


Figure 5.12a - Comparison of curves for Lys A and B (all range)

Figure 5.12b - Comparison of curves for Lys A and B (detail)

behaviour is reverted very close to saturation, in the case of MACRO and Van Genuchten relationships. The differences between the values of moisture content obtained with the adopted curves of each lysimeter are small, but it can help to explain different responses observed in the data set.

The main reason for testing different models for the optimisation of the characteristic curves was to tackle the problem of parameter identification and also to have an idea of model uncertainty. The models selected were the most widely used in the past: Van Genuchten and Brooks-Corey (MACRO is actually a modified Brooks-Corey). The fact that they produce very similar results is neither enough to eliminate the problem of parameter identification nor to estimate a low model uncertainty. However, besides being similar, these results show a good fit to the observed data, which is a good indicative that the methodologies are appropriate for use in the conditions of the experiment.

5.4 - Conclusions

The problem of determination of soil properties was tackled by the combined use of data from physical analysis of soil cores and adjustment of soil characteristic parametric relationships, through optimisation of objective functions applied to the available $\theta(\psi)$ data.

The available data for particle size analysis provided information to identify a sandy loam soil, but the fact that the sample used for this analysis was of only two cores did not allow further statistical analysis.

A falling head permeameter was assembled for the physical analysis of soil cores from the destructive sampling of two lysimeters (deep lysimeter F and shallow lysimeter G). These analysis comprised tests of saturated conductivity, porosity, dry bulk density and void ratio. The results of these tests showed that there is enough statistical evidence to identify a difference in the values of porosity, dry bulk density and void ratio for the top layer of the soil, when compared with the deeper layers. This behaviour can be explained by the higher biological activity in the top soil. Statistical evidence of a significant difference in saturated conductivity, could not be identified, due to the high spatial variation of this variable. However, as the mean values of saturated conductivity for different soil layers present a difference of one or even two orders of magnitude, these values were adopted for simulating vertical heterogeneity in the soil. Also, the presence of structure in the soil caused some of the cores to be rejected as statistical outliers for the analysis of the saturated conductivity. The physical phenomena controlling the

water flow in the cores with structured soil can not be described by capillary theory flow, and the concept of saturated conductivity is not applicable to them.

A methodology for estimating the parameter values and associated uncertainty, based on first-order error analysis, was applied to three different soil moisture parametric curves: Van Genuchten's equation, Brooks-Corey's equation and MACRO model methodology for the single porosity case. All three relationships produced very similar results. Soil moisture characteristic curves fitted under the assumption of homogeneous soil produced errors of same magnitude of those given by curves assuming different sets of parameters along the soil profile. This fact leads to the adoption of only one curve for the whole depth profile. Also, the use of different saturated moisture contents for the top and bottom layers of the soil, as suggested by the porosity data obtained from the destructive tests of lysimeters F and G, showed not to produce better results than the use of one fixed value for the whole profile, given by the optimisation methodology. Finally, the uncertainties due to input parameter error were quite small when compared to the data variation, suggesting that other sources of uncertainty, such as data error (due to measurement inaccuracies or to spatial variability) or uncertainty in the model itself, should be investigated.

CHAPTER 6 - APPLICATION OF SPW1hyst TO THE SELECTED EVENTS

6.1 - Introduction

Infiltration and soil water movement models have been discussed for many years. According to Beven and Germann (1981), most of these models use approaches based on Darcy's law and the Richards' equation, and, although Darcy's law is itself an empirical approximation, such models have been well proven in the past. Edwards et al. (1979), refer to several works where the Richards' equation has been successfully used to describe unsaturated soil water flow under laboratory conditions and under controlled field conditions. Failures of the Richards' equation to describe unsaturated water movement, however, are also reported in the literature. According to Edwards et al. (1979), many reports indicate that agricultural chemicals sometimes move through an undisturbed soil profile much faster than can be explained with capillary water flow theory.

The importance of rapid flow processes to describe unsaturated water flow in the Imperial College's lysimeter experiment at Silwood Park was shown in chapter 4, as the majority of the noticeable events of the experimental station present evidence of preferential or rapid water flow. It is important to evaluate the capacity of models based on the Richards' equation to properly represent these events.

In chapter 5 it was demonstrated that there is not enough statistical evidence to assume significant difference among the saturated conductivities of the different soil layers of the lysimeters. However, the data presented and discussed in that chapter clearly shows a difference of one or even two orders of magnitude between the conductivities values for the three analyzed layers, justifying the need to study the influence of this vertical heterogeneity.

In the present chapter, model SPW1hyst is employed in order to test the strengths and limitations of the traditional models of water flow in the unsaturated zone, based on Richards' equation. Model SPW1hyst, as previously described in chapter 3, is an adaptation of model SPW1, in order to incorporate the effects of air entrapment and hysteresis in the soil characteristic curve. It was also adapted in order to be able to run MACRO methodology in one flow domain. The model was applied to the events selected and described in chapter 4, alternatively including or neglecting the effects of hysteresis, and also to assess the effect of vertical heterogeneity of saturated conductivity of the soil in the lysimeters.

6.2 - Non-hysteretic simulations using parameters fitted to observed $\theta(\psi)$ and K_s data

In chapter 5, values for the soil properties of the lysimeters of Imperial College's experimental station were determined by the combined use of data from physical analysis of soil cores and observed $\theta(\psi)$ data. The fitted parameter values for different soil characteristic curves that can be used by model SPW1hyst are summarised in table 6.1. The saturated hydraulic conductivity of the soil is adopted as 6 cm/h for a homogeneous soil profile and, when considering heterogeneity, as $K_{s1}=20.6$ cm/h, $K_{s2}=0.4$ cm/h and $K_{s3}=0.03$ cm/h for depths 0 to 25 cm, 25 to 50 cm and 50 to 70 cm, respectively. When using MACRO methodology, the value of the boundary conductivity (K_b) is fixed as 0.01 cm/h.

Table 6.1 - Parameters fitted to observed $\theta(\psi)$ and K_s data

Soil Characteristic Curve	Parameter	Parameter Value	
		Lysimeter A	Lysimeter B
Van Genuchten	α (1/cm)	0.06	0.07
	n (-)	1.70	1.48
	θ_r (cm ³ /cm ³)	0.05	0.05
	θ_s (cm ³ /cm ³)	0.42	0.42
Brooks-Corey	λ (-)	0.49	0.42
	θ_r (cm ³ /cm ³)	0.05	0.05
	θ_s (cm ³ /cm ³)	0.42	0.42
	P_h (cm)	-10.0	-10.0
MACRO Single Porosity	λ (-)	0.46	0.35
	θ_r (cm ³ /cm ³)	0.05	0.05
	θ_s (cm ³ /cm ³)	0.42	0.42
	θ_b (cm ³ /cm ³)	0.41	0.39
	ψ_b (cm)	-10.0	-10.0

A grid of 35 elements with fixed thickness of 2 cm was adopted, and the initial conditions (matric potential) for each element were obtained by fitting polynomial approximations to the measured data from the tensiometers of a deep lysimeter at 10, 20, 30, 40, 50 and 60 cm depth. The unsaturated hydraulic conductivity curve when using Van Genuchten's or Brooks-Corey's characteristic curves was described using Mualem's (1976a) relationship. SPW1hyst was run in non-hysteretic mode taking into account root uptake in response to imposed hourly evapotranspiration rates, obtained from daily totals computed using the Penman model. The daily totals were divided by 12 and the results were applied to the period of 6 am to 6 pm. The time-dependent root density profile was represented by fitting an exponential distribution to the weekly borescope measurements of wheat root densities (Butler and Wheater, 1993). The lower boundary condition adopted was of a fixed pressure of 5 cm

above the base. Rainfall information was provided by the automatic weather station located at the experimental station. The results of the simulations of the 12 selected events are summarised in table 6.2.

Table 6.2 - Non-hysteretic SPW1hyst simulations - param fitted to obs $\theta(\psi)$ and Ks data

Event			L y s	Soil characteristic parametric relationship											
				Van Genuchten				Brooks-Corey				MACRO - Single Porosity			
				Homogeneous		Heterogeneous		Homogeneous		Heterogeneous		Homogeneous		Heterogeneous	
				R ² (p)	R ² (f)	R ² (p)	R ² (f)	R ² (p)	R ² (f)	R ² (p)	R ² (f)	R ² (p)	R ² (f)	R ² (p)	R ² (f)
R A P I D F L O W	90158	A	0.69	-156	0.51	-1.8	0.36	-271	0.40	0.24	-0.5	-1.3	-0.5	-2.5	
		B	0.59	-210	0.63	-3.1	0.28	-828	0.43	0.12	-0.3	-3.0	-0.3	-3.7	
	90230	A	0.29	-31	0.26	0.47	0.13	-22	0.16	-0.3	0.62	0.17	0.62	0.20	
		B	0.28	0.46	0.36	-3.0	0.05	-2.7	0.19	-0.1	0.03	-2.4	0.04	-2.8	
	90291	A	0.79	0.73	0.84	-3.2	0.62	-0.6	0.83	-1.3	0.26	-3.3	0.26	-3.3	
		B	0.84	-0.3	0.73	-2.8	0.63	0.55	0.67	-1.9	0.61	-1.3	0.62	-2.6	
	91017	A	0.53	-0.9	0.70	0.02	0.48	-1.4	0.70	0.81	0.22	0.48	0.22	0.60	
		B	0.53	0.84	0.75	-2.9	0.27	0.75	0.57	-0.5	0.49	-2.9	0.50	-3.0	
	91119	A	0.86	-1.3	0.76	-2.7	0.66	0.28	0.69	-2.4	0.40	-3.0	0.41	-2.8	
		B	0.77	0.32	0.71	-2.1	0.46	0.60	0.61	-1.3	0.56	-3.5	0.57	-2.1	
	91136	A	0.97	-526	0.89	-31	0.84	< -999	0.85	-51	0.77	-26	0.77	-67	
		B	0.97	-99	0.91	-17	0.81	< -999	0.89	-46	0.63	< -999	0.63	-3.3	
	91198	A	0.90	-480	0.78	0.73	0.72	-398	0.73	-17	0.20	-8.0	0.21	-2.5	
		B	0.92	-46	0.86	-1.4	0.68	-86	0.81	-1.7	0.46	-2.5	0.46	-1.1	
	91211	A	0.88	-4.9	0.82	-3.4	0.76	-2.2	0.81	-3.3	0.15	-5.5	0.16	-4.3	
		B	0.92	-1.7	0.86	-2.4	0.72	-1.6	0.83	-1.9	0.13	-2.2	0.13	-2.2	
$\bar{x}$ s	A	0.74	-96	0.70	-1.4	0.57	-99	0.65	-3.3	0.27	-2.9	0.27	-2.1		
	B	0.23	178	0.21	1.73	0.24	165	0.24	6.20	0.38	3.06	0.38	1.81		
$\bar{x}$ s	A	0.73	-37	0.73	-2.5	0.49	-131	0.63	-1.0	0.33	-2.5	0.33	-2.5		
	B	0.24	78	0.17	0.61	0.27	309	0.23	0.87	0.34	0.70	0.34	0.82		
S L O W F L O W	90129	A	0.49	-24	0.48	-2.5	0.21	-51	0.36	-1.1	0.59	0.91	0.61	-2.6	
		B	0.46	-10	0.47	-7.7	-0.004	-107	0.23	-2.5	-1.9	-28	0.90	-22	
	91108	A	0.83	-131	0.80	0.58	0.70	-129	0.76	-0.9	-1.7	0.21	-1.7	0.81	
		B	0.66	-81	0.70	-1.7	0.48	-119	0.60	-1.4	0.42	-0.4	0.42	-1.3	
	91165	A	0.91	-17	0.86	-1.0	0.86	-16	0.87	0.72	-0.1	0.58	-0.1	-0.9	
		B	0.87	-10	0.84	-2.0	0.74	-15	0.84	0.79	0.09	-0.6	0.10	-1.4	
	91204	A	0.90	-146	0.89	-0.6	0.84	-151	0.88	0.01	0.49	0.67	0.49	0.71	
		B	0.91	-23	0.92	-2.3	0.78	-41	0.89	0.76	0.57	-1.3	0.57	-2.1	
	$\bar{x}$ s	A	0.78	-80	0.74	-2.1	0.65	-87	0.72	-0.3	-0.2	0.59	-0.2	-0.5	
		B	0.20	69	0.19	0.35	0.30	64	0.24	0.84	1.06	0.29	1.06	1.61	
$\bar{x}$ s	A	0.73	-31	0.73	-3.4	0.50	-71	0.64	-0.6	-0.2	-7.6	0.50	-6.7		
	B	0.21	34	0.20	2.86	0.36	50	0.30	1.64	1.15	13.6	0.33	10.2		

R²(p) = Coefficient of determination for the fit of simulated and observed matric potentials

R²(f) = Coefficient of determination for the fit of simulated and observed bottom inflow

$\bar{x}$ = mean value - event 91136 (outlier) not considered when computing statistics for R²(f)

s = standard deviation - event 91136 (outlier) not considered when computing statistics for R²(f)

Obs.: Homogeneous or heterogeneous conditions refer to saturated hydraulic conductivity values

The values presented in table 6.2 clearly show that the model, when using the parameters obtained from the fitted moisture characteristic curves and experimentally determined saturated conductivity, can not properly represent the observed bottom inflow. For both Van Genuchten's and Brook-Corey's equations, the mean values of the coefficients of determination,

$R^2(f)$, are negative or very small, suggesting that the fit is poor. When using Van Genuchten's or Brook-Corey's soil characteristic relationships, there is a significant improvement in the results for the bottom inflow under heterogeneous conditions for all slow flow events. However, a different effect is observed for the rapid flow events: although the mean values of the coefficient of determination are clearly better for the heterogeneous simulations, this is not necessarily true if each event is analyzed separately. When Van Genuchten's equation is used, events 90158, 91136 and 91198 show better results under heterogeneous conditions for both lysimeters; events 90230, 91017 and 91211 show better outcomes under heterogeneous conditions for lysimeter A and under homogeneous conditions for lysimeter B; and events 90291 and 91119 present better bottom inflow representation under homogeneous conditions. When using Brooks-Corey's relationship, a better representation of bottom inflow, for both lysimeters, was obtained under heterogeneous conditions for events 90158, 90230, 91136 and 91198; event 91017 showed better results under heterogeneous conditions for lysimeter A and under homogeneous conditions for lysimeter B; and events 90291, 91119 and 91211 have their bottom inflow better represented by homogeneous conditions. Simulations using MACRO's methodology showed results of the same order of magnitude as those observed for the simulations under heterogeneous conditions using the other two characteristic equations and no clear improvement was observed when using heterogeneity in the saturated hydraulic conductivity.

The responses observed with the use of MACRO's methodology were obtained for similar boundary and saturated water contents, which induced the simulations to be mostly performed for matric potentials and water contents smaller than the boundary values. Consequently, the simulated conductivity is generally less than the boundary conductivity values, where the saturated conductivity has no effect. This can also be an indication that smaller values of saturated conductivities would be more appropriate to represent the observed data. The poor results obtained for all soil characteristic relationships show that there is a problem in the model conceptualisation or in the parameter values. The improvement and also the diversity of responses observed when heterogeneity was considered could be an indication that other combinations of parameters are able to provide better results for the simulations.

The representation of matric potentials was not strongly affected by the inclusion of heterogeneity in the hydraulic conductivity. For MACRO's methodology, there is marginal or no improvement in the results when using heterogeneous conditions, except for lysimeter B in event 90129, where a significantly better outcome is provided by the heterogeneous simulation. Simulations using MACRO methodology generally provided poor representations of the matric potentials, with values of the coefficient of determination ranging from -1.9 to 0.77 (mean value:

0.13; standard deviation: 0.67) for homogeneous conditions and from -1.7 to 0.90 (mean value: 0.25; standard deviation: 0.53) for heterogeneous simulations. The use of Brooks-Corey's relationship with a heterogeneous representation led to minor improvements compared to homogeneous conditions (except, again, for lysimeter B in event 90129). The results were generally better than those obtained with MACRO methodology, with values of the coefficient of determination varying from -0.004 to 0.86 (mean value: 0.54; standard deviation: 0.27) for homogeneous conditions and from 0.16 to 0.89 (mean value: 0.65; standard deviation: 0.23) for heterogeneous simulations. When using Van Genuchten's equation, the simulated matric potentials were not significantly affected by heterogeneity in the hydraulic conductivity, presenting slightly better results alternatively for homogeneous or heterogeneous conditions. The coefficient of determination fluctuated between 0.28 and 0.97 (mean value: 0.74; standard deviation: 0.21) for homogeneous conditions and between 0.26 to 0.92 (mean value: 0.72; standard deviation: 0.18) for heterogeneous simulations, suggesting that Van Genuchten's equation provided a better fit for the matric potentials than the other soil characteristic parametric relationships utilised.

Three of these events were chosen to be discussed in detail: rapid flow events 90158 and 91211, and slow flow event 91165. Event 90158 was chosen because, as in event 90230, it presents very dry initial conditions, different pattern of responses for lysimeters A and B, and a steady flow of water from the common reservoir to the lysimeters. Event 91211 was chosen because it presents similar behaviour to the other selected rapid flow events responding to rainfall input (90291, 91017, 91119, and 91198): dry initial conditions (but not as dry as in events 90158 and 90230); matric potentials responding very quickly to the rainfall inputs along the whole soil profile (rising and recessing quickly, except for the top layer, where a quick rise is followed by a slow recession curve); and flow of water out of the lysimeter and into the common reservoir, coincident with the rapid increase of water tensions. Event 91136 is the only rapid flow event which can not be represented by these two, and will be analyzed in section 6.3.1. Event 91165 was chosen as an example of a typical slow flow event: responses to a low rainfall noticeable only for the top tensiometer; constant flow of water from the common reservoir to the lysimeters; and diurnal effects caused by evapotranspiration clearly observed for the whole depth profile. The results of the simulations for these three events compared to the observed bottom inflow and tensiometer data of deep lysimeters A and B at the depths 10 cm, 30 cm and 50 cm are presented in figures 6.1 to 6.6.

An important feature observed for these figures is that Van Genuchten's and Brooks-Corey's simulations show a rise in the matric potentials at the top layer starting immediately

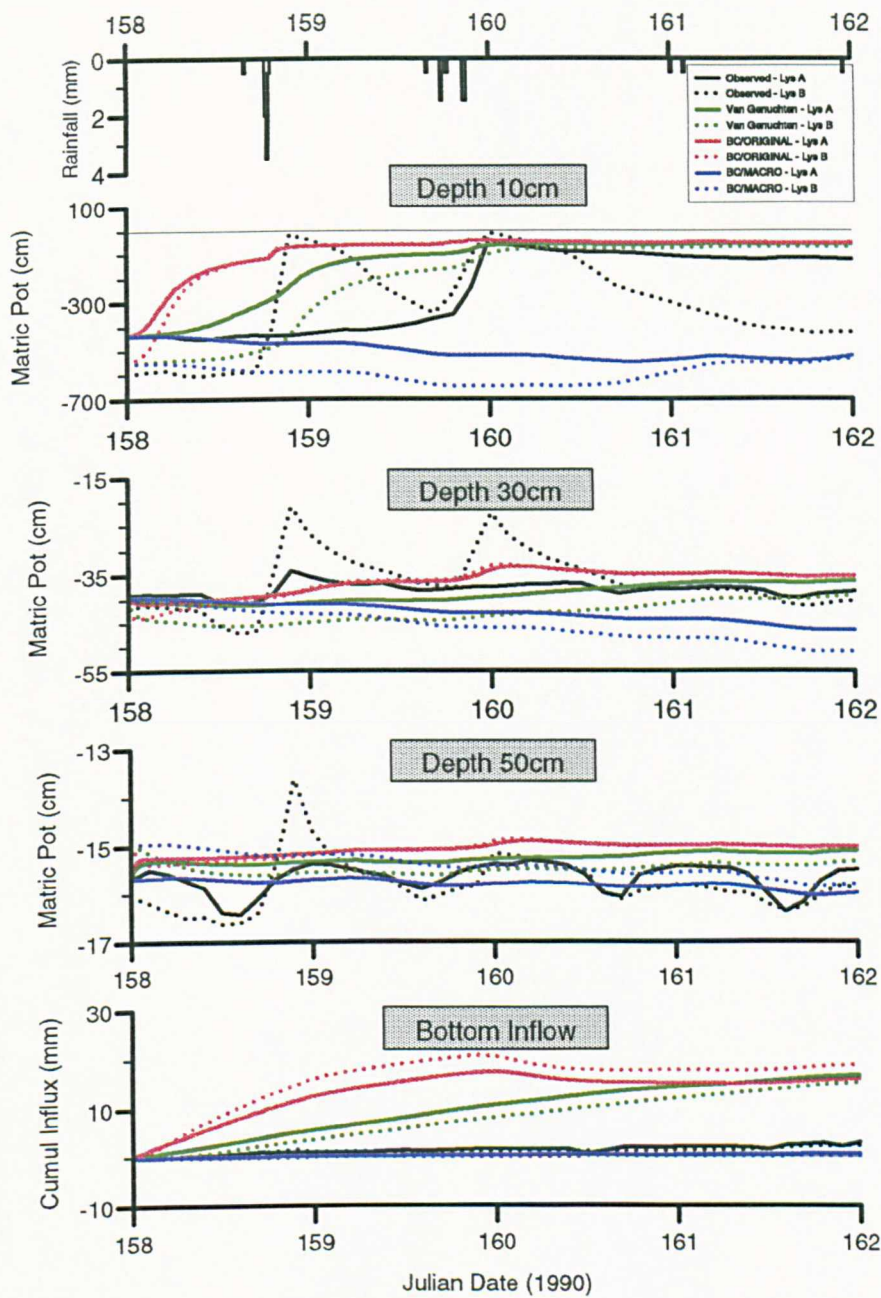


Figure 6.1 - SPW1hyst simulations of event 90158:
non-hysteretic, homogeneous conditions, parameters fitted to observed $\theta(\psi)$ and K_s data

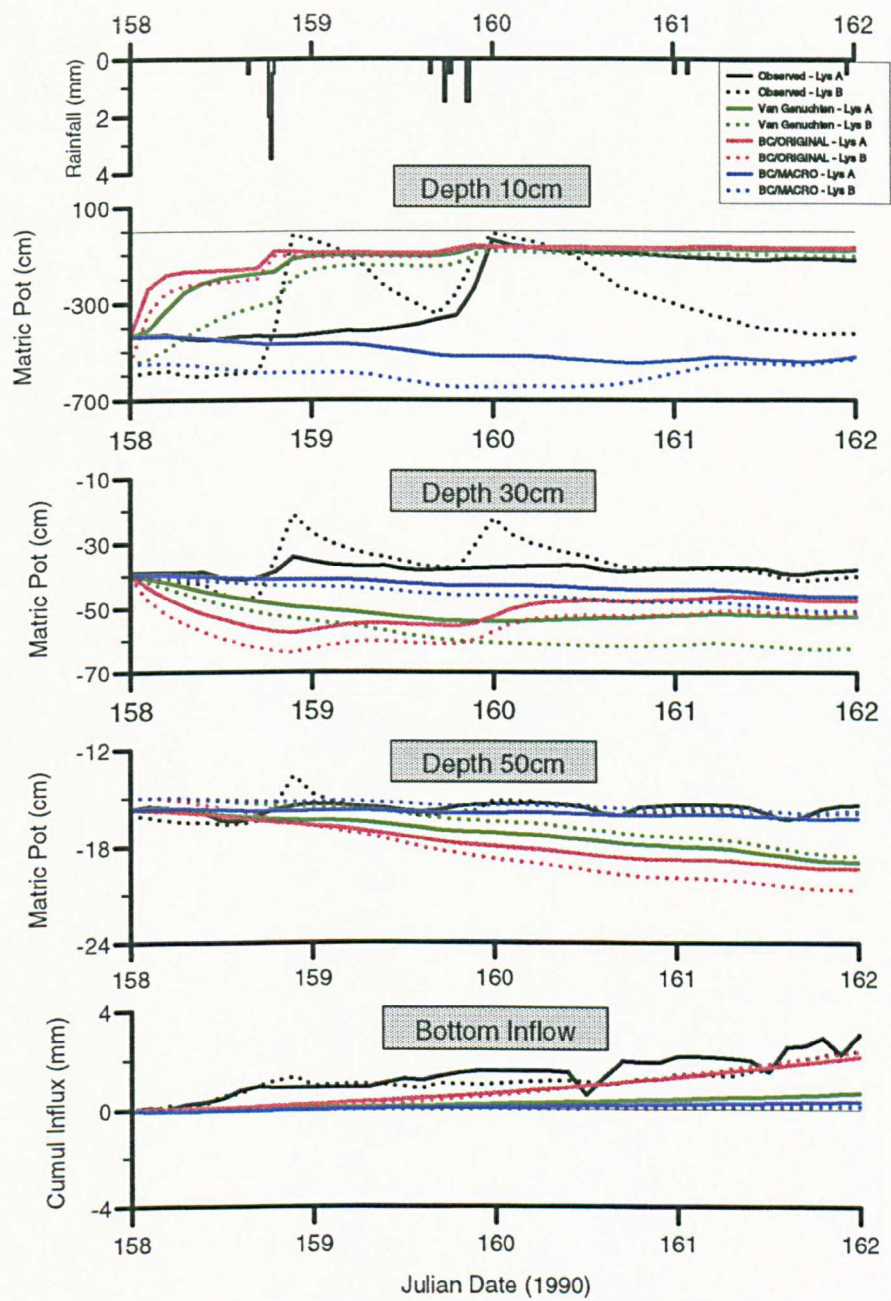


Figure 6.2 - SPWlhyst simulations of event 90158:

non-hysteretic, heterogeneous conditions, parameters fitted to observed $\theta(\psi)$ and K_s data

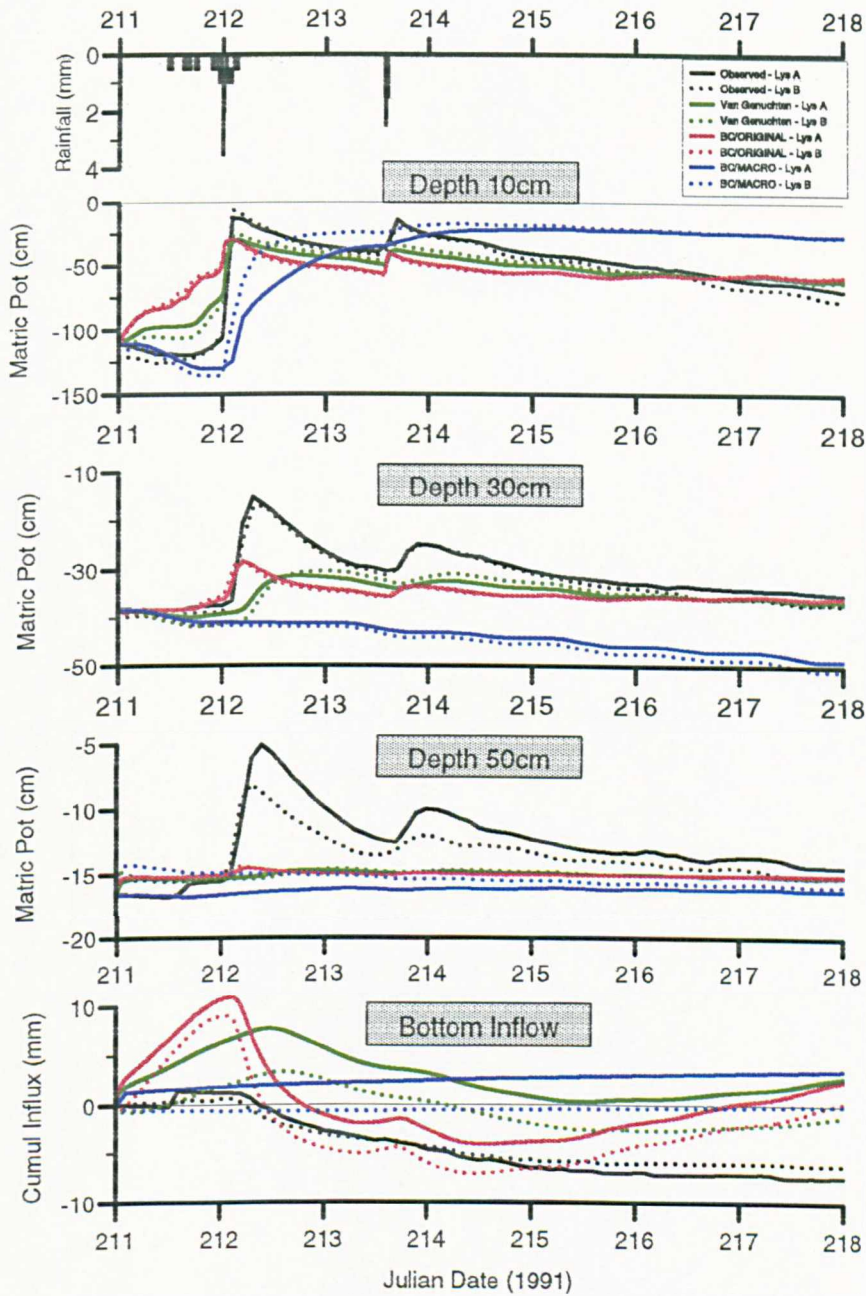


Figure 6.3 - SPW1hyst simulations of event 91211:

non-hysteretic, homogeneous conditions, parameters fitted to observed $\theta(\psi)$ and K_s data

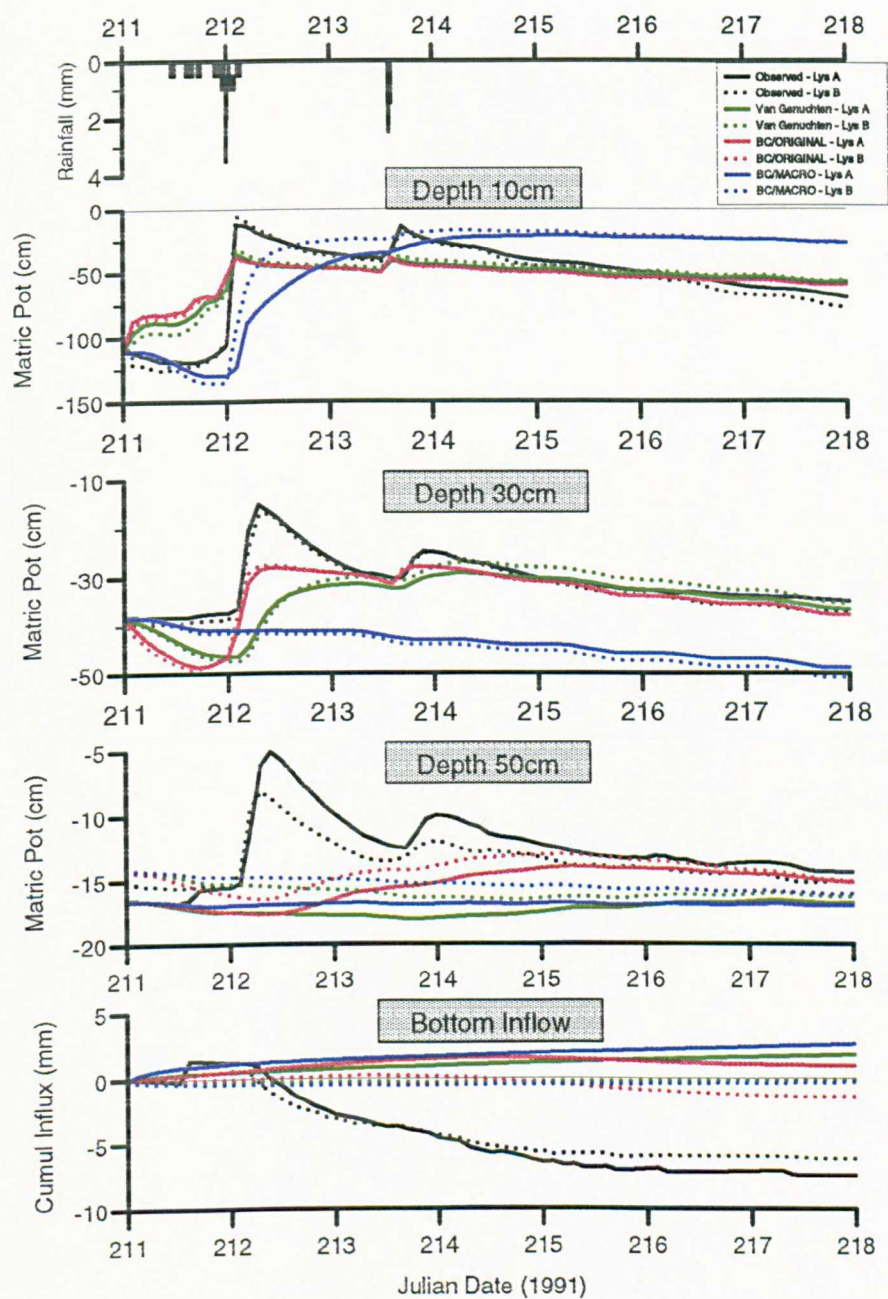


Figure 6.4 - SPW1hyst simulations of event 91211:

non-hysteretic, heterogeneous conditions, parameters fitted to observed $\theta(\psi)$ and K_s data

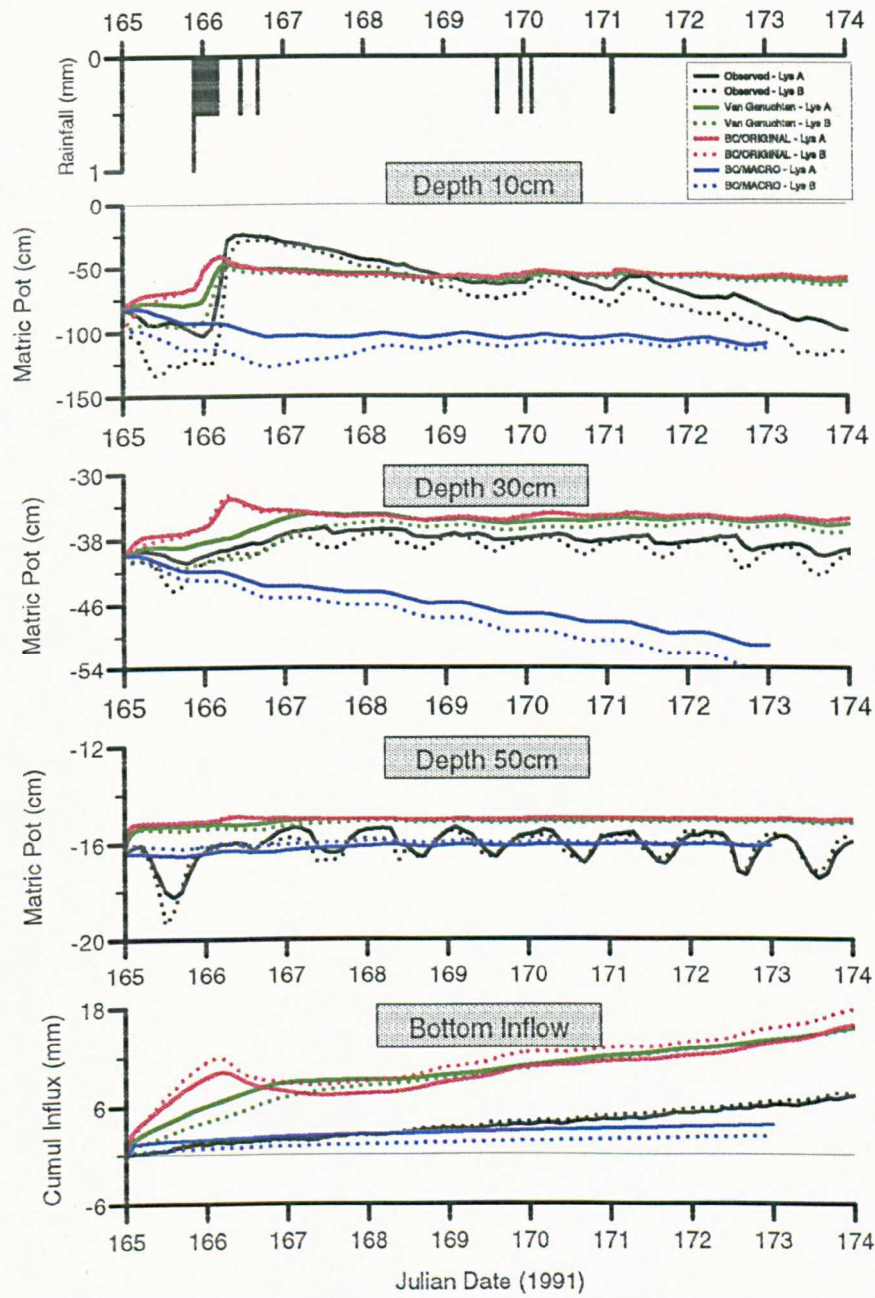


Figure 6.5 - SPWlhyst simulations of event 91165:

non-hysteretic, homogeneous conditions, parameters fitted to observed $\theta(\psi)$ and K_s data

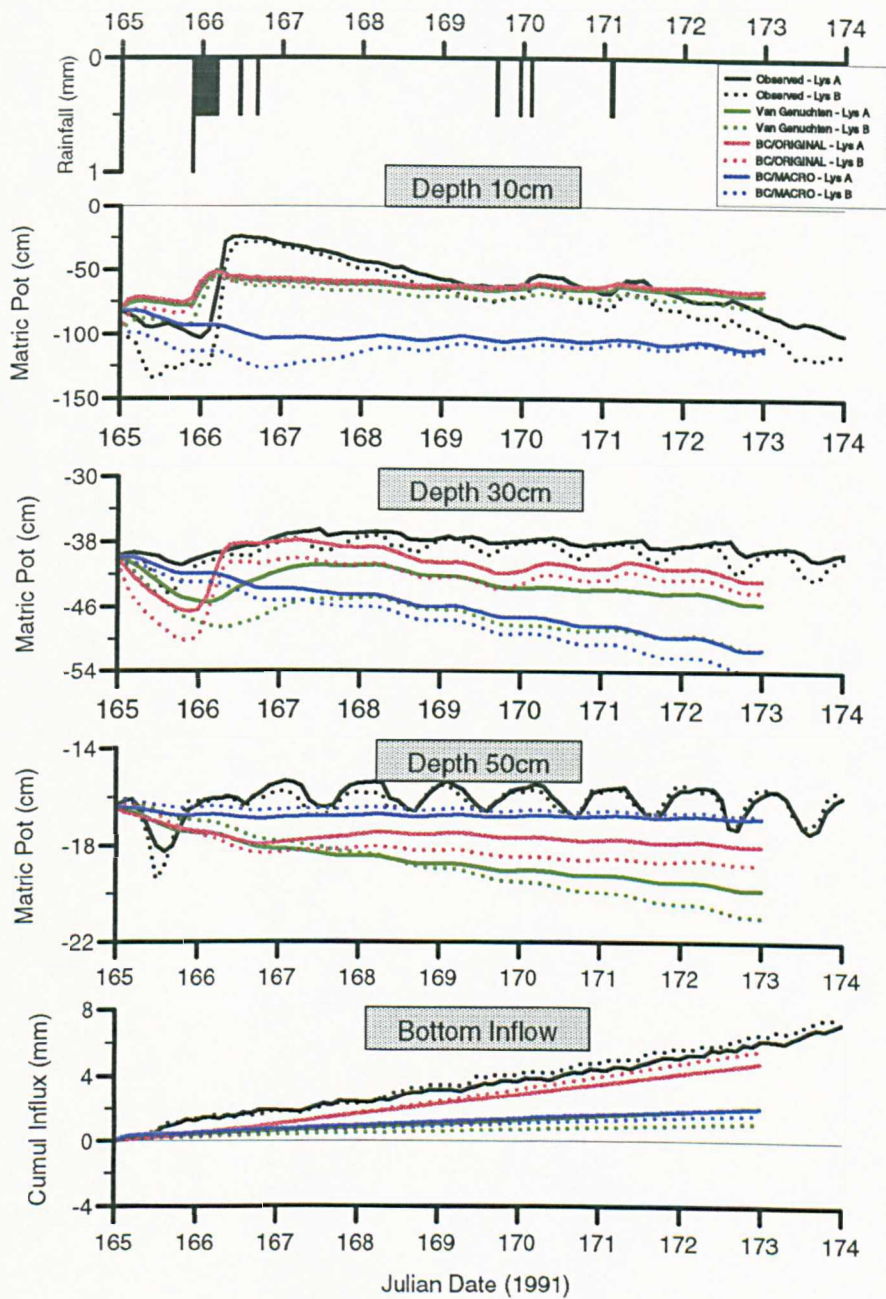


Figure 6.6 - SPW1hyst simulations of event 91165:
non-hysteretic, heterogeneous conditions, parameters fitted to observed $\theta(\psi)$ and K_s data

after the beginning of the simulations, even before any rainfall input. Under homogeneous conditions, this rise is coincident with bottom inflow of water into the lysimeters; under heterogeneous conditions, there is a reduction in the matric potentials at the middle of the profile coinciding with the rise at the top. These responses were caused by the initial conditions, which were obtained from measured data. The soil was not in hydrostatic equilibrium, with higher total potential at deeper layers. The differences in total potential induced movement of water from the bottom to the top of the profile. Under homogeneous conditions, this movement of water in the soil generated the overestimations in inflow from the common reservoir into the lysimeters. Under heterogeneous conditions, the small value of saturated conductivity in the deeper layers brought restrictions to the water movement in this region of the profile. Consequently, the supply of water to the top layers was taken from the middle of the profile, causing a reduction on the matric potentials at these layers, until the beginning of the rainfall. The simulations using MACRO's characteristic curve did not present this behaviour because they were controlled by the low values of the boundary conductivity (0.01 cm/h), which allowed only slow water movement along the soil profile.

As previously commented, the representation of the bottom inflows for simulations of event 90158 using Van Genuchten's or Brooks-Corey's equations presented better results when heterogeneity in the saturated hydraulic conductivity was considered. There is an overestimation under homogeneous conditions and small underestimation for the heterogeneous simulations. When MACRO's methodology was adopted, the results were slightly worse for heterogeneous conditions. Figure 6.1 shows that MACRO's simulation managed to provide a much closer representation to the observed data when using homogeneous conditions than the other two characteristic curves. A comparison of the bottom inflows in figures 6.1 and 6.2 reveals that the heterogeneous conditions led to Van Genuchten's simulations (green lines) with results very close to those using MACRO's characteristic curve (blue lines). Brooks-Corey's simulations (red lines) for heterogeneous saturated hydraulic conductivities present the best results, with a very good fit to the observed data for the last third part of the event. As MACRO's simulations were not improved by heterogeneity, it seems that they gave reasonably good results because they were actually controlled by the boundary conductivity instead of the saturated conductivity values. This suggests that the reason for the amelioration of results with heterogeneous conditions for Van Genuchten's and Brooks-Corey's representations could be rather due to the reduction in the saturated conductivity in the deeper layers than because of its heterogeneity.

A comparison of matric potential representations in figures 6.1 and 6.2 demonstrates that results using MACRO's characteristic curve were insensitive to the changes in the saturated conductivity values, while Van Genuchten's and Brooks-Corey's representations were actually worsened by heterogeneous conditions for middle and deep layers, as a consequence of the

initial conditions, as commented above. Also, the simulations of the top layer completely failed to represent the observed data in the first half of the event (up to the end of day 90160). These results reinforce the hypothesis that, in order to simulate these rapid flow events, there is a problem in the model conceptualisation or in the parameter values and that other combinations of parameters and processes should be tried.

Figures 6.3 and 6.4 show the simulation results for event 91211. The results of bottom inflow are better for homogeneous conditions, as they managed to represent the general observed shape of response, but overestimated the real values, while the heterogeneous simulations produced a very flat (and still overestimative) response. This qualitative difference in responses was not properly represented by the R^2 estimates because this statistic stresses the deviations between observed and simulated values by considering the square value of these differences and, consequently, can miss important features, as an amelioration in the shape of response. The matric potential simulations were better represented by the heterogeneous conditions, using Van Genuchten or Brooks-Corey, in the final half of the event (after the last important rainfall input, on day 91213) specially for the middle and deep layers. Before that, the homogeneous simulations better succeed in representing the observed data, mainly for the shapes at middle and deep layers. Matric potential representations for MACRO's methodology were not significantly affected by the changes in the saturated conductivity values. Again, the effect of the initial conditions helps to explain these diverse behaviours. As commented above, the differences in total potential in the beginning of the simulations induced water flow in the soil from the bottom to the top of the profile. Both the overestimation in bottom inflow under homogeneous condition, and the representation of matric potentials, under heterogeneous conditions, at the middle of the profile before day 91213 were caused by this soil water movement. The MACRO simulations presented similar results for the matric potentials under homogeneous and heterogeneous conditions because they were mostly controlled by the boundary conductivity. These observations again suggest that other combinations of parameters and processes should be tried in order to better represent the observed rapid flow events.

For event 91165 (figures 6.5 and 6.6), there is a significant improvement in the results for the bottom inflow under heterogeneous conditions when using Van Genuchten's or Brooks-Corey's soil characteristic relationships, as the homogeneous conditions produced overestimated responses, while the heterogeneous gave slightly underestimates. Simulations using MACRO's methodology showed only small differences between homogeneous and heterogeneous representations, with both results being similar to those observed for the simulations under heterogeneous conditions using the other two characteristic equations. As for event 90158,

Brooks-Corey's simulations under heterogeneous saturated hydraulic conductivities presented the best results for the bottom inflow.

The representation of matric potentials of event 91165 when using MACRO's methodology was only marginally affected by the inclusion of heterogeneity in the hydraulic conductivity. For Brooks-Corey's and Van Genuchten's relationships, the results for the top layer were not significantly affected by heterogeneity. For the middle and bottom layers, the homogeneous representation led to overestimates and the heterogeneous simulations provided underestimates, but none of them is clearly better than the other. The results can be considered reasonably good, as the main shapes of response were reproduced and the deviations between observed and simulated values were small. The initial conditions again can help to explain the differences, but their influence was reduced because the total potential variation along the soil profile in the beginning of the event is much smaller than in the previous events.

The results obtained for the simulations of event 91165 suggest that SPW1hyst can properly represent slow flow events, when initial conditions are close to hydrostatic equilibrium. However, the bottom inflow results with and without heterogeneity in the saturated conductivities presented similar features to those already commented for the other two events, which, again, can justify a search for other combinations of parameters and processes in order to obtain a better representation of the observations. The differences between observed and simulated values, although small, reinforce this hypothesis.

6.3 - A numerical study of the effects of hysteresis and air entrapment

The results presented in section 6.2 justify the need to consider other combinations of parameters and processes than those obtained from observed $\theta(\psi)$ and K_s data, in order to better represent the events observed at the experimental station. The successive cycles of wetting and drainage naturally occurring in the lysimeters suggest the necessity of taking into account the hysteretic nature of the hydraulic properties of the soil. A methodology for simulating air entrapment and hysteresis effects in the soil characteristic curve, described in chapter 3, was already adapted and tested in order to run in conjunction with the original SPW1 model, constituting model SPW1hyst.

In the next sections, the significance of hysteresis is investigated through the application of SPW1hyst, in both hysteretic and non-hysteretic modes, to event 91136, where injection of a relatively small volume of water below the water table was observed to generate a significant

perturbation of soil water states, which could not be explained by a non-hysteretic single porosity soil-plant-water model such as SPW1.

6.3.1 - Event 91136: re-dosing of the lysimeters (an unscheduled water table rise)

As already commented in chapter 4, event 91136 presents a fundamental difference from the others, which is that the hydraulic perturbation was caused by water added through the base of the lysimeters, instead of being a response to rainfall input. During the first radiochemical re-dosing of the lysimeters (16-17 May 1991 - Julian date: 91136-91137), the addition of 3 litres of water through the base of the lysimeters over a 2 hours period caused a sharp rise in the lower tensiometers of all four instrumented lysimeters, followed by a less rapid fall back to the original values. The lowest tensiometer readings suggest water table rises of 16.3, 21.8, 9.2 and 12.4 cm for lysimeters A, B, C and D, respectively. The very sensitive responses in all lysimeters, with an apparent water table rise of up to 21.8 cm (for lysimeter B), can not be explained by treating the soil as a uniform porous medium, strongly suggesting preferential flow mechanisms.

In order to analyze the effects of the water table response, model simulations were undertaken for both hysteretic and non-hysteretic conditions. As in section 6.2, a grid of 35 elements with fixed thickness of 2 cm was adopted, and SPW1hyst was run taking into account root uptake in response to imposed hourly evapotranspiration rates, obtained from daily totals computed using the Penman model. Rainfall information was provided by the automatic weather station located at the experimental station. Model SPW1hyst was run under non-hysteretic conditions using Van Genuchten's moisture retention curve with the parameters fitted using observed $\theta(\psi)$ and K_s data for lysimeter B (table 6.1) and Mualem's unsaturated hydraulic conductivity curve, with saturated conductivity of 6 cm/h. The soil was assumed to be initially in hydrostatic equilibrium for a water table located 5 cm above the base of the lysimeter and the lower boundary conditions were derived from information available from the re-dosing, taking the form of 5 distinct phases, as presented in table 6.3. For the hysteretic simulation, a new set of characteristic curves was selected. These were obtained by adopting the fitted parameters as those of the main drying curve, and defining the wetting curve by decreasing the value of its maximum moisture content, and thus introducing air entrapment into the system. The hypothesis for this representation is that, as the water was introduced relatively quickly into the system, it rose through preferential path flows, causing the entrapment of air. The main wetting curve presents maximum moisture content (θ_w) equal to $0.20 \text{ m}^3/\text{m}^3$, which represents a reduction of over 50% of the original saturated moisture content. These curves are presented in figure 6.7.

Table 6.3 - Lower boundary conditions for simulations of event 91136

Julian Date		Boundary Condition	
Start time	End Time	Type	Value
136.30	136.40	Flux	+0.0 cm/min
136.40	136.48	Flux	+0.0010483 cm/min
136.48	136.49	Flux	+0.004193 cm/min
136.49	136.57	Flux	+0.0 cm/min
136.57	136.90	Pressure	+5.0 cm

When analyzing this same event, Butler (1991b) tested the hypothesis of by-pass or preferential flow mechanisms by using a non-hysteretic simulation and increasing the boundary fluxes by a scaling factor of 7.5 (i.e. the total volume of water added to the lysimeter during redosing became 22.5 litres). This would be similar to flushing the original 3 litres of water through a much smaller area, equivalent to that of the preferential pathways.

Figure 6.8 shows the results of SPW1hyst simulations under non-hysteretic conditions, with original and scaled boundary fluxes, compared to hysteretic conditions and the observed data. The results obtained with the original boundary fluxes for non-hysteretic conditions showed changes in the simulated matric potentials that were substantially less than those observed. The maximum rise of the simulated water table, 2.5 cm, was about a tenth of the observed data. With the consideration of hysteresis and air entrapment, the simulation presented results remarkably similar to both observed data and non-hysteretic simulations using the scaled boundary fluxes, with good agreement in both the overall shape and magnitude of the matric potential responses. The only major discrepancy that can be noticed is that the hysteretic simulation shows a more rapid fall in the matric potentials at the beginning of the last phase of the event. This was due to the fact that this phase marks a sudden change of simulated boundary condition type from flux zero to a fixed pressure, when, in reality, this change is not as immediate. The non-hysteretic simulation presented a slower fall because there was much more water available in the simulated system, as the volumes had been increased by a factor of 7.5.

These results seem to confirm the existence of preferential flow paths during the event. As the substrate solution was introduced, the water rose through these preferential path flows, causing the entrapment of air, that was represented by lowering the main wetting curve, or by increasing the volume of water added to the lysimeter.

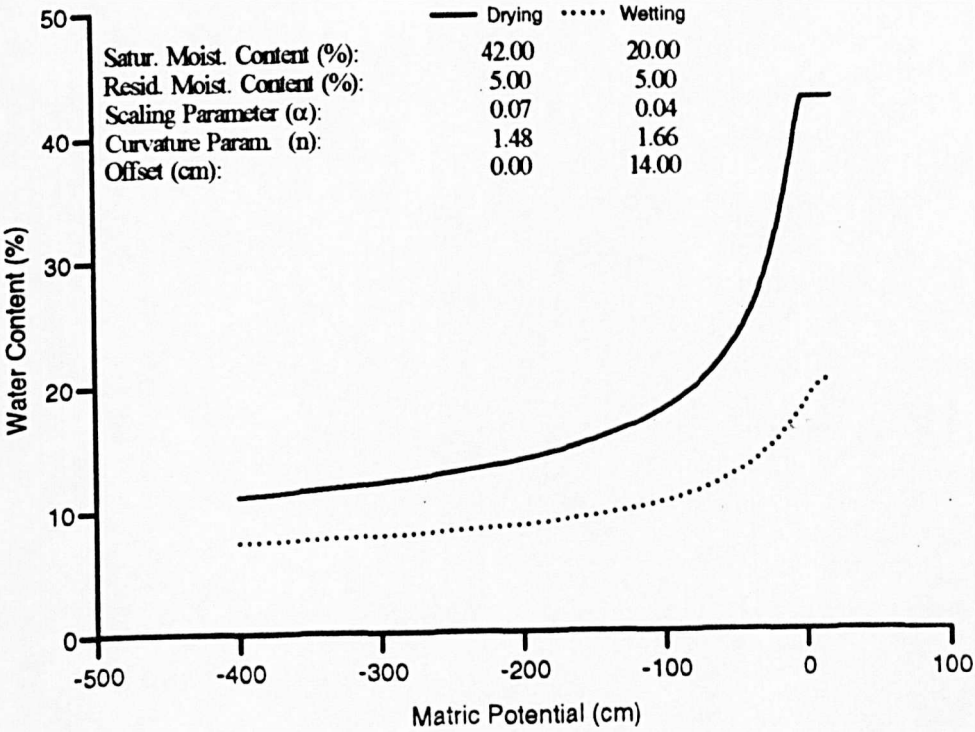


Figure 6.7 - Main characteristic curves for hysteretic simulation of event 91136

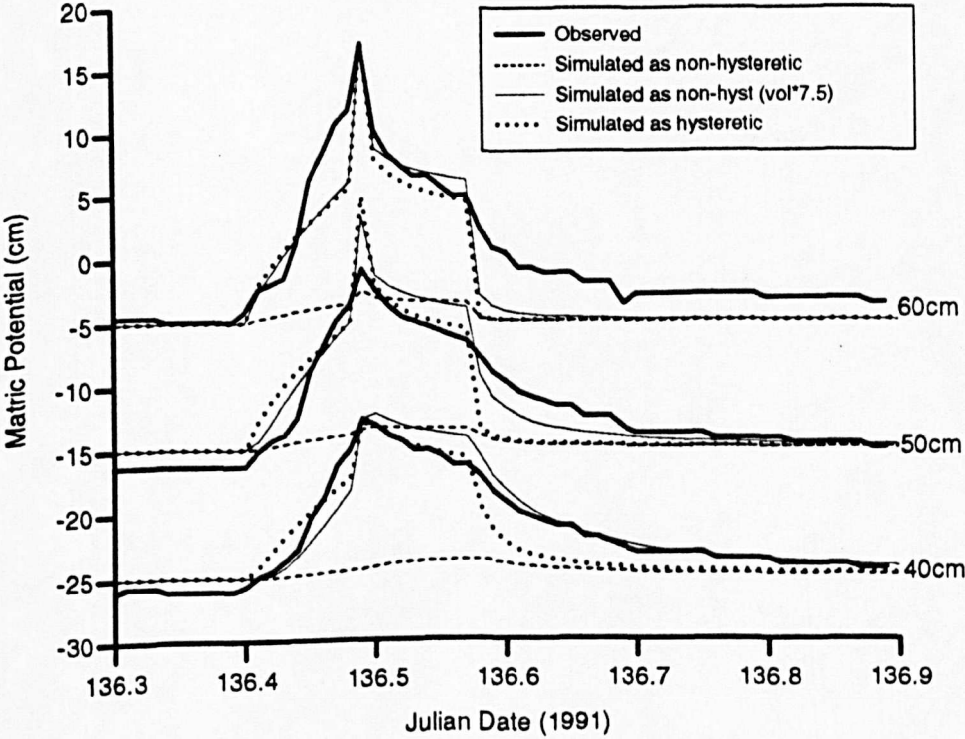


Figure 6.8 - SPWlhyst simulations of event 91136 using curves as presented in figure 6.7

6.3.2 - Application of the parameters fitted for event 91136 to the other selected events

The same set of parameters adopted in section 6.3.1 for the hysteretic simulation of event 91136 is now applied to the other selected events. This is to verify the validity of the hysteretic representation but also to test if this particular set of parameters is able to represent hysteretic conditions in any event or if it is a combination of parameters valid only for the conditions observed for event 91136.

The general conditions and driving variables necessary for the simulations were the same as adopted for the non-hysteretic simulations using parameters fitted to observed $\theta(\psi)$ and K_s data (section 6.2), employing Van Genuchten's soil characteristic parametric relationship: a grid of 35 elements with fixed thickness of 2 cm; initial conditions obtained by fitting polynomial approximations to the measured data from the tensiometers; Mualem's unsaturated hydraulic conductivity; evapotranspiration rates obtained from daily totals computed using the Penman model; root density profile represented by an exponential distribution; lower boundary condition of a fixed pressure of 5 cm above the base; and rainfall information provided by the automatic weather station located at the experimental station.

The statistics summarising the results of the hysteretic simulations compared to the non-hysteretic results obtained using Van Genuchten's equation are presented in table 6.4.

The hysteretic simulations of the selected events using the parameters fitted for event 91136 showed significant improvement in the representation of bottom inflows for almost all events (except for event 90291 and for lysimeter B in event 90230) when compared to the original homogeneous non-hysteretic simulations. These results were accompanied by slight worsening of the results for the matric potentials, for all events except for event 91204 and for lysimeter A in event 91017. These outcomes seem to indicate that air entrapment and hysteresis in the soil characteristic curve can be used to explain part of the observed variations in the bottom inflows that can not be represented by the original model, but has minor influence for matric potentials.

A comparison with the heterogeneous non-hysteretic simulations shows that the coefficients of determination for the bottom inflows of the hysteretic simulations were generally smaller than those provided by the inclusion of heterogeneity (except for event 91119, for lysimeter A in event 90291, and for lysimeter B in events 91017 and 90129). When comparing matric potential outcomes, events 91119, 91198, 91211, and lysimeter A in events 91165 and

91204 showed better representation by the hysteretic simulations, although the mean values present slightly higher estimates for the heterogeneous non-hysteretic simulations. These results suggest that other combinations of parameters and processes than hysteretic simulations using parameters fitted for event 91136 should be tested.

Table 6.4 - Hysteretic SPW1hyst simulations using parameters fitted for event 91136

Event			Lys	Non-hysteretic				Hysteretic	
				Homogeneous		Heterogeneous		Homogeneous	
				R ² (p)	R ² (f)	R ² (p)	R ² (f)	R ² (p)	R ² (f)
RAPID FLOW	90158	A	0.69	-156	0.51	-1.8	0.42	-27	
		B	0.59	-210	0.63	-3.1	0.51	-39	
	90230	A	0.29	-31	0.26	0.47	0.17	-7.8	
		B	0.28	0.46	0.36	-3.0	0.17	-5.7	
	90291	A	0.79	0.73	0.84	-3.2	0.77	0.33	
		B	0.84	-0.3	0.73	-2.8	0.62	-4.3	
	91017	A	0.53	-0.9	0.70	0.02	0.61	-0.9	
		B	0.53	0.84	0.75	-2.9	0.52	0.88	
	91119	A	0.86	-1.3	0.76	-2.7	0.80	0.94	
		B	0.77	0.32	0.71	-2.1	0.75	0.93	
	91198	A	0.90	-480	0.78	0.73	0.85	-26	
		B	0.92	-46	0.86	-1.4	0.89	-42	
	91211	A	0.88	-4.9	0.82	-3.4	0.87	-0.3	
		B	0.92	-1.7	0.86	-2.4	0.91	0.76	
	$\bar{x}$ s	A	0.71	-96	0.67	-1.4	0.64	-8.7	
			0.22	178	0.21	1.73	0.26	13	
$\bar{x}$ s	B	0.69	-37	0.70	-2.5	0.62	-13		
		0.24	78	0.17	0.61	0.26	19		
SLOW FLOW	90129	A	0.49	-24	0.48	-2.5	0.34	-4.1	
		B	0.46	-10	0.47	-7.7	0.19	-0.1	
	91108	A	0.83	-131	0.80	0.58	0.75	-25	
		B	0.66	-81	0.70	-1.7	0.61	-39	
	91165	A	0.91	-17	0.86	-1.0	0.89	-6.7	
		B	0.87	-10	0.84	-2.0	0.83	-6.0	
	91204	A	0.90	-146	0.89	-0.6	0.92	-97	
		B	0.91	-23	0.92	-2.3	0.91	-20	
	$\bar{x}$ s	A	0.78	-80	0.74	-2.1	0.73	-33	
			0.20	69	0.19	0.35	0.27	44	
	$\bar{x}$ s	B	0.73	-31	0.73	-3.4	0.64	-16	
			0.21	34	0.20	2.86	0.32	17	

$R^2(p)$ = Coefficient of determination for the fit of simulated and observed matric potentials

$R^2(f)$ = Coefficient of determination for the fit of simulated and observed bottom inflow

$\bar{x}$ = mean value

s = standard deviation

Obs.: Simulations using Van Genuchten's soil characteristic curve

Homogeneous or heterogeneous conditions refer to saturated hydraulic conductivity values

6.4 - Parameter optimisation per event

The results presented in sections 6.2 and 6.3 suggest that the use of heterogeneity in the saturated hydraulic conductivity and hysteresis in the soil characteristic curve can help to improve the representation of the observed events at Imperial College's lysimeter experiment at Silwood Park. However, they also give indications that there is still the need to consider other combinations of parameters and processes than those already tested.

In the following sections, a methodology for optimising SPW1hyst parameters per event is described and applied to the selected events, for homogeneous and heterogeneous conditions, hysteretic and non-hysteretic simulations. The methodology is employed using Van Genuchten's and Brooks-Corey's equations only, as MACRO methodology showed to be controlled by the boundary hydraulic conductivity value. MACRO simulations will be discussed in chapter 7.

6.4.1 - Methodology for parameter optimisation

The issue of estimating parameters in soil hydraulic property models was already addressed in chapter 5. In section 5.3 a methodology for estimation of parameter values based on first-order error analysis was presented and applied to the available $\theta(\psi)$ data. The main principles described in chapter 5 are now applied to the determination of set of parameters optimising the error between simulated and observed matric potentials and bottom inflow, for each of the selected events.

An optimisation program was developed in a FORTRAN code in order to obtain the minimum of an objective function through the use of NAG (Numerical Algorithms Group, 1987) routine E04CCF or E04JAF. As already described in chapter 5, routine E04CCF minimises a general function $F(x)$ of m independent variables by the Simplex method. Routine E04JAF uses a quasi-Newton method for finding a minimum of a function $F(x)$, subject to fixed upper and lower bounds on the independent variables $x_1, x_2, \dots, x_m$, using functions values only.

The optimisation program is set so that the objective function to be minimised can be the quadratic error, the absolute error or the difference of reciprocals between observed and simulated values. The observed values to account for the objective function evaluation can be the matric potential, the boundary influx or both simultaneously. When both sets of observed values are considered simultaneously, the errors for each of them are non-dimensionalised by its respective mean, and the objective function is obtained as a mean value of these non-

dimensionalised errors. The observed values to account for in the optimisation, the parameters to be optimised, and initial values for all parameters are given as input, together with lower and upper bounds for all optimised parameters. Any combination of parameters can be used for optimisation. At each iteration, the optimisation program runs the SPW1hyst model, computes the objective function and selects the next iteration values of the parameters being optimised, until a maximum number of iterations or the conditions for a minimum are reached. If the SPW1hyst simulation fails for a combination of parameters, the tolerances of the model (error tolerance and reversal point tolerance) are increased and SPW1hyst is run again, for the same combination of parameters. This procedure is repeated until the simulation succeeds or the maximum limits of the tolerances (fixed as inputs) are reached. The tolerances are reset to their initial values, and a new set of parameters is tested. If the simulation fails even at the maximum tolerance levels, the objective function value is set as 9999. The output of the program, for the optimised set of parameters, are the value of all parameters (with an indication if they were optimised or not) and their lower and upper bounds, the objective function results and the coefficient of determination, both for matric potentials and for bottom influx, and the simulated values of boundary inflow and matric potential. The values of the tolerances adopted for each successful iteration are also provided.

6.4.2 - Application to selected events and discussion of results

After testing the three available objective functions, the quadratic error was selected, and the optimisation model was run, for each event, choosing several different combinations of parameters to be optimised, in hysteretic or non-hysteretic mode, homogeneous or heterogeneous conditions. The heterogeneous mode was optimised by fitting the saturated hydraulic conductivity at depths 0 to 25 cm, 25 to 50 cm, and 50 to 70 cm as three independent parameters. The number of parameters to be optimised at each run was kept small (generally less than 4), in order to facilitate the interpretation of each parameter's effects in the simulations, and also to avoid excessively long times of simulation. The lower and upper bounds adopted for the optimisations are presented in table 6.5.

The response surface of the optimisation function was revealed to be very flat, with several local minima. Consequently, different 'optimum' conditions could be found for different initial values of the parameters, as the optimisation routines frequently were not able to find a global minimum. For this reason, for each test, the model was run, for both Simplex and quasi-Newton optimisation routines, using various different sets of initial values for the parameters, and the best result was adopted as minimum value. It is important to emphasise that this

procedure does not guarantee that the solution found is the global minimum.

Table 6.5 - Bounds for the optimisations

Equation	Parameter	Lower value	Upper value
Van Genuchten's soil characteristic	α (1/cm)	0.01	0.50
	n (-)	1.00	3.00
	θ_r (cm ³ /cm ³)	0.01	0.10
	θ_s (cm ³ /cm ³)	0.20	0.60
Brooks-Corey's soil characteristic	λ (-)	0.01	0.90
	θ_r (cm ³ /cm ³)	0.01	0.10
	θ_s (cm ³ /cm ³)	0.20	0.60
	P_b (cm)	-50.0	0.00
Mualem's conductivity curve	Ks (cm/h)	0.01	99.0

6.4.2.1 - Non-hysteretic simulations

The optimisation model was applied to the selected events in non-hysteretic mode, for both homogeneous and heterogeneous conditions, using different combinations of optimised parameters, and accounting separately matric potential or boundary influx for the objective function evaluation. The results for each event are presented in Appendix VI, tables VI.1 to VI.12. For the great majority of the simulations, when matric potentials were optimised, the fit between observed and simulated bottom influx was very poor; when the bottom influx was optimised, some simulations produced reasonable and even good fit (sometimes with R^2 bigger than 0.9) between observed and simulated matric potentials. For this reason, simultaneous optimisations of matric potentials and bottom influx were performed. The results for each event are presented in Appendix VI, tables VI.13 to VI.24. The mean values and standard deviations of these results are summarised in table 6.6, for the selected rapid flow events, and in table 6.7, for the selected slow flow events.

The mean values of the coefficients of determination for homogeneous conditions, both for rapid and slow flow events, show clear improvement when compared to the original non-hysteretic homogeneous SPW1hyst simulations using parameters fitted to observed $\theta(\psi)$ and Ks data (table 6.2). The means of the means $R^2(p)$ showed on table 6.6 for non-hysteretic homogeneous simulations of the selected rapid flow events are 0.77 for lysimeter A and 0.64 for lysimeter B; the means of the means $R^2(f)$ for the same conditions are -1.3 for lysimeter A and -2.4 for lysimeter B. These values not only compare favourably with the homogeneous results of table 6.2 but are also very similar to those obtained for original non-hysteretic heterogeneous simulations. The results for non-hysteretic homogeneous optimisations of the slow

Table 6.6 - SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Means and standard dev. from non-hysteretic simulations of selected rapid flow events

Simulation	L	S	Optimised parameters							$R^2(p)$	$R^2(f)$
			α 1/cm	n -	λ -	ψ_b cm	Ks_1 cm/h	Ks_2 cm/h	Ks_3 cm/h		
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	4.67	4.67	4.67	0.70	-0.3
		s	*	*	*	*	5.46	5.46	5.46	0.14	1.77
		x	*	*	*	*	9.34	9.34	9.34	0.54	0.53
	B	s	*	*	*	*	7.22	7.22	7.22	0.26	0.55
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
	V2	A	0.15	1.25	*	*	*	*	*	0.79	0.75
		s	0.16	0.25	*	*	*	*	*	0.28	0.33
		x	0.08	1.18	*	*	*	*	*	0.70	0.76
	B	s	0.02	0.14	*	*	*	*	*	0.24	0.19
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
	V3	A	0.13	1.32	*	*	10.20	10.20	10.20	0.90	0.76
		s	0.07	0.35	*	*	6.65	6.65	6.65	0.03	0.30
		x	0.11	1.23	*	*	16.57	16.57	16.57	0.71	0.78
	B	s	0.06	0.20	*	*	12.86	12.86	12.86	0.23	0.19
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
	B1	A	*	*	*	*	1.39	1.39	1.39	0.72	0.10
		s	*	*	*	*	1.62	1.62	1.62	0.18	1.07
		x	*	*	*	*	1.72	1.72	1.72	0.54	0.57
	B	s	*	*	*	*	1.18	1.18	1.18	0.26	0.50
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
	B1A	A	*	*	0.63	*	*	*	*	0.61	-14
		s	*	*	0.40	*	*	*	*	0.24	31
		x	*	*	0.83	*	*	*	*	0.63	-24
	B	s	*	*	0.11	*	*	*	*	0.24	61
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
	B2	A	*	*	0.21	*	0.45	0.45	0.45	0.88	0.87
		s	*	*	0.20	*	0.74	0.74	0.74	0.07	0.09
		x	*	*	0.48	*	2.64	2.64	2.64	0.64	0.76
	B	s	*	*	0.33	*	2.84	2.84	2.84	0.24	0.22
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
	B2A	A	*	*	0.24	-1.99	*	*	*	0.79	0.71
		s	*	*	0.20	1.77	*	*	*	0.30	0.40
		x	*	*	0.43	-4.50	*	*	*	0.71	0.53
	B	s	*	*	0.34	3.36	*	*	*	0.26	0.39
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
	B3	A	*	*	0.39	8.72	20.53	20.53	20.53	0.79	0.79
		s	*	*	0.22	10.50	25.52	25.52	25.52	0.20	0.14
		x	*	*	0.56	6.24	6.98	6.98	6.98	0.64	0.75
	B	s	*	*	0.14	2.88	4.71	4.71	4.71	0.27	0.22
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
NON-HYST HETERO	V3	A	*	*	*	*	13.15	3.15	0.14	0.75	-0.4
		s	*	*	*	*	16.09	2.98	0.19	0.20	1.80
		x	*	*	*	*	31.44	12.85	1.59	0.57	0.69
	B	s	*	*	*	*	22.09	14.26	1.22	0.19	0.29
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
	V5	A	0.07	1.63	*	*	10.74	2.12	0.07	0.75	-0.3
		s	0.04	0.26	*	*	8.54	2.79	0.12	0.22	1.70
		x	0.05	2.00	*	*	24.92	5.96	0.31	0.64	0.62
	B	s	0.03	0.65	*	*	36.08	9.21	0.23	0.27	0.30
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
	B3	A	*	*	*	*	21.02	1.39	0.27	0.71	0.33
		s	*	*	*	*	26.63	1.38	0.44	0.19	0.79
		x	*	*	*	*	26.77	1.20	0.52	0.55	0.67
	B	s	*	*	*	*	25.13	0.72	0.70	0.22	0.35
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*
	B5	A	*	*	0.35	-13.63	26.57	1.68	0.17	0.75	0.87
		s	*	*	0.19	14.36	37.93	1.98	0.31	0.18	0.14
		x	*	*	0.25	-8.77	15.86	0.76	0.17	0.59	0.75
	B	s	*	*	0.17	4.38	18.21	0.38	0.11	0.22	0.27
		x	*	*	*	*	*	*	*	*	*
		s	*	*	*	*	*	*	*	*	*

$R^2(p)$ = Coef of Determination for matric potentials;

* = parameter not optimised;

Obs.: Events 91136 and 91198 (outliers) not considered

$R^2(f)$ = Coef of Determination for bottom inflow;

Sta = statistics: $\bar{x}$ = mean value; s = standard deviation

Table 6.7 - SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Means and standard dev. from non-hysteretic simulations of selected slow flow events

Simulation		L y s	S t a	Optimised parameters						R ² (p)	R ² (f)	
				α 1/cm	n	λ	Ψ_b cm	Ks ₁ cm/h	Ks ₂ cm/h			Ks ₃ cm/h
NON-HYST HOMOGENEOUS	V1	A	$\bar{x}$	*	*	*	*	0.38	0.38	0.38	0.51	0.86
		A	s	*	*	*	*	0.43	0.43	0.43	0.55	0.13
		B	$\bar{x}$	*	*	*	*	1.15	1.15	1.15	0.79	0.41
		B	s	*	*	*	*	1.11	1.11	1.11	0.07	1.14
	V2	A	$\bar{x}$	0.14	1.27	*	*	*	*	*	0.84	0.90
		A	s	0.05	0.18	*	*	*	*	*	0.12	0.13
		B	$\bar{x}$	0.14	1.20	*	*	*	*	*	0.73	0.97
		B	s	0.06	0.14	*	*	*	*	*	0.25	0.04
	V3	A	$\bar{x}$	0.09	1.31	*	*	2.66	2.66	2.66	0.88	0.92
		A	s	0.02	0.26	*	*	2.80	2.80	2.80	0.09	0.10
		B	$\bar{x}$	0.13	1.53	*	*	5.27	5.27	5.27	0.88	0.92
		B	s	0.08	0.45	*	*	3.63	3.63	3.63	0.09	0.14
	B1	A	$\bar{x}$	*	*	*	*	0.15	0.15	0.15	0.53	0.89
		A	s	*	*	*	*	0.17	0.17	0.17	0.49	0.11
		B	$\bar{x}$	*	*	*	*	0.20	0.20	0.20	0.78	0.58
		B	s	*	*	*	*	0.19	0.19	0.19	0.07	0.79
	B1A	A	$\bar{x}$	*	*	0.47	*	*	*	*	0.74	-29
		A	s	*	*	0.50	*	*	*	*	0.13	38
		B	$\bar{x}$	*	*	0.69	*	*	*	*	0.63	-24
		B	s	*	*	0.42	*	*	*	*	0.24	31
	B2	A	$\bar{x}$	*	*	0.37	*	0.16	0.16	0.16	0.86	0.93
		A	s	*	*	0.26	*	0.21	0.21	0.21	0.11	0.11
		B	$\bar{x}$	*	*	0.38	*	0.18	0.18	0.18	0.79	0.78
		B	s	*	*	0.31	*	0.10	0.10	0.10	0.09	0.38
	B2A	A	$\bar{x}$	*	*	0.16	-1.26	*	*	*	0.71	0.82
		A	s	*	*	0.12	1.07	*	*	*	0.18	0.13
		B	$\bar{x}$	*	*	0.19	-1.58	*	*	*	0.68	0.91
		B	s	*	*	0.15	0.39	*	*	*	0.32	0.13
	B3	A	$\bar{x}$	*	*	0.24	-5.77	0.21	0.21	0.21	0.83	0.94
		A	s	*	*	0.17	1.82	0.23	0.23	0.23	0.14	0.07
		B	$\bar{x}$	*	*	0.30	-8.78	3.33	3.33	3.33	0.87	0.92
		B	s	*	*	0.16	12.74	4.20	4.20	4.20	0.11	0.12
NON-HYST HETTER	V3	A	$\bar{x}$	*	*	*	*	5.81	0.99	0.21	0.91	0.90
		A	s	*	*	*	*	6.88	0.58	0.29	0.01	0.15
		B	$\bar{x}$	*	*	*	*	10.00	0.84	0.28	0.89	-0.9
		B	s	*	*	*	*	11.79	0.51	0.24	0.06	3.63
	V5	A	$\bar{x}$	0.07	1.91	*	*	12.43	1.72	0.15	0.91	0.93
		A	s	0.02	0.46	*	*	8.95	2.31	0.12	0.06	0.07
		B	$\bar{x}$	0.15	1.53	*	*	10.68	1.29	0.13	0.89	-0.6
		B	s	0.14	0.34	*	*	10.50	0.43	0.09	0.05	2.96
	B3	A	$\bar{x}$	*	*	*	*	16.93	0.73	0.11	0.88	0.83
		A	s	*	*	*	*	20.17	0.36	0.18	0.01	0.22
		B	$\bar{x}$	*	*	*	*	18.11	1.37	0.03	0.61	0.90
		B	s	*	*	*	*	9.71	1.66	0.01	0.34	0.08
	B5	A	$\bar{x}$	*	*	0.47	-6.70	8.72	0.68	0.15	0.89	0.91
		A	s	*	*	0.19	3.22	11.20	0.84	0.12	0.07	0.09
		B	$\bar{x}$	*	*	0.45	-9.81	22.83	0.87	0.03	0.63	0.91
		B	s	*	*	0.04	0.91	4.67	0.73	0.01	0.33	0.08

R²(p) = Coef of Determination for matric potentials;
* = parameter not optimised;

R²(f) = Coef of Determination for bottom inflow;
Sta = statistics: $\bar{x}$ = mean value; s = standard deviation

flow events (table 6.7) present similar results: the means of the means $R^2(p)$ are 0.74 for lysimeter A and 0.77 for lysimeter B; the means of the means $R^2(f)$ are -2.8 for lysimeter A and -2.3 for lysimeter B. Again, these values compare favourably with the results of table 6.2 for homogeneous conditions and are similar to those obtained for original non-hysteretic heterogeneous simulations.

When the events are optimised under heterogeneous conditions, there is no significant improvement in the values of $R^2(p)$: the means of the means $R^2(p)$ showed on table 6.6 for heterogeneous simulations of the selected rapid flow events are 0.77 for lysimeter A and 0.64 for lysimeter B; the means of the means $R^2(p)$ for heterogeneous simulations of the slow flow events (table 6.7) are 0.90 for lysimeter A and 0.76 for lysimeter B. The results for $R^2(f)$, however, are much better than in the other modes: for the rapid flow events, the means of the means $R^2(f)$ are 0.13 for lysimeter A and 0.68 for lysimeter B; and, for the slow flow events, 0.89 for lysimeter A and 0.08 for lysimeter B.

These results seem to confirm that, given an adequate combination of parameter values, the model is able to provide reasonable results for the simulations of the observed data. However, even if the results are favourable in a bulk analysis, a closer view reveals fundamental problems. The results of the optimisations show a big variation in the optimised values of all parameters tested, which is translated into high values in the relation $|s/\bar{x}|$ for tables 6.6 and 6.7. This big variation could be caused by the local minima being taken as optimum results, but could also be consequence of an inadequacy of the model conceptualisation in representing the observed data. If this is true, physically unrealistic values of the parameters can be selected by the optimisation routine, so that, although the result of the simulation seems to be good, it gives no valid information for the understanding of the processes involved. The variations observed in the optimised parameters are such that, in practical terms, a different set of parameters was fitted to each event, for each simulation. The values of the parameters that produce a maximum agreement between the model and the observed data often show lack of physical basis and attempts to correlate them with other variables (such as initial water content, initial matric potential, previous rainfall, etc.) were not successful. Consequently, the model can not be used for prediction of the lysimeter response. Also, analysis of the mean values of the optimised parameters shown in tables 6.6 and 6.7 is of very limited validity, due to the great variation in the values which generated these means.

In the same way as presented for the non-hysteretic simulations using parameters fitted to observed $\theta(\psi)$ and K_s data (section 6.2), results for events 90158, 91211 and 91165 are

graphically displayed and discussed. For each of these events, two figures are presented: one for non-hysteretic simulations under homogeneous conditions, with the results given by options V2 (optimising Van Genuchten's α and n) and B2A (optimising Brooks-Corey's λ and ψ_b); and the other for non-hysteretic simulations under heterogeneous conditions, showing the results given by options V3 and B3 (optimising the saturated conductivity). Both figures use parameters obtained from simultaneous optimisations of matric potentials and bottom inflow. Table 6.8 presents the values of the optimised parameters for each of the figures.

Table 6.8 - Values of the optimised parameters in figures 6.9 to 6.14

Figure	Event	Simulation	Lys	Optimised parameters							$R^2(p)$	$R^2(f)$
				α 1/cm	n -	λ -	ψ_b cm	Ks_1 cm/h	Ks_2 cm/h	Ks_3 cm/h		
6.9	90158	HOM	V2	A	0.17	1.74	*	*	*	*	0.92	0.86
			B		0.10	1.09	*	*	*	*	0.56	0.41
		B2A	A	*	*	0.37	-2.10	*	*	*	0.89	0.86
			B	*	*	0.11	-0.96	*	*	*	0.54	0.39
6.10	90158	HET	V3	A	*	*	*	1.59	0.51	0.21	0.95	0.78
			B	*	*	*	*	11.51	0.82	0.34	0.65	0.24
		B3	A	*	*	*	*	0.41	0.22	0.08	0.95	0.79
			B	*	*	*	*	1.72	0.41	0.03	0.63	0.12
6.11	91211	HOM	V2	A	0.07	1.13	*	*	*	*	0.89	0.95
			B		0.07	1.16	*	*	*	*	0.96	0.78
		B2A	A	*	*	0.11	-1.50	*	*	*	0.89	0.90
			B	*	*	0.25	-3.10	*	*	*	0.96	0.75
6.12	91211	HET	V3	A	*	*	*	6.87	6.67	0.01	0.85	-2.8
			B	*	*	*	*	67.69	4.84	2.69	0.82	0.45
		B3	A	*	*	*	*	37.98	3.22	0.22	0.72	-1.1
			B	*	*	*	*	59.8	1.06	0.43	0.79	0.32
6.13	91165	HOM	V2	A	0.11	1.14	*	*	*	*	0.96	0.97
			B		0.14	1.20	*	*	*	*	0.91	0.99
		B2A	A	*	*	0.10	-1.00	*	*	*	0.93	0.91
			B	*	*	0.13	-1.23	*	*	*	0.93	0.96
6.14	91165	HET	V3	A	*	*	*	3.28	1.16	0.09	0.91	0.98
			B	*	*	*	*	12.05	1.59	0.21	0.87	0.98
		B3	A	*	*	*	*	23.49	0.76	0.03	0.87	0.97
			B	*	*	*	*	21.98	0.39	0.04	0.84	0.96

$R^2(p)$ = Coef of Determination for matric potentials;

$R^2(f)$ = Coef of Determination for bottom inflow;

* = parameter not optimised

Results for event 90158 are shown in figures 6.9 and 6.10. These simulations present a much better agreement with the observed data than when using parameters fitted to observed moisture characteristic and conductivity data (figures 6.1 and 6.2). The responses for the top layer are very close to the data for lysimeter A, but they still fail in representing the rapid recessions observed for lysimeter B. For middle and bottom layers, again the modeled responses did not reproduce the rapid responses of lysimeter B, but succeeded in portraying the general behaviour registered for lysimeter A. The representation of bottom inflow was very close to the observations, for both lysimeters. These responses were obtained using parameter values quite

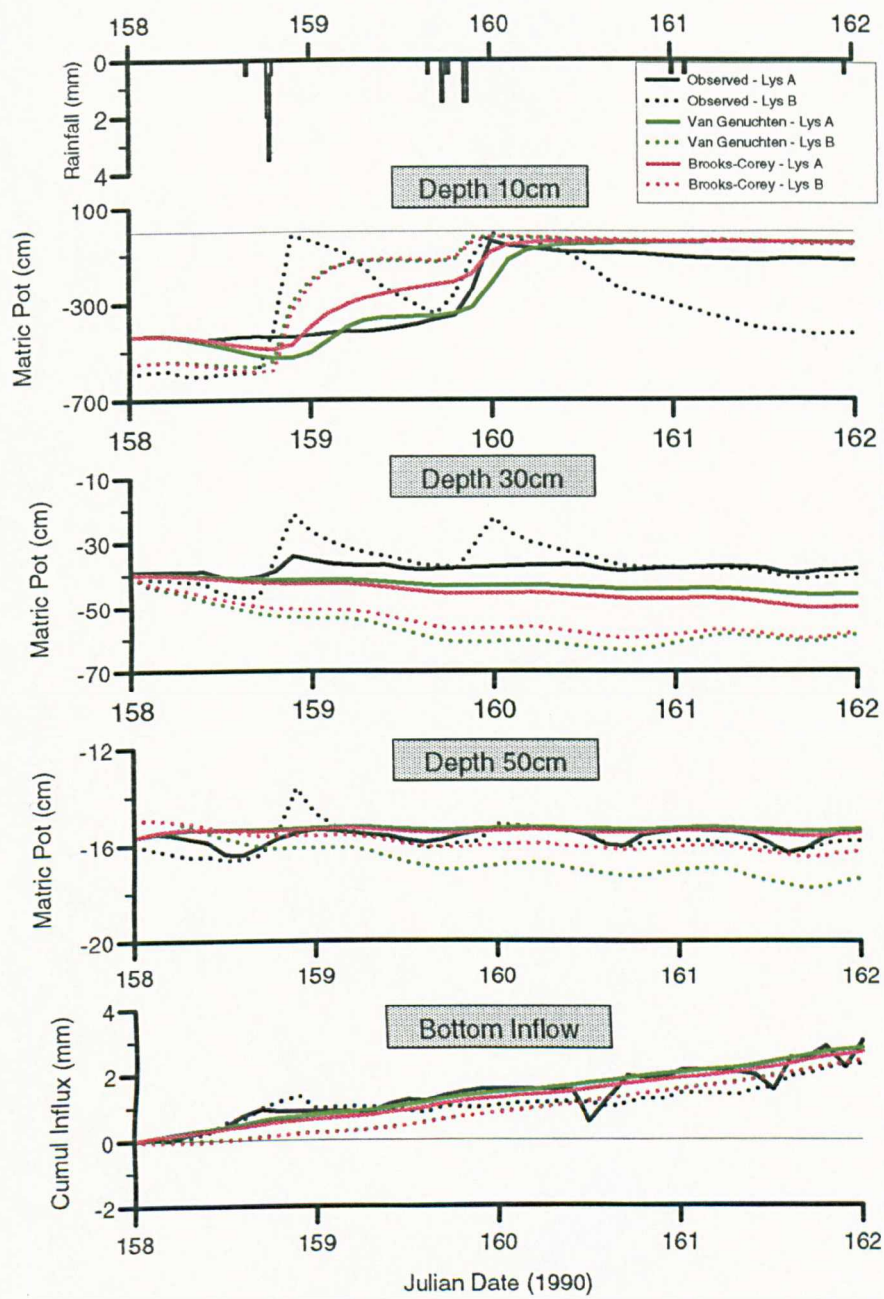


Figure 6.9 - SPW1hyst simulations of event 90158:
non-hysteretic, homogeneous conditions, using optimised parameters

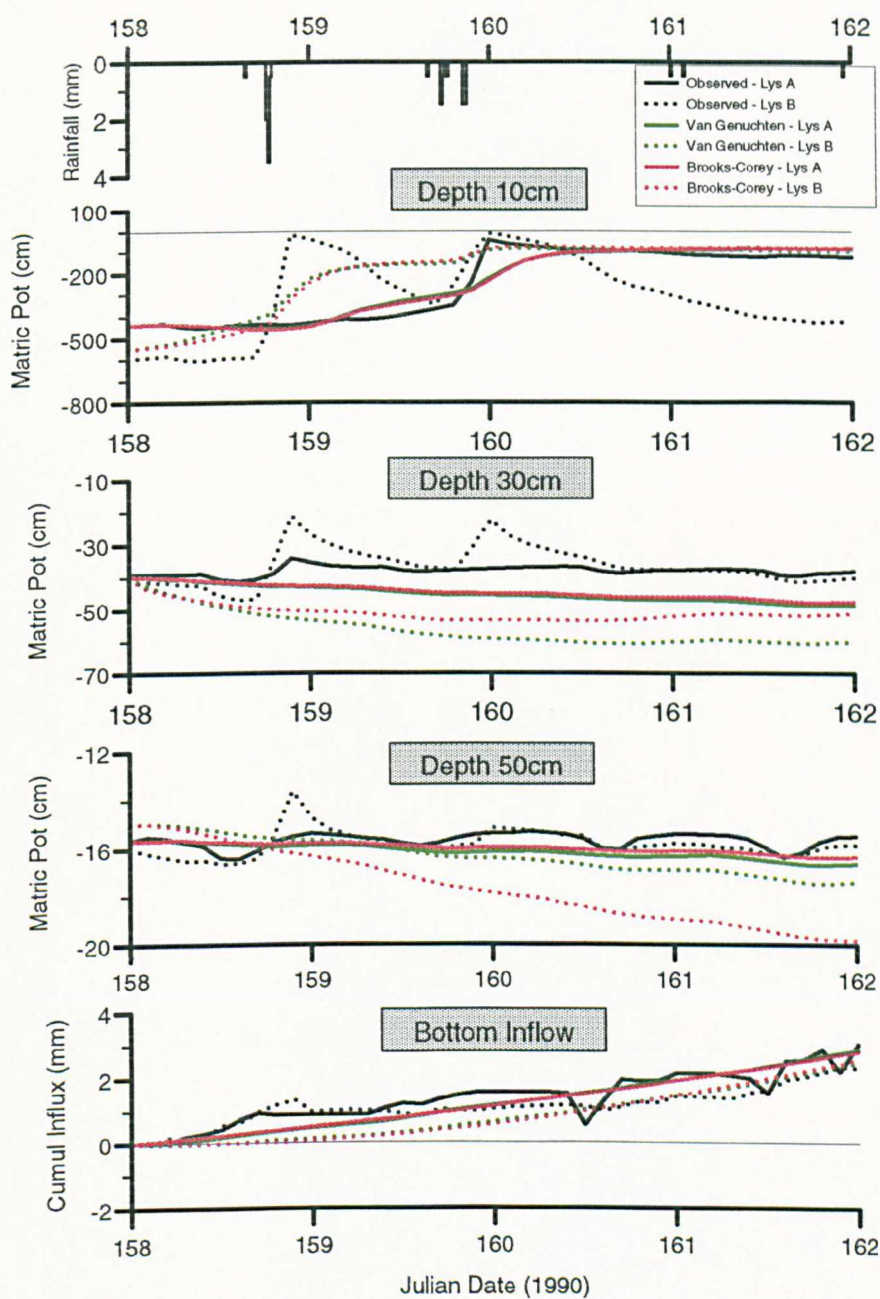


Figure 6.10 - SPW1hyst simulations of event 90158:
non-hysteretic, heterogeneous conditions, using optimised parameters

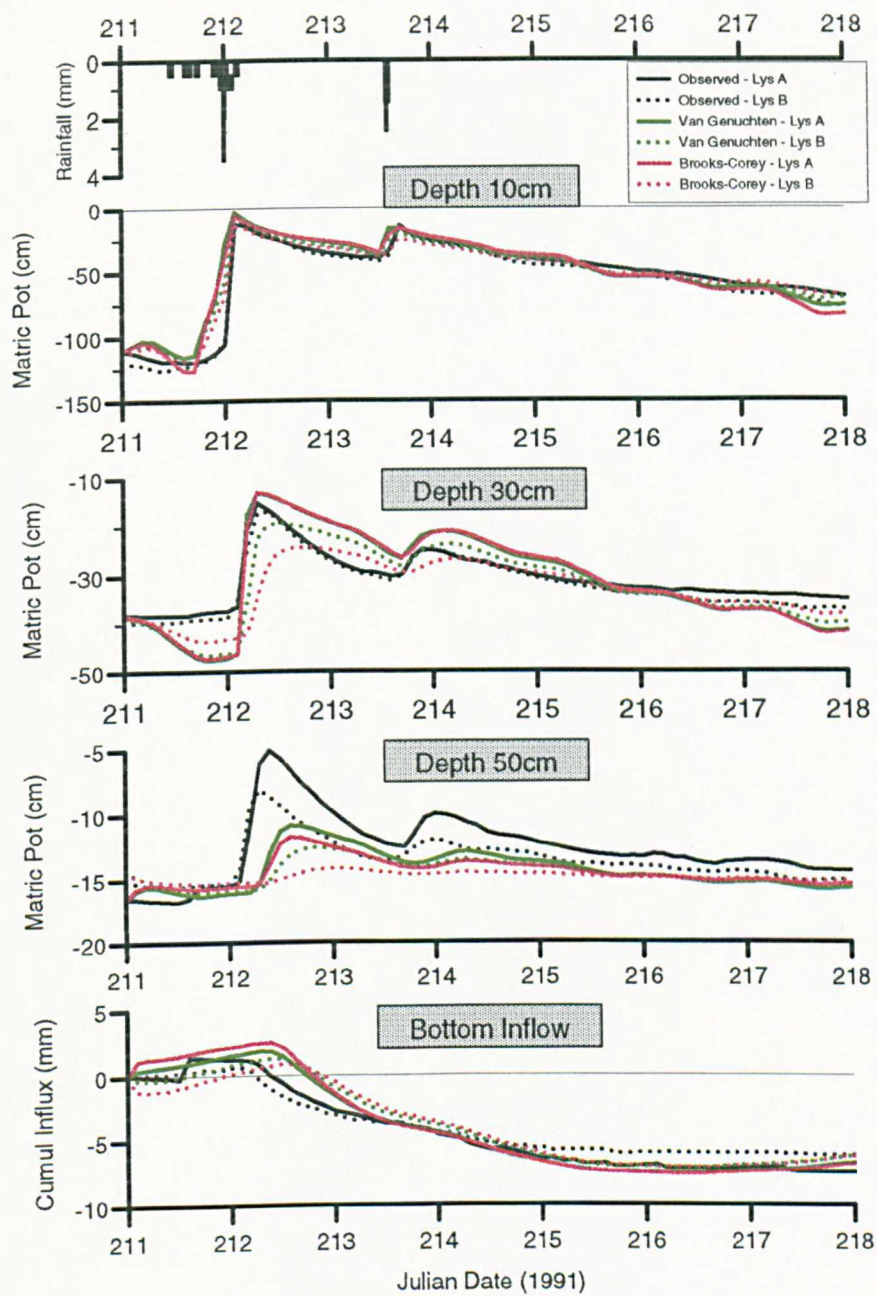


Figure 6.11 - SPWlhyst simulations of event 91211:
non-hysteretic, homogeneous conditions, using optimised parameters

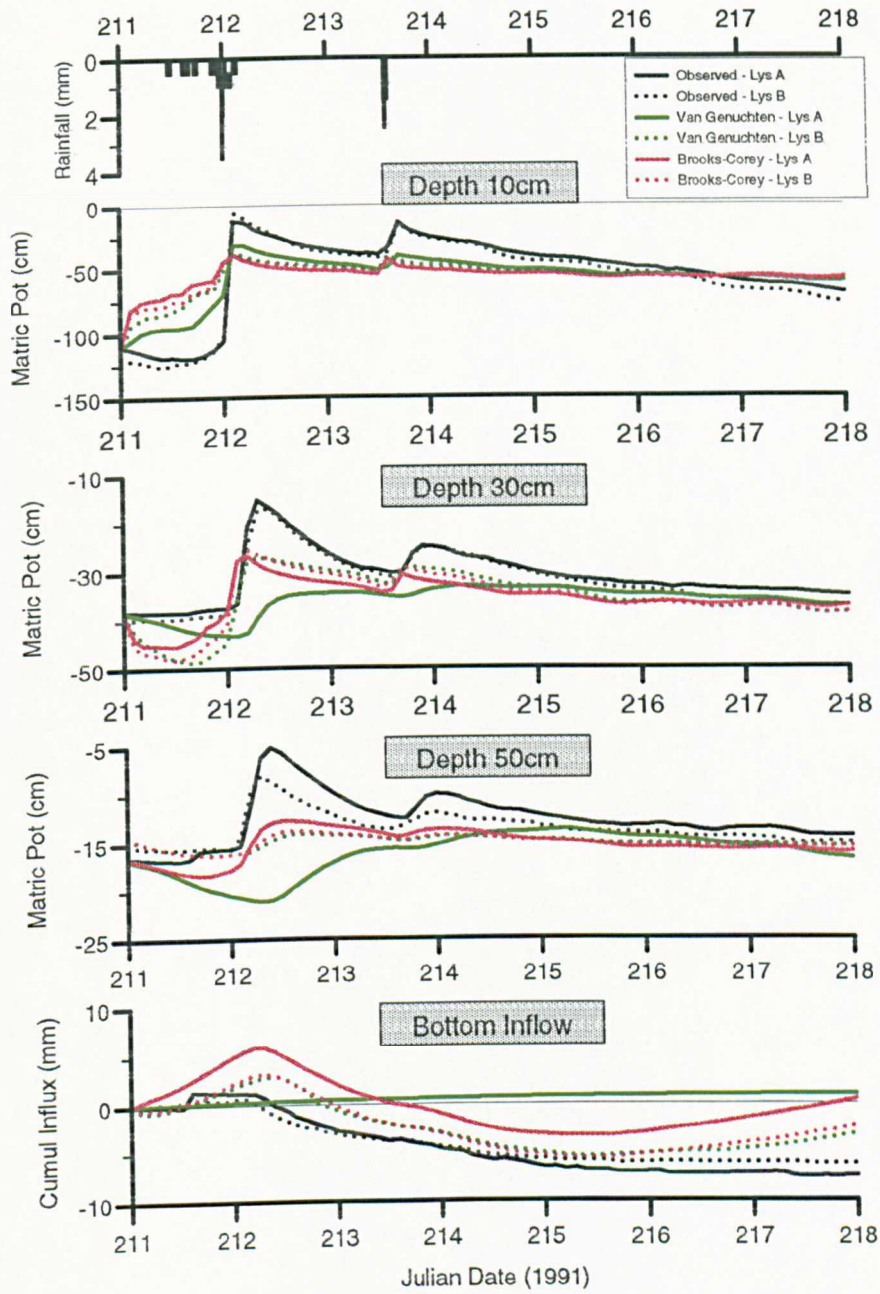


Figure 6.12 - SPWlhyst simulations of event 91211:
non-hysteretic, heterogeneous conditions, using optimised parameters

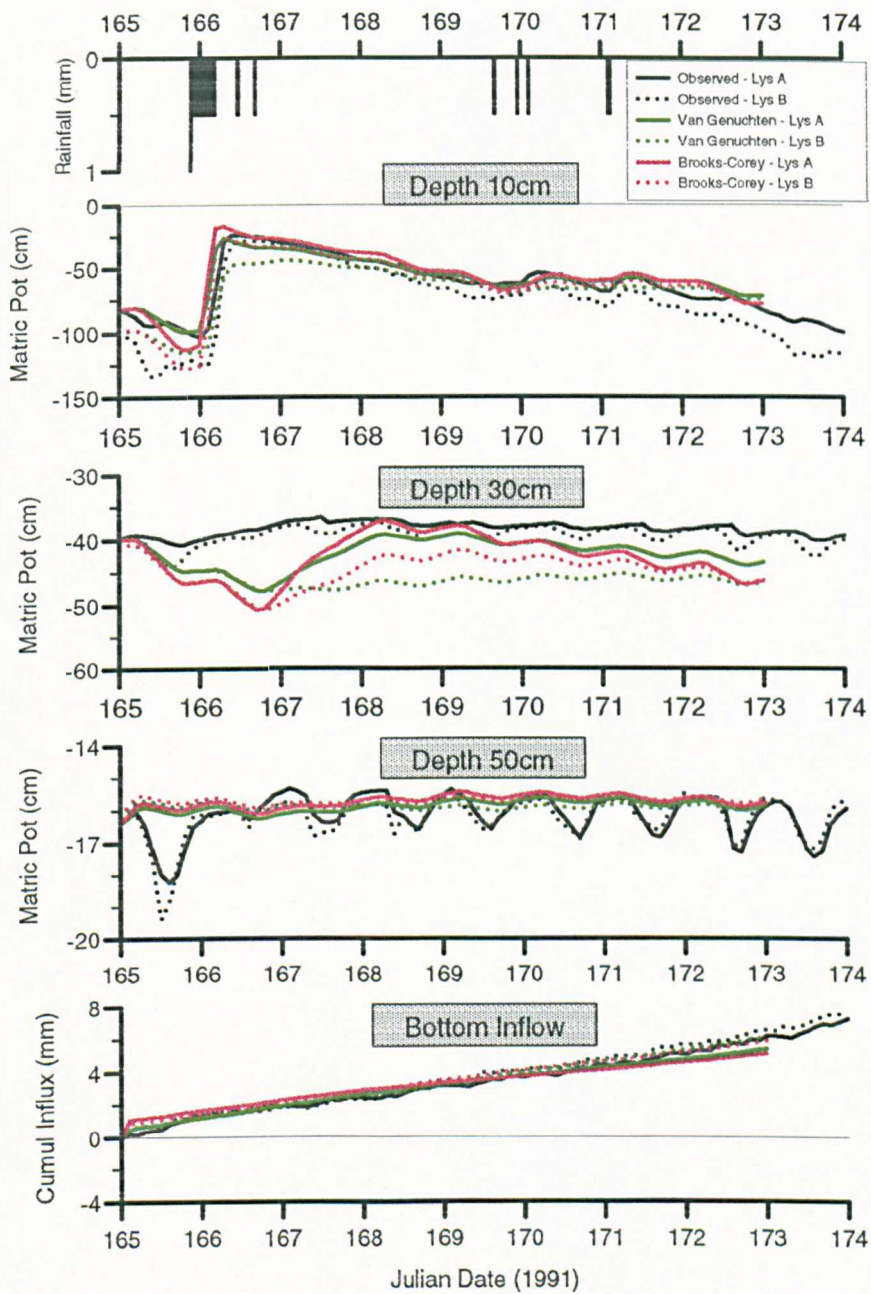


Figure 6.13 - SPWlhyst simulations of event 91165:
non-hysteretic, homogeneous conditions, using optimised parameters

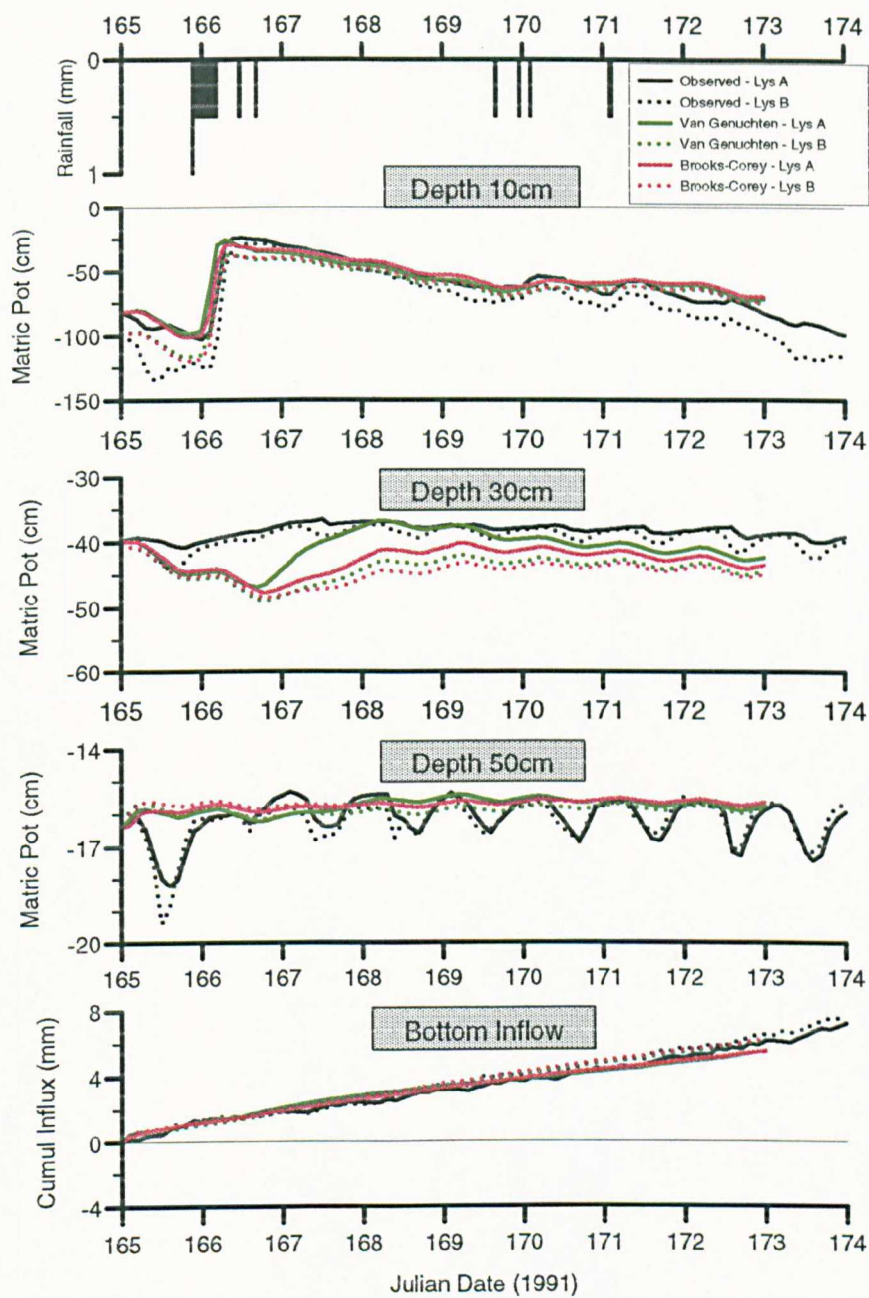


Figure 6.14 - SPW1hyst simulations of event 91165:
non-hysteretic, heterogeneous conditions, using optimised parameters

different from the original values and also different for lysimeters A and B. It is important to observe that, when the saturated conductivities were optimised, small values were always obtained for middle and bottom layers. These values caused restriction to the flow induced by the initial conditions, in a similar way as commented in section 6.2, for heterogeneous simulations. The difficulties in representing rapid responses, even if a major variation in parameters value is allowed, suggest an inadequacy of the model conceptualisation for modelling rapid flows, although problems due to local minima being taken as optimum parameters, or even inconsistencies in the observed data could also have influenced these results.

The responses for event 91211, however, seem to demonstrate that the model can represent rapid flows to some extent. The simulations under homogeneous conditions (figure 6.11) showed a very good fit for the bottom inflow and also for the matric potentials at top and middle layers. For the bottom layer, although the model was not able to meet the peaks observed for the matric potentials, the shape of response shows the influence of the rapid flow. Also, the diurnal variation caused by evapotranspiration is noticeable in the simulated matric potential responses for all layers. These results were achieved with minor alteration in the value of Van Genuchten's parameter α , but significant changes for Van Genuchten's n and Brooks-Corey's λ and ψ_b . The results under heterogeneous conditions (figure 6.12) were not as good, but they still manage to reproduce the general shape of response for Brooks-Corey's simulations, both for bottom inflow and matric potentials at all depths. To obtain this representation, the optimisation routine estimated saturated hydraulic conductivities with differences of one order of magnitude from one layer to the next. The difference observed in the responses shown in figures 6.11 and 6.12 seems to demonstrate that the soil characteristic parameters play a more important role than the saturated hydraulic conductivity in the representation of the matric potentials. This conclusion is consistent with observations from section 6.2, where changes in conductivity values improved the simulation of the bottom inflow by compensating effects of initial conditions, but did not significantly improve the matric potential results.

The results for slow flow event 91165 (figures 6.13 and 6.14), both under homogeneous and heterogeneous conditions, show very good agreement with the observed values for the bottom inflow and for the matric potentials. As for events 91211, the diurnal variation caused by evapotranspiration is noticeable in the simulated matric potential responses for all layers. These results seem to confirm that SPW1hyst can properly represent slow flow events. However, this fit was achieved via a substantial change in parameter values, and these variations, as commented above, bring great difficulties for using the model as a predictive tool.

6.4.2.2 - Hysteretic simulations

The optimisation model was applied to the selected events in hysteretic mode, under homogeneous conditions, optimising simultaneously matric potentials and bottom influx. The results for each event are presented in Appendix VI, tables VI.13 to VI.24. The mean values and standard deviations of these results are summarised in tables 6.9 and 6.10, for the selected rapid and slow flow events, respectively.

A comparison of these results with the hysteretic simulations of the selected events using the parameters fitted for event 91136 (table 6.4) shows that there is significant improvement in the representation of bottom inflows. However, these ameliorations were obtained in conjunction with slight worsening of the results for the simulation of matric potentials. Better results for both driving variables were observed only for simulations V4 and B4, where the saturated hydraulic conductivity is optimised in conjunction with the hysteretic soil characteristic parameters. These results seem to confirm the conclusion from section 6.3, that air entrapment and hysteresis in the soil characteristic curve can help improving the representation of the bottom inflows, but has minor influence for matric potentials.

As for the non-hysteretic simulations, the results of the optimisations show a big variation in the optimised values of all parameters tested, with high values in the relation $|s/\bar{x}|$ for tables 6.9 and 6.10. The exceptions seem to be the main wetting curve maximum moisture content (θ_w^*) for the slow flow events (mean of the mean optimised values of θ_w^* : $0.25 \text{ cm}^3/\text{cm}^3$) and Brooks-Corey's parameter λ (mean of the mean optimised values: 0.57), both presenting values of $|s/\bar{x}|$ around 0.10. Again as observed for the non-hysteretic case, the values of the parameters that produce a maximum agreement between the model and the observed data often show a lack of physical basis and attempts to correlate them with other variables were not successful, bringing difficulties for the use of the model as a predictive tool and also limiting the validity of a detailed analysis of the mean values of the optimised parameters shown in tables 6.9 and 6.10.

The results for hysteretic SPWlhyst simulations V4 and B4 of events 90158, 91211 and 91165, with parameters obtained from simultaneous optimisations of matric potentials and bottom inflow are presented in figures 6.15 to 6.17. Table 6.11 present the values of the optimised parameters for each of the figures.

Table 6.9 - SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Means and standard dev. from hysteretic simulations of selected rapid flow events

Simulation	Lys	Stats	Optimised parameters						$R^2(p)$	$R^2(f)$
			θ_s^w m ³ /m ³	α^w cm ⁻¹	n^w -	λ^w -	ψ_b^w cm	Ks cm/h		
H Y S T E R E T I C H O M O G E N E O U S	V1	A	$\bar{x}$	0.28	*	*	*	*	0.58	-1.7
		A	s	0.07	*	*	*	*	0.27	4.38
		B	$\bar{x}$	0.34	*	*	*	*	0.62	-1.2
		B	s	0.07	*	*	*	*	0.25	4.79
	V2	A	$\bar{x}$	*	0.17	1.63	*	*	0.55	-0.9
		A	s	*	0.13	0.15	*	*	0.28	2.55
		B	$\bar{x}$	*	0.16	1.73	*	*	0.61	-0.4
		B	s	*	0.10	0.61	*	*	0.27	2.71
	V3	A	$\bar{x}$	0.28	0.06	1.73	*	*	0.58	-0.6
		A	s	0.07	0.04	0.12	*	*	0.28	2.23
		B	$\bar{x}$	0.31	0.06	1.90	*	*	0.59	0.33
		B	s	0.08	0.04	0.49	*	*	0.26	1.07
	V4	A	$\bar{x}$	0.31	0.11	1.74	*	*	0.68	0.11
		A	s	0.07	0.07	0.15	*	*	0.30	1.64
		B	$\bar{x}$	0.31	0.09	1.77	*	*	0.67	0.83
		B	s	0.08	0.06	0.60	*	*	0.24	0.24
	B1	A	$\bar{x}$	0.31	*	*	*	*	0.43	-2.5
		A	s	0.08	*	*	*	*	0.28	4.35
		B	$\bar{x}$	0.37	*	*	*	*	0.41	-4.3
		B	s	0.07	*	*	*	*	0.27	10.66
	B2	A	$\bar{x}$	0.34	*	*	0.51	*	0.44	-3.2
		A	s	0.08	*	*	0.06	*	0.25	5.76
		B	$\bar{x}$	0.38	*	*	0.50	*	0.40	-2.3
		B	s	0.08	*	*	0.17	*	0.29	5.79
	B2A	A	$\bar{x}$	*	*	*	0.58	-11.38	0.44	-2.1
		A	s	*	*	*	0.07	9.51	0.26	4.24
		B	$\bar{x}$	*	*	*	0.57	-9.30	0.39	-2.62
		B	s	*	*	*	0.16	3.37	0.29	6.61
	B3	A	$\bar{x}$	0.32	*	*	0.53	-14.37	0.46	-2.0
		A	s	0.08	*	*	0.04	5.64	0.25	3.91
		B	$\bar{x}$	0.33	*	*	0.42	-19.80	0.41	-3.0
		B	s	0.08	*	*	0.08	9.49	0.29	7.42
	B4	A	$\bar{x}$	0.33	*	*	0.53	-13.46	0.67	0.80
		A	s	0.06	*	*	0.06	10.34	0.22	0.23
		B	$\bar{x}$	0.31	*	*	0.58	-24.55	0.67	0.80
		B	s	0.08	*	*	0.17	17.78	0.19	0.25

$R^2(p)$ = Coef of Determination for matric potentials;

* = parameter not optimised;

Obs.: Events 91136 and 91198 (outliers) not considered

$R^2(f)$ = Coef of Determination for bottom inflow;

Stats = statistics: $\bar{x}$ = mean value; s = standard deviation

Table 6.10 - SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Means and standard dev. from hysteretic simulations of selected slow flow events

Simulation	Lys	Stats	Optimised parameters						$R^2(p)$	$R^2(f)$
			θ_s^w m ³ /m ³	α^w cm ⁻¹	n^w -	λ^w -	ψ_b^w cm	Ks cm/h		
H Y S T E R E T I C H O M O G E N E O U S	V1	A	$\bar{x}$	0.24	*	*	*	*	0.67	-15
			s	0.04	*	*	*	*	0.30	28
		B	$\bar{x}$	0.28	*	*	*	*	0.67	-2.6
			s	0.09	*	*	*	*	0.22	3.67
	V2	A	$\bar{x}$	*	0.42	1.65	*	*	0.60	-5.6
			s	*	0.06	0.37	*	*	0.33	10
		B	$\bar{x}$	*	0.36	1.74	*	*	0.58	-0.5
			s	*	0.12	0.19	*	*	0.32	1.12
	V3	A	$\bar{x}$	0.22	0.10	1.64	*	*	0.64	-4.6
			s	0.02	0.05	0.07	*	*	0.29	8.96
		B	$\bar{x}$	0.27	0.18	1.52	*	*	0.59	-0.5
			s	0.10	0.16	0.28	*	*	0.32	1.11
	V4	A	$\bar{x}$	0.27	0.15	1.66	*	*	0.68	-0.2
			s	0.08	0.12	0.08	*	*	0.31	1.78
		B	$\bar{x}$	0.31	0.21	1.71	*	*	0.61	0.53
			s	0.09	0.17	0.15	*	*	0.35	0.53
	B1	A	$\bar{x}$	0.22	*	*	*	*	0.57	-7.6
			s	0.03	*	*	*	*	0.34	12
		B	$\bar{x}$	0.23	*	*	*	*	0.45	-2.0
			s	0.02	*	*	*	*	0.39	1.80
	B2	A	$\bar{x}$	0.22	*	*	0.53	*	0.56	-7.1
			s	0.02	*	*	0.06	*	0.34	12
		B	$\bar{x}$	0.22	*	*	0.69	*	0.44	-1.9
			s	0.02	*	*	0.18	*	0.38	2.0
	B2A	A	$\bar{x}$	*	*	*	0.59	-1.72	0.56	-9.8
			s	*	*	*	0.05	0.66	0.35	17
		B	$\bar{x}$	*	*	*	0.76	-2.66	0.44	-2.0
			s	*	*	*	0.04	1.52	0.38	2.0
	B3	A	$\bar{x}$	0.22	*	*	0.54	-9.43	0.56	-6.9
			s	0.05	*	*	0.10	6.07	0.35	12
		B	$\bar{x}$	0.31	*	*	0.64	-6.07	0.44	-1.7
			s	0.12	*	*	0.19	6.05	0.38	1.82
	B4	A	$\bar{x}$	0.21	*	*	0.50	-13.05	0.59	-6.8
			s	0.01	*	*	0.02	5.44	0.35	12
		B	$\bar{x}$	0.30	*	*	0.65	-7.91	0.44	-1.8
			s	0.11	*	*	0.25	5.99	0.38	1.87

$R^2(p)$ = Coef of Determination for matric potentials;
 * = parameter not optimised;

$R^2(f)$ = Coef of Determination for bottom inflow;
 Stats = statistics: $\bar{x}$ = mean value; s = standard deviation

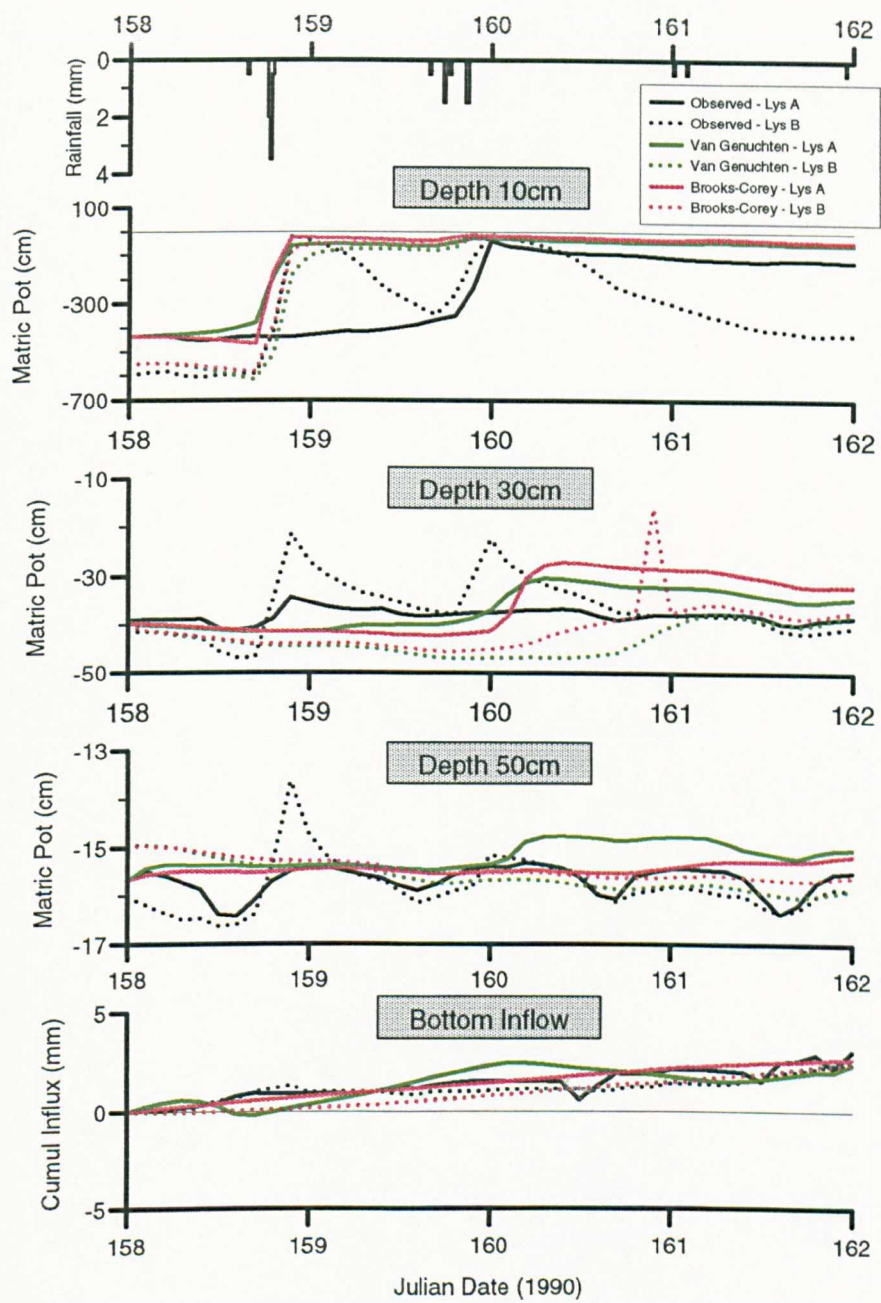


Figure 6.15 - SPWlhyst simulations of event 90158:
hysteretic, homogeneous conditions, using optimised parameters

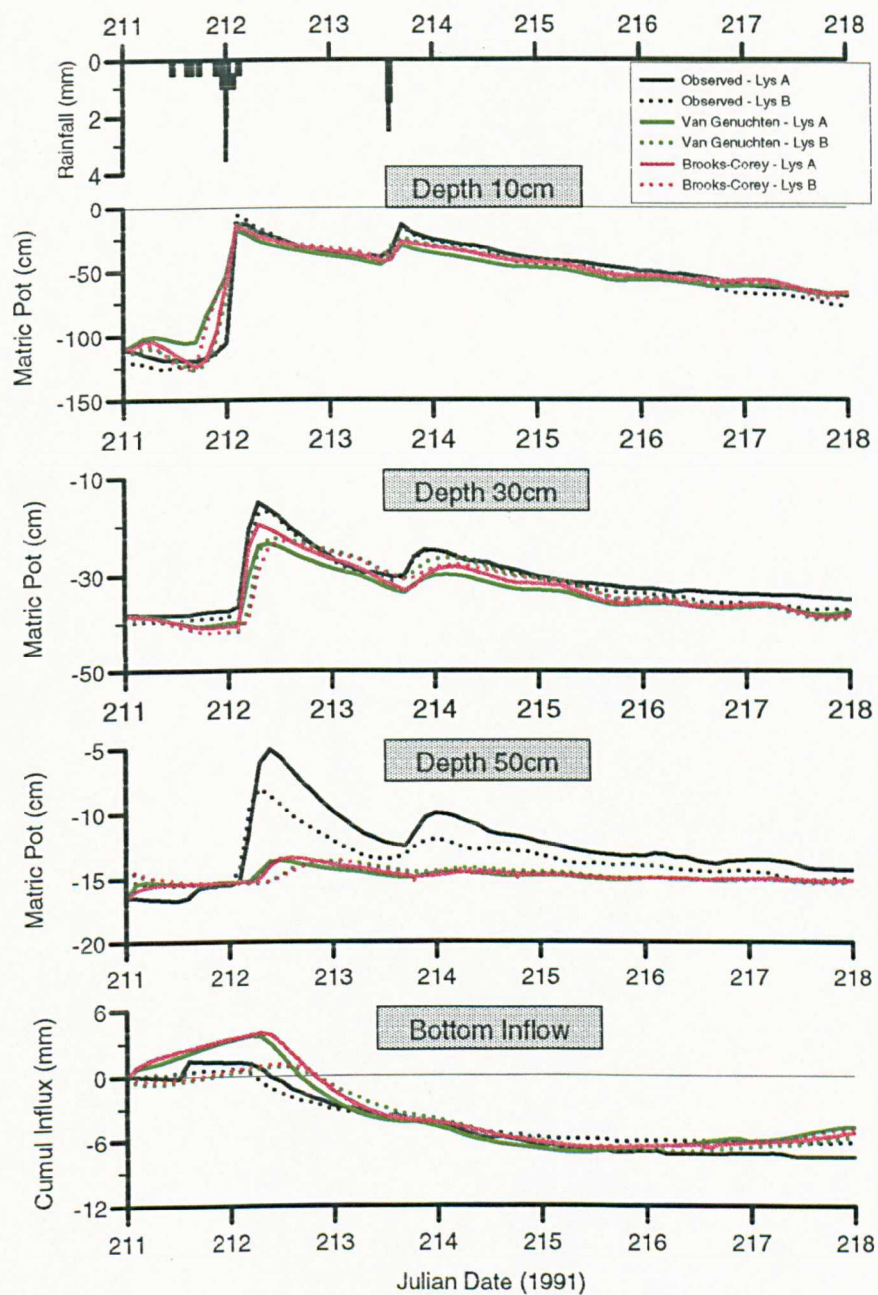


Figure 6.16 - SPW1hyst simulations of event 91211:
hysteretic, homogeneous conditions, using optimised parameters

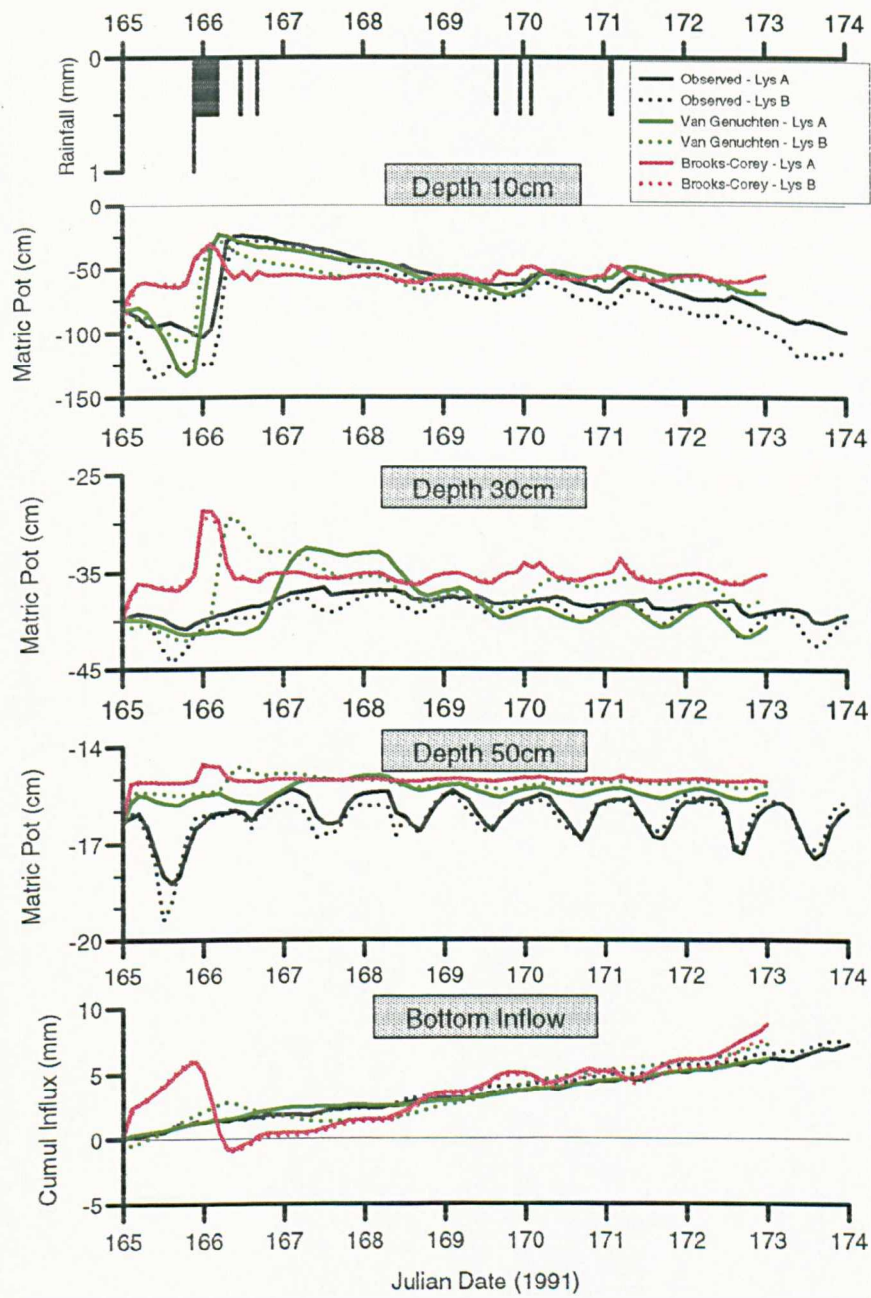


Figure 6.17 - SPWlhyst simulations of event 91165:
hysteretic, homogeneous conditions, using optimised parameters

Table 6.11 - Values of the optimised parameters in figures 6.15 to 6.17

Figure	Event	Simulation		Lys	Optimised parameters						R ² (p)	R ² (f)
					θ_s^w m ² /m ³	α^w cm ⁻¹	n^w -	λ^w -	ψ_s^w cm	Ks cm/h		
6.15	90158	H O M	V4	A	0.28	0.14	1.69	*	*	1.77	0.49	0.34
				B	0.22	0.15	1.30	*	*	0.66	0.54	0.35
		B4	A	0.38	*	*	0.65	-1.50	0.16	0.41	0.82	
			B	0.22	*	*	0.80	-11.9	0.16	0.55	0.32	
6.16	91211	H O M	V4	A	0.38	0.17	1.49	*	*	2.86	0.92	0.81
				B	0.29	0.07	1.61	*	*	2.49	0.97	0.82
		B4	A	0.27	*	*	0.54	-11.5	0.62	0.96	0.78	
			B	0.33	*	*	0.75	-10.0	0.49	0.95	0.84	
6.17	91165	H O M	V4	A	0.38	0.32	1.74	*	*	0.70	0.92	0.98
				B	0.37	0.25	1.66	*	*	5.16	0.83	0.87
		B4	A	0.20	*	*	0.49	-10.0	6.00	0.79	-0.1	
			B	0.20	*	*	0.42	-15.0	6.00	0.69	0.21	

$R^2(p)$ = Coef of Determination for matric potentials;

$R^2(f)$ = Coef of Determination for bottom inflow;

* = parameter not optimised

The results of figure 6.15 show that the hysteretic simulations of event 90158 provided good fit for the bottom inflow. For the matric potentials, the results of the hysteretic simulations present an interesting behaviour. At the top layer, all simulations followed the pattern of response of lysimeter B for the first rainfall input, but failed to reproduce its rapid recession, so that the final half of the simulated event is similar to the observed lysimeter A data. At the middle layer, the matric potentials rise only after the second rainfall input, the same being observed at the bottom layer only for the Van Genuchten's simulation of lysimeter A. It seems that the optimised set of parameters induced a rapid response for the first rainfall input at the top layer, but the amount of water was not enough to reach deeper layers. As the model follows the slow pattern of infiltration predicted by capillary theory, the recession was slow, and the top layer of the soil was still close to saturation when the second rainfall input happened. This contribution was then conducted directly to deeper layers. It is interesting to note that in none of the previous, non-hysteretic, simulations the first rapid rise of matric potentials of lysimeter B was properly reproduced as in this case. However, this response does not mean that the model was reproducing rapid flow mechanisms, as it was influenced by the low values of saturated conductivity optimised in conjunction with the hysteretic soil characteristic parameters.

The hysteretic simulation of event 91211 (figure 6.16) shows similar results to those obtained by the non-hysteretic, homogeneous simulation (section 6.4.2.1): very good fit for the bottom inflow and for the matric potentials at top and middle layers; shape of response at the bottom layer showing the influence of the rapid flow; and diurnal variation caused by evapotranspiration noticeable in the simulated matric potential responses for all layers. The fit

is better for the bottom layer and for the bottom inflow of the non-hysteretic representation, but the hysteretic simulations present better fit at top and middle layers. These results indicate that hysteresis and air entrapment can help to simulate rapid flow responses. However, to obtain good fit, major variations were necessary in the parameter values.

The results for slow flow event 91165 (figure 6.17), show very good agreement to the observed values for the bottom inflow and for the matric potentials only for the simulations for lysimeter A, using Van Genuchten's equation. For the other cases, the model presented an exaggerated sensitivity to the rainfall input, rapidly transmitting these responses down into the soil profile, indicating faster water flow than the observed values. The diurnal variation caused by evapotranspiration is noticeable in the simulated matric potential responses for all layers, in all simulations. These results seem to show that the hysteretic mode can bring difficulties to the representation of matric potentials, as it becomes too sensitive to rainfall inputs, and can suggest faster water flow responses than those observed.

6.5 - Conclusions

Model SPW1hyst was applied to the events selected in chapter 4 in both hysteretic and non-hysteretic mode, under homogeneous and heterogeneous conditions, in order to test how air entrapment and hysteresis in the soil characteristic curve and vertical heterogeneity of saturated water conductivity affect the responses of soil water flow.

When the model was applied using parameters fitted to observed $\theta(\psi)$ and K_s data, poor representations of the observed bottom inflow were obtained. The use of heterogeneous conditions for the saturated conductivity provided significant progress in the results when using Van Genuchten's or Brooks-Corey's soil characteristic curves. However, as simulations using MACRO's methodology showed no clear improvement when considering heterogeneity, it was suggested that the amelioration observed in the other cases could be rather due to the reduction of the saturated conductivity value at deeper layers, than because of its heterogeneity. Detailed analysis of simulations obtained for three selected events gave indications that there is a problem in the model conceptualisation or in the parameter values of SPW1hyst when representing the observed rapid flow events using parameters fitted to observed $\theta(\psi)$ and K_s data. This analysis also suggested that the model can properly represent slow flow events, but other combinations of parameters and processes could be tried in order to improve the results.

The effects of air entrapment and hysteresis in the soil characteristic curve were

investigated by applying SPWlhyst to event 91136. Results for simulations under non-hysteretic mode, using boundary conditions derived from experimental information, were compared to simulations under hysteretic mode and also to a non-hysteretic representation where the boundary fluxes were increased by a scaling factor of 7.5. The excellent fit observed for both the non-hysteretic simulations using the scaled boundary fluxes and the hysteretic representation seems to confirm the existence of preferential flow paths during the event. The set of parameters fitted for the heterogeneous simulation of event 91136 was applied to the other selected events, and the outcomes seem to indicate that air entrapment and hysteresis in the soil characteristic curve can be used to explain the observed variations in the bottom inflows, but has minor influence for matric potentials.

A methodology for optimising SPWlhyst parameters per event was developed and applied to the selected events, for homogeneous and heterogeneous conditions, and under hysteretic and non-hysteretic mode. The optimisation response surface was very flat, so that it was not possible to guarantee that the solutions found for each case correspond to global minima. The results seem to show that, given an adequate combination of parameter values, the model is able to provide good results for the simulations. However, a big variation in the estimates of the optimised parameters from event to event was observed. The values of the parameters that produce a maximum agreement between the simulations and the observed data often lack physical basis and attempts to correlate them with other variables were not successful, bringing difficulty for the use of the model as a predictive tool. Detailed analysis of results obtained under non-hysteretic mode for the same three selected events previously studied seem to confirm that SPWlhyst can properly represent slow flow events. These results also showed that the soil characteristic parameters seem to play a more important role than the saturated hydraulic conductivity in the representation of the matric potentials. The hysteretic simulations showed that this mechanism can help to simulate rapid flow responses, but can bring difficulties to the representation of matric potentials for slow flow events.

A fundamental problem remains for the determination of a unique set of parameters able to optimise the representation of observed matric potentials and bottom inflow for the whole set of selected events. The results from the various conceptualisations seem to show that, although good fits to the observed data can be obtained by the use of an adequate combination of parameter values, there are still inadequacies in the model conceptualisation. Evidence of preferential flow suggests the necessity of dual porosity models in order to simulate the soil water flow processes.

CHAPTER 7 - APPLICATION OF MACRO TO THE SELECTED EVENTS

7.1 - Introduction

As commented in chapter 4, nearly 70% of all rainfall events observed in lysimeter experiments at Silwood Park present fast and sharp response along the whole depth profile of the lysimeters, providing indications of preferential or rapid flow. A detailed analysis of a selection of these events seems to confirm this hypothesis. In chapter 6, simulations using model SPW1hyst, a single porosity model based on the Richards' equation, were performed for these selected events, under different combinations of processes and parameter values. These simulations showed an inadequacy of the model conceptualization for representing rapid flows and provided further evidence of preferential flow, suggesting the necessity of dual porosity models in order to better represent the observed phenomena.

For a long time, the importance of macropores in the movement of water has been recognised. In chapter 2, it was shown that its relevance was observed in numerous theoretical and experimental researches, ranging from a first work identified in 1864 to several recent experiments. As result of these and many other works, various models for simulating macroporous flow were developed, as described and commented on in chapter 3.

In the present chapter, MACRO, a dual porosity model, already described in chapter 3, is applied to simulate the same selected events dealt with in the previous sections. The model was employed in both single and dual porosity modes, in order to assess the importance of macroporous flow. The effects of vertical heterogeneity in the saturated conductivity values were also investigated.

7.2 - Parametrisation

7.2.1 - Adopted parameter values

The same values for the soil properties of the lysimeters of Imperial College's experimental station determined in chapter 5 using observed $\theta(\psi)$ and K_s data, and adopted for model SPW1hyst in chapter 6, are now used as input parameters for the MACRO model. The value of the effective diffusion pathlength (d) was obtained through model calibration and is discussed in section 7.2.2. The remaining parameters that could not be obtained from the conditions adopted in chapters 5 and 6 were determined from literature values, as suggested by

An analysis of equation 3.5 shows that the MACRO model does not consider positive water potentials in the micropores. For this reason, ψ_{mi} assumes a constant value under saturated conditions. This value is determined by the saturated water content and the boundary potential and implies an increase in the total potential with elevation, inducing water movement in the micropores and, consequently, affecting the simulated bottom inflows. In order to avoid this effect and to compensate for this limitation in MACRO's formulation, the solution adopted was to simulate the soil profile down to a maximum depth such that unsaturated conditions are ensured. The effect of the bottom layers of the lysimeters was considered by choosing a boundary condition of a fixed pressure, equivalent to the difference in depth from the water table to the bottom of the lower simulated layer. This difference should be bigger than the boundary potential, in order to avoid saturated conditions. This simplification is made possible because the matric potentials in the bottom layers present only small variations, allowing the consideration of a fixed pressure at a depth above, but close to, the water table level.

A grid of 11 elements was adopted, with the top element 2.5 cm thick and the other 10 elements with thickness of 5 cm, so that their centres coincide with the measured variables, up to a total depth of 52.5 cm. As the water table is located at a depth of 65 cm (5 cm above the bottom of the lysimeters), the lower boundary condition was defined as a constant water pressure of -12.5 cm of H_2O . The initial conditions (water contents) were obtained from the SPW1hyst simulations, so that both model performances could be comparable. For the same reason, the evapotranspiration rates were derived as daily totals computed using the Penman model and the hourly rainfall input was provided by the data from the automatic weather station located at the experimental station.

7.2.2 - Calibration of the effective diffusion pathlength (d)

As already presented in chapter 3, the MACRO model computes water exchange between macro- and micropore domains using equation 3.8, which implies a rectangular-slab geometry for the aggregates. A key parameter for the estimation of the water exchange is the effective diffusion pathlength (d, equal to half the aggregate width). A model calibration was performed in order to define its value for the simulations.

The calibration was performed by running the MACRO model for the selected events, in dual porosity mode, under the conditions described in section 7.2.1 and assuming homogeneity in the saturated conductivity values. Values of d were tested in the range from 1 to 20 cm. Figure 7.1 shows the results of these simulations for event 91211 of lysimeter A, with

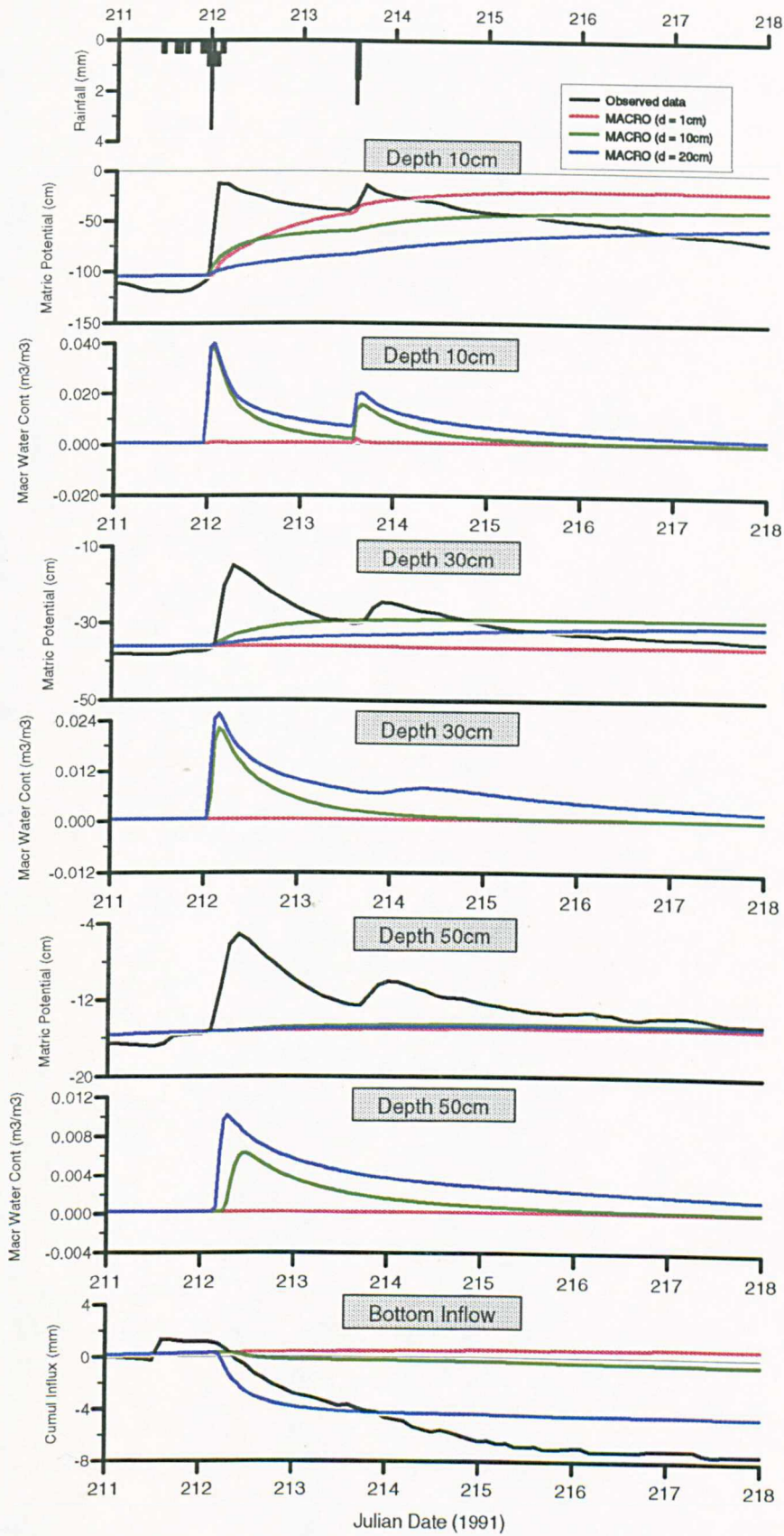


Figure 7.1 - Calibration of the effective diffusion pathlength (d): Event 91211 - Lysimeter A

values of d equal to 1, 10 and 20 cm.

The water exchange is inversely proportional to d^2 . When d is increased, less water is transmitted from the macropores to the matrix, and, consequently, the macropore water content reaches higher values and lasts longer. Also, the effect of the simulated macropore flow is propagated deeper in the profile for bigger values of d .

The model showed a significant sensitivity to the value of this parameter. The results of the simulations of event 91211 show that, for d equal to 1 cm, almost no effect of macropore flow can be noticed. For d equal to 10 cm, macropore water is simulated along the whole depth profile and is rapidly transmitted to the bottom of the lysimeter. Besides that, it seems that the shape of the rapid responses observed in the tensiometer data is reproduced by the patterns of the simulated macropore water contents, and that the micropore matric potentials tend to reasonably represent the observed tensiometer responses when the macropore water content is zero. This behaviour gives an indication that the soil water potential measurements were influenced by macropore flow and could help to explain the observed data. However, for $d=10\text{cm}$, the simulated values of the bottom inflow are too small when compared with the observed data. For d equal to 20 cm, a much closer agreement of the bottom inflows was observed. Bigger values of d would further increase these effects, but they would also imply an aggregate width too large for the type of soil in the lysimeters, as an expected value would be around 5cm. Jarvis (1994) adopted $d=4\text{cm}$ in an example using three different hypothetical soils: clay, loam and sand. The top value in the tested range, $d=20\text{cm}$, is already a high value for this soil. However, it was adopted for the simulations of the selected events due to the results obtained in the calibration and also taking into account the empiricism in the water exchange relation adopted in the model. In this way, d is defined in order to reduce the water exchange between domains, so that most of the macropore water is routed through the soil profile directly to the bottom of the lysimeter. Finally, it is important to emphasise that spatial and temporal variability in this parameter can be expected.

7.3 - Application to the selected events and discussion of results

The MACRO model was applied to the same events already simulated with SPW1hyst, except for the first re-dosing of the lysimeters (event 91136). This event was not simulated because it was not possible to reproduce its boundary conditions using the available version of MACRO. The simulations were performed using the set of parameters presented in section 7.2, for single and dual porosity modes, both under homogeneous and heterogeneous conditions.

7.3.1 - Comparison of simulations under homogeneous and heterogeneous conditions

The results of MACRO simulations, comparing homogeneous and heterogeneous conditions, are now presented, for the same three events discussed in detail for the SPW1hyst simulations, in chapter 6. The outputs obtained for the bottom inflow and for micropore matric potentials and macropore water content, at depths 10, 30 and 50 cm, are shown in figure 7.2 for slow flow event 91165, and in figures 7.3 and 7.4, for rapid flow events 90158 and 91211, respectively. The bottom inflow results refer to total (micropore + macropore) seepage.

A common characteristic among the simulations of the matric potentials of all selected events is that there is small difference between the homogeneous and the heterogeneous results. As already commented in chapter 6, these responses are due to the fact that the MACRO model representation in the micropore range is controlled by the boundary hydraulic conductivity value, which was kept constant for all simulations.

For the slow flow events, there is either no macropore response at all, or the macropore water content appears only at the top layer, as in event 91165 (figure 7.2). An explanation for this behaviour is that, even for the slow flow events, some preferential flow can happen in response to rainfall input. However, the lateral losses from the walls of the macropores into the matrix would take this excess of water and it would go no deeper than the few top layers. So, no macropore water is transmitted to the bottom of the lysimeters, and consequently the simulated bottom inflows are due only to micropore water, being the same for the single porosity, the dual porosity and the heterogeneous representations. An inflow from the common reservoir to the lysimeters is simulated, in order to compensate for evapotranspiration effects. However, the magnitude of this simulated inflow is much smaller than the observed data, probably due to limitations in the model conceptualisation to deal with these effects. These limitations will be discussed in section 7.3.2.

The simulation of event 90158 (figure 7.3) follows exactly the pattern described for slow flow events. This happens because the simulation is reproducing the behaviour observed at lysimeter A, where, as commented in section 4.3.1, the observed tensions are consistent with the principles of slow capillary flow. For this event, only lysimeter B showed evidence of rapid flow, which was not reproduced by the MACRO results.

For the rapid flow events, in general the heterogeneous response is larger in the middle and bottom of the profile, but the simulated bottom boundary flow from the tensiometers to the

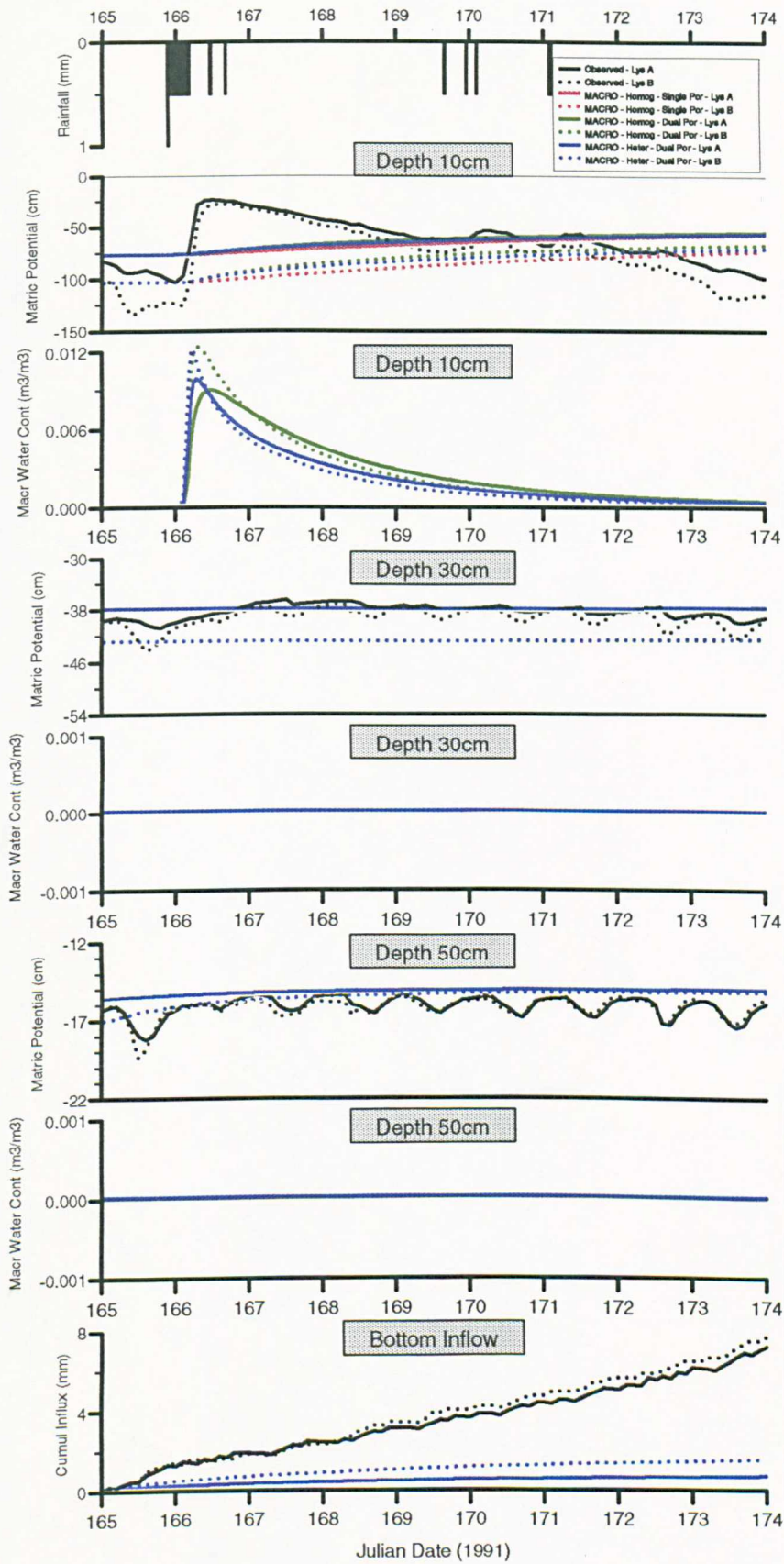


Figure 7.2 - Results of MACRO simulations for event 91165:
comparison of homogeneous and heterogeneous conditions

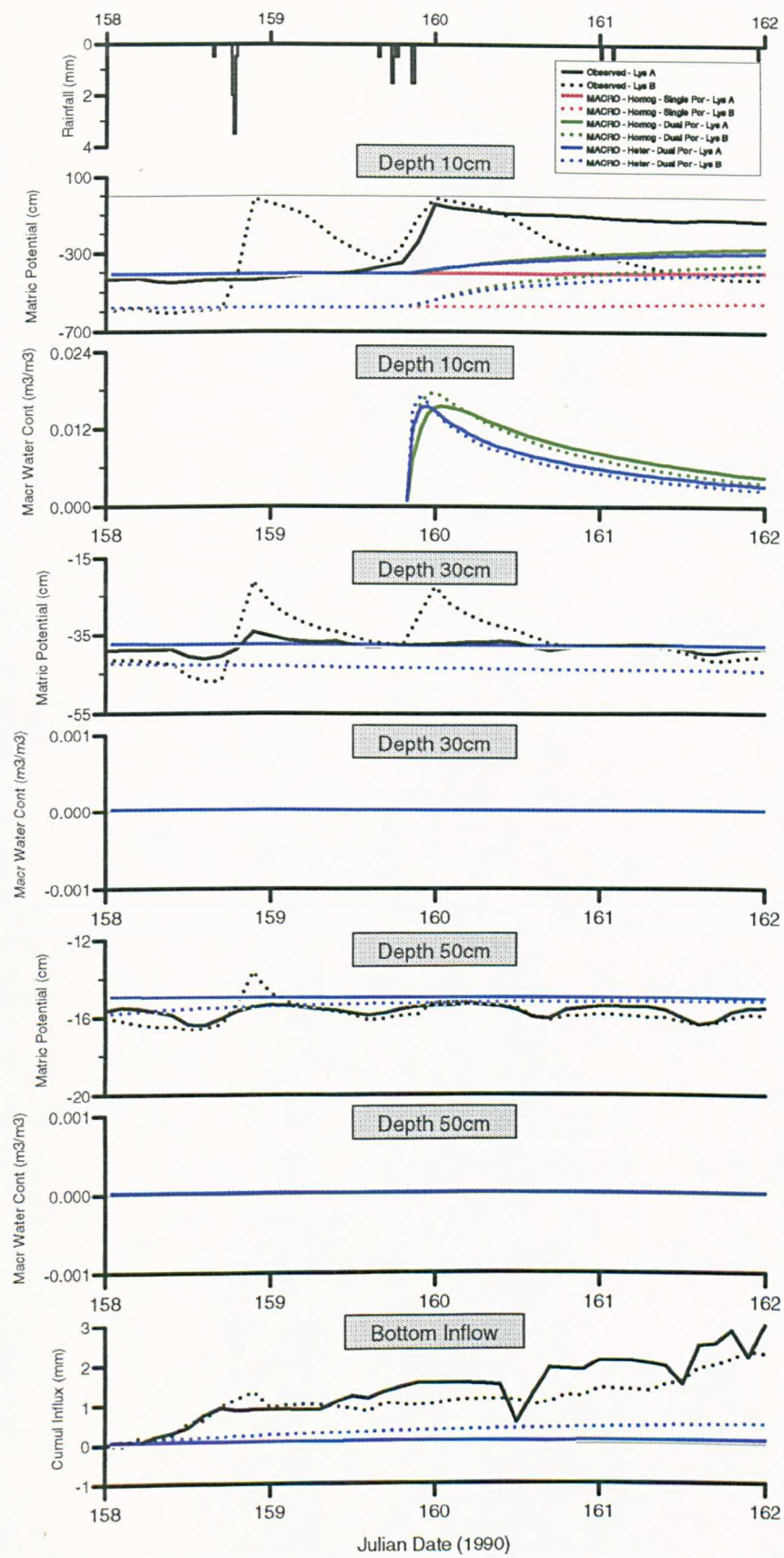


Figure 7.3 - Results of MACRO simulations for event 90158: comparison of homogeneous and heterogeneous conditions

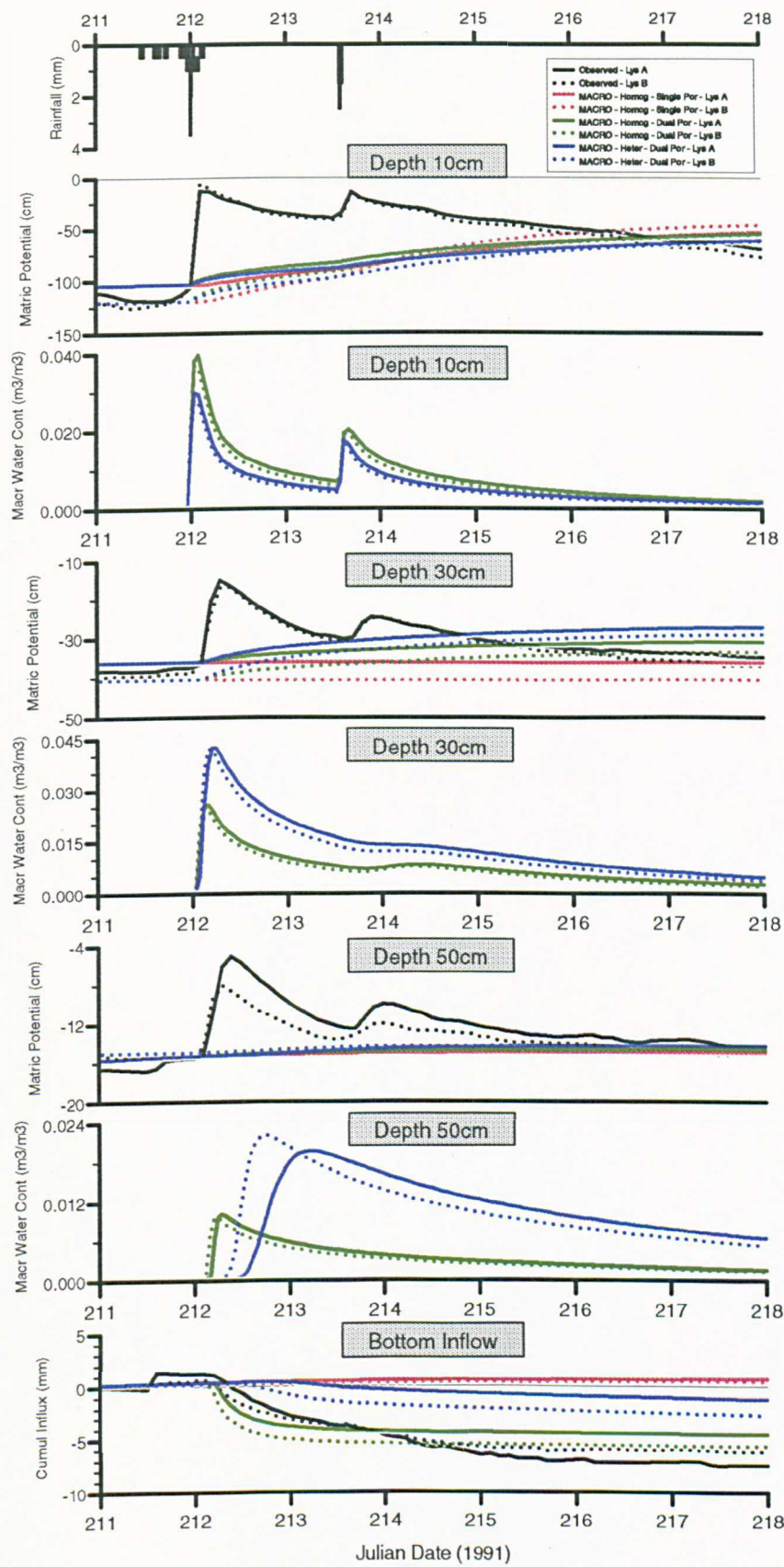


Figure 7.4 - Results of MACRO simulations for event 91211: comparison of homogeneous and heterogeneous conditions

common reservoir is bigger for the homogeneous simulations. This is the behaviour observed for event 91211 (figure 7.4). An interpretation of these results is that, after the macropore flow is initiated, its volume of water is enough to compensate the lateral losses into the matrix, and the flow reaches deeper layers. The water flow in the macropores, as described in section 3.3.2, is computed using Darcy's equation assuming a unit hydraulic gradient, so that it is equal to the hydraulic conductivity. Analysing equations 3.5 and 3.6, it is possible to verify that the macropore conductivity is determined by the difference between saturated and boundary conductivities, while the conductivity in the micropores is controlled by the boundary conductivity only. The value adopted for the boundary conductivity is the same for both homogeneous and heterogeneous representations, but the saturated conductivity varies with depth in the heterogeneous mode. Under heterogeneous conditions, the value of the saturated conductivity of the bottom layer is very close to the boundary conductivity, so that very little macropore flow is possible. Consequently, the macropore water cannot be transmitted through the bottom boundary and it is, therefore, concentrated at the bottom and middle of the depth profile. For the homogeneous simulations the difference between the boundary and the saturated conductivity is constant through the whole soil profile, and the macropore flow can go down to the deeper layers, causing a rapid response in the bottom inflows and reproducing similar values to the observed data.

As commented in section 7.2.2, it seems that the shape of the rapid responses observed in the tensiometer data is reproduced by the patterns of the simulated macropore water contents, while the micropore matric potentials tend to reasonably represent the observed tensiometer responses only when the macropore water content is zero. For event 91211, even the double peak pattern of the tensiometer response is reproduced by the macropore water content at the top and middle layers. This seems to indicate that the tensiometer response could be reproduced by a combination of micro- and macropore effects, implying that the tensiometers were not registering exclusively micropore tensions, but, as they were probably intercepting a preferential water flow path, the data they provide is a result of an increase in macropore water content.

7.3.2 - Analysis of MACRO simulations under homogeneous conditions

Results of the simulations of the selected rapid flow events 90230, 90291, 91017, 91119 and 91198 under homogeneous conditions are presented in figures 7.5, 7.6, 7.7, 7.8 and 7.9, respectively. In these figures, the simulated bottom inflow represented by the red and green lines refer to total (micro+macropore) inflow, while the blue lines show the effect of micropore flow only.

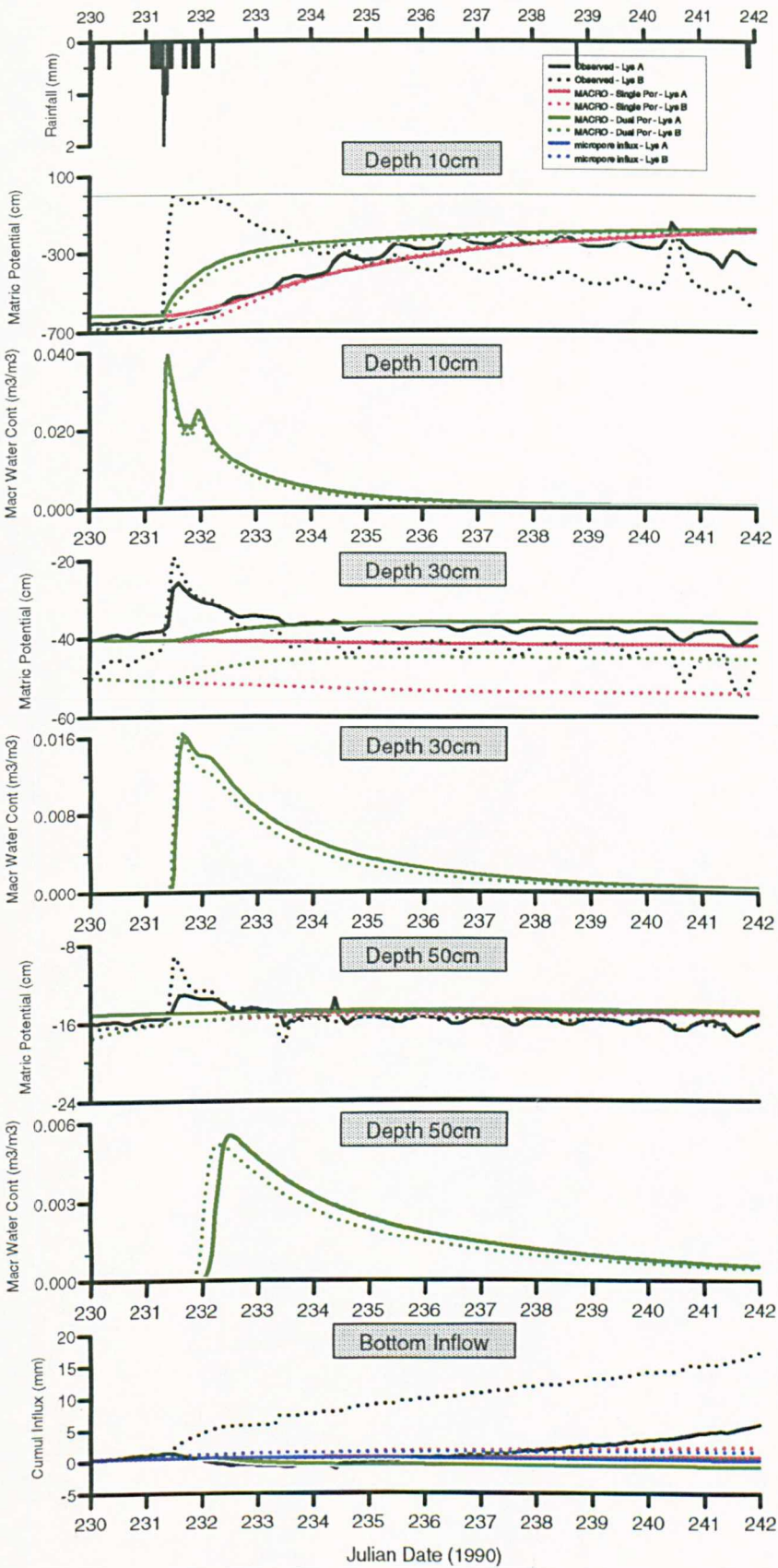


Figure 7.5 - Event 90230: results of MACRO simulations under homogeneous conditions

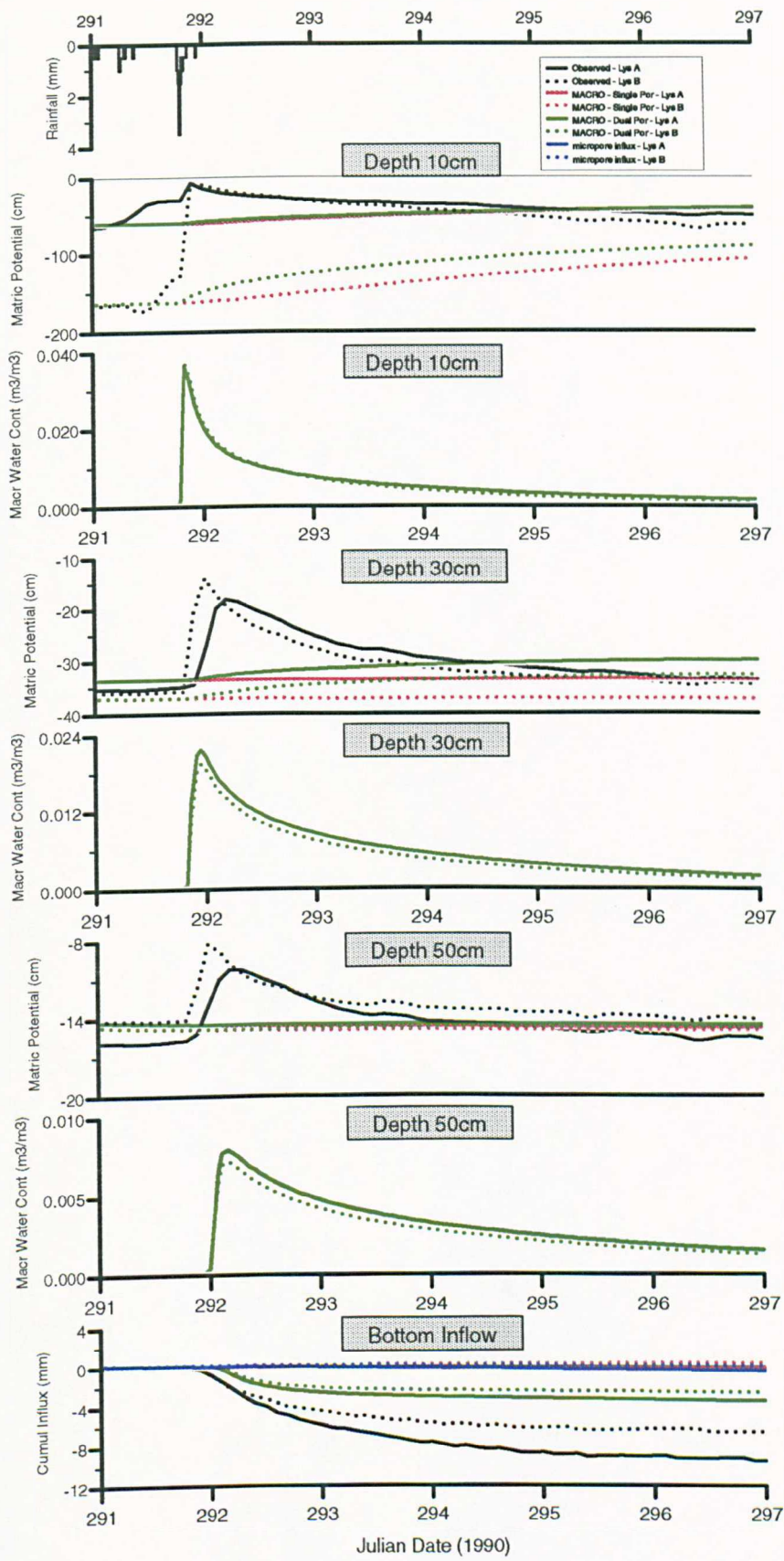


Figure 7.6 - Event 90291: results of MACRO simulations under homogeneous conditions

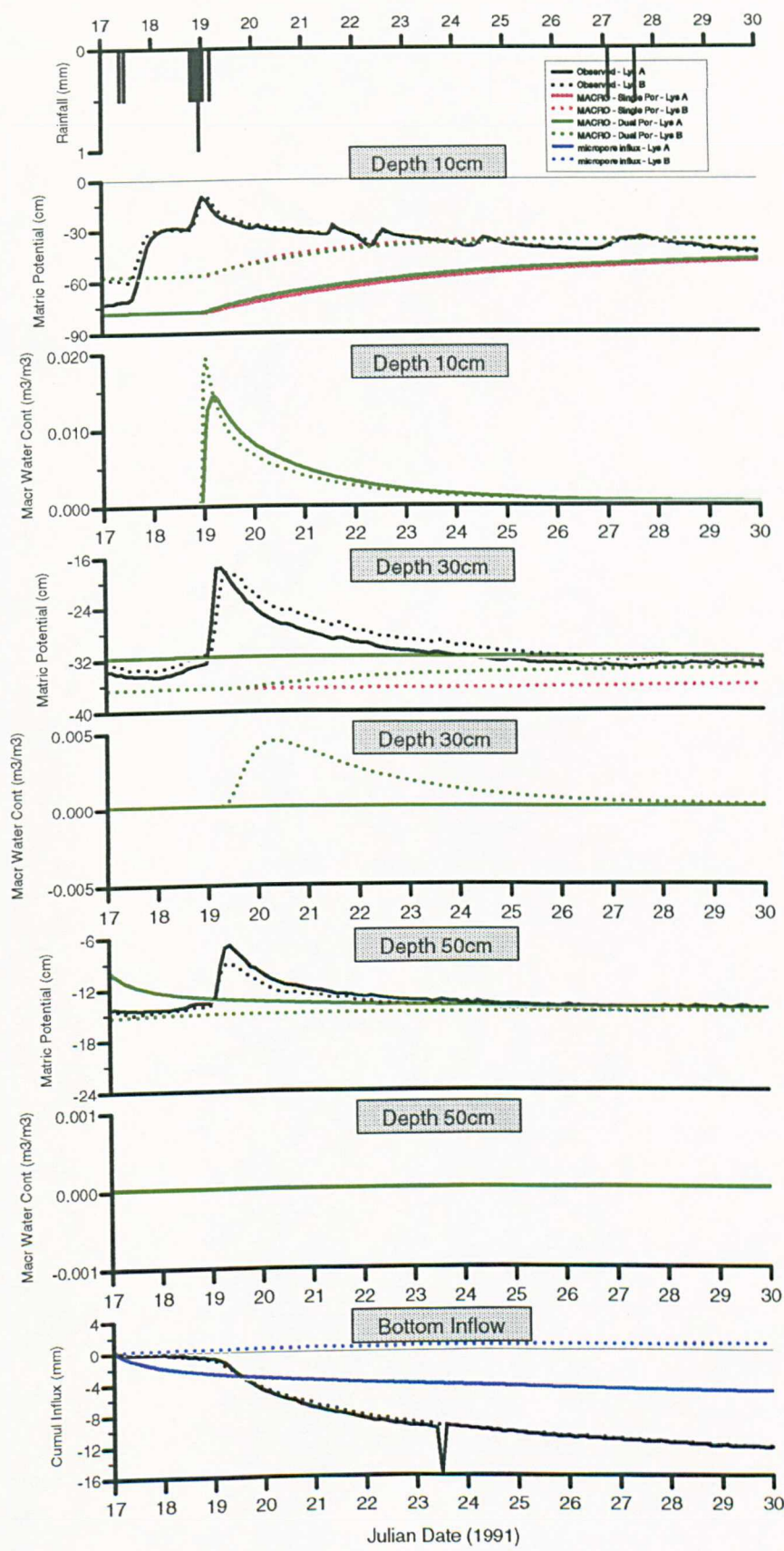


Figure 7.7 - Event 91017: results of MACRO simulations under homogeneous conditions

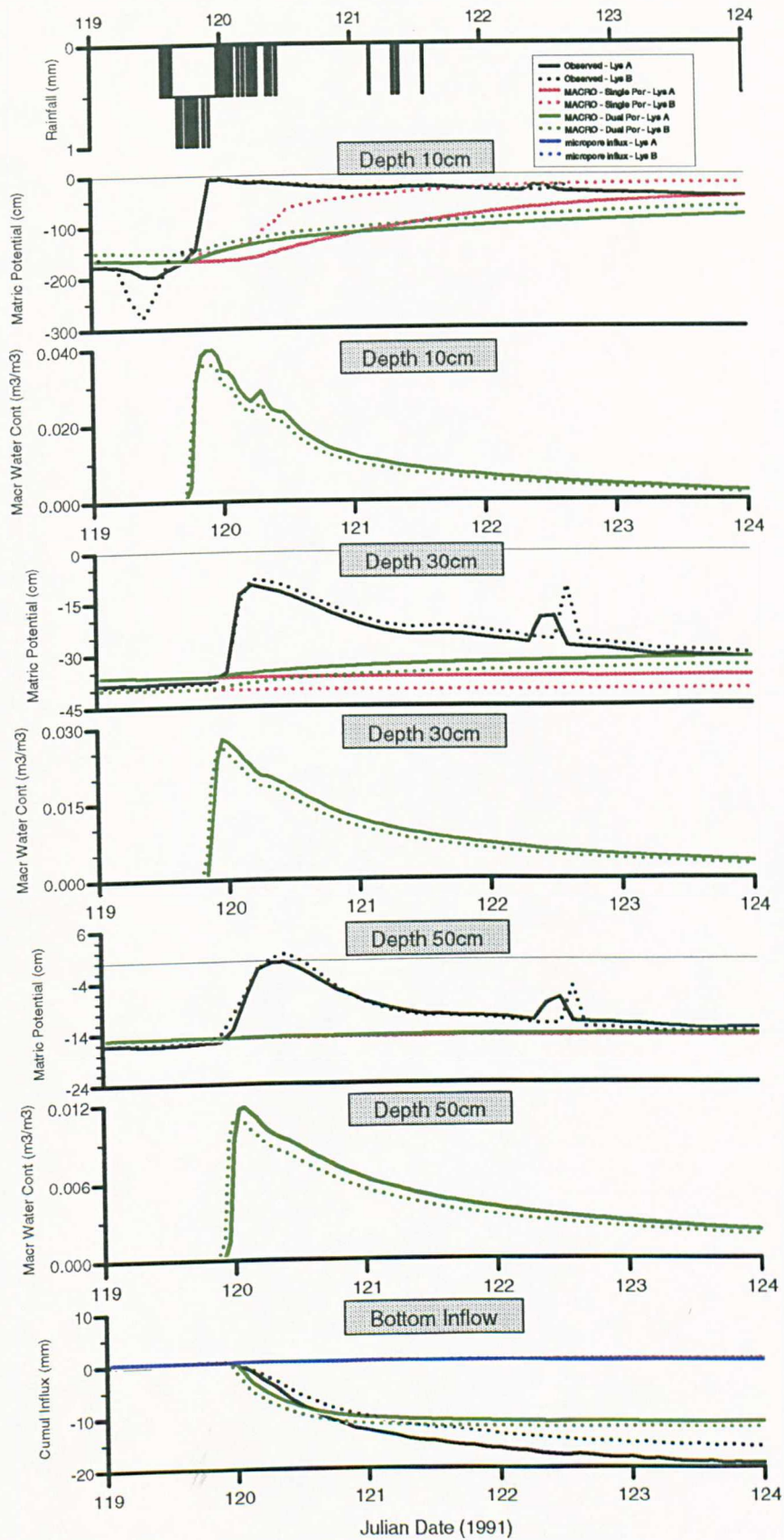


Figure 7.8 - Event 91119: results of MACRO simulations under homogeneous conditions

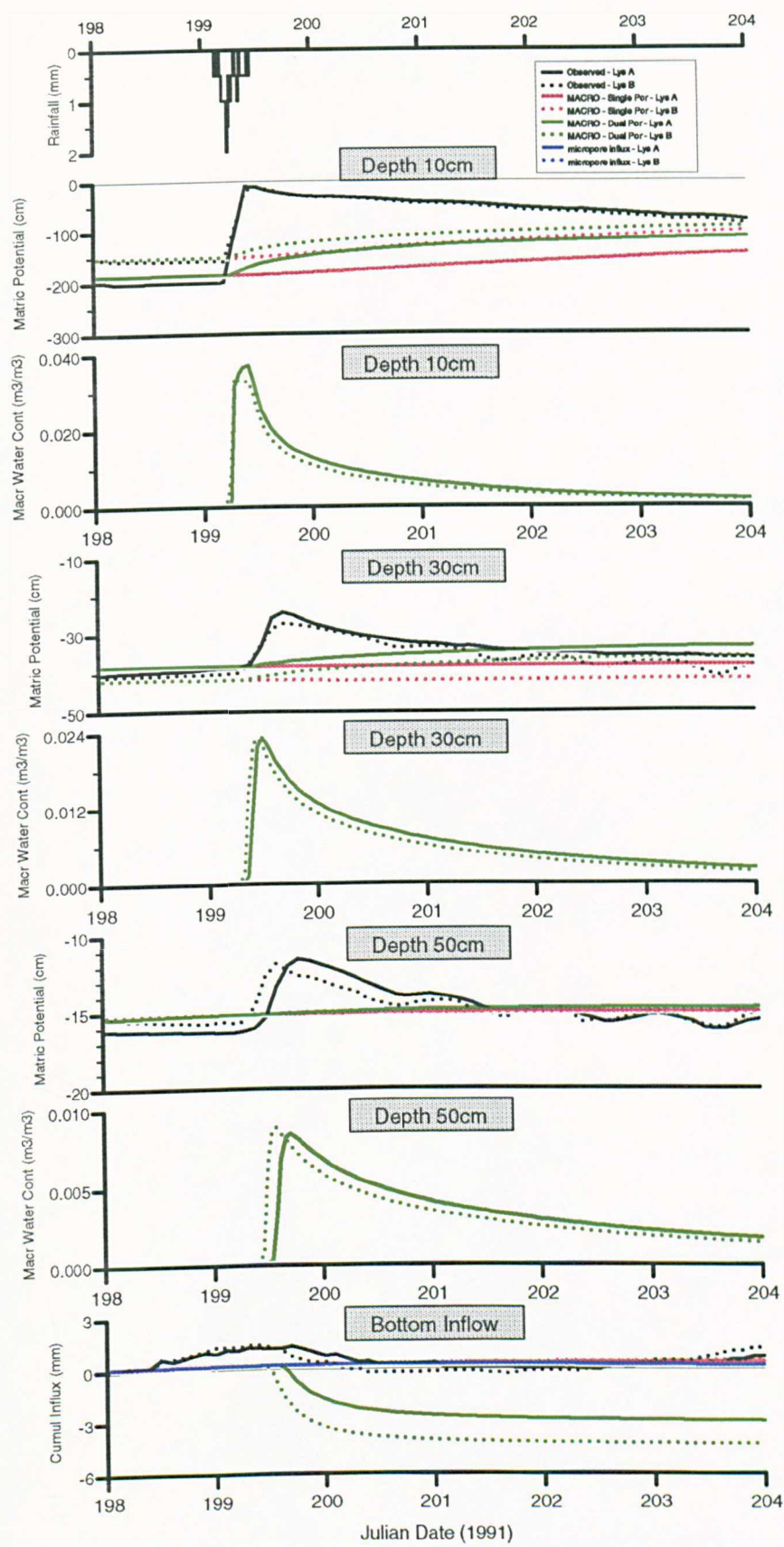


Figure 7.9 - Event 91198: results of MACRO simulations under homogeneous conditions

The simulations of the selected rapid flow events follow patterns similar to those described in section 7.3.1 for event 91211, where the shape of the rapid responses observed in the tensiometer data is reproduced by the simulated macropore water contents, and the micropore matric potentials tend to reasonably represent the observed tensiometer responses when the macropore water content is zero. Another common characteristic of the rapid flow events is a significant difference between the micropore and total influx, with the observed cumulative influx being better represented by the total seepage.

As already commented in chapter 4, the observed responses of event 90230 show different behaviour for lysimeters A and B. At the top layer, lysimeter A presents a pattern consistent with capillary flow, while lysimeter B shows evidence of rapid flow. At deeper layers, both lysimeters present evidences of rapid flow, but the bottom inflow from the common reservoir to lysimeter B is an evidence of slow flow. These apparent inconsistencies in the data, showing evidence of both slow and rapid flow for each lysimeter, bring difficulties to the interpretation of the simulation results. Figure 7.5 shows that, at the top layer, MACRO dual porosity simulations of event 90230 seem to represent the pattern of lysimeter B data, although they fail to reproduce its rapid recession. The simulated macropore water content reproduces the shape of the rapid responses of the tensiometers at the top and the middle of the profile. At the top layer, even the double peak pattern of the tensiometer data is reproduced by the macropore water content simulations. Also, the observed matric potentials of lysimeter A at the top layer are closely matched by the single porosity simulation, suggesting that they are due to capillary flow. When the effects of macropore flow stop, the single and dual porosity simulated values of matric potentials clearly converge to a same value.

The bottom inflow representation, however, presents some problems. Although the simulated values of bottom inflow are close to lysimeter A observations, both total and micropore inflow simulations fail to simulate lysimeter B data. These problems in the representation of bottom inflow can be related to the inconsistencies in the data referred to above, or to problems in the model conceptualisation. Nevertheless, the results showed in figure 7.5 are very significant: the similarities in the shape of the simulated macropore water content and the observed rise in the tensiometer data, including the double peak, and the fact that MACRO's single porosity simulation closely follows lysimeter A data seem to confirm the hypothesis raised in chapter 4 (i.e., the observed tensiometer responses at the top layer of lysimeter A are due to slow capillary flow, while those of lysimeter B correspond to preferential flow).

Events 90291 (figure 7.6) and 91119 (figure 7.8) present all characteristics already identified for the rapid flow events: the simulated micropore matric potentials tend to coincide with the observed tensiometer responses only when the macropore water content is zero, the shape of the rapid responses observed in the tensiometer data is reproduced by the patterns of the simulated macropore water contents along the whole depth profile, and the observed cumulative influx is better represented by the total seepage. Also, a coincidence in time between the effects of macropore flow and the observed peaks is noticeable both for matric potentials and bottom inflow, including the rapid response at 50 cm, that could not be reproduced by traditional single porosity models.

The simulated macropore flow for event 91017 (figure 7.7) reaches no deeper than the middle of the profile and is not transmitted to the bottom of the lysimeter. The simulated bottom inflow of lysimeter A is actually due to initial conditions: the simulated matric potentials at 50cm indicate a drainage at this layer, which induces outflow from the lysimeter to the common reservoir.

The simulations of event 91198 (figure 7.9) show micropore matric potentials similar to the observed tensiometer responses only when the macropore water content is zero, and the simulated macropore water contents reproduce the patterns of the tensiometer data along the whole depth profile. Also, dual and single porosity results seem to converge when the simulated macropore water content tends to zero. However, neither the micropore flow nor the total seepage provide a good fit to the observed bottom inflow. Before the rainfall, evapotranspiration occurs and, in response to that, some bottom inflow is induced. This effect is represented in the simulations, but the intensity observed is much larger than the simulated, so that the observed cumulative influx is much higher than the simulated when the rainfall starts. Immediately after the beginning of the rainfall, an outflow of water, from the lysimeters to the common reservoir, is observed, for both the data and the simulations, in response to rapid flow through the macropores. These results again indicate that the errors in the bottom inflow are due to underestimation of the evapotranspiration effects.

Results of the simulations of selected events 90129, 91108, 91165, 91204, and 90158 are presented in figures 7.10, 7.11, 7.12, 7.13 and 7.14 respectively. The inclusion of event 90158 in this group is because the model reproduces the slow flow observed in lysimeter A, instead of the rapid response of lysimeter B, as already commented in section 7.3.1. These simulations follow the patterns described for slow flow: the macropore flow is zero or limited only to the top layer and the total bottom inflow is equal to the micropore influx. The simulated

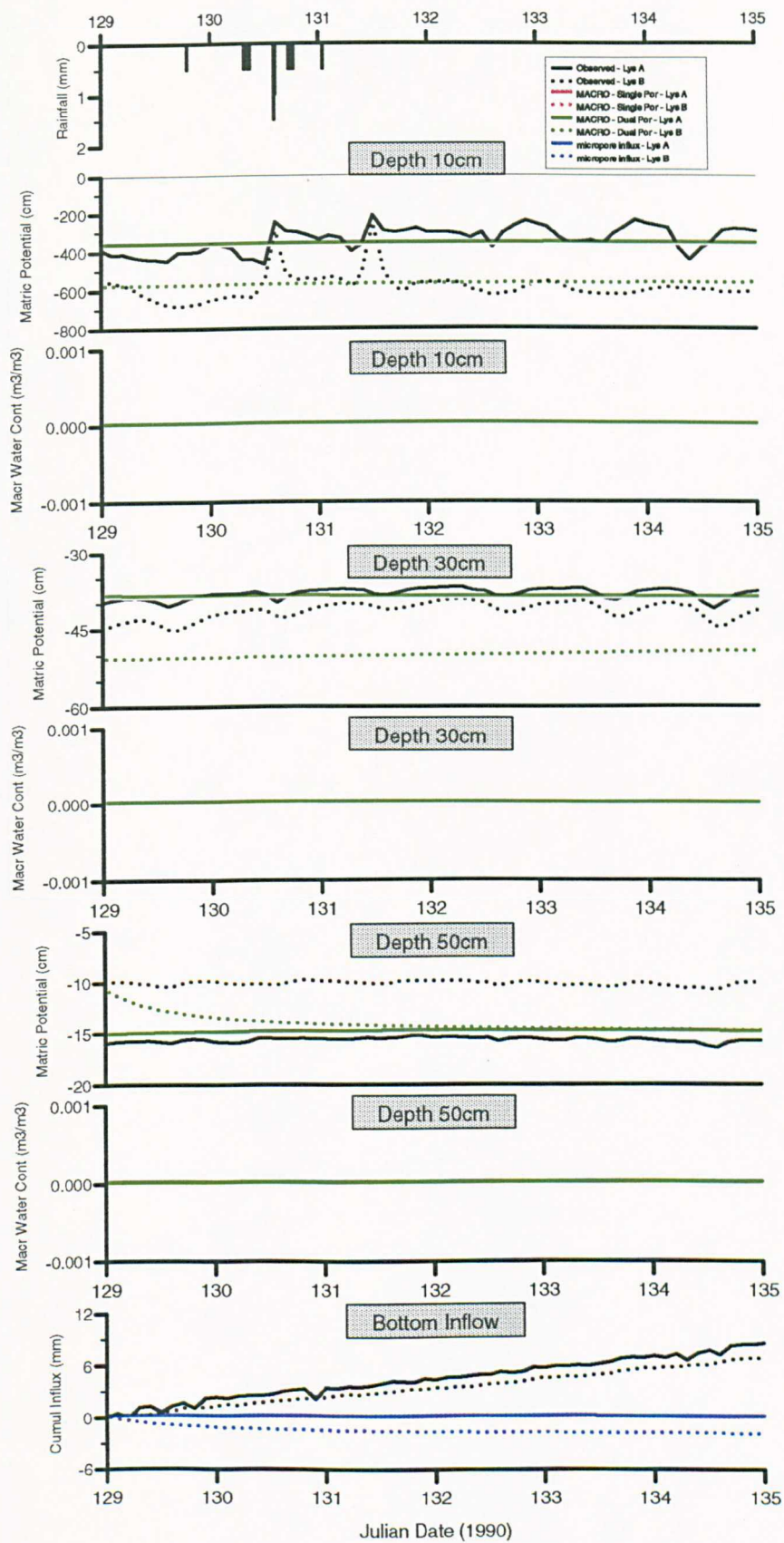


Figure 7.10 - Event 90129: results of MACRO simulations under homogeneous conditions

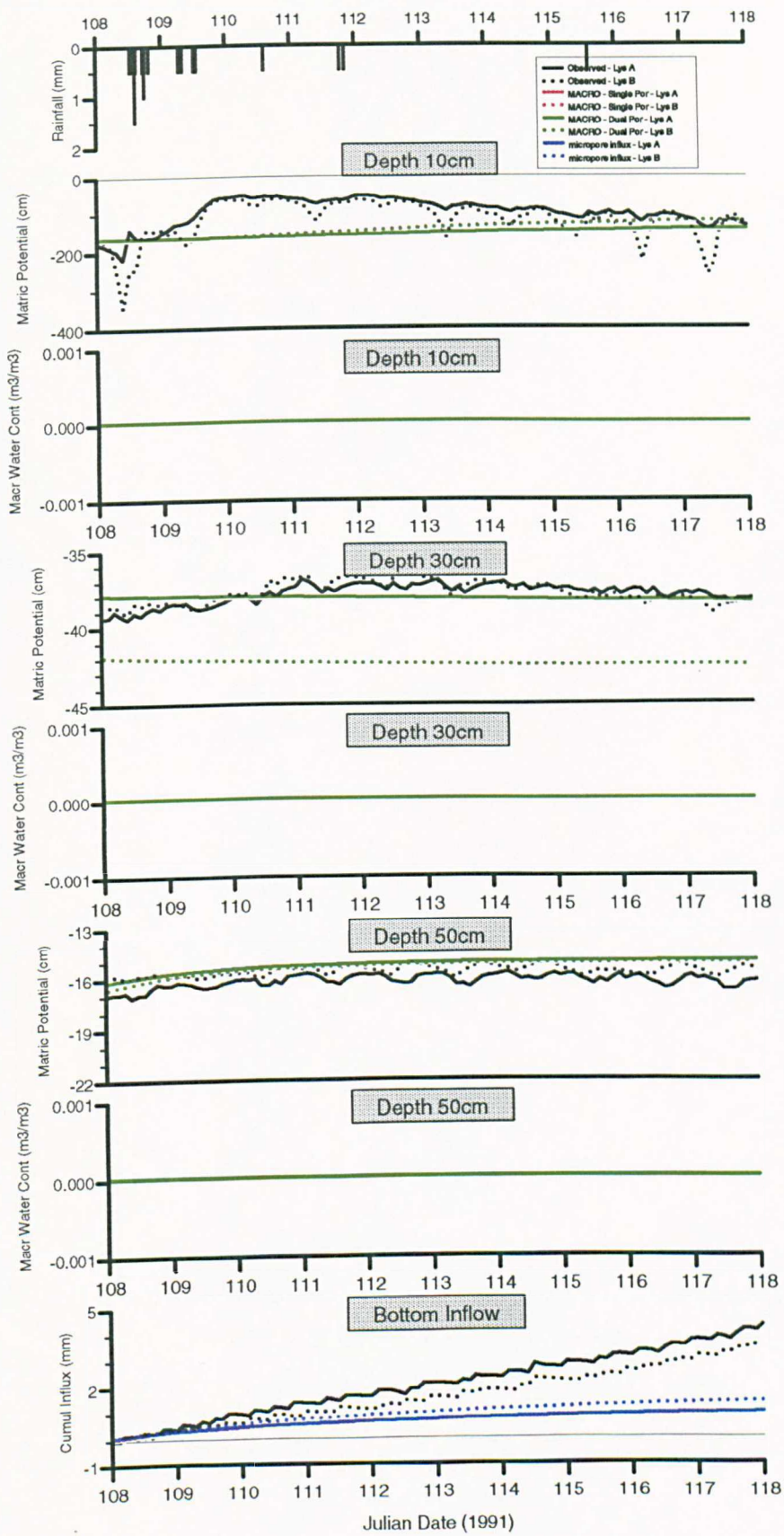


Figure 7.11 - Event 91108: results of MACRO simulations under homogeneous conditions

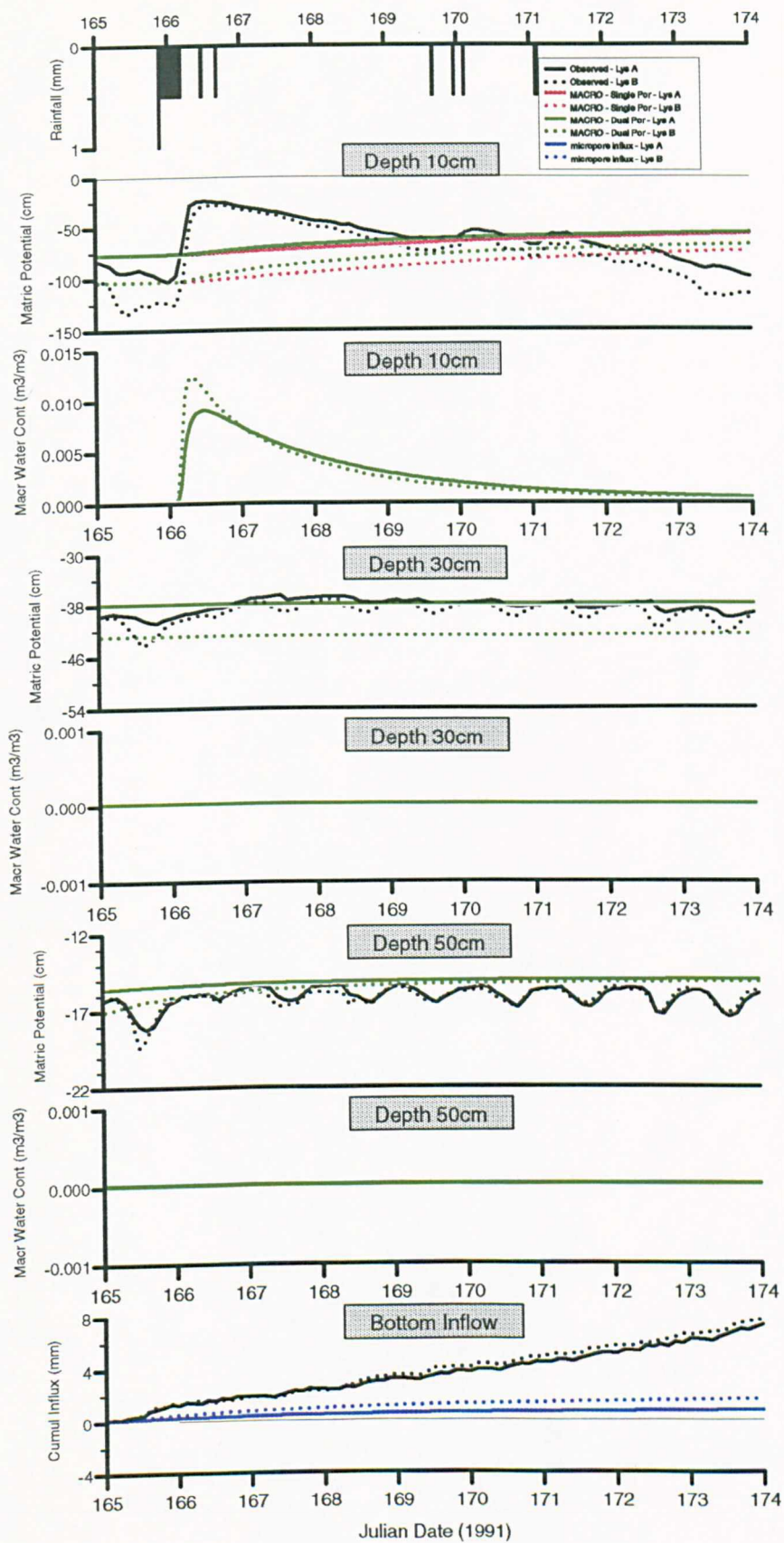


Figure 7.12 - Event 91165: results of MACRO simulations under homogeneous conditions

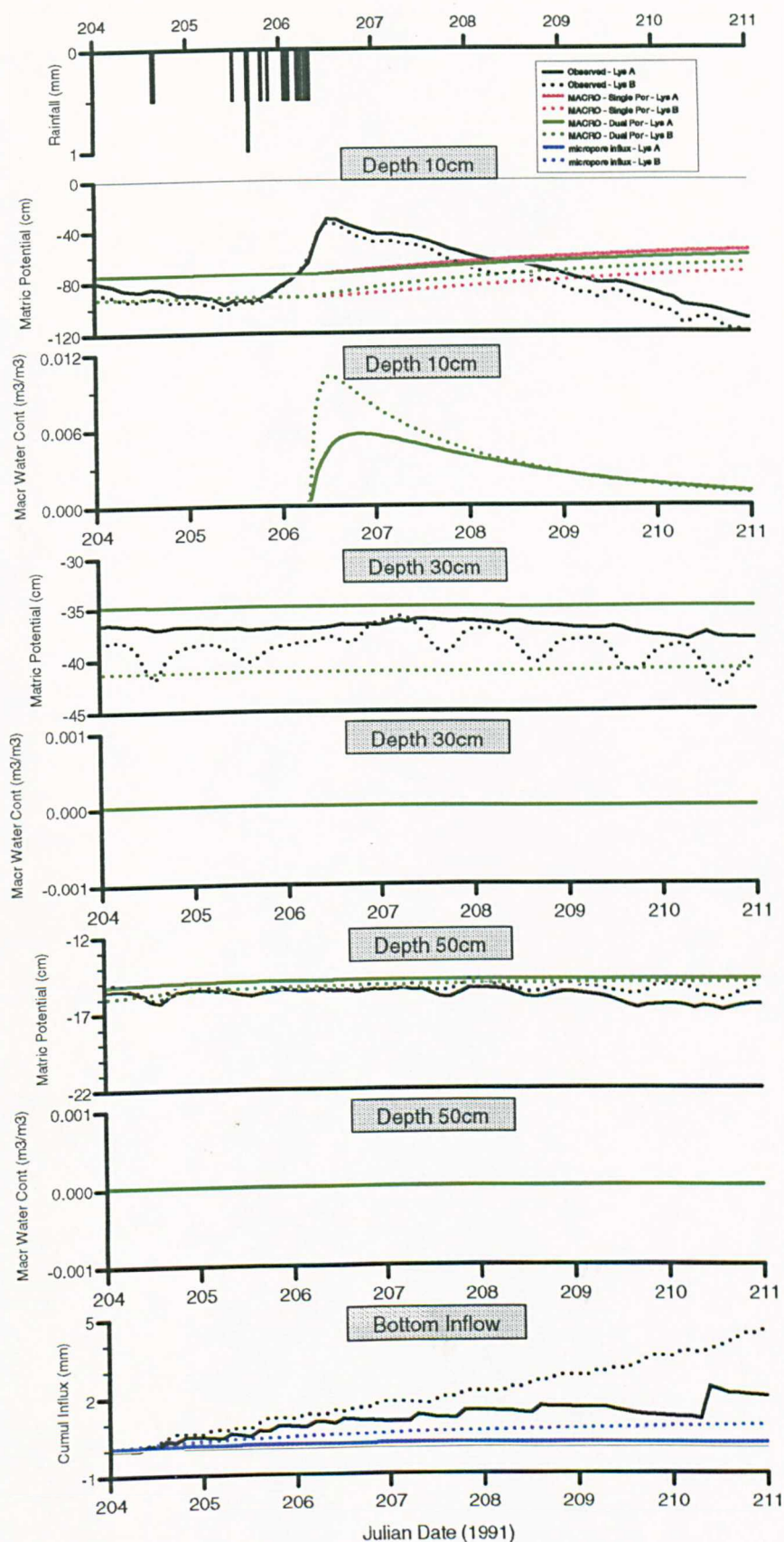


Figure 7.13 - Event 91204: results of MACRO simulations under homogeneous conditions

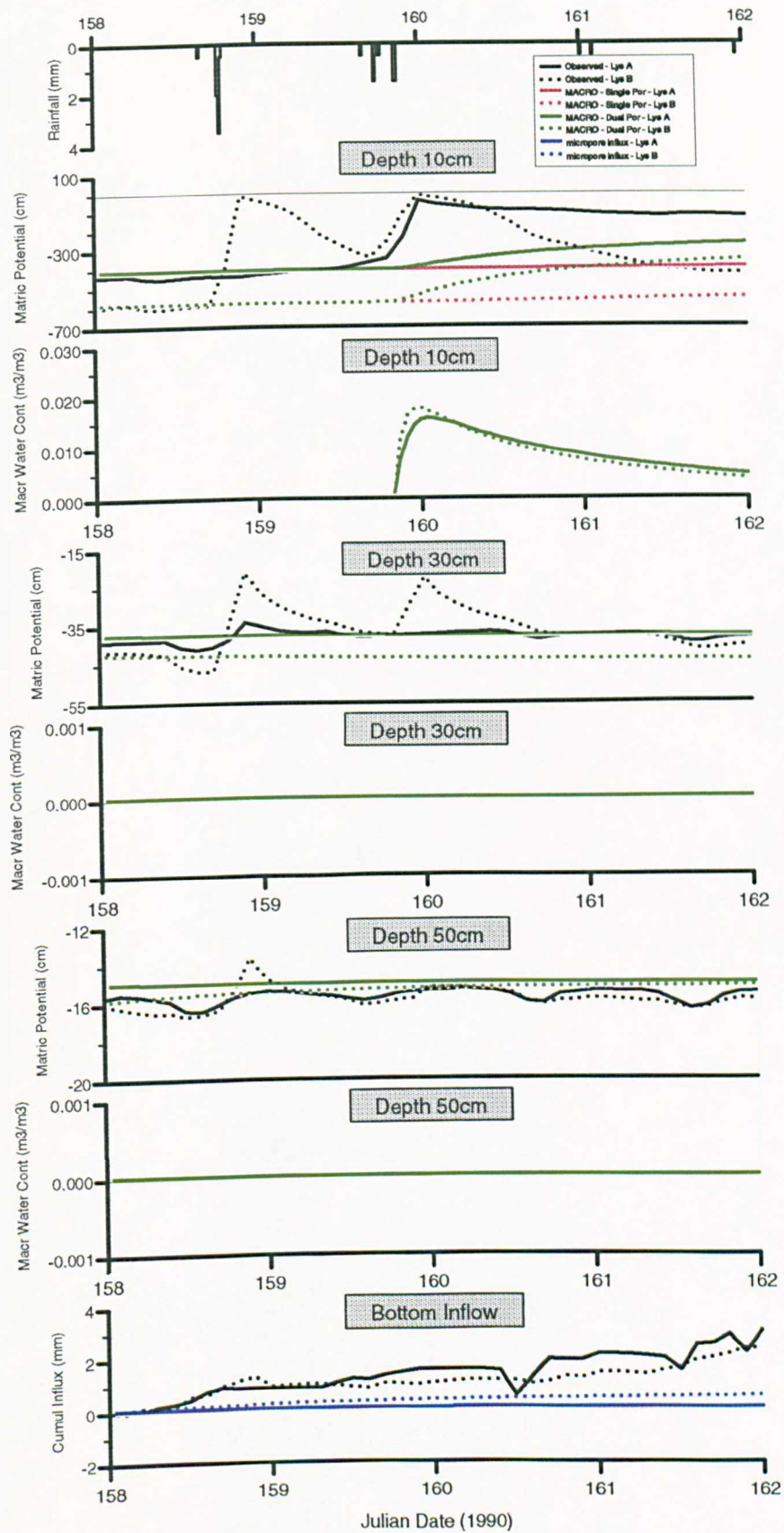


Figure 7.14 - Event 90158: results of MACRO simulations under homogeneous conditions

flow is usually from the common reservoir into the lysimeters, but the observed values are much higher than the simulations, due to the problems on representing water uptake, as commented for event 91198.

These errors in the bottom inflow representation could be caused by problems in the initial conditions or in the model representation of the processes controlling the effects of evapotranspiration, for the conditions adopted in this work. An exercise was performed in order to find the equilibrium situation to be used as initial conditions for the simulations that would allow the water uptake: the parameters relative to root water uptake were changed in order to enhance this effect (the root adaptability factor was reduced to zero; the root distribution factor was reduced to 25 %) and a simulation of a period of one year was performed, considering zero rainfall and a constant actual evaporation of 1 mm/day. The results of this exercise are shown in figure 7. 15.

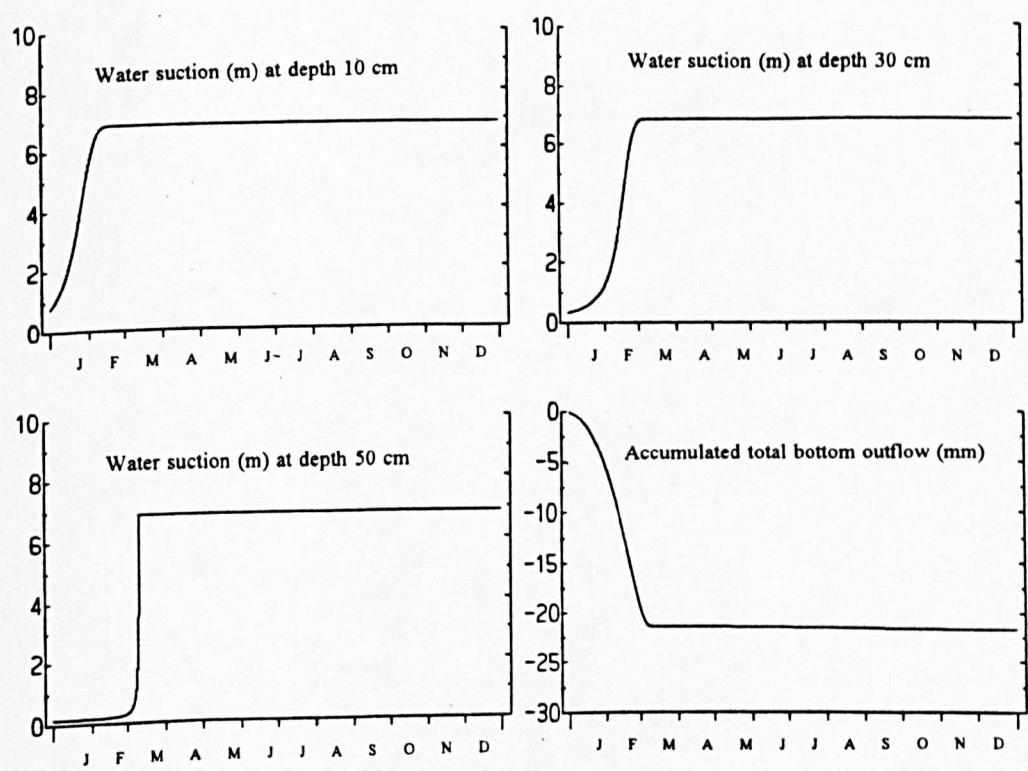


Figure 7.15 - Simulation exercise in order to determine the equilibrium conditions

It can be observed that an increase in the water suctions was transmitted down into the profile, in response to the drying processes due to the evapotranspiration. At the same time, an inflow of water was simulated at the bottom of the lysimeter, tending to a constant rate. When water started to be taken out from the bottom layer, a sudden change in the suction value occurred, at the same time that the bottom inflow ceased. This happened because, with the reduction in water content, also the hydraulic conductivity was reduced. Eventually, the hydraulic conductivity reached a very small value, which does not allow any further inflow, and the equilibrium conditions could not be reached. The results of this exercise show that there is a problem in the model conceptualisation when trying to represent water uptake due to evapotranspiration processes, for the conditions set up in this thesis. For this reason, the observed inflow of water could not be properly reproduced.

These errors are important, and can seriously limit the use of the model, at least under the same conditions adopted here. However, they do not invalidate the conclusions obtained for the matric potentials or even for the bottom inflow of the rapid flow events, as these results are due to macropore flow, which is not affected by the water uptake processes. As could be observed in the results presented so far, the errors in the representation of water uptake were important only when macropore flow was not observed.

7.4 - A physical interpretation of tensiometer measurements

The results of the simulations presented in this chapter provide further evidence that macropore flow influences the tensiometer response and also suggest that the tensiometer measurements correspond to a combined macro- and micropore stimulus. A physical reasoning for this is described below, assuming that the tensiometers are intercepting preferential flow paths.

A tensiometer intercepting a preferential flow path would register a combination of effects from the soil matrix and the macropores. If the macropores are empty, the tensiometer data would reflect micropore tension only. Extremely high suctions could be achieved for tensiometers in equilibrium with a very dry soil matrix. If preferential flow of water from the macropores reaches the porous cups of these tensiometers, this water is immediately sorbed by the porous cup, due to the difference in matric potential between the tensiometers and the macropore water. As the tensiometers in the experimental station were connected to pressure transducers, even a very small macropore water volume could cause a rapid increase in the instrument response. In this case, the tensiometer measurements could change very quickly from

a high suction, relative to the micropore status, to a near-saturation condition, caused by the macropore water. The change in the tensions can achieve one or even two orders of magnitude, as observed in some of the selected rapid flow events. When the preferential flow ceases, the macropore water is rapidly transferred to the soil and, after a relatively short time, the tensiometers go back to the condition of equilibrium with the tensions in the soil matrix. At the end of a rapid flow event, the tensiometers would indicate matric potentials of similar order of magnitude to those registered before the preferential flow occurred. The difference between the tensions before and after the rapid flow event is due to water stored in the soil matrix, coming from both preferential and slow flow.

Under this scenario, it is reasonable to hypothesise that, whenever macropore water occurs, its effect would be dominant in the tensiometer reaction, specially under very dry initial conditions. This hypothesis can explain why the results of MACRO simulations for the macropore water content reproduce the shape of the rapid responses observed in the tensiometer data.

The physical reasoning presented above is consistent with the observed data and also with the results of the simulations performed in this thesis. Therefore, it could be adopted as the theoretical basis for the development of a model combining inputs from both macro- and micropores, in order to test its validity and to obtain a better understanding of the soil water potential measurements and, consequently, of the water flow in unsaturated soils.

A simple way of modelling this effect would be to adopt the simulated micropore matric potentials as the tensiometer response when the macropores are empty, and to consider only macropore input otherwise. The tensiometer response resulting from the change in macropore water content can be interpreted as a fictitious macroporous potential (ψ_{ma}), so that the tension simulated as response of the tensiometer (ψ_{tens}) could be obtained as:

$$\psi_{tens} = \max [\psi_{mi}, \psi_{ma}] \quad (7.1)$$

The main difficulty in such model would be the determination of the fictitious macroporous potential, ψ_{ma} . The conceptualisation presented in the MACRO model is not applicable because it considers laminar flow under gravity in the macropores and consequently ψ_{ma} is not required. A possible solution would be to use an analogy of the solution adopted for MACRO in one flow domain, where the potentials in the macropore region are computed by a

linear function between the boundary potential, ψ_b , and saturation. However, this option would imply that the minimum macropore potential is the boundary value, ψ_b . Therefore, whenever there is a macropore flow, the simulated matric potentials would oscillate between the ψ_b value and zero. In the simulations performed in this thesis, $\psi_b = -10\text{cm}$. This means that the effect of the macropore flow would cause an immediate jump in the matric potentials from the micropore potential, ψ_{mi} , to -10cm . When the macropore water content falls to zero, the simulated matric potentials would immediately decrease to the ψ_{mi} value. The observed tensiometer records do not follow this pattern. Although the change in matric potentials is fast, it is not immediate. Also, values much smaller than -10cm are observed in the top layer, coinciding with non-zero macropore water contents, and the information available is not enough to a priori determine a valid minimum value of the fictitious macropore tension.

A simple scaling of the simulated macropore water contents is not applicable either. An analysis of the events that present a double-peak pattern shows that the simulated θ_{ma} in the second peak is nearly half the value of the first. This would lead to a second peak in the matric potentials much lower than the first. However, for events 90230 and 91211, where a double peak is observed, the registered matric potentials are of same order of magnitude in the first and second peaks. As the simulated micropore tensions are higher at the time of the second peak, it seems that it would be necessary to add the effects of micro- and macropore in order to reproduce the tensiometers response. This addition is not consistent with the physical reasoning used to explain the mechanisms involved in the tensiometer response when intercepting a macropore.

A possible explanation for these difficulties in using MACRO results to simulate the tensiometer response is that this model actually provides a macroscopic representation of the system: the simulated variables are representative of a layer of the soil, and not of a specific pore. The simulated values are equivalent to a mean response of a representative elementary volume (REV) equal to a soil layer, and not to the scale of the real tensiometers and macropores. Also, the empiricism of the functions adopted in MACRO methodology complicates the physical interpretation of its results.

It seems that the MACRO simulations, as well as other preferential flow models, as commented in section 3.5, are important in suggesting that macropores play an important role in the soil water flow and help to understand some of the physical processes entailed. However, the lack of experimental data on the nature of macropore flows, the structure of macropore systems and the interactions between macropores and the matrix do not allow a proper

calibration, validation and interpretation of these results.

7.5 - Conclusions

The MACRO model was applied to the events selected in chapter 4 for single and dual porosity modes, both under homogeneous and heterogeneous conditions, using parameters fitted to observed $\theta(\psi)$ and K_s data, in order to investigate the importance of preferential flow.

The MACRO model requires a big number of input parameters and the information necessary to estimate their value is not always available. This was the case for the effective diffusion pathlength, and, consequently, a calibration was performed. The model showed a significant sensitivity to the value of the effective diffusion pathlength, which can increase the uncertainty in using MACRO when this parameter cannot be easily determined. A deficiency in the representation of water uptake due to evapotranspiration effects, under the conditions adopted for the simulations, was observed in the model and can cause problems for long-term simulations of experimental data.

The macropore matric potentials obtained with MACRO model show good fit to the observed tensiometer data only when the macropore water content is zero. The simulated macropore water contents, when different than zero, seem to reproduce the shape of the rapid responses registered by the tensiometers and to induce a rapid response in the bottom inflow. These results suggest that the observed tensiometer response can be represented by a combination of macro- and micropore effects and show the need to develop a model to simulate the soil/tensiometer system.

A detailed analysis and a physical interpretation of these results provided a theoretical basis for the future development of a model combining inputs from both macro- and micropores, which can allow a better understanding of soil water potential measurements. However, such model could not be formulated because of limitations in the MACRO model and also due to lack of data which would allow the definition, calibration, and validation of an adequate model of a combined macropore/matrix system.

CHAPTER 8 - SUMMARY, CONCLUSIONS AND FUTURE DIRECTIONS

8.1 - The experimental station and available data

Imperial College is undertaking a combined modelling and experimental study at the College's Field Research Station at Silwood Park, near Ascot, England. The experimental station at Silwood Park consists of an automatic weather station and eight concrete lysimeters. It was designed as part of a contract undertaken by Imperial College under the Nirex Safety Assessment Research Program (NSARP) to develop methods to evaluate the risks of possible migration of radionuclides from a proposed repository in the UK for low and intermediate level radioactive wastes.

The lysimeters were filled with a sieved, mixed and homogenised sandy loam soil to a depth of either 40 or 70 cm and a crop of wheat was grown in each one of them. They have controlled water tables at 5 cm above the base of the soil and are provided with equipment for measuring root distribution, redox potential, crop height, leaf area index, pH and soil moisture properties (access tubes for neutron probe, TDR, pressure-transducers + tensiometer systems). The system designed to control the water table level allows the measurement of the flow through the base of the lysimeters, providing full knowledge of the lower boundary condition.

The influx/outflux of water through the base of the lysimeters and the matric potential data were used to identify the pattern of response of the system to rainfall input, with special emphasis to recognising evidences of rapid, or preferential, water flow. Nearly 70% of the events were identified as rapid flow events. A set of 8 of them, where the evidence of rapid flow was significant and representative of the different situations observed in the whole data set, was selected and designated for detailed analysis and mathematical simulations. This set of eight events covers all observed main features in the identified rapid flow events, as the great majority of them present very similar patterns. A set of 4 events where no evidence of preferential flow can be assumed is also identified. Both sets of events were selected in order to assess the performance of different modelling approaches and to test hypotheses describing the physical processes governing the flux of water in the near surface environment.

Values for the particle size distribution, saturated conductivity, porosity, dry bulk density and void ratio were provided by physical analysis of soil cores taken from the lysimeters. The results of these tests showed that there is enough statistical evidence to identify a difference in the values of porosity, dry bulk density and void ratio for the top layer of the soil, when

compared with the deeper layers. This behaviour can be explained by the higher biological activity in the top soil. Statistical evidence of a significant difference in saturated conductivity could not be identified, due to the high spatial variation of this variable. However, as the mean values of saturated conductivity for two adjacent soil layers presented a difference of one or even two orders of magnitude, these values were adopted to simulate vertical heterogeneity in the soil.

Estimates of parameter values and associated uncertainty of three different soil characteristic parametric relationships, under assumption of single porosity, were obtained through the use of first-order error analysis applied to the available $\theta(\psi)$ data, using a Simplex or a quasi-Newton algorithm. This methodology lead to the adoption of a single soil moisture characteristic curve and a fixed value of saturated moisture content for the whole depth profile. The errors produced by sets of parameters considering vertical heterogeneity in the soil properties, as suggested by the physical analysis of soil cores, were of same order of magnitude of those given by homogeneous representations. Also, the uncertainties due to input parameter error were quite small when compared to the data variation, suggesting that other sources of uncertainty, such as data error (due to measurements inaccuracies or to spatial variability) or uncertainty in the model itself, should be investigated.

8.2 - Limitations in the use of Richards' equation based models

The SPW1 model was developed as part of the study that is being undertaken by Imperial College on behalf of UK Nirex Ltd. It is a physically-based soil-plant-water-model which combines a plant water and a soil water sub-models in a single model. The soil water flow model uses the Darcy-Richards' equation to simulate one-dimensional unsaturated flow. SPW1 does not include the representation of preferential water flow or hysteresis in the hydraulic properties of the soil, but it has been shown to be able of handling the types of problems that occur in the field and to perform in a superior manner against an internationally recognised unsaturated flow model.

The SPW1 model was selected to test the strengths and limitations in the use of traditional models of water flow in the unsaturated zone based on the Richards' equation. It was adapted in order to include the moisture characteristic relationship employed in the MACRO model for single porosity mode, for comparison with results using Van Genuchten's and Brooks-Corey's curves. The adapted version was applied to the previously selected events, alternatively considering homogeneous profile or vertical heterogeneity of the saturated conductivity.

When the model was employed using parameters fitted to observed $\theta(\psi)$ and K_s data, an important effect was observed due to the influence of the initial conditions (which were obtained from measured data). As the soil was not in hydrostatic equilibrium in the beginning of the events, the differences in total potential induced movement of water from the bottom to the top of the profile. Under homogeneous conditions, this caused an inflow from the common reservoir into the lysimeters. However, under heterogeneous conditions, a small value of saturated conductivity was estimated for the bottom layers, restricting the flow velocity, so that the water for the top was provided by the middle of the profile, where a reduction on the matric potentials happened. Simulations using MACRO's characteristic curve did not present this behaviour, because they were controlled by the low values of the boundary conductivity, which allowed only slow water movement along the soil profile.

Poor representations of the observed bottom inflow were obtained for a homogeneous soil profile with the parameters fitted to observed $\theta(\psi)$ and K_s data. The use of heterogeneous conditions for the saturated conductivity improved these results, but it was suggested that the amelioration observed was actually due to the reduction of the saturated conductivity value at deeper layers, compensating effects induced by the initial conditions, as commented above. The simulations obtained gave indications that there is a problem in the model conceptualization or in the parameter values of SPW1 when representing the observed rapid flow events using parameters fitted to observed $\theta(\psi)$ and K_s data. This analysis also suggested that the model can properly represent slow flow events, at least when initial conditions are close to hydrostatic equilibrium.

A methodology for optimising SPW1 parameters per event was developed, using a Simplex or quasi-Newton routine to minimise the error between observed and simulated values of matric potential and/or bottom influx. This methodology was applied to the selected events, for homogeneous and heterogeneous conditions, using Van Genuchten's and Brooks-Corey's equations only, as MACRO's methodology was shown to be controlled by the boundary hydraulic conductivity value. Simultaneous optimisations of matric potential and bottom influx were adopted, because, for the great majority of the simulations, when matric potentials were optimised, the fit between observed and simulated bottom influx was very poor; when the bottom influx was optimised, few simulations produced reasonable or good fit between observed and simulated matric potentials. The optimisation response surface was revealed to be very flat, with several local minima, so that it was not possible to ensure that the solutions found for each case correspond to global minima. For this reason, for each event, the model was run for both Simplex and quasi-Newton optimisation routines, using various different sets of initial values

for the parameters, and the minimum value was adopted as the best result. Although this procedure does not guarantee that the solution found is the global minimum, the results of the simulations seem to show that, given an adequate combination of parameter values, the model is able to provide good fits. However, a big variation in the estimates of the optimised parameters from event to event was observed. The values of the parameters that produce a maximum agreement between the simulations and the observed data often lack physical basis and attempts to correlate them with other variables were not successful, bringing difficulty for the use of the model as a predictive tool. Also, problems in the representation of some rapid responses were observed, even with a major variation in parameter values. This suggests an inadequacy of the model conceptualization for simulating rapid flows, although problems due to local minima being taken as optimum parameters, or even inconsistencies in the observed data could also have influenced these results. The simulations with optimised parameters seem to confirm that SPW1 can properly represent slow flow events, but a good fit was frequently achieved via a substantial change in parameter values, again bringing difficulties for the use of the model as a predictive tool. The results also showed that the soil characteristic curve parameters seem to play a more important role than the saturated conductivity in the representation of the matric potentials.

These results indicate that the traditional modelling approach of the Richards' equation to simulate unsaturated flow, as adopted by the SPW1 model, presents weaknesses when trying to represent observed rapid flows. The determination of a unique set of parameters able to optimise the representation of observed matric potentials and bottom inflow for the whole set of selected events can be considered a fundamental problem, implying a possible indication of temporal changes in soil structure, or simply non-uniqueness of the inverse procedure. The evident inadequacies in model conceptualisation suggest the necessity to study modelling approaches not considered in the SPW1 model, such as the effect of hysteresis and also preferential flow.

8.3 - Effects of hysteresis and air entrapment

The limitations of the SPW1 model conceptualisation show that alternative techniques have to be tried. The successive cycles of wetting and drainage naturally occurring in the lysimeters suggest the necessity of taking into account the hysteretic nature of the hydraulic properties of the soil. A model of hysteresis considering air entrapment, based on those presented by Kool and Parker (1987) and Parker and Lenhard (1987) was adapted and tested in order to run in conjunction with the SPW1 model. To describe the scanning curves, it employs

an empirical procedure which rescales main branch functions to pass through appropriate reversal points, enforcing the closure of scanning loops. An empirical procedure is also adopted to incorporate the effects of air entrapment into the model. One of the main advantages of this methodology is its parametric simplicity, which facilitates its implementation with minimal effort, as it does not require any parameter that was not previously included in model SPW1. On the other hand, it had the disadvantage that it is necessary to know two previous reversal points for each scanning branch, bringing the necessity of large storage requirements. Also, when a simulation starts in a scanning curve, these two reversal points have to be known in order to set the initial conditions for simulation. An algorithm to estimate the reversal points was developed, in order to allow the use of the hysteresis model when the previous points are unknown, providing the initial conditions for simulation. The hysteresis model and the initial conditions algorithm have been shown to perform well when tested against experimental and synthetic data. The SPW1 model was adapted in order to incorporate the hysteresis model and the initial conditions algorithms. This new version (also including the methodologies adopted by MACRO to represent, in one flow domain, the soil water retention curve and the unsaturated hydraulic conductivity), called SPW1hyst, was used in this thesis to investigate how air entrapment and hysteresis in the soil characteristic curve affects the unsaturated soil water flow.

The significance of hysteresis and air entrapment was investigated through the application of SPW1hyst, in both hysteretic and non-hysteretic modes, to event 91136, where injection of a relatively small volume of water below the water table was observed to generate a significant perturbation of soil water states in all lysimeters. This event can not be explained by treating the soil as a uniform porous medium, strongly suggesting preferential flow mechanisms. Results for simulations under non-hysteretic mode, using boundary conditions derived from experimental information, were compared to simulations under hysteretic mode and also to a non-hysteretic representation where the boundary fluxes were increased by a scaling factor of 7.5. Both hysteretic and scaled representations imply the existence of preferential flow paths: the scaling of the boundary fluxes is equivalent to flushing the original volume of water through a much smaller area, corresponding to that of the preferential pathways; the hypothesis for introducing hysteresis and air entrapment is that, as the water was introduced into the system, it rose through preferential paths, causing the entrapment of air. The excellent fit observed for both the hysteretic representation and the scaled non-hysteretic simulations seems to confirm these hypothesis. The set of parameters fitted for the hysteretic simulation of event 91136 was applied to the other selected events, and the outcomes seem to indicate that air entrapment and hysteresis in the soil characteristic curve can be used to explain the observed variations in the bottom inflows, but has minor influence for matric potentials.

The methodology developed to optimise SPW1 parameters per event was applied to the selected events in hysteretic mode, under homogeneous conditions, optimising simultaneously matric potentials and bottom influx. A comparison of these results with the hysteretic simulations of the selected events using the parameters fitted for event 91136 showed that significant improvement in the representation of bottom inflows was obtained in conjunction with slight worsening of the results for the simulations of matric potentials, seeming to confirm that air entrapment and hysteresis in the soil characteristic curve can improve the representation of bottom inflows, but has minor influence for matric potentials. The results indicate that hysteresis and air entrapment can help to simulate rapid flow responses, but major variations in the parameter values can be necessary to obtain a good fit. The results for slow flow events seem to show that the hysteretic mode can bring difficulties to the representation of matric potentials, as the model becomes too sensitive to rainfall inputs and can suggest faster water flow responses than those observed.

The problem of determining a unique set of optimised parameters for the whole set of selected events is not solved by the inclusion of hysteresis and air entrapment in the SPW1 model. The results from the various conceptualisations seem to show that, although good fits to the observed data can be obtained by the use of an adequate combination of parameter values, there are still inadequacies in the model. Evidence of preferential flow suggests the necessity of dual porosity models in order to simulate soil water flow processes.

8.4 - Effects of preferential water flow

The MACRO model was selected in order to test the effects of preferential movement in unsaturated water flow. It is a deterministic model of non-steady state water and solute transport in macroporous field soils that can be run in either one or two flow domains. The model includes a comprehensive treatment of most of the processes involved, using simple formulations in order to provide a modelling device that can be easily applied to field soils. Its major disadvantage is its empirical nature.

A key parameter for the estimation of the water exchange is the effective diffusion pathlength (d , equal to half the aggregate width). The model showed a significant sensitivity to the value of this parameter when a calibration was performed in order to define it, which can increase the uncertainty in using this model when this parameter cannot be easily determined. It was also observed that the MACRO model needs a big number of parameters and that the information necessary to estimate their value is not always readily available.

The MACRO model was applied to the selected events for single and dual porosity modes, both under homogeneous and heterogeneous conditions, using parameters fitted to observed $\theta(\psi)$ and K_s data. The shape of the rapid responses observed in the tensiometer data is reproduced by the patterns of the simulated macropore water contents. On the other hand, when the macropore water content is zero, the micropore matrix potentials tend to reasonably represent the observed tensiometer responses. There is small difference between the homogeneous and the heterogeneous results, due to the fact that the MACRO simulations in the micropore range were controlled by the boundary hydraulic conductivity value.

The MACRO simulations seem to indicate that the observed response could be reproduced by a combination of micro- and macropore effects, implying that the tensiometers were intercepting a preferential flow path, and, consequently, they were registering stimulus from both domains. A physical interpretation of these results provides a theoretical basis for the future development of a methodology able to combine macro- and micropore effects in order to represent soil water potential measurements. However, such a model could not be formulated because of limitations in the MACRO conceptualisation and also due to lack of experimental data on the nature of macropore flows, the structure of macropore systems and the interactions between macropores and the matrix.

It should be noticed that these results were obtained using parameters fitted to observed $\theta(\psi)$ and K_s data, under assumption of single porosity, and without any further optimisation, except for the effective diffusion pathlength. This implies that, despite the limitations of their conceptualisation, the use of dual porosity models in order to simulate the soil water flow processes can provide an answer for a problem that could not be solved by the single porosity approaches tested in this thesis: the determination of a unique set of parameters valid for the whole set of selected events. The consistency of the results obtained with this methodology strongly suggests the necessity of a macroporous flow model to represent the observed data, providing even more evidence of the presence of preferential flow.

8.5 - Future research directions

The results obtained in this thesis highlight the difficulties in understanding, measuring and representing the complex processes regulating soil water flow. The successes achieved and the difficulties found suggest future experimental and modelling work in the direction of two mechanisms that are not only non-exclusive, but are closely related to each other: heterogeneity and preferential flow.

A suggestion for future experimental work is the implementation of a procedure for continuous measurement of the soil moisture contents, using the same time resolution adopted for the matric potential data. In the case of the experimental facility at Silwood Park this could be achieved by the use of the TDR associated with a dedicated computer, in order to automatically record the soil moisture. This would allow the use of a simulation optimisation method instead of static $\theta(\psi)$ measurements for the parameter estimation. A proper model calibration would be possible, either by conducting a dynamic flow experiment (i.e., infiltration, redistribution and/or drainage event) or by identifying events where these processes naturally occur, and then to use the observed water content, pressure head and/or boundary flux data to invert the governing initial-boundary value problem. With this dynamic data, mechanisms such as hysteresis could be identified and the methodologies for their representation could be properly validated, calibrated and verified.

Another suggestion for experimental work is the adoption of more than one vertical array for measuring the soil properties and variables, in order to identify possible horizontal variability. Comparisons of vertical profiles of soil water flow variables in different spatial locations inside a same unit, such as a lysimeter, would allow a better identification of heterogeneity in soil properties and could also help in the understanding of preferential flow processes.

The natural variability of aquifer materials means that a detailed deterministic model which represents the actual heterogeneity of the aquifer would require enormous computational resources and would be impractical in terms of the amount of data required. An obvious suggestion for future modelling works is the use of stochastic techniques in order to obtain a better representation of the hydraulic variables and soil properties and also of the uncertainties associated with this variability.

Uncertainty is another issue closely related to the question of heterogeneity. Uncertainty in model predictions can result from three primary sources: (1) uncertainty in the model itself, because of an incomplete understanding of the underlying physical process(es), leading to incorrect and/or oversimplified representation of reality; (2) uncertainty in the model parameters, because of error in estimating parameters; and (3) error in the data, due to measurement error and/or spatial variability in properties of the medium. In the present thesis, a methodology was developed and applied for the estimation of the uncertainties due to input parameter error. The other sources of error, however, were not explicitly analyzed. The development and application of a proper methodology in order to identify and quantify these errors is of fundamental

importance, and could be a major line of action in future works.

It is also suggested to adapt SPW1 model in order to incorporate the representation of preferential flow, and allow comparison between these processes and water flow in the soil matrix. Although this comparison is possible with MACRO model, the empirical nature of the relations adopted in this model can bring difficulties for the understanding of the real physical processes involved. SPW1, being a physically-based model, can provide a better basis for the interpretation of these phenomena.

Finally, the need for a model able to simulate the soil/tensiometer system was shown by the results of MACRO simulations. Consequently, the development of a model that represents tensiometer data using a combination of macro- and micropores effects is suggested. Such model can be used to test the physical interpretation provided in this thesis for the observed rapid water flow events and can allow a better understanding of soil water potential measurements and of the processes controlling preferential movement of water in the soil.

References:

- Abeliuk, R. and Wheeler, H.S. 1990. Parameter identification of solute transport models for unsaturated soils. *Journal of Hydrology*, Vol. 117, pp.199-224.
- Alexander, L. and Skaggs, R.W. 1986. Predicting unsaturated hydraulic conductivity from the soil water characteristic. *Transactions of the ASAE*, Vol. 29, No.1, pp. 176-184.
- Alexander, L. and Skaggs, R.W. 1987. Predicting unsaturated hydraulic conductivity from soil texture. *Journal of Irrigation and Drainage Engineering*, Vol. 113, No. 2, pp. 184-197
- Anderson, J.L. and Bouma, J. 1973. Relationships between saturated hydraulic conductivity and morphometric data of an argillic horizon. *Soil Science Society of America Proceedings*, Vol.37, pp. 408-413.
- Anderson, M.P., Ward, D.S., Lapalla, E.G. and Prickett, T.A. 1993. Computer models for subsurface water. In: Maidment, D.R., ed. *Handbook of hydrology*. McGraw-Hill Inc, New York, Chapter 22.
- Arya, L.M. and Paris, J.F. 1981. A physicoempirical model to predict the soil characteristic from particle-size distribution and bulk density data. *Soil Science Society of America Journal*, Vol. 45, pp. 1023-1030.
- Aziz, K. and Setari, S. 1979. *Petroleum reservoir simulation*, Applied Science, Barking, United Kingdom.
- Babel, M.S., Loof, R. and Das Gupta, A. 1995. Fingering preferential flow in unsaturated homogeneous coarse sands. *Hydrological Sciences Journal*, Vol. 40, No. 1, pp. 1-17
- Bakr, A.A., Gelhar, L.W., Gutjahr, A.L., and MacMillan, J.R. 1978. Stochastic analysis of spatial variability in subsurface flows. 1. Comparison of one- and three-dimensional flows. *Water Resources Research*, Vol. 14, No. 2, pp. 263-952.
- Bard, Y. 1974. *Nonlinear parameter estimation*. Academic Press, New York, N.Y., 341 pp.

- Barnett, V. and Lewis, T. 1984. *Outliers in statistical data*. 2nd edition, John Wiley and Sons, Chichester, 463 pp.
- Bear, J. 1972. *Dynamics of fluids in porous media*. Elsevier Science, New York, 764 pp.
- Beck, J.V. and Arnold, K.J. 1977. *Parameter estimation in engineering and science*. Wiley, New York, N.Y., 501 pp.
- Beck, M.B. 1987. Water quality modeling: a review of the analysis of uncertainty. *Water Resources Research*, Vol. 23, No. 8, pp. 1393-1442.
- Bell, J.P. 1987. *Neutron probe practice*. Institute of Hydrology Report 19. Third Edition. Wallingford, 51 pp.
- Benjamin, J.C. and Cornell, C.A. 1970. *Probability, statistics and decision for civil engineers*. McGraw-Hill, New York, 684 pp.
- Beven, K. 1981. Micro-, meso-, macroporosity and channelling flow phenomena in soils. *Soil Science Society of America Journal*, Vol. 45, pp. 1245.
- Beven, K.J. and Clarke, R.T. 1986. On the variations of infiltration into a homogeneous soil matrix containing a population of macropores. *Water Resources Research*, Vol. 22, No. 3, pp.383-388.
- Beven, K. and Germann, P. 1981. Water flow in soil macropores. II. A combined flow model. *Journal of Soil Science*, Vol. 32, pp. 14-38.
- Beven, K. and Germann, P. 1982. Macropore and water flow in soils. *Water Resources Research*, Vol. 18, No. 5, pp. 1311-1325.
- Binley, A., Elgy, J. and Beven, K. 1989. A physically based model of heterogeneous hillslopes. 1. Runoff production. *Water Resources Research*, Vol. 25, No. 6, pp. 1219-1226.
- Booltink, H.W.G. and Bouma, J. 1993. Sensitivity analysis of precesses affecting bypass flow. *Hydrological Processes*, Vol. 7, pp. 33-43.

Bouma, J. 1981. Comment on "Micro-, meso-, and macroporosity of soil". *Soil Science Society of America Journal*, Vol. 45, pp. 1244-1245.

Bouma, J. and Decker, L.W. 1978. A case study on infiltration into dry clay soil. I. Morphological observations. *Geoderma*, Vol. 20, pp. 27-40.

Bouma, J., Decker, L.W., and Haans, J.C.F. 1980. Measurement of depth to water table in a heavy clay soil. *Soil Science*, Vol 130, No. 5, pp.264-270.

Box, G.E.P. and Jenkins, G.M. 1970. *Time series analysis*. Holden-Day, San Francisco, California, 553 pp.

Brooks, R.H. and Corey, A.T. 1964. Hydraulic properties of porous media. *Hydrology Papers* 3, Colorado State University, Fort Collins, 28 pp.

Brooks, R.H. and Corey, A.T. 1966. Properties of porous media affecting fluid flow. *Journal of the Irrigation and Drainage Division*, ASCE, Vol. 92, No. IR2, pp. 61-88.

Brusseau, M.L. and Rao, P.S.C. 1990. Modeling solute transport in structured soils: a review. *Geoderma*, Vol. 46, pp. 169-192.

Burdine, N.T. 1953. Relative permeability calculations from pore size distribution data. *Transactions of the Society of Petroleum Engineers of AIME*, Vol.198, pp. 71-78

Burman, B. and Pochop, L.O. 1994. *Evaporation, evapotranspiration and climatic data*. Elsevier, Amsterdam, 278 pp.

Burne, S. 1991. *Experimental and numerical modelling studies of radionuclide transport in the near-surface environment. Report I: design and construction of the experimental lysimeter facility*. Imperial College internal report: IC/REP/DES/LYS/8.0/9111.

Burne, S. 1993. *Experimental and numerical modelling studies of radionuclide transport in the near-surface environment. Report X: summary of hydrological data - April 1190 to December 1990*. Imperial College internal report: IC/D90/LYS/SUM/2.0/9307.

Burne, S., Wheater, H.S., Butler, A.P., Johnston, P.M., Wadey, P., Shaw G. and Bell, J.N.B. 1994. Radionuclide transport above a near-surface water table: I. An automated lysimeter facility for near-surface contaminant transport studies. *Journal of Environmental Quality*, Vol.23, No. 6, pp. 1318-1329.

Butler, A.P. 1991a. *Documentation for the Imperial College coupled Soil-Plant-Water model (SPW1v3)*, Imperial College internal report: IC/MAN/MDL/SPW/1.3/9101.

Butler, A.P. 1991b. *A modelling study of the unscheduled water table rise which occurred during the 1991 re-dosing*, Imperial College internal report: IC/NTE/MDL/WTR/1.1/9110.

Butler, A.P. and Wheater, H.S. 1993. *Modelling radionuclide transport and uptake in vegetated soils. I. Analysis and application of numerical model studies of ^{22}Na uptake by winter wheat in soil lysimeters*, Imperial College internal report: IC/REP/MDL/LYS/2.3/9303.

Campbell, G.S. 1974. A simple method for determining unsaturated conductivity from moisture retention data. *Soil Science*, Vol. 117, No. 6, pp. 311-314.

Carneiro, C. and De Jong, E. 1985. In situ determination of the slope of the calibration curve of a neutron probe using a volumetric technique. *Soil Science*, Vol. 139, No. 3, pp. 250-254.

Carrera, J. and Neuman, S.P. 1986. Estimation of aquifer parameters under transient and steady state conditions. 2. Uniqueness, stability, and solution algorithms. *Water Resources Research*, Vol. 22, pp. 211-227.

Chacksfield, M. 1994. Personal Communication. Unpublished technical note. Centre for Analytical Research in the Environment, Silwood Park, Imperial College.

Channon, J.M. 1988. *Design and instrumentation of lysimeter layout for studies of radionuclide transport in the near-surface environment*, MSc Thesis, Imperial College, University of London, 100 pp.

Chen, C. and Wagenet, R.J. 1992. Simulation of water and chemicals in macropore soils. Part 1. Representation of the equivalent macropore influence and its effect on soilwater flow. *Journal of Hydrology*, Vol. 130, pp. 105-126.

Chevallier, P. 1988. *Complexité hydrologique du petit bassin versant; exemple en savane humide Booro-Borotu (Côte d'Ivoire)*. PhD Thesis, Université des Sciences et Technique du Languedoc, Montpellier, France, 331 pp.

Childs, E.C. 1969. *The physical basis of soil water phenomena*. Willey-Interscience, New York, 493 pp.

Clarke, R.T. 1973. *Mathematical models in hydrology*. Irrigation and Drainage Paper No. 19, FAO.

Clement, T.P., Wise, W.R. and Molz, F.J. 1994. A physically based, two-dimensional, finite-difference algorithm for modelling variably saturated flow. *Journal of Hydrology*, Vol. 161, pp.71-90.

Cordova, J.R. and Bras, R.L. 1981. Physically based probabilistic models of infiltration, soil moisture, and actual evapotranspiration. *Water Resources Research*, Vol. 17, No. 1, pp. 93-106.

Corwin, D.L., Waggoner, B.L., and Rhoades, J.D. 1991. A functional model of solute transport that accounts for bypass. *Journal of Environmental Quality*, Vol. 20, pp. 647-658.

Coulomb, C. and Dever, L. 1994. Evolution saisonnière des modalités de transfert d'eau et de solutés dans un sol argileux drainé: étude isotropique et chimique. *Hydrological Sciences Journal*, Vol. 39, No. 3, pp. 217-232.

Dagan, G. and Bresler, E. 1983. Unsaturated flow in spatially variable fields. 1. Derivation of models of infiltration and redistribution. *Water Resources Research*, Vol. 19, No. 2, pp. 413-420.

Dane, J.H. and Wierenga, P.J. 1975. Effect of hysteresis on the prediction of infiltration, redistribution and drainage of water in a layered soil. *Journal of Hydrology*, Vol. 25, pp. 229-242.

DeVries, J. and Chow, T.L. 1978. Hydrological behaviour of a forested mountain soil in coastal British Columbia. *Water Resources Research*, Vol. 14, No. 15, pp. 935-942.

- Edwards, W.M., Van der Ploeg, R.R., and Ehlers, W. 1979. A numerical study of the effects of noncapillary-sized pores upon infiltration. *Soil Science Society of America Journal*, Vol. 43, pp. 851-856.
- Ehlers, W. 1975. Observations on earthworm channels and infiltration on tilled and untilled loess soil. *Soil Science*, Vol. 119, pp. 242-249.
- El-Kadi, A.I. 1987. Variability of infiltration under uncertainty in unsaturated zone parameters. *Journal of Hydrology*, Vol. 90, pp. 61-80.
- Faybishenko, B.A. 1995. Hydraulic behaviour of quasi-saturated soils in the presence of entrapped air: laboratory experiments. *Water Resources Research*, Vol. 31, No. 10, pp. 2421-2435.
- Fayer, M.J. and Simmons, C.S. 1995. Modified soil water retention functions for all matric suctions. *Water Resources Research*, Vol. 31, No. 5, pp.1233-1238.
- Feddes, R.A., Bresler, E. and Neuman, S.P. 1974. Field test of a modified numerical model for water uptake by root systems. *Water Resources Research*, Vol. 10, pp. 1199-1206.
- Feddes, R.A., Kabat, P., Van Bakel, P.J.T., Bronswijk, J.J.B., and Halbertsma, J. 1988. Modelling water dynamics in the unsaturated zone - state of the art. *Journal of Hydrology*, Vol.100, pp. 69-111.
- Feddes, R.A., Kowalik, P., Kolinska-Malinka, K. and Zaradny, H. 1976. Simulation of field water uptake by plants using a soil water dependent root extraction function. *Journal of Hydrology*, Vol. 31, pp. 13-26.
- Feddes, R.A. and Rijtema, P.E. 1972. Water withdrawal by plant roots. *Journal of Hydrology*, Vol. 17, pp. 33-59.
- Finsterle, S. and Pruess, K. 1995. Solving the estimation-identification problem in two-phase flow modelling. *Water Resources Research*, Vol. 31, No. 4, pp. 913-924.

Flury, M., Flühler, H., Jury, W.A. and Leuenberger, J. 1994. Susceptibility of soils to preferential flow of water: a field study. *Water Resources Research*, Vol. 30, No. 7, pp.1945-1954.

Fredlund, D.G. and Rahardjo, H. 1993. *Soil mechanics for unsaturated soils*. John Wiley and Sons Inc., New York, 517 pp.

Freeze, R.A. 1969. The mechanism of natural ground-water recharge and discharge. 1. One-dimensional, vertical, unsteady, unsaturated flow above a recharging or discharging ground-water flow system. *Water Resources Research*, Vol. 5, No. 1, pp. 153-171.

Freeze, R.A. 1971. Three-dimensional, transient, saturated-unsaturated flow in a groundwater basin. *Water Resources Research*, Vol. 7, No. 2, pp. 347-366.

Freeze, R.A. 1980. A stochastic-conceptual analysis of rainfall-runoff processes on a hillslope. *Water Resources Research*, Vol. 16, No. 2, pp. 391-408.

Frind, E.O. and Verge, M.J. 1978. Three-dimensional modeling of groundwater flow systems. *Water Resources Research*, Vol. 14, No. 5, pp. 844-856.

Gardner, W.R. 1960. Dynamic aspects of soil availability to plants. *Soil Science*, Vol. 89, pp.63-73.

Gelhar, L.W. 1986. Stochastic subsurface hydrology. From theory to applications. *Water Resources Research*, Vol. 22, No. 9, pp. 135S-145S.

Gelhar, L.W., Gutjahr, A.L., and Naff, R.L. 1979. Stochastic analysis of macrodispersion in a stratified aquifer. *Water Resources Research*, Vol. 15, No. 6, pp. 1387-1397.

Gerke, H.H. and Van Genuchten, M.T. 1993. A dual-porosity model for simulating the preferential movement of water and solutes in structured porous media. *Water Resources Research*, Vol. 29, No. 2, pp. 305-319.

Germann, P.F. 1985. Kinematic wave approach to infiltration and drainage into and from soil macropores. *Transactions of the ASAE*, Vol. 28, No. 3, pp. 745-749.

Germann, P.F. 1986. Rapid drainage response to precipitation. *Hydrological Processes*, Vol.1, pp. 3-13.

Germann, P.F. 1990. Preferential flow and the generation of runoff. 1. Boundary layer flow theory. *Water Resources Research*, Vol. 26, No. 12, pp. 3055-3063.

Germann, P. and Beven, K. 1981. Water flow in soil macropores. I. An experimental approach. *Journal of Soil Science*, Vol. 32, pp. 1-13.

Germann, P.F. and Beven, K. 1985. Kinematic wave approximation to infiltration into soils with sorbing macropores. *Water Resources Research*, Vol. 21, No. 7, pp. 990-996.

Germann, P.F. and Beven, K. 1986. A distribution function approach to water flow in soil macropores based on kinematic wave theory. *Journal of Hydrology*, Vol. 83, pp. 173-183

Grant, S.A., Jabro, J.D., Fritton, D.D., and Baker, D.E. 1991. A stochastic model of infiltration which simulates "macropore" soil water flow. *Water Resources Research*, Vol. 27, No. 7, pp.1439-1446.

Green, J.R. and Margerison, D. 1978. *Statistical treatment of experimental data*. Elsevier, Amsterdam, 382 pp.

Green, W.H. and Ampt, G.A. 1911. Studies on soil physics: I. Flow of air and water through soils. *Journal of Agricultural Sciences*, Vol. 4, pp. 1-24.

Hammermeister, D.P., Kling, G.F. and Vomocil, J.A. 1982. Perched water tables on hillsides in Western Oregon: II. Preferential downslope movement of water and anions. *Soil Science Society of America Journal*, Vol. 46, pp. 819-826.

Hanks, R.J. and Bowers, S.A. 1962. Numerical solution of the moisture flow equation for infiltration into layered soils. *Soil Science Society of America Proceedings*, Vol. 26, No. 6, pp.530-534.

Hanks, R.J., Klute, A. and Bresler, E. 1969. A numerical method for estimating infiltration, redistribution, drainage, and evaporation of water from soil. *Water Resources Research*, Vol. 5, No.5, pp. 1064-1069.

Haverkamp, R. and Parlange, J.-Y. 1986. Predicting the water-retention curve from particle-size distribution: 1. Sandy soils without organic matter. *Soil Science*, Vol. 142, No. 6, pp. 325-339.

Haverkamp, R., Vauclin, M., Touma, J., Wierenga, P.J. and Vachaud, G. 1977. A comparison of numerical simulation models for one-dimensional infiltration. *Soil Science Society of America Journal*, Vol. 41, pp. 285-294.

Haverkamp, R., Vauclin, M. and Vachaud, G. 1984. Error analysis in estimating soil water content from neutron probe measurements: 1. Local standpoint. *Soil Science*, Vol. 137, No. 2, pp. 78-90

Hillel, D. 1980. *Fundamentals of Soil Science*. Academic Press, New York, 413 pp.

Hillel, D., Talpaz, H. and Van Keulen, H. 1976. A macroscopic-scale model of water uptake by a nonuniform root system and of water and salt movement in the soil profile. *Soil Science*, Vol. 121, pp. 242-255.

Himmelblau, D.M. 1970. *Process analysis by statistical methods*. John Wiley and Sons, Inc., New York.

Hoelscher, J.R., Nuttle, W.K. and Harvey, J.W. 1993. The calibration and use of pressure transducers in tensiometer systems. *Hydrological Processes*, Vol. 7, pp. 205-211.

Hoogmoed, W.B. and Bouma, J. 1980. A simulation model for predicting infiltration into cracked clay soil. *Soil Science Society of America Journal*, Vol. 44, pp. 458-461.

Hopmans, J.W., Schukking, H., and Torfs, P.J.J.F. 1988. Two-dimensional steady state unsaturated water flow in heterogeneous soils with autocorrelated soil hydraulic properties. *Water Resources Research*, Vol. 24, No. 12, pp. 2005-2017.

Huyakorn, P.S. and Pinder, G.F. 1983. *Computational methods in subsurface flow*. Academic Press, New York, 473 pp.

Huyakorn, P.S., Springer, E.P., Guvanasen, V. and Wadsworth, T.D. 1986. A three-dimensional finite-element model for simulating water flow in variably saturated porous media. *Water Resources Research*, Vol. 22, No. 13, pp. 1790-1808.

- Huyakorn, P.S., Thomas, S.D. and Thompson, B.M. 1984. Techniques for making finite elements competitive in modeling flow in variably saturated porous media. *Water Resources Research*, Vol. 20, No. 8, pp. 1099-1115.
- Jarvis, N.J. 1989. A simple empirical model of root water uptake. *Journal of Hydrology*, Vol.107, pp. 57-72.
- Jarvis, N. 1991. *MACRO - A model of water movement and solute transport in macroporous soils*. Swedish University of Agricultural Sciences, Uppsala, Sweden, 58 pp.
- Jarvis, N. 1994. *The MACRO model (version 3.1). Technical description and sample simulations*. Swedish University of Agricultural Sciences, Uppsala, Sweden, 51 pp.
- Jarvis, N.J., Jansson, P-E., Dik, P.E., and Messing, I. 1991. Modelling water and solute transport in macroporous soil. I. Model description and sensitivity analysis. *Journal of Soil Science*, Vol. 42, pp. 59-70.
- Jaynes, D.B. 1984. Comparison of soil-water hysteresis models. *Journal of Hydrology*, Vol.75, pp. 287-299.
- Jenkins, G.M. and Watts, D.G. 1968. *Spectral analysis and its applications*. Holden-Day, San Francisco. 525 pp.
- Jury, W.A. 1982. Simulation of solute transport using a transfer function model. *Water Resources Research*, Vol. 18, No. 2, pp. 363-368.
- Jury, W.A., Sposito, G., and White, R.E. 1986. A transfer function model of solute transport through soil. I. Fundamental concepts. *Water Resources Research*, Vol. 22, No. 2, pp. 243-247.
- Kaluarachchi, J.J and Parker, J.C. 1987a. Effects of hysteresis with air entrapment on water flow in the unsaturated zone. *Water Resources Research*, Vol. 23, No. 10, pp. 1967-1976.
- Kaluarachchi, J.J and Parker, J.C. 1987b. Finite element analysis of water flow in variably saturated soil. *Journal of Hydrology*, Vol. 90, pp. 269-291.

- Kaluvarachchi, J.J and Parker, J.C. 1989. An efficient element method for modeling multiphase flow. *Water Resources Research*, Vol. 25, No. 1, pp. 43-54.
- Karavokyris, I. 1990. *The modelling of water dynamics in field soil-plant systems*. PhD Thesis, Imperial College, University of London, 377 pp.
- Karavokyris, I., Butler, A.P., and Wheeler, H.S. 1990. The development and validation of a coupled soil-plant-water model (SPW1), *Nirex Safety Series Report NSS/R225*, UK Nirex Ltd.
- Kauark Leite, L.A. 1990. *Réflexions sur l'utilité des modèles mathématiques dans la gestion de la pollution diffuse d'origine agricole*. PhD Thesis, ENPC, Paris, 451 pp.
- Kiefer, E.-M. 1993. A conceptual-stochastic model of unsaturated flow in heterogeneous soils. *Journal of Hydrology*, Vol. 143, pp. 3-18.
- Kirkland, M.R., Hills, R.G. and Wierenga, P.J. 1992. Algorithms for solving Richards' equation for variably saturated soil. *Water Resources Research*, Vol. 28, No. 8, pp. 2049-2058.
- Klute, A. and Heermann, D.F. 1974. Soil water profile development under a periodic boundary condition. *Soil Science*, Vol. 117, pp. 265-271.
- Kool, J.B. and Parker, J.C. 1987. Development and evaluation of closed-form expressions for hysteretic soil hydraulic properties. *Water Resources Research*, Vol. 23, No. 1, pp. 105-114.
- Kool, J.B., Parker, J.C. and Van Genuchten, M.Th. 1987. Parameter estimation for unsaturated flow and transport models - a review. *Journal of Hydrology*, Vol. 91, pp. 255-293.
- Kung, K.-J.S. 1992. Laboratory observation of funnel flow mechanism and its influence on solute transport. *Journal of Environmental Quality*, Vol 22, pp. 91-102
- Kusogi, K. 1994. Three-parameter lognormal distribution model for soil water retention. *Water Resources Research*, Vol. 30, No. 4, pp. 891-901.
- Land, C.S. 1968. Calculation of imbibition relative permeability for two- and three-phase flow from rock properties. *Transactions of the Society of Petroleum Engineers of AIME*, Vol. 243, pp. 149-156.

- Leaney, F.W., Smettem, K.R.J. and Chittleborough, D.J. 1993. Estimating the contribution of preferential flow to subsurface runoff from a hillslope using deuterium and chloride. *Journal of Hydrology*, Vol. 147, pp. 83-103.
- Lenhard, R.J. and Parker, J.C. 1987. A model for hysteretic constitutive relations governing multiphase flow. 2. Permeability-saturation relations. *Water Resources Research*, Vol. 23, No.12, pp. 2197-2206.
- Lenhard, R.J., Parker, J.C. and Kaluarachchi, J.J. 1991. Comparing simulated and experimental hysteretic two-phase transient fluid flow phenomena. *Water Resources Research*, Vol. 27, No.8, pp. 2113-2124.
- Lenhard, R.J., Parker, J.C. and Mishra, S. 1989. On the correspondence between Brooks-Corey and Van Genuchten models. *Journal of Irrigation and Drainage Engineering*, Vol. 115, No. 4, pp. 744-751.
- Luxmoore, R.J. 1981. Micro-, meso-, and macroporosity of soil. *Soil Science Society of America Journal*, Vol. 45, pp. 671-672.
- Mangold, D.C. and Tsang, C.F. 1991. A summary of subsurface hydrological and hydrochemical models. *Reviews of Geophysics*, Vol. 29, No. 1, pp. 51-79.
- Marshall, T.J. and Holmes, J.W. 1988. *Soil physics*. Second edition. Cambridge University Press, Cambridge, 374 pp.
- Michiels, P., Hartmann, R. and De Strooper, E. 1989. Comparisons of the unsaturated hydraulic conductivity of a coarse-textured soil as determined in the field, in the laboratory, and with mathematical models. *Soil Science*, Vol. 147, No. 4, pp. 299-304.
- Milly, P.C.D. 1987. Estimation of Brooks-Corey parameters from water retention data. *Water Resources Research*, Vol. 23, No. 6, pp. 1085-1089.
- Mishra, S. and Parker, J.C. 1989. Effects of parameter uncertainty on predictions of unsaturated flow. *Journal of Hydrology*, Vol 108, pp. 19-33.

Mishra, S., Parker, J.C. and Singhal, N. 1989. Estimation of soil hydraulic properties and their uncertainty from particle size distribution data. *Journal of Hydrology*, Vol 108, pp. 1-18.

Mishra, S., Parker, J.C., and Zhu, J.L. 1990. An algorithm for generating spatially autocorrelated unsaturated flow properties. *Computers and Geosciences*, Vol. 16, No. 5, pp. 697-703.

Molz, F.J. 1981. Models of water transport in the soil-plant system: a review. *Water Resources Research*, Vol. 17, No. 5, pp. 1245-1260.

Molz, F.J. and Remson, I. 1970. Extraction term models of soil moisture use by transpiring plants. *Water Resources Research*, Vol. 6, pp. 1346-1356.

Monteith, J.L. 1965. Evaporation and environment. *Proceedings of Symposium on Experimental Biology*, Vol 19, pp. 205-234.

Monteith, J.L., ed. 1975. *Vegetation and the atmosphere. Volume 1 - Principles*. Academic Press, London, 278 pp.

Mualem, Y. 1973. Modified approach to capillary hysteresis based on a similarity hypothesis. *Water Resources Research*, Vol. 9, No. 5, pp. 1324-1331.

Mualem, Y. 1974. A conceptual model of hysteresis. *Water Resources Research*, Vol. 10, No.3, pp. 514-520.

Mualem, Y. 1976a. A new model for predicting the hydraulic conductivity of unsaturated porous media. *Water Resources Research*, Vol. 12, No. 3, pp. 513-522.

Mualem, Y. 1976b. Hysteretical models for prediction of the hydraulic conductivity of unsaturated porous media. *Water Resources Research*, Vol. 12, No. 6, pp. 1248-1254.

Mualem, Y. 1977. Extension of the similarity hypothesis used for modeling the soil water characteristics. *Water Resources Research*, Vol. 13, No. 4, pp. 773-780.

Mualem, Y. 1984a. A modified dependent-domain theory of hysteresis. *Soil Science*, Vol. 137, No. 5, pp. 283-291.

Mualem, Y. 1984b. Prediction of the soil boundary wetting curve. *Soil Science*, Vol. 137, No.12, pp. 379-390.

Mualem, Y. and Dagan, G. 1975. A dependent domain of capillary hysteresis. *Water Resources Research*, Vol. 11, No. 3, pp. 452-460.

Mualem, Y. and Miller, E.E. 1979. A hysteresis model based on an explicit domain-dependence function. *Soil Science Society of America Journal*, Vol. 43, pp. 1067-1073.

Mualem, Y. and Morel-Seytoux, H.J. 1979a. Capillary pressure. In: Fairbridge, R.W. and Finkl, Jr, C.W. *The Encyclopedia of Soil Science. Part I*. Dowden, Hutchinson and Ross, Inc., Stroudsburg, Pennsylvania, pp. 49-61.

Mualem, Y. and Morel-Seytoux, H.J. 1979b. Permeability. In: Fairbridge, R.W. and Finkl, Jr, C.W. *The Encyclopedia of Soil Science. Part I*. Dowden, Hutchinson and Ross, Inc., Stroudsburg, Pennsylvania, pp. 359-369.

Nachabe, M.H. and Illangasekare, T. 1994. Use of tension infiltrometer data with unsaturated hydraulic conductivity models. *Ground Water*, Vol. 32, No. 6, pp.1017-1021.

Návar, J., Turton, D.J. and Miller, E. 1995. Estimating macropore and matrix flow using the hydrograph separation procedure in an experimental forest plot. *Hydrological Processes*, Vol.9, pp. 743-753.

Nelder, J.A. and Mead, R. 1965. A simplex method for function minimisation. *Computer Journal*, Vol. 7, pp. 308-313.

Neuman, S.P. 1973. Saturated-unsaturated seepage by finite elements. *Proceedings of the ASCE, Journal of Hydraulics Division*, Vol. 99, No. HY 12, pp. 2233-2250.

Nielsen, D.R., Van Genuchten, M. Th., and Biggar, J.W. 1986. Water flow and solute transport processes in the unsaturated zone. *Water Resources Research*, Vol. 22, No. 9, pp. 89S-108S.

Numerical Algorithms Group. 1987. Minimizing or maximizing a function. In: Numerical Algorithms Group. 1987. *The NAG Fortran library manual - Mark 12*. Numerical Algorithms Group Limited, Oxford, UK. Vol. 3, Chapter E04.

- Nwabuzor, S.S. 1984. *Soil water dynamics under field crops*. PhD Thesis, Imperial College, University of London, 255 pp.
- Ogden, C.B., Wagenet, R.J., Van Es, H.M., and Hutson, J.L. 1992. Quantification and modeling of macropore drainage. *Geoderma*, Vol. 55, pp. 17-35.
- Palmier, L.R. 1995. *Hydrological aspects of landfill waste management - a case-study of the Drigg low-level radioactive waste depository*. PhD Thesis, Imperial College, University of London, 428 pp.
- Paniconi, C., Aldama, A.A. and Wood, E.F. 1991. Numerical evaluation of iterative and noniterative methods for the solution of the nonlinear Richards equation. *Water Resources Research*, Vol. 27, No. 6, pp. 1147-1163.
- Paniconi, C. and Wood, E.F. 1993. A detailed model for simulation of catchment scale subsurface hydrologic processes. *Water Resources Research*, Vol. 29, No. 6, pp. 1601-1620.
- Parissopoulos, G.A. and Wheeler, H.S. 1988. On numerical errors associated with the iterative alternating direction implicit (IADI) finite difference solution of the two dimensional saturated-unsaturated flow (Richards) equation. *Hydrological Processes*, Vol. 2, pp. 187-201.
- Parissopoulos, G.A. and Wheeler, H.S. 1992. Effects of hysteresis on groundwater recharge from ephemeral flows. *Water Resources Research*, Vol. 28, No. 11, pp. 3055-3061
- Parker, J.C. and Lenhard, R.J. 1987. A model for hysteretic constitutive relations governing multiphase flow. 1. Saturation-pressure relations. *Water Resources Research*, Vol. 23, No. 12, pp. 2187-2196.
- Parlange, J.-Y. 1976. Capillary hysteresis and the relationship between drying and wetting curves. *Water Resources Research*, Vol. 12, No. 2, pp. 224-228.
- Penman, H.L. 1948. Natural evaporation from open water, bare soil and grass. *Proceedings of the Royal Society of London, Series A*, Vol. 193, pp. 120-145.
- Penman, H.L. 1956. Evaporation: an introductory survey. *Netherlands Journal of Agricultural Science*, Vol. 1, pp. 9-29.

- Philip, J.R. 1957. The theory of infiltration. 1. The infiltration equation and its solution. *Soil Science*, Vol. 83, pp. 345-357.
- Phillip, J.R. 1991. Horizontal redistribution with capillary hysteresis. *Water Resources Research*, Vol. 27, No. 7, pp. 1459-1469.
- Pilgrim, D.H., Huff, D.D., and Steele, T.D. 1978. A field evaluation of subsurface and surface runoff. *Journal of Hydrology*, Vol. 38, pp. 319-341.
- Poulovassilis, A. 1962. Hysteresis of pore water, an application of the concept of independent domains. *Soil Science*, Vol. 93, pp. 405-412.
- Poulovassilis, A. 1970. The effect of the entrapped air on the hysteresis curves of a porous body and on its hydraulic conductivity. *Soil Science*, Vol. 109, No. 3, pp. 154-162.
- Poulovassilis, A. and Childs, E.C. 1971. The hysteresis of pore water: the non-independence of domains. *Soil Science*, Vol. 112, pp. 301-312.
- Protopapas, A.L. and Bras, R.L. 1990. Uncertainty propagation with numerical models for flow and transport in the unsaturated zone. *Water Resources Research*, Vol. 26, No. 20, pp. 2463-2474.
- Pullan, A.J. 1990. The quasilinear approximation for unsaturated porous media flow. *Water Resources Research*, Vol. 26, No. 6, pp. 1219-1234.
- Ragab, R. and Cooper, J.D. 1993. Variability of unsaturated zone water transport parameters: implications for hydrological modelling. 2. Predicted vs. in situ measurements and evaluation of methods. *Journal of Hydrology*, Vol. 148, pp.133-147.
- Rawls, W.J., Ahuja, L.R., Brakensiek, D.L. and Shirmohammadi, A. 1993. Infiltration and soil water movement. In: Maidment, D.R., ed. *Handbook of hydrology*. McGraw-Hill Inc, New York, Chapter 5.
- Rawls, W.J. and Brakensiek, D.L. 1982. Estimating soil water retention from soil properties. *Journal of Irrigation and Drainage Division*, ASCE, Vol. 108, pp 166-171.

Rawls, W.J. and Brakensiek, D.L. 1985. Prediction of soil water properties for hydrologic modeling. In: James, E.B. and Wred, T.J. ed. *Watershed Management in the Eighties*. Denver, Colorado, pp. 293-299..

Rice, R.C., Jaynes, D.B., and Bowman, R.S. 1991. Preferential flow of solutes and herbicide under irrigated fields. *Transactions of the ASAE*, Vol. 34, No. 3, pp. 914-918.

Ross, P.J. 1990. Efficient numerical models for infiltration using Richards' equation. *Water Resources Research*, Vol. 26, No. 2, pp. 279-290.

Rossi, C. and Nimmo, J.R. 1994. Modeling of soil water retention from saturation to oven dryness. *Water Resources Research*, Vol. 30, No. 3, pp. 701-708.

Rubin, J. and Steinhardt, R. 1963. Soil water relations during rain infiltration. I. Theory. *Soil Science Society of America Proceedings*, Vol. 27, No. 3, pp. 246-251.

Russell, R.S. 1977. *Plant root systems. Their function and interaction with the soil*. McGraw Hill Book Company Limited, London, 298 pp.

Russo, D., Bresler, E., Shani, U. and Parker, J.C. 1991. Analises of infiltration in relation to determining soil hydraulic properties by invrse problem methodology. *Water Resources Research*, Vol. 27, No. 6, pp.1361-1373.

Russo, D., Jury, W.A. and Butters, G.L. 1989. Numerical analysis of solute transport during irrigation: 1. The effect of hysteresis and profile heterogeneity. *Water Resources Research*, Vol.25, No. 10, pp. 2109-2118.

Ruygrock, P.A. 1988. Evaluation of the gamma and neutron radiation scattering and transmission methods for soil density and moisture determination. *Geotechnical Testing Journal*, GTJODJ, Vol. 11, No.1, pp. 3-19.

Saxton, K.E., Rawls, W.J., Romberger, J.S. and Papendick, R.I. 1986. Estimating soil-water characteristics from texture. *Soil Science Society of America Journal*, Vol. 50, pp. 1031-1036.

Sharma, M.L. 1985. Estimating evapotranspiration. In: Hillel, D., ed. *Advances in Irrigation*, Academic Press, Orlando, pp.213- 281.

Shuttleworth, W.J. 1993. Evaporation. In: Maidment, D.R., ed. *Handbook of hydrology*. McGraw-Hill Inc, New York, Chapter 5.

Silver, M.L. 1980. Automated data acquisition, transducers, and dynamic recording for the geotechnical testing laboratory. *Soil Science*, Vol. 137, No. 2, pp. 78-90

Silvestri, V., Sarkis, G. Bekkouche, N., Soulie, M. and Tabib, C. 1991. Laboratory and field calibration of a neutron depth moisture gauge for use in high water content soils, *Geotechnical Testing Journal*, GTJODJ, Vol. 14, No.1, pp. 64-70.

Skopp, J. 1981. Comment on "Micro-, meso-, and macroporosity of soil". *Soil Science Society of America Journal*, Vol. 45, pp. 1246.

Smettem, K.R.J., Chittleborough, D.J., Richards, B.G. and Leaney, F.W. 1991. The influence of macropores on runoff generation from a hillslope soil with a contrasting textural class. *Journal of Hydrology*, Vol. 122, pp. 235-252.

Smettem, K.R.J. and Collis-George, N. 1985a. The influence of cylindrical macropores on steady-state infiltration in a soil under pasture. *Journal of Hydrology*, Vol. 79, pp. 107-114.

Smettem, K.R.J. and Collis-George, N. 1985b. Prediction of steady-state ponded infiltration distribution in a soil with vertical macropores. *Journal of Hydrology*, Vol. 79, pp. 115-122.

Smettem, K.R.J. and Ross, P.J. 1992. Measurement and prediction of water movement in a field soil: the matrix-macropore dichotomy. *Hydrological Processes*, Vol. 6, pp. 1-10.

Srivastava, R. and Yeh, T.C.J. 1991. Analytical solutions for one-dimensional, transient infiltration toward the water table in homogeneous and layered soils. *Water Resources Research*, Vol. 27, No. 5, pp. 753-762.

Stannard, D.I. 1992. Tensiometers - theory, construction, and use, *Geotechnical Testing Journal*, GTJODJ, Vol. 15, No.1, pp. 48-58.

Steenhuis, T.S., Parlange, J.-Y. and Andreini, M.S. 1990. A numerical model for preferential solute movement in structured soils. *Geoderma*, Vol. 46, pp.193-208.

- Thomas, D.L. and Beasley, D.B. 1986. A physically-based forest hydrology model. I: Development and sensitivity of components. *Transactions of the ASAE*, Vol. 29, No. 4, pp. 962-972.
- Thomas, G.W. and Phillips, R.E. 1979. Consequences of water movement in macropores. *Journal of Environmental Quality*, Vol. 8, No. 2, pp. 149-152.
- Topp, G.C. 1971. Soil-water hysteresis: the domain theory extended to pore interaction conditions. *Soil Science Society of America Proceedings*, Vol. 35, pp. 219-225.
- Topp, G.C. and Davis, J.L. 1985a. Time-domain reflectometry (TDR) and its application to irrigation scheduling. In: Hillel, D., ed. *Advances in Irrigation*, Academic Press, Orlando, Vol.3, pp. 107- 127.
- Topp, G.C. and Davis, J.L. 1985b. Measurement of soil water content using time-domain reflectometry (TDR): a field evaluation. *Soil Science Society of America Journal*, Vol. 49, pp. 19-24.
- Topp, G.C., Davis, J.L. and Annan, A.P. 1980. Electromagnetic determination of soil water content: measurements in coaxial transmission lines. *Water Resources Research*, Vol. 16, No 3, pp. 574-582
- Tucci, C.E.M. 1986. *Modelos matemáticos em hidrologia e hidráulica*. RBE, Rio de Janeiro, 3 Vol.
- Vachaud, G., Vauclin, M. and Colombani, J. 1981. Bilan hydrique dans le Sud-Tunisien. I. Caractérisation expérimentale des transferts dans la zone non-saturée. *Journal of Hydrology*, Vol.49, pp. 31-52.
- Van Genuchten, M.Th. 1978. *Mass transport in saturated-unsaturated media: one-dimension solutions*. Research report 78-WR-11, Water Resources Program, Department of Civil Engineering, Princeton University.
- Van Genuchten, M.Th. 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Science Society of America Journal*, Vol. 44, pp. 892-898.

Vauclin, M., Haverkamp, R. and Vachaud, G. 1979. *Résolution numérique d'une équation de diffusion non linéaire - Application à l'infiltration de l'eau dans les sols non saturés*. Presses Universitaires de Grenoble, France, 183 pp.

Vauclin, M. and Vachaud, G. 1981. Bilan hydrique dans le Sud-Tunisien. II. Modélisation numérique et prévision des transferts hydriques en sol stratifié. *Journal of Hydrology*, Vol.49, pp. 53-73.

Vereecken, H., Maes, J. and Feyen, J. 1990. Estimating unsaturated hydraulic conductivity from easily measured soil properties. *Soil Science*, Vol. 149, No. 1, pp. 1-12

Vereecken, H., Maes, J., Feyen, J. and Darius, P. 1989. Estimating the soil moisture retention characteristic from texture, bulk density, and carbon content. *Soil Science*, Vol. 148, No. 6, pp.389-403.

Viaene, P., Vereecken, H., Diels, J. and Feyen, J. 1994. A statistical analysis of six hysteresis models for the moisture retention characteristic. *Soil Science*, Vol. 157, No. 6, pp. 345-355.

Wadey, P. 1991. *Quality assurance for biological and radiochemical procedures at the lysimeter facility*, Imperial College internal report: IC/REP/QAP/LYS/1.0/9107.

Ward, R.C. and Robinson, M. 1990. *Principles of hydrology*. Third edition. McGraw-Hill Book Company Ltd., London, UK, 365 pp.

Warrick, A.W., Islas, A. and Lomen, D.O. 1991. An analytical solution to Richards' equation for time-varying infiltration. *Water Resources Research*, Vol. 27, No. 5, pp. 763-766.

Wheater, H.S., Jakeman, A.J. and Beven, K.J. 1993. Progress and directions in rainfall-runoff modelling. In: Jakeman, A.J., Beck, M.B. and McAleer, M.J., ed. *Modelling changes in environmental systems*, pp. 101-161.

Whisler, F.D., Klute, A. and Millington, R.J. 1968. Analysis of steady state evapotranspiration from a soil column. *Soil Science Society of America Proceedings*, Vol. 32, pp. 167-174.

White, R.E. and Magesan, G.N. 1991. A stochastic-empirical approach to modelling nitrate leaching. *Soil Use and Management*, Vol. 7, No. 2, pp. 85-94.

Yeh, T.-C.J. 1992. Stochastic modelling of groundwater flow and solute transport in aquifers. *Hydrological Processes*, Vol. 6, pp. 369-395.

Yeh, T.-C.J., Gelhar, L.W. and Gutjahr, A.L. 1985a. Stochastic analysis of unsaturated flow in heterogeneous soils. 1. Statistically Isotropic media. *Water Resources Research*, Vol. 21, No.4, pp. 447-456.

Yeh, T.-C.J., Gelhar, L.W. and Gutjahr, A.L. 1985b. Stochastic analysis of unsaturated flow in heterogeneous soils. 2. Statistically anisotropic media with variable α . *Water Resources Research*, Vol. 21, No. 4, pp. 457-464.

Yeh, T.-C.J., Gelhar, L.W. and Gutjahr, A.L. 1985c. Stochastic analysis of unsaturated flow in heterogeneous soils. 3. Observations and applications. *Water Resources Research*, Vol. 21, No.4, pp. 465-471.

Yeh, T.-C.J., Srivastava, R., Guzman, A. and Harter, T. 1993. A numerical model for water flow and chemical transport in variably saturated porous media. *Groundwater*, Vol. 31, No. 4, pp. 634-644.

Yevjevich, V. 1974. Determinism and stochasticity in hydrology. *Journal of Hydrology*, Vol.22, pp. 225-238.

Zhu, J.L., Mishra, S., and Parker, J.C. 1990. Effective properties for modeling unsaturated flow in large scale heterogeneous porous media. In: Roth, K.; Flühler, H.; Jury, W.A.; Parker, J.C., ed. *Field-scale water and solute flux in soils*. Birkhäuser, Basel, Switzerland, pp. 261-268.

APPENDIX I

Matric potential data for lysimeters A and B

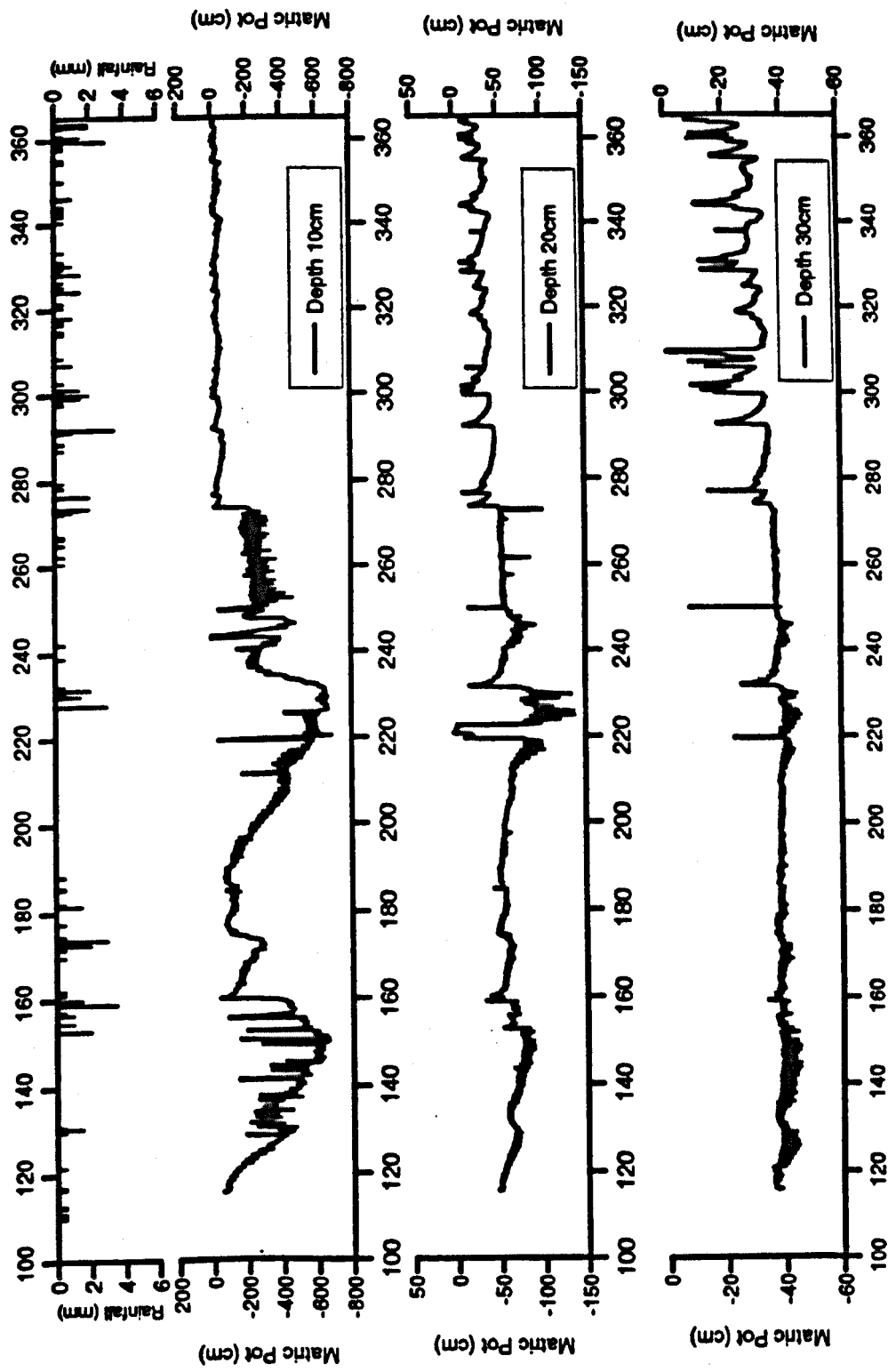


Figure I.1 Matric potentials - Lysimeter A - 1990

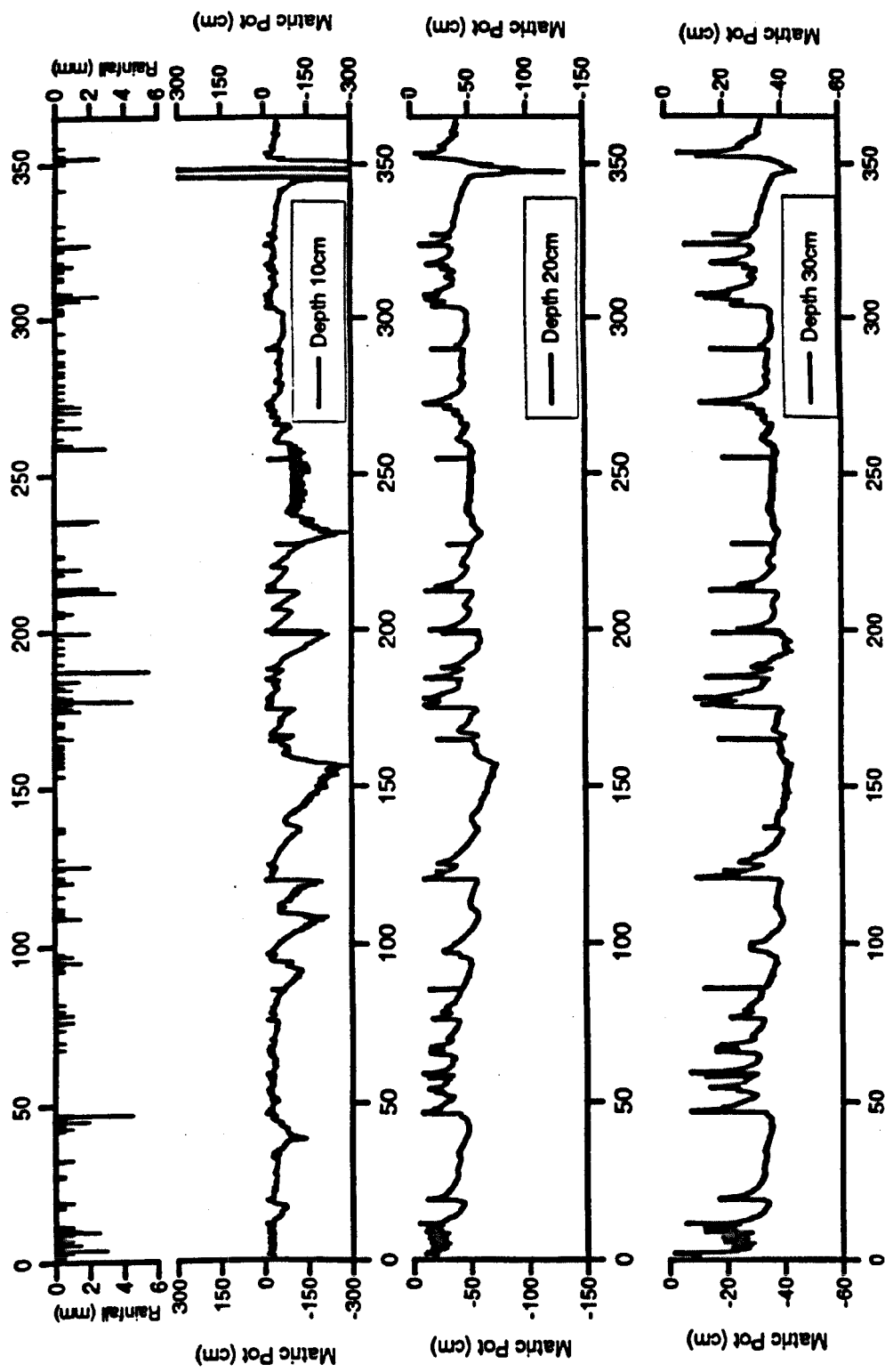


Figure I.2 Matric potentials - Lysimeter A - 1991

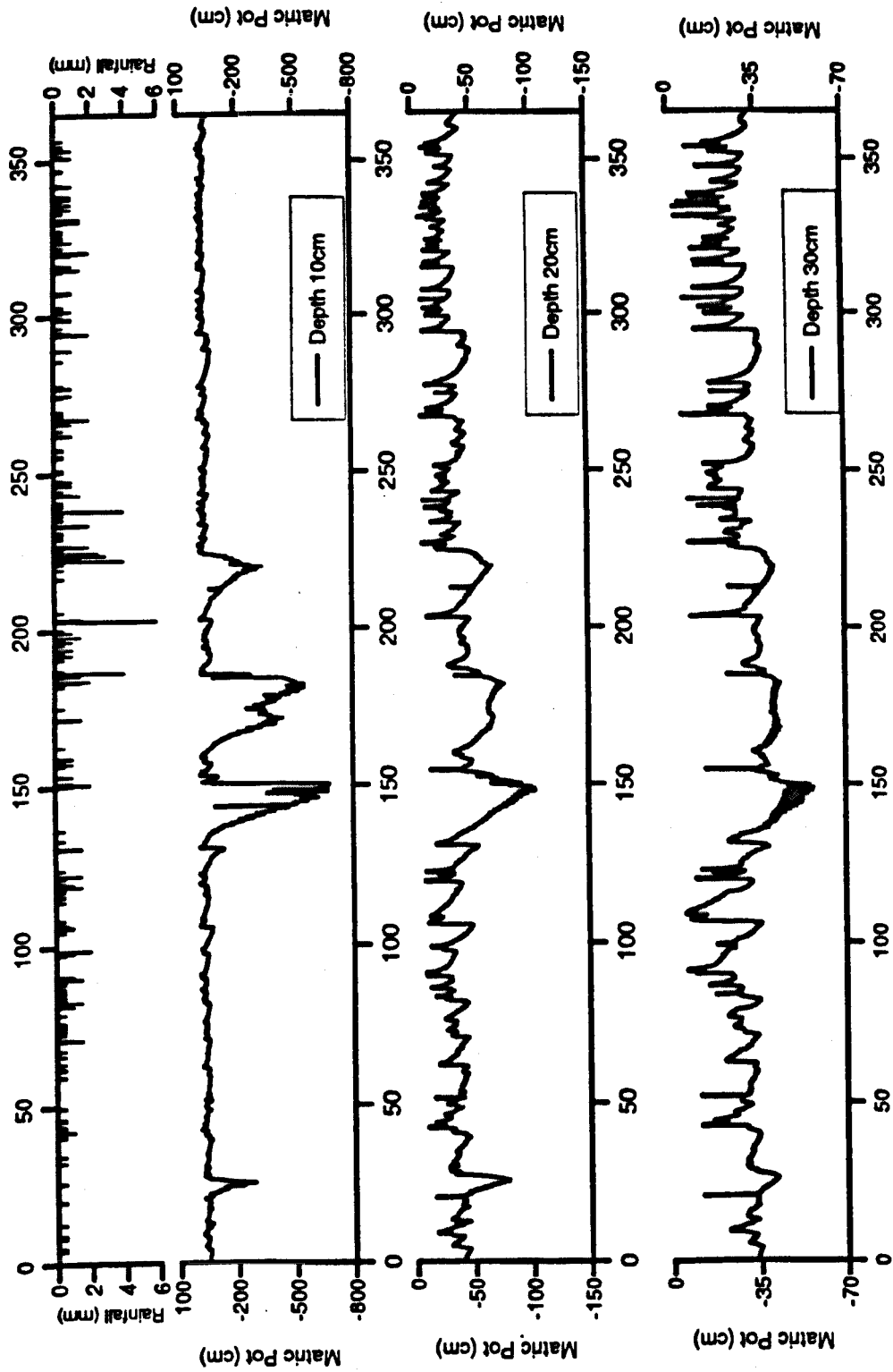


Figure I.3 Matric potentials - Lysimeter A - 1992

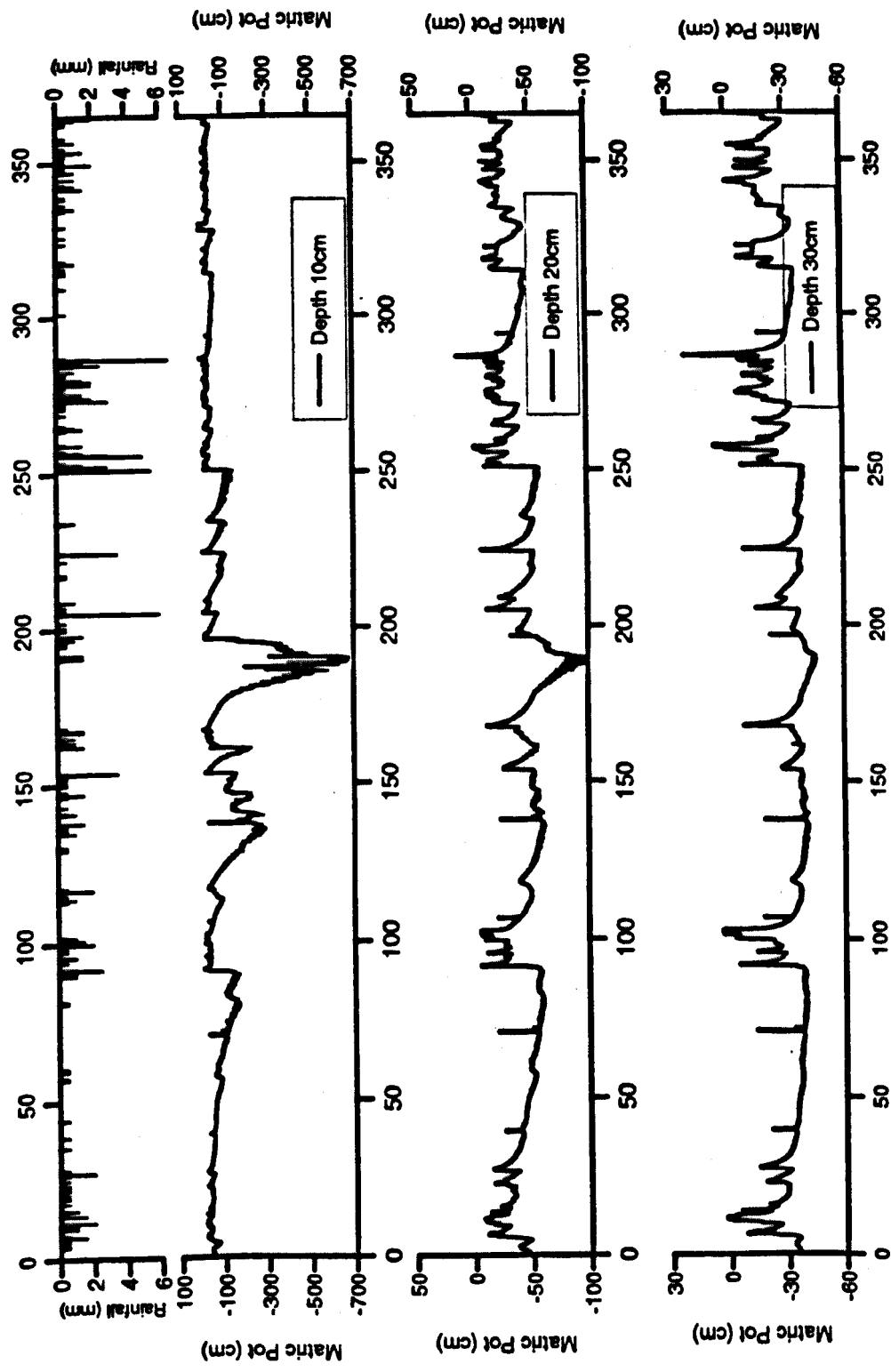


Figure I.4 Matric potentials - Lysimeter A - 1993

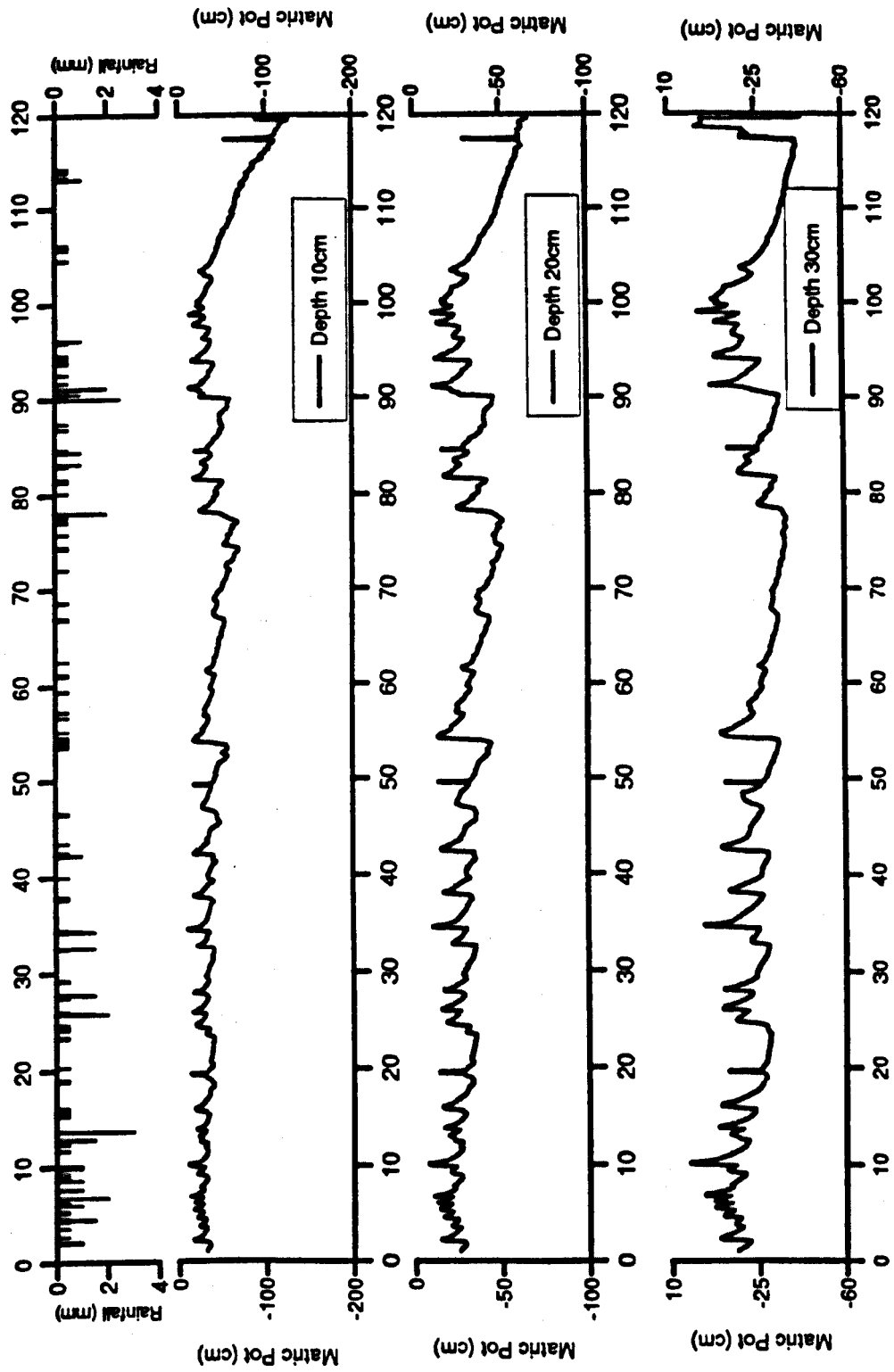


Figure 1.5 Matric potentials - Lysimeter A - 1994

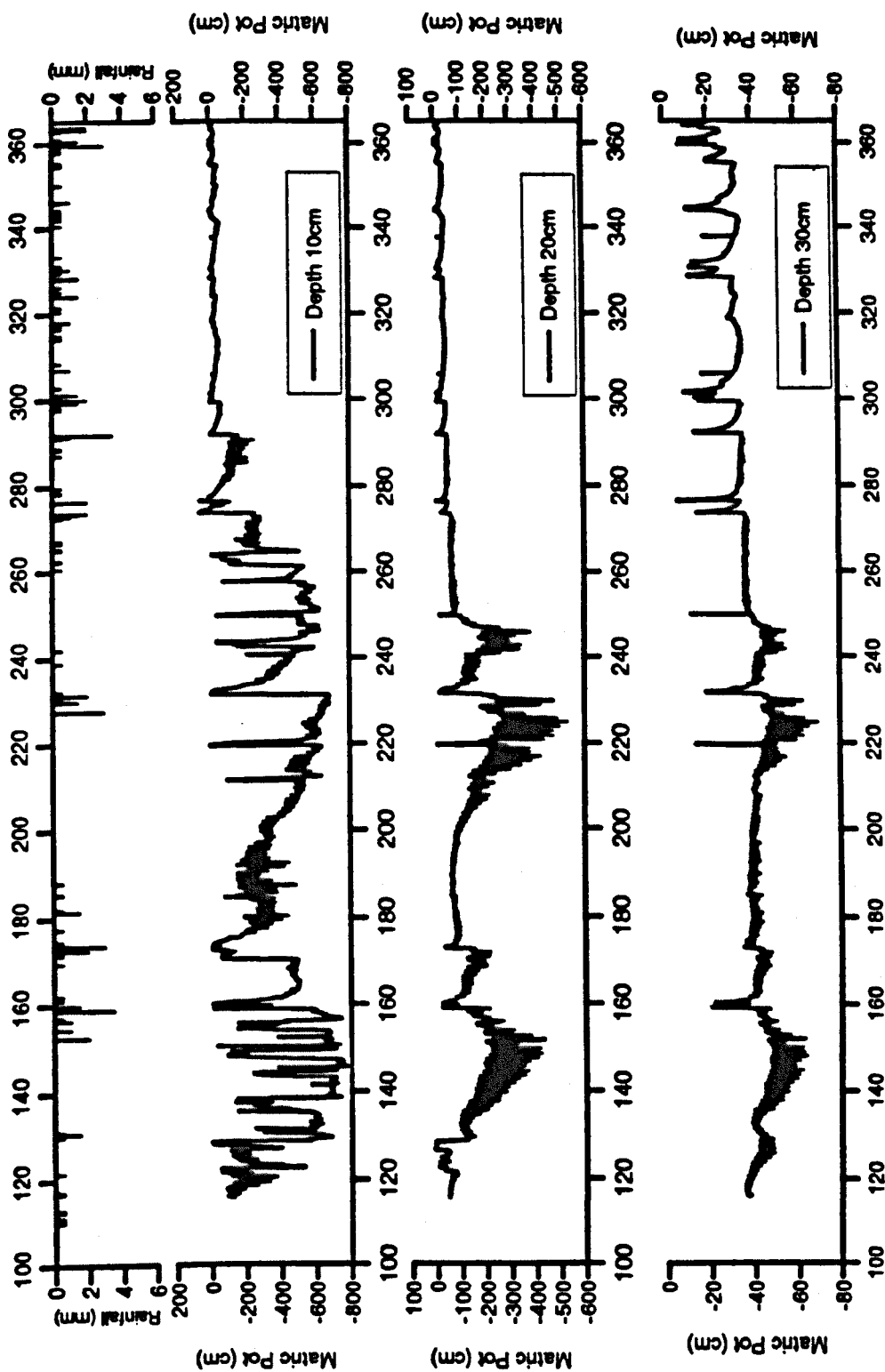


Figure I.6 Matric potentials - Lysimeter B - 1990

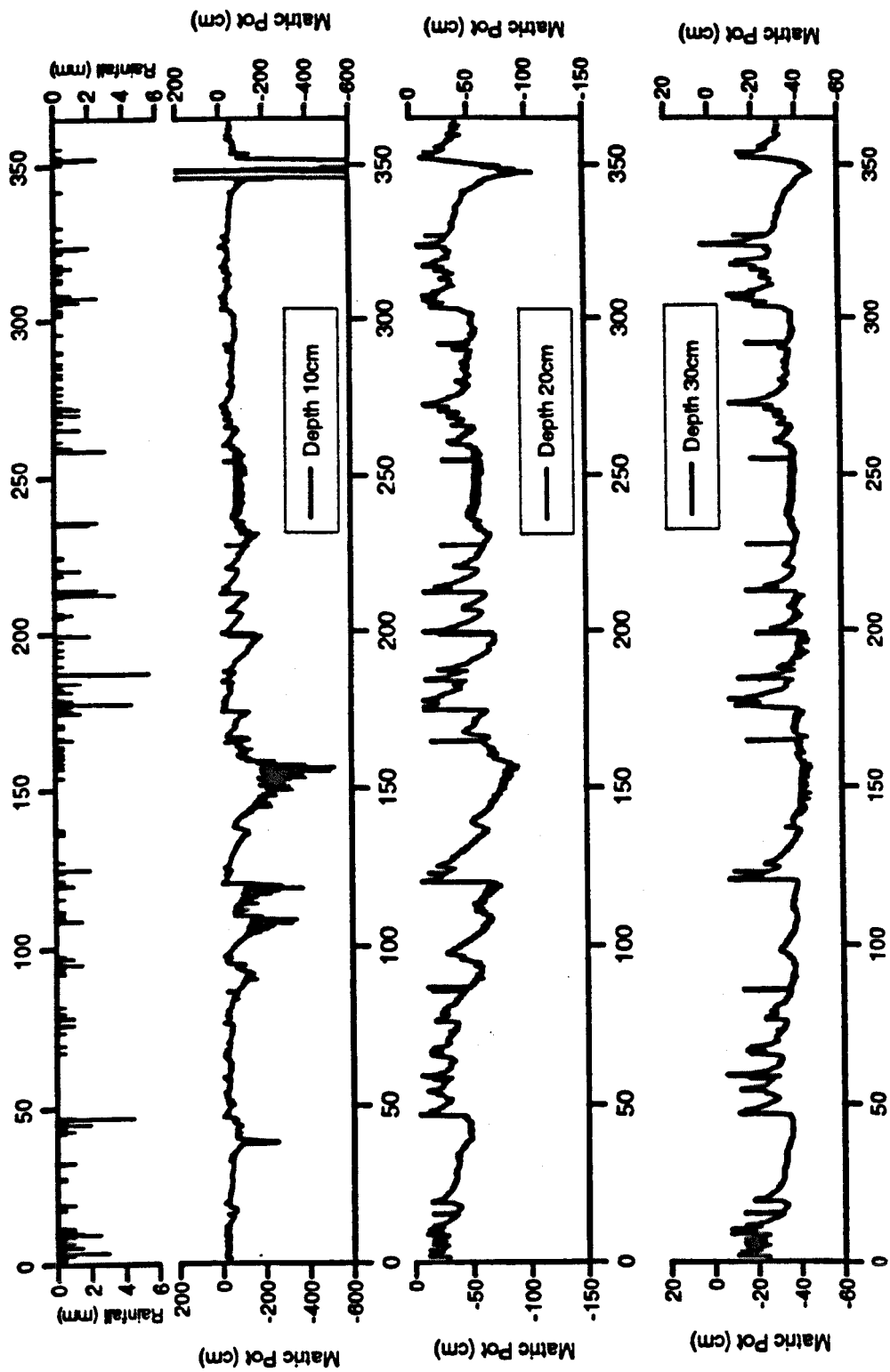


Figure 1.7 Matric potentials - Lysimeter B - 1991

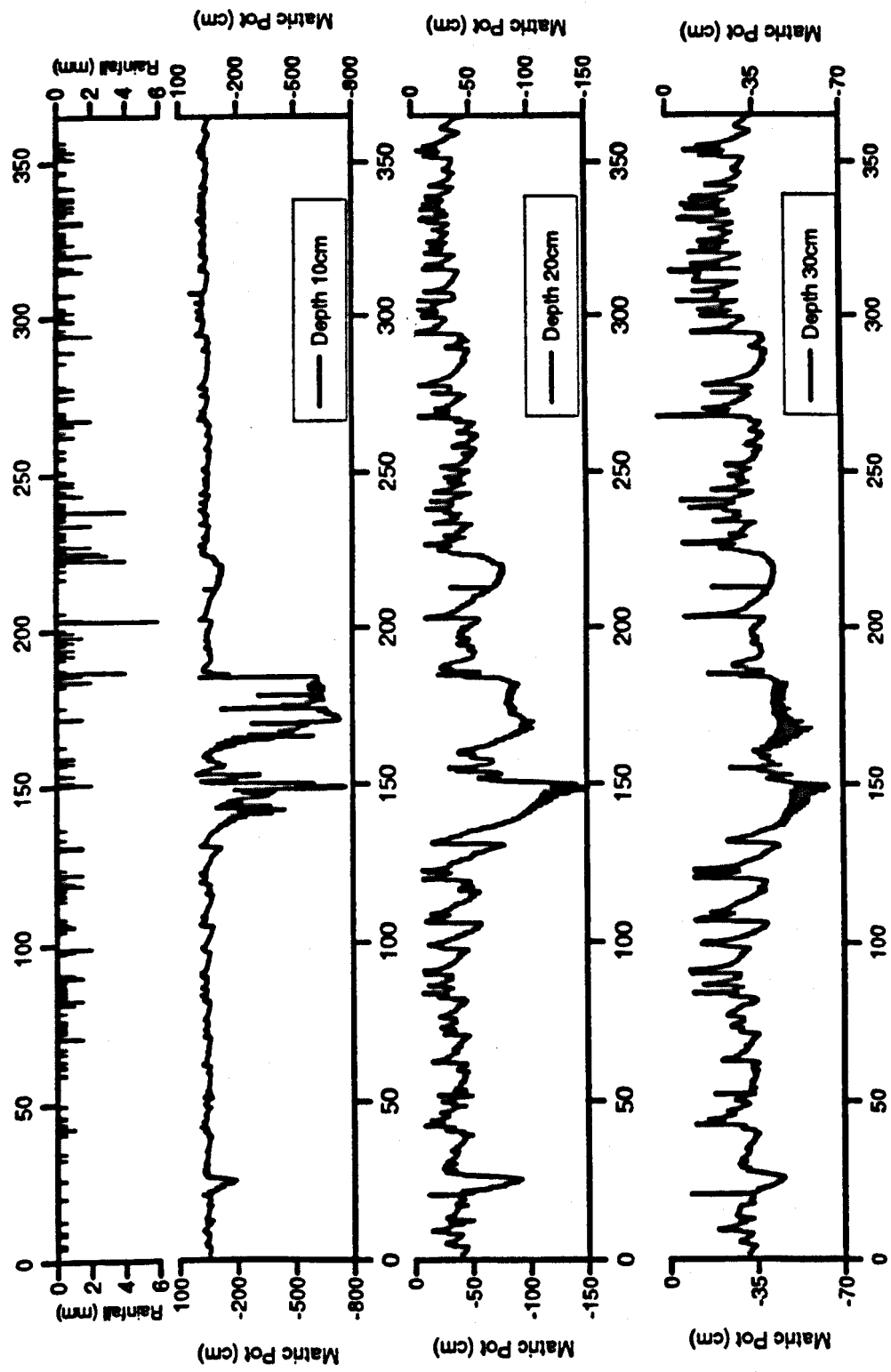


Figure 1.8 Matric potentials - Lysimeter B - 1992

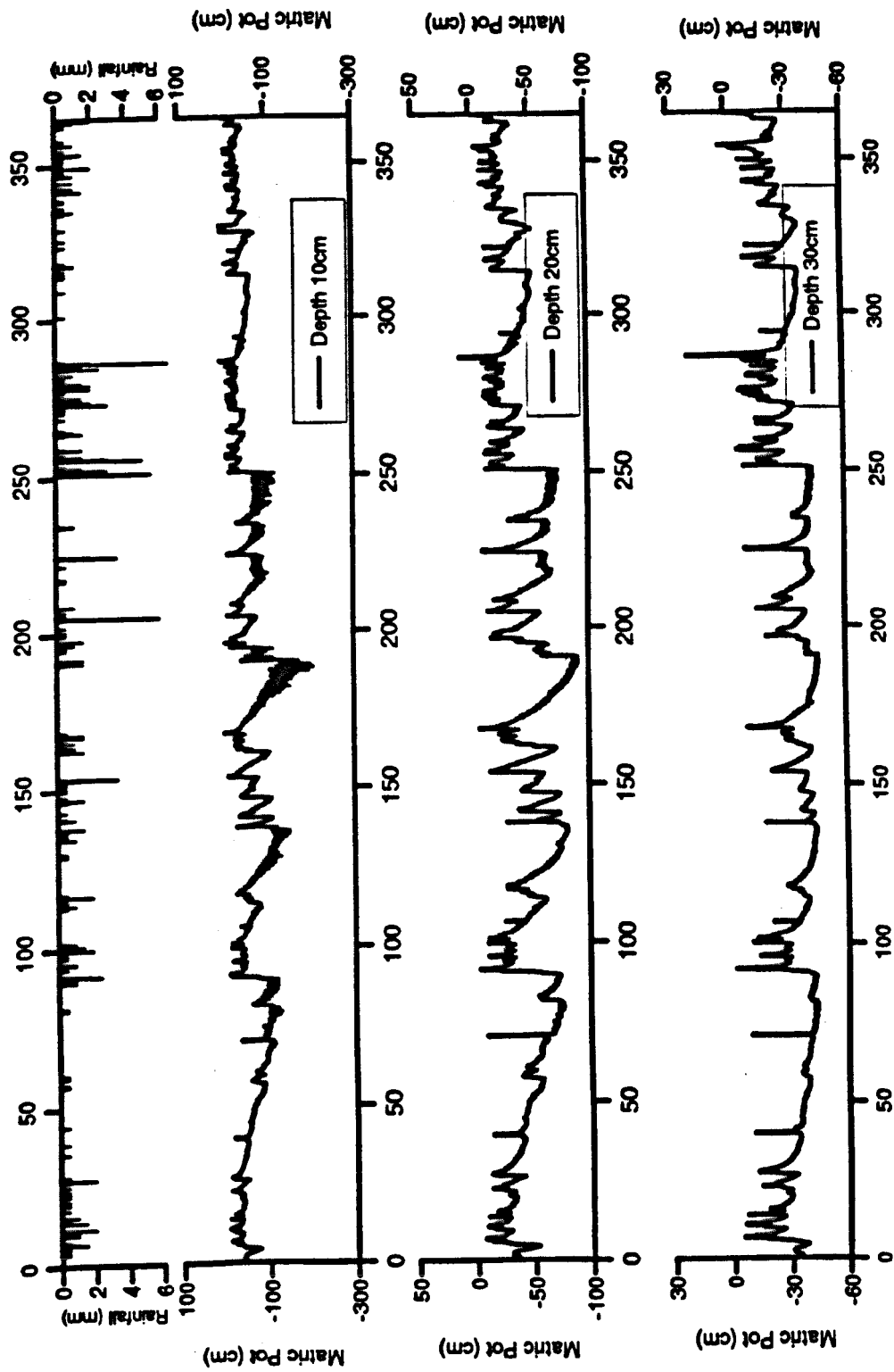


Figure I.9 Matric potentials - Lysimeter B - 1993

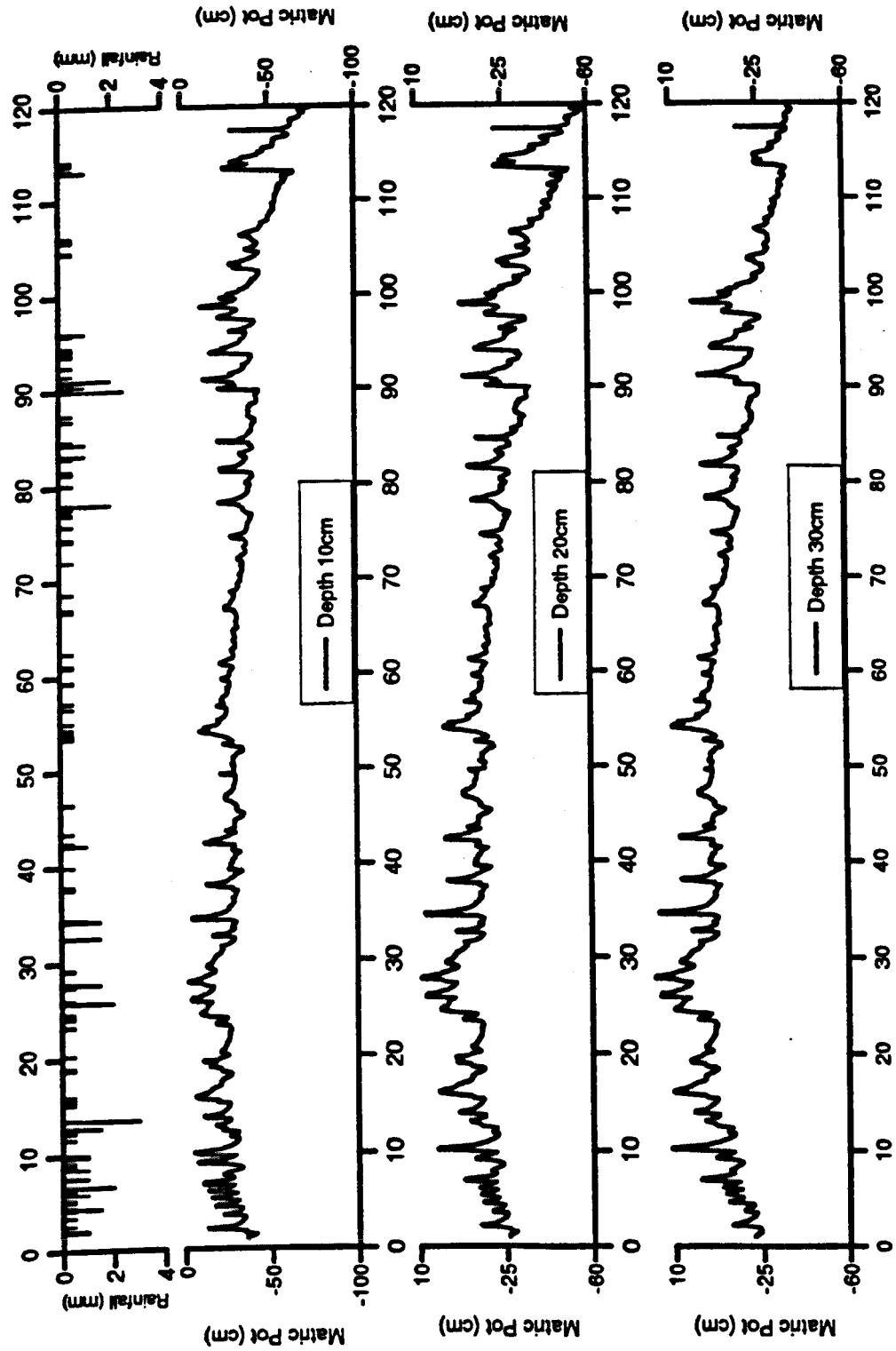


Figure I.10 Matric potentials - Lysimeter B - 1994

APPENDIX II

Soil particle size analysis using hydrometer method

SOIL PARTICLE SIZE ANALYSIS USING HYDROMETER METHOD

Source: Personal communication by Chacksfield (1994)

The soil sample to be analyzed is oven dried at 105°C and then passed through a 2mm sieve. A 50.0g sub-sample of this sieved soil is taken and placed in an 800ml glass beaker. To this is added 200ml de-ionised water and 15ml 1.0M di-sodium ethandioate solution. This mixture is allowed to stand overnight, and then dispersed using an electrical stirrer and baffle. The suspension is then transferred into a 1000ml measuring cylinder and diluted up to the 1000ml mark. The measuring cylinder is sealed, shaken thoroughly, and unsealed.

The shaken suspension is then allowed to stand for four minutes, at which time a Boyoucos soil hydrometer is placed into the measuring cylinder. After the suspension had been standing for five minutes a reading of particle concentrations (concentration C1, in g/l) in the suspension is taken from the hydrometer. The temperature of the suspension is also taken at this time (temperature T1), to account for changes in density of the water due to temperature.

The hydrometer is removed and the measuring cylinder again sealed, shaken and unsealed. The suspension is allowed to settle for five hours, after which hydrometer and temperature readings are taken again (concentration C2 and temperature T2, respectively).

The effect of the di-sodium ethandioate on the apparent particle concentration of the suspensions is determined by floating the hydrometer in a 'blank' solution of 15ml of the di-sodium ethandioate in 200ml de-ionised water. A thermometer reading is taken and a temperature correction is applied to this result. The reading on the hydrometer is the zero offset of the di-sodium ethandioate.

A temperature correction of +0.3g/l per degree centigrade of the solution above the zero offset due to the presence of the di-sodium ethandioate is applied to each result.

The value of concentration C1 is due to the presence of suspended silt and clay particles, whereas the value of concentration C2 is due only to suspended clay particles. Hence, C1-C2 is the concentration of silt particles in the suspension.

Once the mass of silt and clay have been determined, the remainder of the original 50g is assumed to be entirely sand.

APPENDIX III
Instructions for using the falling head permeameter

INSTRUCTIONS FOR USING THE FALLING HEAD PERMEAMETER

This apparatus, shown in figure III.1, comprises a permeability cell, a set of core cutters, a standpipe panel, a soaking tank, a funnel and silicone tubing. It is used to measure the permeability (or saturated hydraulic conductivity) of clays, silts and fine sand. This method of permeability determination measures the hydraulic gradient and quantity of water flowing into the sample using a varying head of water during the test. The permeability cell supplied is for use with undisturbed samples in 10cm diameter and 13cm high core cutters. The standpipe panel holds 6 glass tubes, each of them approximately 1m long and with bores of 27.4mm, 22.1mm, 13.1mm, 10mm, 5.3mm and 3.4mm. A stopwatch and a balance are also necessary to perform the test.

1. Preparing the cores

After collecting the samples, trim them in the core cutter and assure that they are completely saturated with water. To do that, soak them into water by placing them in a soaking tank and slowly filling the tank with de-aired water, so that the cores are wetted from the bottom to the top, eliminating all the air from the pores. This task can be performed overnight, in order to assure there is no entrapped air. The water is de-aired by boiling.

Assemble the cell about the core cutter ensuring that a metal gauze disc is fitted at each end of the cutter and also that the cell top is filled with steel wool. Attach the tubing as shown in figure 1, choosing the relevant standpipe tube, with all the three clips closed. Ensure that all the air is eliminated from the tubing and that no air is introduced into the core.

2. Performing a single test

Fill the funnel with de-aired water. Select an initial (maximum) head of water (usually around 50cm). Don't forget that the head is measured from the soaking tank overflow weir (add the offset to the readings on the scale; for the setup in the hydrology laboratory, the offset is 2cm). Open clips A and B to fill the standpipe tube just over the adopted maximum head. Close clip A and open clip C. Allow the water to fall to the initial head on the standpipe and then start the stopwatch. Note the time taken for the water level in the tube to reach several intermediate levels, until the final one, coincident with the zero of the scale. Close all the clips and repeat the test at least three times. If necessary, choose a different diameter for the standpipe tube.

Weigh the wet sample, allow it to dry completely in an oven and weigh it again, in order to determinate the porosity, dry bulk density and void ratio of the core.

3. Calculations

Using Darcy's Law,

$$v = -Ki \Rightarrow \frac{dV}{Adt} = -K \frac{h}{L} \quad (\text{III.1})$$

where: v is the Darcy velocity; K is the saturated soil hydraulic conductivity; i is the hydraulic head gradient; dV is the volume of the water which passes through the sample in time dt ; A is the cross-sectional area of the sample; h is the hydraulic head; L is the length of the soil sample (in the direction of flux).

The volume of water that passes through the sample is equal to the volume variation in the

standpipe, and thus the equation can be written as:

$$\frac{a}{A} \int \frac{dh}{h} = - \frac{K}{L} \int dt \quad (\text{III.2})$$

where a is the cross sectional area of the standpipe. Integrating the equation between the instants $t=t_0$ and $t=t_1$, when the height of the water column in the standpipe is h_0 and h_1 , respectively, and defining D as the diameter of the core and d as the internal diameter of the standpipe, we obtain

$$K = \frac{d^2 L}{D^2 (t_1 - t_0)} \ln\left(\frac{h_0}{h_1}\right) \quad (\text{III.3})$$

Use equation III.3 in order to estimate the saturated hydraulic conductivity of the sample.

The porosity, dry bulk density and void ratio of the core are defined by the following equations.

Porosity:

$$f = \frac{V_G + V_L}{V_T} = \frac{(M_{\text{wet}} - M_{\text{dry}})}{(\pi R^2 L)} \quad (\text{III.4})$$

Dry Bulk Density:

$$\rho_b = \frac{M_s}{V_T} = \frac{M_{\text{dry}}}{(\pi R^2 L)} \quad (\text{III.5})$$

Void Ratio:

$$e = \frac{V_L}{V_s} = \frac{f}{1-f} \quad (\text{III.6})$$

where R is the radius of the core; V_G , V_L , V_s and V_T are the volume of gases, liquids, solids and the total volume, respectively; M_G , M_L , M_s and M_T are the corresponding masses; and M_{wet} and M_{dry} are the measured masses for the core wet and dry.

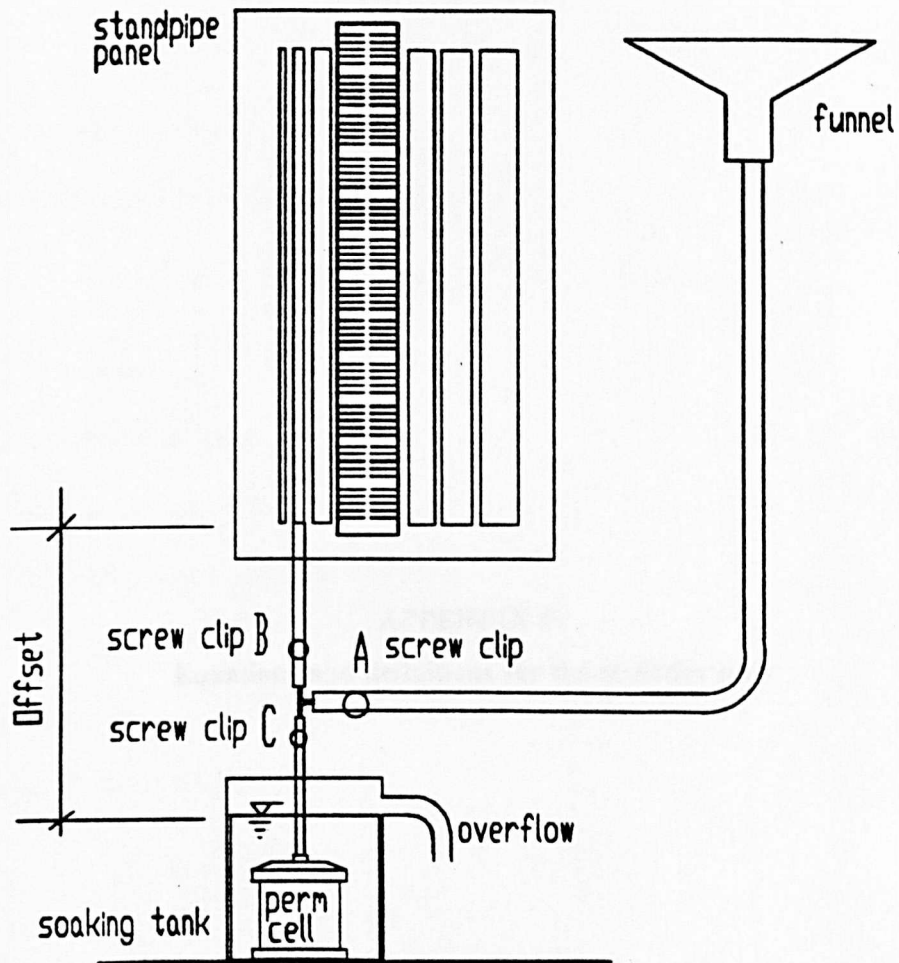


Figure III.1 - Schematic of the falling head permeameter

APPENDIX IV
Equations and definitions for the statistics tests

EQUATIONS AND DEFINITIONS FOR THE STATISTICS TESTS

Source: Benjamin and Cornell (1970); Green and Margerison (1978)

X : random variable

$f_X(x)$: probabilistic density function (pdf)

$m_X^{(n)}$: n^{th} moment of the random variable X

$$m_X^{(n)} = E[X^n] = \int_{-\infty}^{\infty} x^n f_X(x) dx$$

$\mu \equiv m_X^{(1)}$: random variable mean

$\mu_X^{(n)}$: Moments about the mean (central moments)

$$\mu_X^{(n)} = E[(X - m_X)^n] = \int_{-\infty}^{\infty} (x - m_X)^n f_X(x) dx$$

$\sigma^2 \equiv \mu_X^{(2)}$: variance

$V = \sigma/\mu$: coefficient of variation

$\gamma_1 = \mu_X^{(3)}/\sigma^3$: coefficient of skewness

$\gamma_2 = \mu_X^{(4)}/\sigma^4$: coefficient of kurtosis (flatness)

x : observed value

$\bar{x}$: sample mean

m_n : sample n^{th} moment about the mean

$$m_n = 1/n \sum_i (x_i - \bar{x})^n$$

s^2 : sample variance

$$s^2 = \frac{n}{n-1} m_2$$

s : sample standard deviation

$v = |s/\bar{x}|$: sample coefficient of variation

$g_1 = m_3/s^3$: sample coefficient of skewness

$g_2 = m_4/s^4$: sample coefficient of kurtosis (flatness)

Gamma distribution:

$$\mu = K/\lambda;$$

$$\sigma^2 = k/\lambda;$$

$$V = K^{-1/2};$$

$$\gamma_1 = 2 K^{-1/2}$$

Exponential distribution:

It is a Gamma distribution with $K = 1$:

$$V = 1;$$

$$\gamma_1 = 2;$$

$$\gamma_2 = 9$$

Normal distribution:

Odd moments (and skewness) equal zero;

Kurtosis: $\gamma_2 = 3$ ($\gamma_2 > 3$ means flat; $\gamma_2 < 3$ means peaked)

Log-Normal distribution:

$$Y = \ln X$$

Y is treated as a random variable with a normal distribution

Test between means drawn from two samples - normal distributions (X and Y) with unequal unknown variances:

$$H_0: \mu_x = \mu_y$$

$$H_1: \mu_x \neq \mu_y$$

Student's t-distribution for

$$T = \frac{\bar{x} - \bar{y}}{\sqrt{\frac{S_x^2}{n_x} + \frac{S_y^2}{n_y}}}$$

$$\frac{1}{f} = \frac{1}{f_x} \left(\frac{S_x^2/n_x}{S_x^2/n_x + S_y^2/n_y} \right)^2 + \frac{1}{f_y} \left(\frac{S_y^2/n_y}{S_x^2/n_x + S_y^2/n_y} \right)^2$$

$$f_x = n_x - 1 ; f_y = n_y - 1$$

$$P\left[-t\left(\frac{\alpha}{2}, f\right) < t < +t\left(\frac{\alpha}{2}, f\right) \right] = 1 - \alpha$$

APPENDIX V**Discordancy tests for outliers in univariate normal samples****Equations, definitions and tables**

DISCORDANCY TESTS FOR OUTLIERS IN UNIVARIATE NORMAL SAMPLES EQUATIONS, DEFINITIONS AND TABLES

Source: Barnett and Lewis (1984)

n : sample size

μ : random variable mean

$\bar{x}$: sample mean

σ^2 : variance

s^2 : sample variance

S^2 : sum of squares: $S^2 = (n-1)s^2 = \sum (x_i - \bar{x})^2$

P : probability

T : test statistic

t : sample T value

$t_{(n)}$: Student's t with n degrees of freedom

F and G : Normal distributions, $F \sim N(\mu, \sigma^2)$, $G \sim N(\mu+a, \sigma^2)$

a : location-slippage

k : number of upper outliers

Working hypothesis (null hypothesis):

$$H_0: x_{(j)} \in F$$

Alternative hypothesis (labelled slippage):

$$H_1: x_{(1)}, \dots, x_{(n-k)} \in F$$

$$x_{(n-k+1)}, \dots, x_{(n-1)}, x_{(n)} \in G$$

$SP(t)$:significance probability attaching to an observed value t of a discordancy statistic T . It is the probability that, on the working hypothesis, T takes values more discordant than t (generally, $T > t$)

TEST N1 - Discordancy test for a single upper outlier $x_{(n)}$ in a normal sample with μ and σ^2 unknown

Test statistic:

$t = T_{N1}$ = internally studentized deviation from the mean

$$T_{N1} = \frac{x_{(n)} - \bar{x}}{s}$$

Inequality:

$$SP(t) \leq n P[t_{n-2} > (\frac{n(n-2)}{(n-1)^2 - nt^2})^{1/2}]$$

Tabulated significance levels: Table V.1 (Barnett and Lewis, 1984); values of T_{N1} bigger than the tabulated are significant.

Properties of test: N1 is the maximum likelihood test for a location-slippage alternative in which one observation arises from a normal distribution $N(\mu+a, \sigma^2)$, $a > 0$. For this alternative, it has the optimal property of being the scale- and location-invariant test of given size which maximizes the probability of identifying the contaminant as a discordant outlier. Vulnerable to masking effect when there is more than one contaminant. Not very suitable for consecutive use when testing several outliers.

Table V.1 Critical values for 5% and 1% tests of discordancy for a single outlier in a normal sample, using the deviation from the sample mean or population mean, studentized or standardized, as test statistic (after Barnett and Lewis, 1984)

N1		
<i>n</i>	5%	1%
3	1.15	1.15
4	1.46	1.49
5	1.67	1.75
6	1.82	1.94
7	1.94	2.10
8	2.03	2.22
9	2.11	2.32
10	2.18	2.41
12	2.29	2.55
14	2.37	2.66
15	2.41	2.71
16	2.44	2.75
18	2.50	2.82
20	2.56	2.88
30	2.74	3.10
40	2.87	3.24
50	2.96	3.34
60	3.03	3.41
100	3.21	3.60
120	3.27	3.66

TEST N4 - Discordancy test for k upper outliers $x_{(n-k+1)}, \dots, x_{(n-1)}, x_{(n)}$ in a normal sample with μ and σ^2 unknown

Test statistic:
 $t = T_{N4} = (\text{reduced sum of squares})/(\text{total sum of squares})$

$$T_{N4} = \frac{(S_{n-k+1, \dots, n-1, n})^2}{S^2} = \frac{(n-k+1) (s_{n-k+1, \dots, n-1, n})^2}{(n-1) s^2}$$

Tabulated significance levels: Table V. 2 (Barnett and Lewis, 1984); values of T_{N4} smaller than the tabulated are significant.

Properties of test: N4 is the maximum likelihood test for a location-slippage alternative in which k observations arise from separate normal distributions, each with variance σ^2 , but distinct means, all exceeding μ . There is indication that N4 is more robust than N3 (T_{N3} is the sum of internally studentized deviations from the mean) against departures from the relevant alternative. Also better performance, in terms of proportion of contaminants correctly identified as discordant, than consecutive procedures using N14 (T_{N14} is the sample skewness), and much better performance than consecutive procedures using N1. Detailed descriptions of N3, N14 and other discordancy tests can be found in Barnett and Lewis (1984).

Table V.2 Critical values for 5% and 1% tests of discordancy for k upper outliers in a normal sampler (after Barnett and Lewis, 1984)

N4					
k = 2		k = 3		k = 4	
5%	1%	5%	1%	5%	1%
0.019	0.0034				
0.056	0.019				
0.102	0.044	0.032	0.010		
0.148	0.075	0.064	0.028		
0.191	0.108	0.099	0.048	0.045	0.018
0.231	0.141	0.129	0.070	0.070	0.032
0.300	0.204	0.196	0.120	0.125	0.070
0.357	0.261	0.250	0.172	0.174	0.113
0.405	0.310	0.300	0.219	0.219	0.151
0.446	0.353	0.337	0.260	0.259	0.192
0.480	0.391	0.377	0.300	0.299	0.231
0.601	0.527	0.506	0.434	0.434	0.369
0.672	0.610	0.588	0.522	0.523	0.460
0.720	0.667	0.646	0.592	0.588	0.531
0.833	0.802				

APPENDIX VI
Results of the parameter optimisations

Table VI.1 - SPW1hyst optimisation of rapid flow event 90158

Simulation		V	L	Optimised parameters									R ² (p)	R ² (f)
				α 1/cm	n	λ -	ψ_b cm	θ_s m ³ /m ³	θ_r m ³ /m ³	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	P	A	*	*	*	*	*	*	1.61	1.61	1.61	0.96	-14
		P	B	*	*	*	*	*	*	7.58	7.58	7.58	0.59	-302
		f	A	*	*	*	*	*	*	0.34	0.34	0.34	0.63	0.83
		f	B	*	*	*	*	*	*	0.61	0.61	0.61	0.18	0.34
	V2	P	A	0.13	1.48	*	*	*	*	*	*	*	0.95	-1.0
		P	B	0.07	1.19	*	*	*	*	*	*	*	0.61	-51
		f	A	0.17	2.01	*	*	*	*	*	*	*	0.78	0.88
		f	B	0.10	1.09	*	*	*	*	*	*	*	0.56	0.41
	V3	P	A	0.05	1.79	*	*	*	*	1.01	1.01	1.01	0.96	-22
		P	B	0.01	1.30	*	*	*	*	0.12	0.12	0.12	0.63	-34
		f	A	0.15	1.82	*	*	*	*	3.98	3.98	3.98	0.90	0.88
		f	B	0.22	1.07	*	*	*	*	37.13	37.13	37.13	0.55	0.44
	V4	P	A	0.07	1.89	*	*	0.60	0.03	*	*	*	0.96	-86
		P	B	0.06	1.16	*	*	0.60	0.09	*	*	*	0.62	-87
		f	A	0.18	2.03	*	*	0.37	0.02	*	*	*	0.75	0.88
		f	B	0.17	1.52	*	*	0.40	0.06	*	*	*	0.30	0.37
	B1	P	A	*	*	*	*	*	*	0.43	0.43	0.43	0.96	-6.0
		P	B	*	*	*	*	*	*	0.95	0.95	0.95	0.60	-205
		f	A	*	*	*	*	*	*	0.14	0.14	0.14	0.78	0.85
		f	B	*	*	*	*	*	*	0.12	0.12	0.12	0.48	0.24
	B2	P	A	*	*	0.30	-1.25	*	*	*	*	*	0.92	-0.4
		P	B	*	*	0.22	-2.94	*	*	*	*	*	0.60	-46
		f	A	*	*	0.59	-2.89	*	*	*	*	*	0.82	0.87
		f	B	*	*	0.81	-4.11	*	*	*	*	*	0.37	0.43
	B3	P	A	*	*	0.90	-21.3	*	*	0.24	0.24	0.24	0.96	-47
		P	B	*	*	0.25	-2.26	*	*	14.63	14.63	14.63	0.60	-45
		f	A	*	*	0.56	-2.68	*	*	7.21	7.21	7.21	0.80	0.87
		f	B	*	*	0.80	-4.09	*	*	6.08	6.08	6.08	0.38	0.43
NON-HYST HETERO	V3	P	A	*	*	*	*	*	*	1.59	1.59	0.67	0.96	-8.2
		P	B	*	*	*	*	*	*	12.12	0.08	0.01	0.66	-3.5
		f	A	*	*	*	*	*	*	0.46	0.40	0.27	0.73	0.81
		f	B	*	*	*	*	*	*	11.25	0.61	0.57	0.65	0.30
	V5	P	A	0.03	2.18	*	*	*	*	0.40	0.40	0.07	0.96	-7.0
		P	B	0.06	1.81	*	*	*	*	13.58	0.10	0.10	0.66	-1.2
		f	A	0.07	1.72	*	*	*	*	18.07	0.97	0.17	0.58	0.78
		f	B	0.07	1.46	*	*	*	*	54.18	1.70	0.19	0.51	0.30
	B3	P	A	*	*	*	*	*	*	0.43	0.43	0.11	0.96	-0.6
		P	B	*	*	*	*	*	*	2.35	0.01	0.01	0.66	-3.6
		f	A	*	*	*	*	*	*	0.41	0.22	0.08	0.95	0.79
		f	B	*	*	*	*	*	*	24.41	0.41	0.03	0.42	0.13
	B5	P	A	*	*	0.30	-6.75	*	*	0.35	0.35	0.35	0.95	0.28
		P	B	*	*	0.86	-14.1	*	*	5.67	0.06	0.06	0.66	-1.53
		f	A	*	*	0.58	-8.34	*	*	0.97	0.39	0.11	0.94	0.82
		f	B	*	*	0.41	-9.97	*	*	24.21	0.46	0.02	0.41	0.25

Var = optimised variable
p = matric potential
f = bottom inflow
* = parameter not optimised

Table VI.2 - SPW1hyst optimisation of rapid flow event 90230

Simulation		V	a	L	y	Optimised parameters						R ² (p)	R ² (f)		
						α 1/cm	n	λ -	ψ_s cm	θ_s m ² /m ³	θ_r m ² /m ³			Ks ₁ cm/h	Ks ₂ cm/h
NON-HYST HOMOGENEOUS	V1	p	A	*	*	*	*	*	*	0.09	0.09	0.09	0.57	0.33	
			B	*	*	*	*	*	*	*	1.78	1.78	1.78	0.30	0.96
			A	*	*	*	*	*	*	*	0.14	0.14	0.14	0.51	0.37
			B	*	*	*	*	*	*	*	1.83	1.83	1.83	0.30	0.96
	V2	p	A	0.09	1.43	*	*	*	*	*	*	*	*	0.32	-10
			B	0.09	1.39	*	*	*	*	*	*	*	*	0.28	0.80
			A	0.21	1.18	*	*	*	*	*	*	*	*	0.23	0.33
			B	0.10	1.42	*	*	*	*	*	*	*	*	0.28	0.83
	V3	p	A	0.20	1.98	*	*	*	*	0.01	0.01	0.01	0.93	0.18	
			B	0.01	1.74	*	*	*	*	0.01	0.01	0.01	0.50	0.24	
			A	0.20	1.98	*	*	*	*	0.01	0.01	0.01	0.93	0.18	
			B	0.05	1.48	*	*	*	*	0.60	0.60	0.60	0.33	0.99	
	V4	p	A	0.50	1.26	*	*	0.59	0.01	*	*	*	0.69	-0.5	
			B	0.11	1.27	*	*	0.60	0.01	*	*	*	0.35	0.95	
			A	0.15	1.11	*	*	0.55	0.01	*	*	*	0.29	0.43	
			B	0.11	1.30	*	*	0.58	0.05	*	*	*	0.34	0.97	
	B1	p	A	*	*	*	*	*	*	0.05	0.05	0.05	0.46	0.41	
			B	*	*	*	*	*	*	0.29	0.29	0.29	0.28	0.91	
			A	*	*	*	*	*	*	0.05	0.05	0.05	0.46	0.41	
			B	*	*	*	*	*	*	0.29	0.29	0.29	0.28	0.91	
	B2	p	A	*	*	0.60	-6.79	*	*	*	*	*	0.28	-4.8	
			B	*	*	0.52	-6.19	*	*	*	*	*	0.26	-0.1	
			A	*	*	0.28	-1.14	*	*	*	*	*	0.18	-0.1	
			B	*	*	0.45	-5.64	*	*	*	*	*	0.26	-0.1	
	B3	p	A	*	*	0.64	-10.1	*	*	0.01	0.01	0.01	0.79	0.06	
			B	*	*	0.90	-38.6	*	*	0.02	0.02	0.02	0.34	0.12	
			A	*	*	0.60	-26.1	*	*	0.01	0.01	0.01	0.77	0.65	
			B	*	*	0.84	-17.1	*	*	0.15	0.15	0.15	0.25	0.98	
NON-HYST HETTER	V3	p	A	*	*	*	*	*	*	0.05	0.05	0.03	0.66	0.13	
			B	*	*	*	*	*	*	*	11.04	0.05	0.05	0.42	-3.0
			A	*	*	*	*	*	*	*	2.47	1.34	0.02	0.35	0.62
			B	*	*	*	*	*	*	*	54.75	3.39	0.34	0.20	0.97
	V5	p	A	0.02	1.81	*	*	*	*	0.07	0.07	0.07	0.61	-3.8	
			B	0.02	1.62	*	*	*	*	0.35	0.01	0.01	0.53	-2.5	
			A	0.04	1.60	*	*	*	*	0.56	0.54	0.02	0.43	0.68	
			B	0.02	1.35	*	*	*	*	16.03	1.91	0.05	0.13	0.99	
	B3	p	A	*	*	*	*	*	*	0.09	0.05	0.03	0.40	0.42	
			B	*	*	*	*	*	*	0.94	0.01	0.01	0.37	-3.1	
			A	*	*	*	*	*	*	0.20	0.19	0.02	0.36	0.64	
			B	*	*	*	*	*	*	25.18	0.61	0.08	0.15	0.95	
	B5	p	A	*	*	0.48	-11.2	*	*	0.08	0.04	0.03	0.42	0.50	
			B	*	*	0.89	-19.0	*	*	4.50	0.03	0.02	0.36	-2.0	
			A	*	*	0.52	-12.1	*	*	32.10	0.13	0.01	0.16	0.64	
			B	*	*	0.40	-14.4	*	*	40.60	0.63	0.02	0.10	0.98	

Var = optimised variable
p = matric potential
f = bottom inflow
* = parameter not optimised

Table VI.3 - SPW1hyst optimisation of rapid flow event 90291

Simulation	V	a	L	Optimised parameters									R ² (p)	R ² (f)
				α 1/cm	n	λ	Ψ_b cm	θ_r m ³ /m ³	θ_r m ³ /m ³	K _{s1} cm/h	K _{s2} cm/h	K _{s3} cm/h		
NON-HYST HOMOGENEOUS	V1	p	A	*	*	*	*	*	*	2.53	2.53	2.53	0.88	0.23
		p	B	*	*	*	*	*	*	1.97	1.97	1.97	0.89	-2.1
		f	A	*	*	*	*	*	*	4.88	4.88	4.88	0.83	0.79
		f	B	*	*	*	*	*	*	23.93	23.93	23.93	0.70	0.72
	V2	p	A	0.08	1.21	*	*	*	*	*	*	*	0.99	0.74
		p	B	0.08	2.00	*	*	*	*	*	*	*	0.90	0.06
		f	A	0.06	1.86	*	*	*	*	*	*	*	0.81	0.79
		f	B	0.05	1.28	*	*	*	*	*	*	*	0.75	0.83
	V3	p	A	0.07	1.21	*	*	*	*	5.00	5.00	5.00	0.99	0.75
		p	B	0.08	2.01	*	*	*	*	4.98	4.98	4.98	0.91	-0.2
		f	A	0.06	1.78	*	*	*	*	5.99	5.99	5.99	0.82	0.80
		f	B	0.08	1.41	*	*	*	*	26.40	26.40	26.40	0.73	0.84
	V4	p	A	0.10	1.36	*	*	0.31	0.05	*	*	*	0.99	0.72
		p	B	0.08	1.96	*	*	0.44	0.03	*	*	*	0.90	-0.5
		f	A	0.05	1.91	*	*	0.53	0.05	*	*	*	0.65	0.89
		f	B	0.05	1.55	*	*	0.37	0.09	*	*	*	0.74	0.84
	B1	p	A	*	*	*	*	*	*	0.84	0.84	0.84	0.91	0.40
		p	B	*	*	*	*	*	*	0.26	0.26	0.26	0.88	-2.0
		f	A	*	*	*	*	*	*	1.36	1.36	1.36	0.88	0.75
		f	B	*	*	*	*	*	*	2.63	2.63	2.63	0.72	0.81
	B2	p	A	*	*	0.22	-2.77	*	*	*	*	*	0.99	0.69
		p	B	*	*	0.72	-5.84	*	*	*	*	*	0.88	0.39
		f	A	*	*	0.55	-5.46	*	*	*	*	*	0.96	0.74
		f	B	*	*	0.55	-9.64	*	*	*	*	*	0.75	0.84
	B3	p	A	*	*	0.30	-1.98	*	*	22.81	22.81	22.81	0.98	0.67
		p	B	*	*	0.89	-11.5	*	*	1.25	1.25	1.25	0.90	-0.7
		f	A	*	*	0.49	-3.86	*	*	4.58	4.58	4.58	0.98	0.75
		f	B	*	*	0.59	-10.4	*	*	5.35	5.35	5.35	0.73	0.83
NON-HYST HETERO	V3	p	A	*	*	*	*	*	*	4.24	0.96	0.11	0.87	-2.4
		p	B	*	*	*	*	*	*	1.94	1.93	0.04	0.89	-2.8
		f	A	*	*	*	*	*	*	27.41	3.95	0.49	0.75	0.83
		f	B	*	*	*	*	*	*	45.46	38.49	1.38	0.65	0.70
	V5	p	A	0.08	1.28	*	*	*	*	8.23	5.65	0.59	0.95	0.19
		p	B	0.05	2.60	*	*	*	*	2.54	2.53	0.02	0.91	-2.9
		f	A	0.01	1.57	*	*	*	*	8.56	0.82	0.01	0.57	0.96
		f	B	0.05	2.97	*	*	*	*	11.32	2.85	0.22	0.81	0.44
	B3	p	A	*	*	*	*	*	*	1.54	0.30	0.12	0.90	-1.0
		p	B	*	*	*	*	*	*	0.39	0.39	0.14	0.89	-2.2
		f	A	*	*	*	*	*	*	82.19	3.51	0.08	0.66	0.91
		f	B	*	*	*	*	*	*	81.10	1.51	1.49	0.63	0.89
	B5	p	A	*	*	0.19	-3.80	*	*	2.27	2.27	2.24	0.93	0.68
		p	B	*	*	0.90	-12.2	*	*	1.04	0.35	0.05	0.90	-2.2
		f	A	*	*	0.48	-39.2	*	*	28.15	0.56	0.04	0.70	0.99
		f	B	*	*	0.23	-12.6	*	*	36.40	0.59	0.12	0.62	0.86

Var = optimised variable
p = matric potential
f = bottom inflow
* = parameter not optimised

Table VI.4 - SPW1hyst optimisation of rapid flow event 91017

Simulation		V	L	Optimised parameters									R ² (p)	R ² (f)
				α 1/cm	n -	λ -	ψ_b cm	θ_s m ³ /m ³	θ_r m ³ /m ³	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	p	A	*	*	*	*	*	*	1.31	1.31	1.31	0.62	0.03
			B	*	*	*	*	*	*	1.08	1.08	1.08	0.77	-1.4
		f	A	*	*	*	*	*	*	0.15	0.15	0.15	0.43	0.61
			B	*	*	*	*	*	*	9.58	9.58	9.58	0.44	0.91
	V2	p	A	0.07	1.07	*	*	*	*	*	*	*	0.90	0.72
			B	0.09	1.09	*	*	*	*	*	*	*	0.93	0.20
		f	A	0.05	1.14	*	*	*	*	*	*	*	0.73	0.89
			B	0.06	1.75	*	*	*	*	*	*	*	0.41	0.96
	V3	p	A	0.13	1.06	*	*	*	*	25.34	25.34	25.34	0.91	0.82
			B	0.13	1.08	*	*	*	*	15.50	15.50	15.50	0.93	0.28
		f	A	0.07	1.09	*	*	*	*	9.54	9.54	9.54	0.86	0.85
			B	0.07	1.70	*	*	*	*	9.65	9.65	9.65	0.44	0.96
	V4	p	A	0.09	1.10	*	*	0.31	0.04	*	*	*	0.91	0.77
			B	0.14	1.18	*	*	0.30	0.10	*	*	*	0.94	0.31
		f	A	0.05	1.14	*	*	0.50	0.06	*	*	*	0.71	0.88
			B	0.06	1.64	*	*	0.38	0.08	*	*	*	0.46	0.95
	B1	p	A	*	*	*	*	*	*	0.38	0.38	0.38	0.67	0.29
			B	*	*	*	*	*	*	0.16	0.16	0.16	0.78	-1.4
		f	A	*	*	*	*	*	*	0.08	0.08	0.08	0.55	0.69
			B	*	*	*	*	*	*	1.88	1.88	1.88	0.43	0.91
	B2	p	A	*	*	0.05	-0.82	*	*	*	*	*	0.92	0.81
			B	*	*	0.08	-0.97	*	*	*	*	*	0.94	0.39
		f	A	*	*	0.03	-0.61	*	*	*	*	*	0.91	0.87
			B	*	*	0.57	-7.51	*	*	*	*	*	0.48	0.93
	B3	p	A	*	*	0.51	-1.44	*	*	98.97	98.97	98.97	0.87	-13
			B	*	*	0.07	-0.66	*	*	13.08	13.08	13.08	0.94	0.46
		f	A	*	*	0.43	-19.6	*	*	0.49	0.49	0.49	0.50	0.82
			B	*	*	0.87	-9.48	*	*	7.39	7.39	7.39	0.48	0.94
NON-HYST HETERO	V3	p	A	*	*	*	*	*	*	12.27	0.29	0.05	0.70	0.54
			B	*	*	*	*	*	*	23.65	0.01	0.01	0.80	-3.2
		f	A	*	*	*	*	*	*	94.23	86.94	0.07	0.61	0.93
			B	*	*	*	*	*	*	40.07	7.68	1.44	0.39	0.91
	V5	p	A	0.03	1.12	*	*	*	*	0.88	0.87	0.23	0.87	0.40
			B	0.12	1.30	*	*	*	*	32.23	0.69	0.06	0.82	-3.1
		f	A	0.04	1.56	*	*	*	*	94.16	4.43	0.13	0.55	0.94
			B	0.03	2.40	*	*	*	*	77.20	2.15	0.12	0.30	0.92
	B3	p	A	*	*	*	*	*	*	34.84	0.05	0.05	0.74	0.65
			B	*	*	*	*	*	*	28.11	0.01	0.01	0.79	-3.2
		f	A	*	*	*	*	*	*	89.37	15.65	0.03	0.59	0.95
			B	*	*	*	*	*	*	24.20	1.56	0.19	0.35	0.91
	B5	p	A	*	*	0.06	-1.69	*	*	2.27	2.27	0.10	0.89	0.87
			B	*	*	0.06	-2.75	*	*	0.54	0.53	0.08	0.92	0.20
		f	A	*	*	0.41	-14.1	*	*	74.72	0.72	0.06	0.55	0.96
			B	*	*	0.78	-11.5	*	*	45.03	2.63	0.19	0.35	0.95

Var - optimised variable
p - matric potential
f - bottom inflow
* - parameter not optimised

Table VI.5 - SPW1hyst optimisation of rapid flow event 91119

Simulation	V a r	L y s	Optimised parameters									R ² (p)	R ² (f)
			α 1/cm	n -	λ -	Ψ_0 cm	θ_1 m ³ /m ³	θ_r m ³ /m ³	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	p	*	*	*	*	*	*	3.00	3.00	3.00	0.90	-2.5
		B	*	*	*	*	*	*	2.53	2.53	2.53	0.81	-1.1
		A	*	*	*	*	*	*	29.85	29.85	29.85	0.57	-0.1
		f	*	*	*	*	*	*	16.94	16.94	16.94	0.63	0.89
	V2	p	0.08	1.94	*	*	*	*	*	*	*	0.93	-2.3
		B	0.08	2.17	*	*	*	*	*	*	*	0.84	-0.5
		A	0.07	1.08	*	*	*	*	*	*	*	0.86	1.00
		f	0.09	1.10	*	*	*	*	*	*	*	0.79	0.97
	V3	p	0.20	1.49	*	*	*	*	47.01	47.01	47.01	0.94	-1.0
		B	0.12	2.03	*	*	*	*	14.73	14.73	14.73	0.85	0.18
		A	0.28	1.07	*	*	*	*	98.20	98.20	98.20	0.86	1.00
		f	0.12	1.12	*	*	*	*	14.64	14.64	14.64	0.81	0.94
	V4	p	0.10	1.54	*	*	0.35	0.06	*	*	*	0.95	-0.7
		B	0.10	1.92	*	*	0.37	0.08	*	*	*	0.85	0.21
		A	0.11	1.11	*	*	0.32	0.06	*	*	*	0.84	1.00
		f	0.06	1.45	*	*	0.38	0.09	*	*	*	0.70	0.92
	B1	p	*	*	*	*	*	*	0.85	0.85	0.85	0.92	-2.0
		B	*	*	*	*	*	*	0.35	0.35	0.35	0.81	-1.0
		A	*	*	*	*	*	*	8.01	8.01	8.01	0.61	0.31
		f	*	*	*	*	*	*	2.16	2.16	2.16	0.64	0.89
	B2	p	*	*	0.47	-4.19	*	*	*	*	*	0.94	-1.0
		B	*	*	0.82	-5.94	*	*	*	*	*	0.85	0.26
		A	*	*	0.04	-0.42	*	*	*	*	*	0.73	1.00
		f	*	*	0.31	-5.35	*	*	*	*	*	0.71	0.95
	B3	p	*	*	0.54	-4.97	*	*	5.32	5.32	5.32	0.94	-1.0
		B	*	*	0.85	-5.97	*	*	6.29	6.29	6.29	0.85	0.39
		A	*	*	0.04	-0.21	*	*	23.37	23.37	23.37	0.72	1.00
		f	*	*	0.59	-7.98	*	*	7.03	7.03	7.03	0.71	0.91
NON-HYST HETERO	V3	p	*	*	*	*	*	*	2.87	2.87	0.89	0.90	-2.8
		B	*	*	*	*	*	*	2.55	2.52	0.96	0.81	-1.3
		A	*	*	*	*	*	*	82.90	19.96	0.01	0.56	-2.6
		f	*	*	*	*	*	*	94.46	54.85	0.98	0.44	0.93
	V5	p	0.10	1.93	*	*	*	*	17.98	5.28	0.02	0.92	-2.8
		B	0.10	2.14	*	*	*	*	12.59	1.70	0.16	0.84	-1.7
		A	0.08	1.04	*	*	*	*	61.89	0.76	0.01	0.36	-2.5
		f	0.10	2.53	*	*	*	*	98.15	24.44	0.17	0.82	0.34
	B3	p	*	*	*	*	*	*	0.82	0.47	0.20	0.91	-2.9
		B	*	*	*	*	*	*	0.50	0.17	0.10	0.80	-2.2
		A	*	*	*	*	*	*	81.33	5.20	0.93	0.48	0.36
		f	*	*	*	*	*	*	51.34	1.35	1.04	0.51	0.94
	B5	p	*	*	0.30	-4.54	*	*	2.09	2.09	0.64	0.94	-1.3
		B	*	*	0.88	-7.74	*	*	3.59	0.66	0.01	0.83	-2.2
		A	*	*	0.05	-0.69	*	*	74.55	2.87	0.67	0.69	1.00
		f	*	*	0.20	-10.8	*	*	36.87	0.79	0.08	0.50	0.94

Var = optimised variable
p = matric potential
f = bottom inflow
* = parameter not optimised

Table VI.6 - SPW1hyst optimisation of rapid flow event 91136

Simulation	V a r	L y s	Optimised parameters									R ² (p)	R ² (f)
			α 1/cm	n -	λ -	ψ_b cm	θ_s m ³ /m ³	θ_r m ³ /m ³	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	p	A	*	*	*	*	*	3.75	3.75	3.75	0.99	-292
			B	*	*	*	*	*	6.82	6.82	6.82	0.97	-134
		f	A	*	*	*	*	*	0.07	0.07	0.07	0.81	-22
			B	*	*	*	*	*	1.31	1.31	1.31	0.81	-2.0
	V2	p	A	0.05	2.48	*	*	*	*	*	*	1.00	-712
			B	0.07	1.53	*	*	*	*	*	*	0.97	-154
		f	A	0.37	1.18	*	*	*	*	*	*	0.63	-12
			B	0.12	1.12	*	*	*	*	*	*	0.84	0.01
	V3	p	A	0.05	2.44	*	*	*	7.58	7.58	7.58	1.00	-689
			B	0.11	1.95	*	*	*	46.35	46.35	46.35	0.98	-50
		f	A	0.23	1.18	*	*	*	1.06	1.06	1.06	0.67	-15
			B	0.07	1.65	*	*	*	1.32	1.32	1.32	-2.0	0.79
	V4	p	A	0.06	2.08	*	*	0.30	*	*	*	0.99	-345
			B	0.08	1.52	*	*	0.30	*	*	*	0.98	-53
		f	A	0.23	1.55	*	*	0.33	*	*	*	-33	0.32
			B	0.10	1.48	*	*	0.42	*	*	*	-3	0.89
	B1	p	A	*	*	*	*	*	1.21	1.21	1.21	0.99	-255
			B	*	*	*	*	*	0.96	0.96	0.96	0.97	-154
		f	A	*	*	*	*	*	0.01	0.01	0.01	0.75	-39
			B	*	*	*	*	*	0.23	0.23	0.23	0.79	-9.0
	B2	p	A	*	*	0.90	-9.81	*	*	*	*	0.99	-460
			B	*	*	0.60	-7.54	*	*	*	*	0.98	-83
		f	A	*	*	0.83	-0.87	*	*	*	*	<-999	-39
			B	*	*	0.10	-1.32	*	*	*	*	0.94	-2.6
	B3	p	A	*	*	0.90	-10.9	*	*	4.16	4.16	0.99	-442
			B	*	*	0.31	-3.57	*	*	9.90	9.90	0.98	-30
		f	A	*	*	0.74	-4.88	*	*	0.10	0.10	0.52	-41
			B	*	*	0.62	-7.97	*	*	1.29	1.29	0.80	-1.7
NON-HYST HETERO	V3	p	A	*	*	*	*	*	3.96	3.55	1.16	0.99	-205
			B	*	*	*	*	*	6.55	6.39	0.10	0.97	-9.2
		f	A	*	*	*	*	*	84.78	0.11	0.09	0.86	-22
			B	*	*	*	*	*	21.48	1.14	0.60	0.92	-1.4
	V5	p	A	0.05	1.90	*	*	*	1.99	1.19	0.06	0.98	-43
			B	0.05	1.69	*	*	*	2.74	2.71	0.05	0.97	-25
		f	A	0.11	1.23	*	*	*	73.56	0.49	0.18	0.86	-18
			B	0.08	1.31	*	*	*	24.26	0.60	0.21	0.91	-0.9
	B3	p	A	*	*	*	*	*	1.11	1.10	0.04	0.98	-63
			B	*	*	*	*	*	1.29	1.29	0.07	0.98	-68
		f	A	*	*	*	*	*	46.07	0.01	0.01	0.84	-39
			B	*	*	*	*	*	0.18	0.18	0.18	0.76	-9.0
	B5	p	A	*	*	0.90	-9.73	*	*	6.13	6.12	0.99	-198
			B	*	*	0.63	-8.21	*	*	5.14	5.03	0.98	-37
		f	A	*	*	0.07	-3.08	*	*	31.18	0.68	0.82	-20
			B	*	*	0.35	-6.68	*	*	2.95	0.55	0.95	-2.5

Var = optimised variable
p = matric potential
f = bottom inflow
* = parameter not optimised

Table VI.7 - SPW1hyst optimisation of rapid flow event 91198

Simulation		V a r	L y s	Optimised parameters									R ² (p)	R ² (f)
				α 1/cm	n -	λ -	ψ_b cm	θ_s m ³ /m ³	θ_r m ³ /m ³	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	p	A	*	*	*	*	*	*	3.10	3.10	3.10	0.94	-391
			B	*	*	*	*	*	*	3.75	3.75	3.75	0.92	-45
		f	A	*	*	*	*	*	*	0.11	0.11	0.11	0.41	-11
			B	*	*	*	*	*	*	0.23	0.23	0.23	0.58	-1.2
	V2	p	A	0.06	2.11	*	*	*	*	*	*	*	0.97	-373
			B	0.06	2.13	*	*	*	*	*	*	*	0.94	<-999
		f	A	0.48	1.06	*	*	*	*	*	*	*	0.49	-0.3
			B	0.24	1.07	*	*	*	*	*	*	*	-0.7	0.58
	V3	p	A	0.14	1.77	*	*	*	*	41.19	41.19	41.19	0.98	-134
			B	0.08	2.04	*	*	*	*	14.62	14.62	14.62	0.95	-12
		f	A	0.40	1.10	*	*	*	*	2.48	2.48	2.48	0.54	-0.7
			B	0.24	1.06	*	*	*	*	5.71	5.71	5.71	-0.7	0.56
	V4	p	A	0.08	1.80	*	*	0.30	0.07	*	*	*	0.98	-33
			B	0.09	1.69	*	*	0.30	0.10	*	*	*	0.97	-17
		f	A	0.22	1.08	*	*	0.32	0.05	*	*	*	0.72	-0.5
			B	0.25	1.11	*	*	0.37	0.09	*	*	*	0.65	-0.8
	B1	p	A	*	*	*	*	*	*	0.93	0.93	0.93	0.95	-275
			B	*	*	*	*	*	*	0.56	0.56	0.56	0.93	-35
		f	A	*	*	*	*	*	*	0.01	0.01	0.01	-0.1	-1.1
			B	*	*	*	*	*	*	1.26	1.26	1.26	0.90	-31
	B2	p	A	*	*	0.90	-9.23	*	*	*	*	*	0.98	-312
			B	*	*	0.89	-8.99	*	*	*	*	*	0.95	-7
		f	A	*	*	0.10	-0.99	*	*	*	*	*	0.92	-2.4
			B	*	*	0.20	-2.58	*	*	*	*	*	0.95	-0.9
	B3	p	A	*	*	0.63	-3.48	*	*	44.66	44.66	44.66	0.98	-45
			B	*	*	0.90	-5.39	*	*	43.50	43.50	43.50	0.97	-60
		f	A	*	*	0.53	-1.05	*	*	7.37	7.37	7.37	0.30	-24
			B	*	*	0.24	-2.43	*	*	9.29	9.29	9.29	0.95	-0.9
NON-HYST HETERO	V3	p	A	*	*	*	*	*	*	3.07	0.87	0.19	0.91	-61
			B	*	*	*	*	*	*	4.10	4.10	0.09	0.92	-1.7
		f	A	*	*	*	*	*	*	28.19	0.34	0.01	0.76	-0.5
			B	*	*	*	*	*	*	3.14	2.51	0.05	0.92	-0.8
	V5	p	A	0.07	2.19	*	*	*	*	11.75	11.74	2.19	0.97	-269
			B	0.08	2.62	*	*	*	*	21.07	6.04	0.63	0.95	-4.3
		f	A	0.21	1.20	*	*	*	*	45.76	0.66	0.01	0.92	-0.3
			B	0.02	1.31	*	*	*	*	89.24	0.06	0.01	0.83	-0.4
	B3	p	A	*	*	*	*	*	*	0.87	0.56	0.07	0.94	-75
			B	*	*	*	*	*	*	0.83	0.25	0.05	0.92	-4.4
		f	A	*	*	*	*	*	*	15.92	0.01	0.01	0.74	-1.1
			B	*	*	*	*	*	*	45.89	0.14	0.01	0.82	-0.3
	B5	p	A	*	*	0.71	-6.98	*	*	6.65	0.51	0.04	0.96	-9.7
			B	*	*	0.90	-10.3	*	*	4.31	0.43	0.01	0.93	-0.5
		f	A	*	*	.10	-5.17	*	*	11.98	4.87	0.02	0.93	-0.3
			B	*	*	0.58	-9.89	*	*	30.74	0.29	0.01	0.83	-0.3

Var = optimised variable
p = matric potential
f = bottom inflow
* = parameter not optimised

Table VI.8 - SPW1hyst optimisation of rapid flow event 91211

Simulation	V	L	Optimised parameters									R ² (p)	R ² (f)
			α	n	λ	ψ_b	θ_s	θ_r	Ks ₁	Ks ₂	Ks ₃		
			1/cm	-	-	cm	m ³ /m ³	m ³ /m ³	cm/h	cm/h	cm/h		
NON-HYST HOMOGENEOUS	V1	p	A	*	*	*	*	*	3.19	3.19	3.19	0.90	-7.3
		p	B	*	*	*	*	*	4.88	4.88	4.88	0.92	-2.3
		f	A	*	*	*	*	*	15.02	15.02	15.02	0.79	-1.8
		f	B	*	*	*	*	*	14.10	14.10	14.10	0.86	-0.5
	V2	p	A	0.08	1.21	*	*	*	*	*	*	0.95	-0.5
		p	B	0.07	1.18	*	*	*	*	*	*	0.96	0.77
		f	A	0.09	1.08	*	*	*	*	*	*	0.78	0.98
		f	B	0.07	1.17	*	*	*	*	*	*	0.96	0.78
	V3	p	A	0.11	1.21	*	*	*	10.36	10.36	10.36	0.95	-0.5
		p	B	0.10	1.17	*	*	*	12.93	12.93	12.93	0.96	0.77
		f	A	0.15	1.06	*	*	*	11.21	11.21	11.21	0.64	0.98
		f	B	0.09	1.08	*	*	*	4.23	4.23	4.23	0.75	0.85
	V4	p	A	0.10	1.68	*	*	0.30	*	*	*	0.96	-0.2
		p	B	0.10	1.54	*	*	0.30	*	*	*	0.97	0.67
		f	A	0.08	1.63	*	*	0.30	*	*	*	0.93	0.80
		f	B	0.08	1.19	*	*	0.39	*	*	*	0.96	0.78
	B1	p	A	*	*	*	*	*	1.02	1.02	1.02	0.92	-5.3
		p	B	*	*	*	*	*	0.66	0.66	0.66	0.92	-1.7
		f	A	*	*	*	*	*	4.13	4.13	4.13	-2.0	0.81
		f	B	*	*	*	*	*	1.78	1.78	1.78	0.87	0.00
	B2	p	A	*	*	0.45	-4.52	*	*	*	*	0.95	-3.0
		p	B	*	*	0.19	-2.52	*	*	*	*	0.96	0.75
		f	A	*	*	0.04	-0.41	*	*	*	*	0.47	0.98
		f	B	*	*	0.19	-2.34	*	*	*	*	0.80	0.95
	B3	p	A	*	*	0.66	-4.08	*	*	20.51	20.51	0.96	-2.4
		p	B	*	*	0.22	-1.71	*	*	19.69	19.69	0.96	0.46
		f	A	*	*	0.02	-0.05	*	*	23.03	23.03	-0.8	0.99
		f	B	*	*	0.41	-3.68	*	*	11.81	11.81	0.75	0.96
NON-HYST HETERO	V3	p	A	*	*	*	*	*	3.18	3.18	3.18	0.90	-7.3
		p	B	*	*	*	*	*	5.07	5.00	4.61	0.92	-2.2
		f	A	*	*	*	*	*	14.86	3.97	0.01	0.81	-2.7
		f	B	*	*	*	*	*	67.69	4.84	2.69	0.82	0.45
	V5	p	A	0.07	2.42	*	*	*	17.08	0.66	0.41	0.91	-9.7
		p	B	0.06	1.19	*	*	*	4.81	4.80	0.76	0.95	0.58
		f	A	0.08	1.16	*	*	*	18.49	8.63	0.01	0.83	-2.3
		f	B	0.05	1.19	*	*	*	4.81	4.80	0.76	0.93	0.79
	B3	p	A	*	*	*	*	*	1.06	0.37	0.11	0.90	-6.1
		p	B	*	*	*	*	*	1.01	0.40	0.40	0.91	-2.8
		f	A	*	*	*	*	*	86.89	10.65	0.16	0.67	-1.0
		f	B	*	*	*	*	*	70.37	1.58	0.23	0.77	0.36
	B5	p	A	*	*	0.24	-3.52	*	*	3.39	3.39	0.95	-1.4
		p	B	*	*	0.17	-5.49	*	*	1.12	1.11	0.95	0.28
		f	A	*	*	0.15	-5.55	*	*	77.71	2.28	0.74	0.96
		f	B	*	*	0.14	-9.04	*	*	65.18	2.00	0.75	0.92

Var = optimised variable
p = matric potential
f = bottom inflow
* = parameter not optimised

Table VI.9 - SPW1hyst optimisation of slow flow event 90129

Simulation		V	a	r	L	y	s	Optimised parameters						R ² (p)	R ² (f)
								α 1/cm	n	λ -	ψ_s cm	θ_s m ³ /m ³	θ_r m ³ /m ³		
NON - HYST HOMOGENEOUS	V1	p	A	*	*	*	*	*	*	0.87	0.87	0.87	0.92	0.91	
			B	*	*	*	*	*	*	0.61	0.61	0.61	0.96	-12	
		f	A	*	*	*	*	*	*	1.01	1.01	1.01	0.91	0.97	
			B	*	*	*	*	*	*	3.14	3.14	3.14	0.67	-1.2	
	V2	p	A	0.18	1.30	*	*	*	*	*	*	*	0.90	-0.1	
			B	0.23	1.26	*	*	*	*	*	*	*	0.93	-23	
		f	A	0.11	1.46	*	*	*	*	*	*	*	0.85	0.98	
			B	0.03	1.05	*	*	*	*	*	*	*	0.31	0.95	
	V3	p	A	0.02	1.89	*	*	*	*	0.03	0.03	0.03	0.95	0.03	
			B	0.01	1.70	*	*	*	*	0.02	0.02	0.02	0.97	-1.8	
		f	A	0.10	1.55	*	*	*	*	3.65	3.65	3.65	0.88	0.98	
			B	0.05	1.05	*	*	*	*	9.28	9.28	9.28	0.31	0.94	
	V4	p	A	0.12	1.38	*	*	*	0.60	0.02	*	*	*	0.95	0.97
			B	0.15	1.35	*	*	*	0.60	0.01	*	*	*	0.97	-39
		f	A	0.11	1.52	*	*	*	0.38	0.10	*	*	*	0.70	0.98
			B	0.08	1.79	*	*	*	0.30	0.10	*	*	*	-0.04	0.08
	B1	p	A	*	*	*	*	*	*	0.25	0.25	0.25	0.92	0.55	
			B	*	*	*	*	*	*	0.09	0.09	0.09	0.95	-7.6	
		f	A	*	*	*	*	*	*	0.41	0.41	0.41	0.88	0.97	
			B	*	*	*	*	*	*	0.38	0.38	0.38	0.70	-0.2	
	B2	p	A	*	*	0.23	-0.89	*	*	*	*	*	0.82	-0.87	
			B	*	*	0.19	-0.59	*	*	*	*	*	0.87	-41	
		f	A	*	*	0.34	-2.84	*	*	*	*	*	0.73	0.96	
			B	*	*	0.06	-1.80	*	*	*	*	*	0.22	0.72	
	B3	p	A	*	*	0.31	-15.0	*	*	0.04	0.04	0.04	0.93	-1.0	
			B	*	*	0.44	-32.0	*	*	0.01	0.01	0.01	0.97	0.37	
		f	A	*	*	0.23	-2.58	*	*	4.33	4.33	4.33	0.70	0.97	
			B	*	*	0.50	-27.8	*	*	0.02	0.02	0.02	0.96	0.75	
NON - HYST HETTER	V3	p	A	*	*	*	*	*	*	0.88	0.65	0.01	0.92	-3.1	
			B	*	*	*	*	*	*	0.60	0.59	0.05	0.96	-8.7	
		f	A	*	*	*	*	*	*	1.07	1.06	0.90	0.91	0.97	
			B	*	*	*	*	*	*	57.78	5.69	0.01	0.18	-5.9	
	V5	p	A	0.08	1.40	*	*	*	*	1.25	1.25	0.06	0.93	-2.4	
			B	0.09	1.39	*	*	*	*	1.16	1.16	0.04	0.95	-8.6	
		f	A	0.08	2.21	*	*	*	*	7.04	5.55	0.57	-2.2	0.98	
			B	0.01	1.12	*	*	*	*	21.29	3.42	0.03	0.10	0.99	
	B3	p	A	*	*	*	*	*	*	0.39	0.39	0.38	0.88	0.96	
			B	*	*	*	*	*	*	39.03	0.01	0.01	0.41	-6.1	
		f	A	*	*	*	*	*	*	0.39	0.39	0.38	0.88	0.96	
			B	*	*	*	*	*	*	97.95	36.58	0.02	-0.03	0.94	
	B5	p	A	*	*	0.42	-4.94	*	*	0.84	0.84	0.03	0.89	-2.3	
			B	*	*	0.26	-2.61	*	*	0.62	0.62	0.15	0.92	-24	
		f	A	*	*	0.49	-8.45	*	*	26.61	0.70	0.13	0.36	0.87	
			B	*	*	0.22	-12.6	*	*	36.94	5.53	0.01	0.01	0.97	

Var = optimised variable

p = matric potential

f = bottom inflow

* = parameter not optimised

Table VI.10 - SPW1hyst optimisation of slow flow event 91108

Simulation	V	L	Optimised parameters									R ² (p)	R ² (f)
			α	n	λ	ψ_0	θ_0	θ_r	Ks ₁	Ks ₂	Ks ₃		
			1/cm	-	-	cm	m ³ /m ³	m ³ /m ³	cm/h	cm/h	cm/h		
NON-HYST HOMOGENEOUS	V1	p	A	*	*	*	*	*	1.78	1.78	1.78	0.92	-48
			B	*	*	*	*	*	0.96	0.96	0.96	0.81	-3.0
		f	A	*	*	*	*	*	0.08	0.08	0.08	-0.9	0.89
			B	*	*	*	*	*	0.42	0.42	0.42	0.77	0.98
	V2	p	A	0.12	1.34	*	*	*	*	*	*	0.93	-12
			B	0.15	1.41	*	*	*	*	*	*	0.79	-0.6
		f	A	0.12	1.10	*	*	*	*	*	*	0.83	0.96
			B	0.19	1.48	*	*	*	*	*	*	0.76	0.99
	V3	p	A	0.13	1.36	*	*	*	6.97	6.97	6.97	0.93	-13
			B	0.04	1.40	*	*	*	0.27	0.27	0.27	0.81	-1.0
		f	A	0.04	1.12	*	*	*	0.94	0.94	0.94	0.85	0.99
			B	0.20	1.47	*	*	*	5.94	5.94	5.94	0.76	0.99
	V4	p	A	0.12	1.35	*	*	0.43	*	*	*	0.93	-11
			B	0.13	1.27	*	*	0.60	*	*	*	0.82	-3.0
		f	A	0.20	1.11	*	*	0.58	*	*	*	0.67	0.74
			B	0.19	1.48	*	*	0.42	*	*	*	0.76	0.99
	B1	p	A	*	*	*	*	*	0.47	0.47	0.47	0.93	-29
			B	*	*	*	*	*	0.12	0.12	0.12	0.81	-1.0
		f	A	*	*	*	*	*	0.03	0.03	0.03	-0.2	0.96
			B	*	*	*	*	*	0.06	0.06	0.06	0.78	0.99
	B2	p	A	*	*	0.36	-2.61	*	*	*	*	0.91	-14
			B	*	*	0.35	-2.23	*	*	*	*	0.74	0.11
		f	A	*	*	0.07	-0.62	*	*	*	*	0.69	0.72
			B	*	*	0.40	-2.01	*	*	*	*	0.71	0.99
	B3	p	A	*	*	0.32	-6.31	*	*	0.58	0.58	0.93	-12
			B	*	*	0.38	-8.68	*	*	0.19	0.19	0.81	-1.6
		f	A	*	*	0.10	-5.80	*	*	0.08	0.08	0.86	0.97
			B	*	*	0.35	-2.06	*	*	4.07	4.07	0.72	0.99
NON-HYST HETERO	V3	p	A	*	*	*	*	*	2.03	1.09	0.43	0.98	-20
			B	*	*	*	*	*	1.06	0.60	0.08	0.81	0.20
		f	A	*	*	*	*	*	32.26	0.95	0.04	0.78	0.99
			B	*	*	*	*	*	98.39	0.39	0.28	0.68	0.97
	V5	p	A	0.12	1.46	*	*	*	6.47	6.45	1.26	0.93	-16
			B	0.05	1.61	*	*	*	0.61	0.48	0.10	0.81	0.45
		f	A	0.06	1.78	*	*	*	42.29	1.05	0.04	0.78	0.98
			B	0.06	1.51	*	*	*	37.29	0.36	0.15	0.68	0.94
	B3	p	A	*	*	*	*	*	0.53	0.36	0.22	0.93	-19
			B	*	*	*	*	*	44.49	0.01	0.01	0.69	-1.3
		f	A	*	*	*	*	*	27.63	0.44	0.01	0.76	0.96
			B	*	*	*	*	*	25.85	0.44	0.01	0.60	0.93
	B5	p	A	*	*	0.50	-8.52	*	*	0.77	0.60	0.93	-11
			B	*	*	0.35	-14.7	*	*	0.05	0.05	0.81	0.88
		f	A	*	*	0.50	-7.84	*	*	25.15	0.38	0.78	0.99
			B	*	*	0.50	-8.61	*	*	22.10	0.42	0.64	0.95

Var = optimised variable

p = matric potential

f = bottom inflow

* = parameter not optimised

Table VI.11 - SPW1hyst optimisation of slow flow event 91165

Simulation	V a r	L y s	Optimised parameters									R ² (p)	R ² (f)
			α 1/cm	n -	λ -	ψ_s cm	θ_s m ³ /m ³	θ_r m ³ /m ³	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	p	*	*	*	*	*	*	2.62	2.62	2.62	0.91	-11
		B	*	*	*	*	*	*	2.34	2.34	2.34	0.91	-3.0
		A	*	*	*	*	*	*	0.25	0.25	0.25	0.64	0.98
		f	*	*	*	*	*	*	0.67	0.67	0.67	0.79	0.99
	V2	p	0.10	1.16	*	*	*	*	*	*	*	0.96	0.90
		B	0.10	1.16	*	*	*	*	*	*	*	0.94	0.96
		A	0.13	1.17	*	*	*	*	*	*	*	0.94	0.98
		f	0.13	1.20	*	*	*	*	*	*	*	0.92	0.99
	V3	p	0.16	1.17	*	*	*	*	17.01	17.01	17.01	0.97	0.74
		B	0.16	1.17	*	*	*	*	14.97	14.97	14.97	0.94	0.90
		A	0.07	1.22	*	*	*	*	1.36	1.36	1.36	0.92	0.99
		f	0.14	1.18	*	*	*	*	7.59	7.59	7.59	0.93	0.99
	V4	p	0.11	1.66	*	*	0.30	0.06	*	*	*	0.96	-1.0
		B	0.13	1.29	*	*	0.36	0.10	*	*	*	0.94	0.84
		A	0.16	1.23	*	*	0.35	0.08	*	*	*	0.94	0.97
		f	0.15	1.28	*	*	0.36	0.09	*	*	*	0.93	0.98
	B1	p	*	*	*	*	*	*	0.80	0.80	0.80	0.93	-8.0
		B	*	*	*	*	*	*	0.33	0.33	0.33	0.92	-2.0
		A	*	*	*	*	*	*	0.09	0.09	0.09	0.66	0.98
		f	*	*	*	*	*	*	0.11	0.11	0.11	0.83	0.99
	B2	p	*	*	0.20	-1.97	*	*	*	*	*	0.97	-0.4
		B	*	*	0.23	-2.04	*	*	*	*	*	0.94	0.11
		A	*	*	0.11	-0.96	*	*	*	*	*	0.91	0.92
		f	*	*	0.13	-1.23	*	*	*	*	*	0.93	0.96
	B3	p	*	*	0.27	-1.46	*	*	22.10	22.10	22.10	0.96	-1.0
		B	*	*	0.24	-1.38	*	*	17.17	17.17	17.17	0.94	0.33
		A	*	*	0.13	-5.00	*	*	0.25	0.25	0.25	0.95	0.98
		f	*	*	0.16	-4.17	*	*	0.46	0.46	0.46	0.93	0.98
NON-HYST HETERO	V3	p	*	*	*	*	*	*	3.02	3.01	0.25	0.92	-3.1
		B	*	*	*	*	*	*	2.77	2.21	0.52	0.91	-0.3
		A	*	*	*	*	*	*	25.57	0.52	0.14	0.86	0.99
		f	*	*	*	*	*	*	30.51	1.63	0.21	0.85	0.99
	V5	p	0.09	2.49	*	*	*	*	27.69	4.36	0.25	0.95	-0.4
		B	0.14	2.01	*	*	*	*	63.66	10.37	0.42	0.93	0.90
		A	0.07	1.67	*	*	*	*	16.24	0.80	0.17	0.88	0.99
		f	0.05	1.60	*	*	*	*	22.06	0.42	0.15	0.84	0.98
	B3	p	*	*	*	*	*	*	0.84	0.49	0.11	0.93	-1.1
		B	*	*	*	*	*	*	0.54	0.39	0.04	0.91	0.95
		A	*	*	*	*	*	*	20.82	0.79	0.03	0.87	0.97
		f	*	*	*	*	*	*	20.56	1.24	0.03	0.81	0.96
	B5	p	*	*	0.16	-3.92	*	*	1.02	0.80	0.34	0.96	0.86
		B	*	*	0.40	-2.14	*	*	21.09	20.49	1.56	0.94	0.50
		A	*	*	0.53	-8.40	*	*	0.73	0.37	0.06	0.90	0.99
		f	*	*	0.40	-10.3	*	*	9.69	1.74	0.02	0.81	0.97

Var = optimised variable

p = matric potential

f = bottom inflow

* = parameter not optimised

Table VI.12 - SPW1hyst optimisation of slow flow event 91204

Simulation	Var	Lys	Optimised parameters									R ² (p)	R ² (f)
			α 1/cm	n	λ	ψ_b cm	θ_i m ³ /m ³	θ_r m ³ /m ³	K_{s1} cm/h	K_{s2} cm/h	K_{s3} cm/h		
NON-HYST HOMOGENEOUS	V1	p	*	*	*	*	*	*	1.69	1.69	1.69	0.94	-60
		B	*	*	*	*	*	*	2.34	2.34	2.34	0.94	-6
		A	*	*	*	*	*	*	0.12	0.12	0.12	0.75	0.76
		f	*	*	*	*	*	*	0.70	0.70	0.70	0.87	0.96
	V2	p	0.11	1.37	*	*	*	*	*	*	*	0.95	-30
		B	0.10	1.25	*	*	*	*	*	*	*	0.94	-2
		A	0.29	1.20	*	*	*	*	*	*	*	0.58	0.78
		f	0.15	1.97	*	*	*	*	*	*	*	0.51	0.99
	V3	p	0.14	1.40	*	*	*	*	11.88	11.88	11.88	0.95	-35
		B	0.07	1.24	*	*	*	*	2.78	2.78	2.78	0.94	-1.3
		A	0.16	1.33	*	*	*	*	0.99	0.99	0.99	0.69	0.81
		f	0.14	1.64	*	*	*	*	3.35	3.35	3.35	0.78	0.98
	V4	p	0.10	1.71	*	*	0.39	0.10	*	*	*	0.95	-43
		B	0.07	1.14	*	*	0.60	0.02	*	*	*	0.94	-1.2
		A	0.37	1.31	*	*	0.34	0.10	*	*	*	0.07	0.78
		f	0.17	1.42	*	*	0.41	0.06	*	*	*	0.83	0.98
	B1	p	*	*	*	*	*	*	0.54	0.54	0.54	0.94	-48
		B	*	*	*	*	*	*	0.33	0.33	0.33	0.93	-4.0
		A	*	*	*	*	*	*	0.05	0.05	0.05	0.75	0.74
		f	*	*	*	*	*	*	0.12	0.12	0.12	0.88	0.94
	B2	p	*	*	0.57	-4.91	*	*	*	*	*	0.95	-53
		B	*	*	0.28	-2.80	*	*	*	*	*	0.94	-2.5
		A	*	*	0.11	-0.58	*	*	*	*	*	0.49	0.70
		f	*	*	0.68	-3.33	*	*	*	*	*	0.50	0.99
	B3	p	*	*	0.56	-4.68	*	*	6.36	6.36	6.36	0.94	-48
		B	*	*	0.26	-4.48	*	*	1.60	1.60	1.60	0.94	-2.6
		A	*	*	0.26	-4.00	*	*	0.12	0.12	0.12	0.63	0.84
		f	*	*	0.74	-3.48	*	*	6.65	6.65	6.65	0.46	0.99
NON-HYST HETERO	V3	p	*	*	*	*	*	*	2.16	0.51	0.10	0.93	0.08
		B	*	*	*	*	*	*	3.67	1.25	0.62	0.94	0.26
		A	*	*	*	*	*	*	1.04	0.12	0.09	0.91	0.75
		f	*	*	*	*	*	*	25.88	0.65	0.59	0.92	0.95
	V5	p	0.07	2.68	*	*	*	*	11.82	1.22	0.11	0.95	-4.6
		B	0.12	1.89	*	*	*	*	50.06	4.90	0.33	0.94	0.10
		A	0.10	1.73	*	*	*	*	10.98	0.20	0.19	0.93	0.84
		f	0.06	1.94	*	*	*	*	27.99	0.28	0.28	0.91	0.95
	B3	p	*	*	*	*	*	*	32.13	0.03	0.01	0.89	-0.8
		B	*	*	*	*	*	*	24.52	0.02	0.02	0.92	-1.6
		A	*	*	*	*	*	*	76.46	0.20	0.02	0.89	0.50
		f	*	*	*	*	*	*	97.09	10.55	0.02	0.82	0.98
	B5	p	*	*	0.67	-7.83	*	*	2.55	1.21	0.37	0.94	-28
		B	*	*	0.78	-7.81	*	*	8.35	0.52	0.02	0.94	-1.8
		A	*	*	0.64	-5.83	*	*	7.48	0.08	0.08	0.93	0.88
		f	*	*	0.41	-10.2	*	*	31.4	0.66	0.03	0.87	0.92

Var = optimised variable

p = matric potential

f = bottom inflow

* = parameter not optimised

Table VI.13-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for rapid flow event 90158

Simulation		Lys	Optimised parameters												R ² (p)	R ² (f)
			α 1/cm	n -	λ -	ψ_b cm	θ_s^w m ³ /m ³	α^w cm ⁻¹	n ^w -	λ^w -	ψ_b^w cm	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	*	0.42	0.42	0.42	0.71	0.74
		B	*	*	*	*	*	*	*	*	*	0.66	0.66	0.66	0.19	0.33
	V2	A	0.17	1.74	*	*	*	*	*	*	*	*	*	*	0.92	0.86
		B	0.10	1.09	*	*	*	*	*	*	*	*	*	*	0.56	0.41
	V3	A	0.23	1.40	*	*	*	*	*	*	*	13.0	13.0	13.0	0.94	0.84
		B	0.22	1.07	*	*	*	*	*	*	*	37.1	37.1	37.1	0.55	0.44
	B1	A	*	*	*	*	*	*	*	*	*	0.16	0.16	0.16	0.82	0.77
		B	*	*	*	*	*	*	*	*	*	0.16	0.16	0.16	0.23	0.21
	B1A	A	*	*	0.90	*	*	*	*	*	*	*	*	*	0.63	-76
		B	*	*	0.90	*	*	*	*	*	*	*	*	*	0.57	-149
	B2	A	*	*	0.25	*	*	*	*	*	*	0.10	0.10	0.10	0.94	0.79
		B	*	*	0.08	*	*	*	*	*	*	0.04	0.04	0.04	0.57	0.33
	B2A	A	*	*	0.37	-2.10	*	*	*	*	*	*	*	*	0.89	0.86
		B	*	*	0.11	-0.96	*	*	*	*	*	*	*	*	0.54	0.39
	B3	A	*	*	0.58	-2.82	*	*	*	*	*	5.41	5.41	5.41	0.85	0.86
		B	*	*	0.76	-4.00	*	*	*	*	*	6.72	6.72	6.72	0.42	0.38
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	*	1.59	0.51	0.21	0.95	0.78
		B	*	*	*	*	*	*	*	*	*	11.51	0.82	0.34	0.65	0.24
	V5	A	0.08	1.53	*	*	*	*	*	*	*	2.39	2.09	0.31	0.95	0.72
		B	0.06	1.55	*	*	*	*	*	*	*	7.13	0.35	0.32	0.65	0.30
	B3	A	*	*	*	*	*	*	*	*	*	0.41	0.22	0.08	0.95	0.79
		B	*	*	*	*	*	*	*	*	*	1.72	0.41	0.03	0.63	0.12
	B5	A	*	*	0.46	-8.29	*	*	*	*	*	0.56	0.47	0.09	0.95	0.78
		B	*	*	0.08	-2.67	*	*	*	*	*	1.41	0.93	0.17	0.57	0.21
HYSTERIC HOMOGENEOUS	V1	A	*	*	*	*	0.20	*	*	*	*	*	*	*	0.33	-10
		B	*	*	*	*	0.20	*	*	*	*	*	*	*	0.45	-11
	V2	A	*	*	*	*	*	0.37	1.73	*	*	*	*	*	0.26	-4.8
		B	*	*	*	*	*	0.34	1.69	*	*	*	*	*	0.36	-5.9
	V3	A	*	*	*	*	0.22	0.12	1.68	*	*	*	*	*	0.29	-3.6
		B	*	*	*	*	0.21	0.09	1.74	*	*	*	*	*	0.34	-1.8
	V4	A	*	*	*	*	0.28	0.14	1.69	*	*	1.77	1.77	1.77	0.49	0.34
		B	*	*	*	*	0.22	0.15	1.30	*	*	0.66	0.66	0.66	0.54	0.35
	B1	A	*	*	*	*	0.20	*	*	*	*	*	*	*	0.08	-9.9
		B	*	*	*	*	0.22	*	*	*	*	*	*	*	0.16	-26
	B2	A	*	*	*	*	0.20	*	*	0.48	*	*	*	*	0.18	-14
		B	*	*	*	*	0.23	*	*	0.83	*	*	*	*	0.11	-14
	B2A	A	*	*	*	*	*	*	*	0.63	-2.54	*	*	*	0.18	-9.3
		B	*	*	*	*	*	*	*	0.80	-2.53	*	*	*	0.10	-16
	B3	A	*	*	*	*	0.21	*	*	0.52	-9.84	*	*	*	0.22	-8.4
		B	*	*	*	*	0.20	*	*	0.54	-10.2	*	*	*	0.12	-18
	B4	A	*	*	*	*	0.38	*	*	0.65	-1.50	0.16	0.16	0.16	0.41	0.82
		B	*	*	*	*	0.22	*	*	0.80	-11.9	0.16	0.16	0.16	0.55	0.32

* = parameter not optimised; R²(p) = Coef of Determination for matric potentials; R²(f) = Coef of Determination for bottom inflow

Table VI.14-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for rapid flow event 90230

Simulation		Lys	Optimised parameters												R ² (p)	R ² (f)
			α 1/cm	n	λ -	ψ_b cm	θ_b^w m ³ /m ³	α^w cm ⁻¹	n ^w -	λ^w -	ψ_b^w cm	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	*	0.09	0.09	0.09	0.56	0.33
		B	*	*	*	*	*	*	*	*	*	1.50	1.50	1.50	0.30	0.90
	V2	A	0.46	1.20	*	*	*	*	*	*	*	*	*	*	0.22	0.10
		B	0.10	1.40	*	*	*	*	*	*	*	*	*	*	0.28	0.83
	V3	A	0.20	1.98	*	*	*	*	*	*	*	0.01	0.01	0.01	0.93	0.18
		B	0.05	1.45	*	*	*	*	*	*	*	0.90	0.90	0.90	0.32	0.98
	B1	A	*	*	*	*	*	*	*	*	*	0.05	0.05	0.05	0.44	0.41
		B	*	*	*	*	*	*	*	*	*	0.38	0.38	0.38	0.28	0.91
	B1A	A	*	*	0.90	*	*	*	*	*	*	*	*	*	0.27	-5.6
		B	*	*	0.79	*	*	*	*	*	*	*	*	*	0.26	-0.6
	B2	A	*	*	0.10	*	*	*	*	*	*	0.10	0.10	0.10	0.91	0.95
		B	*	*	0.38	*	*	*	*	*	*	0.34	0.34	0.34	0.28	0.92
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	*	0.63	0.62	0.04	0.40	0.61
		B	*	*	*	*	*	*	*	*	*	8.81	2.09	0.94	0.30	0.96
	V5	A	0.05	1.66	*	*	*	*	*	*	*	0.69	0.66	0.02	0.41	0.65
		B	0.04	2.01	*	*	*	*	*	*	*	12.7	0.38	0.25	0.31	0.98
	B3	A	*	*	*	*	*	*	*	*	*	0.20	0.19	0.02	0.36	0.64
		B	*	*	*	*	*	*	*	*	*	13.2	0.48	0.10	0.19	0.94
	B5	A	*	*	0.46	-14.9	*	*	*	*	*	0.05	0.05	0.01	0.42	0.64
		B	*	*	0.58	-14.1	*	*	*	*	*	1.19	0.19	0.11	0.32	0.90
HYSTERETIC HOMOGENEOUS	V1	A	*	*	*	*	0.29	*	*	*	*	*	*	*	0.20	-3.4
		B	*	*	*	*	0.38	*	*	*	*	*	*	*	0.27	0.27
	V2	A	*	*	*	*	*	0.12	1.75	*	*	*	*	*	0.17	-3.4
		B	*	*	*	*	*	0.09	1.53	*	*	*	*	*	0.26	0.23
	V3	A	*	*	*	*	0.26	0.04	1.81	*	*	*	*	*	0.20	-3.4
		B	*	*	*	*	0.35	0.04	1.78	*	*	*	*	*	0.25	0.28
	V4	A	*	*	*	*	0.29	0.05	1.70	*	*	6.04	6.04	6.04	0.21	-3.2
		B	*	*	*	*	0.40	0.03	1.56	*	*	1.64	1.64	1.64	0.34	0.98
	B1	A	*	*	*	*	0.33	*	*	*	*	*	*	*	0.09	-5.7
		B	*	*	*	*	0.38	*	*	*	*	*	*	*	0.07	-1.4
	B2	A	*	*	*	*	0.34	*	*	0.53	*	*	*	*	0.09	-5.5
		B	*	*	*	*	0.38	*	*	0.43	*	*	*	*	0.07	-1.5
	B2A	A	*	*	*	*	*	*	*	0.69	-7.26	*	*	*	0.07	-5.1
		B	*	*	*	*	*	*	*	0.66	-9.79	*	*	*	0.04	-1.3
	B3	A	*	*	*	*	0.29	*	*	0.53	-14.9	*	*	*	0.09	-5.4
		B	*	*	*	*	0.26	*	*	0.44	-28.2	*	*	*	0.07	-1.2
	B4	A	*	*	*	*	0.31	*	*	0.48	-12.0	0.07	0.07	0.07	0.61	0.35
		B	*	*	*	*	0.36	*	*	0.62	-43.5	0.29	0.29	0.29	0.47	0.98

* = parameter not optimised; R²(p) = Coef of Determination for matric potentials; R²(f) = Coef of Determination for bottom inflow

Table VI.15-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for rapid flow event 90291

Simulation		Lys	Optimised parameters												$R^2(p)$	$R^2(f)$
			α 1/cm	n -	λ -	ψ_b cm	θ_s^w m ³ /m ³	α^w cm ⁻¹	n^w -	λ^w -	ψ_b^w cm	Ks_1 cm/h	Ks_2 cm/h	Ks_3 cm/h		
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	*	4.50	4.50	4.50	0.84	0.79
		B	*	*	*	*	*	*	*	*	*	18.0	18.0	18.0	0.73	0.70
	V2	A	0.08	1.21	*	*	*	*	*	*	*	*	*	*	0.98	0.78
		B	0.05	1.28	*	*	*	*	*	*	*	*	*	*	0.75	0.83
	V3	A	0.08	1.21	*	*	*	*	*	*	*	5.27	5.27	5.27	0.98	0.78
		B	0.10	1.50	*	*	*	*	*	*	*	25.7	25.7	25.7	0.78	0.81
	B1	A	*	*	*	*	*	*	*	*	*	1.31	1.31	1.31	0.89	0.75
		B	*	*	*	*	*	*	*	*	*	3.00	3.00	3.00	0.74	0.79
	B1A	A	*	*	0.85	*	*	*	*	*	*	*	*	*	0.82	0.59
		B	*	*	0.63	*	*	*	*	*	*	*	*	*	0.75	0.81
	B2	A	*	*	0.61	*	*	*	*	*	*	1.96	1.96	1.96	0.88	0.75
		B	*	*	0.66	*	*	*	*	*	*	4.92	4.92	4.92	0.78	0.79
	B2A	A	*	*	0.55	-5.46	*	*	*	*	*	*	*	*	0.96	0.74
		B	*	*	0.71	-6.21	*	*	*	*	*	*	*	*	0.86	0.60
	B3	A	*	*	0.49	-3.96	*	*	*	*	*	11.68	11.68	11.68	0.98	0.75
		B	*	*	0.65	-6.67	*	*	*	*	*	4.33	4.33	4.33	0.87	0.60
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	*	27.41	3.95	0.49	0.75	0.83
		B	*	*	*	*	*	*	*	*	*	45.56	38.49	1.38	0.65	0.70
	V5	A	0.01	1.57	*	*	*	*	*	*	*	8.56	0.82	0.01	0.57	0.96
		B	0.05	2.97	*	*	*	*	*	*	*	11.32	2.85	0.22	0.81	0.44
	B3	A	*	*	*	*	*	*	*	*	*	66.56	1.10	0.12	0.74	0.83
		B	*	*	*	*	*	*	*	*	*	29.70	2.13	0.44	0.63	0.84
	B5	A	*	*	0.45	-41.4	*	*	*	*	*	36.86	0.83	0.03	0.72	0.99
		B	*	*	0.24	-12.0	*	*	*	*	*	17.77	1.24	0.10	0.61	0.85
HYSTERIC HOMOGENEOUS	V1	A	*	*	*	*	0.39	*	*	*	*	*	*	*	0.80	0.77
		B	*	*	*	*	0.37	*	*	*	*	*	*	*	0.81	0.79
	V2	A	*	*	*	*	*	0.03	1.76	*	*	*	*	*	0.77	0.92
		B	*	*	*	*	*	0.12	1.41	*	*	*	*	*	0.81	0.77
	V3	A	*	*	*	*	0.41	0.02	1.88	*	*	*	*	*	0.76	0.94
		B	*	*	*	*	0.40	0.10	1.81	*	*	*	*	*	0.73	0.87
	V4	A	*	*	*	*	0.22	0.08	1.94	*	*	0.66	0.66	0.66	0.96	0.91
		B	*	*	*	*	0.31	0.04	1.56	*	*	6.47	6.47	6.47	0.81	0.92
	B1	A	*	*	*	*	0.42	*	*	*	*	*	*	*	0.62	-0.6
		B	*	*	*	*	0.39	*	*	*	*	*	*	*	0.65	0.75
	B2	A	*	*	*	*	0.41	*	*	0.48	*	*	*	*	0.59	0.47
		B	*	*	*	*	0.42	*	*	0.41	*	*	*	*	0.66	0.73
	B2A	A	*	*	*	*	*	*	*	0.50	-26.9	*	*	*	0.63	0.97
		B	*	*	*	*	*	*	*	0.45	-10.4	*	*	*	0.66	0.71
	B3	A	*	*	*	*	0.29	*	*	0.51	-21.4	*	*	*	0.61	0.28
		B	*	*	*	*	0.41	*	*	0.43	-11.5	*	*	*	0.67	0.72
	B4	A	*	*	*	*	0.26	*	*	0.50	-29.7	4.62	4.62	4.62	0.63	0.96
		B	*	*	*	*	0.40	*	*	0.46	-9.97	2.14	2.14	2.14	0.75	0.80

* = parameter not optimised; $R^2(p)$ = Coef of Determination for matric potentials; $R^2(f)$ = Coef of Determination for bottom inflow

Table VI.16-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for rapid flow event 91017

Simulation	Lys	Optimised parameters												$R^2(p)$	$R^2(f)$
		α 1/cm	n -	λ -	ψ_b cm	$\theta_{s,w}$ m ³ /m ³	α'' cm ⁻¹	n'' -	λ'' -	$\psi_{b,w}$ cm	$K_{s,1}$ cm/h	$K_{s,2}$ cm/h	$K_{s,3}$ cm/h		
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	0.23	0.23	0.23	0.49	0.58
		B	*	*	*	*	*	*	*	*	7.58	7.58	7.58	0.48	0.90
	V2	A	0.06	1.09	*	*	*	*	*	*	*	*	*	0.86	0.83
		B	0.05	1.04	*	*	*	*	*	*	*	*	*	0.85	0.74
	V3	A	0.07	1.09	*	*	*	*	*	*	9.54	9.54	9.54	0.86	0.85
		B	0.07	1.05	*	*	*	*	*	*	10.4	10.4	10.4	0.85	0.75
	B1	A	*	*	*	*	*	*	*	*	0.09	0.09	0.09	0.57	0.67
		B	*	*	*	*	*	*	*	*	1.88	1.88	1.88	0.43	0.91
	B1A	A	*	*	0.05	*	*	*	*	*	*	*	*	0.41	0.63
		B	*	*	0.89	*	*	*	*	*	*	*	*	0.49	0.93
	B2	A	*	*	0.09	*	*	*	*	*	0.17	0.17	0.17	0.75	0.89
		B	*	*	0.74	*	*	*	*	*	3.75	3.75	3.75	0.49	0.91
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	38.98	6.54	0.07	0.64	0.91
		B	*	*	*	*	*	*	*	*	26.43	18.66	0.72	0.38	0.91
	V5	A	0.08	1.93	*	*	*	*	*	*	22.32	0.80	0.06	0.73	0.84
		B	0.02	1.77	*	*	*	*	*	*	15.42	2.91	0.12	0.32	0.89
	B3	A	*	*	*	*	*	*	*	*	17.70	0.58	0.03	0.68	0.91
		B	*	*	*	*	*	*	*	*	52.98	1.19	0.19	0.37	0.91
	B5	A	*	*	0.52	-5.41	*	*	*	*	18.03	0.62	0.03	0.79	0.89
		B	*	*	0.25	-11.3	*	*	*	*	44.46	0.96	0.07	0.37	0.88
HYSTERIC HOMOGENEOUS	V1	A	*	*	*	*	0.21	*	*	*	*	*	*	0.54	0.75
		B	*	*	*	*	0.36	*	*	*	*	*	*	0.52	0.87
	V2	A	*	*	*	*	*	0.03	1.39	*	*	*	*	0.54	0.81
		B	*	*	*	*	*	0.07	2.96	*	*	*	*	0.52	0.94
	V3	A	*	*	*	*	0.28	0.09	1.53	*	*	*	*	0.56	0.78
		B	*	*	*	*	0.22	0.02	2.86	*	*	*	*	0.51	0.93
	V4	A	*	*	*	*	0.28	0.04	1.83	*	*	3.74	3.74	0.62	0.82
		B	*	*	*	*	0.42	0.07	2.96	*	*	6.00	6.00	0.52	0.94
	B1	A	*	*	*	*	0.25	*	*	*	*	*	*	0.46	0.67
		B	*	*	*	*	0.42	*	*	*	*	*	*	0.29	0.78
	B2	A	*	*	*	*	0.40	*	*	0.48	*	*	*	0.48	-0.5
		B	*	*	*	*	0.41	*	*	0.41	*	*	*	0.29	0.78
	B2A	A	*	*	*	*	*	*	*	0.52	-19.2	*	*	0.48	0.77
		B	*	*	*	*	*	*	*	0.42	-10.8	*	*	0.28	0.79
	B3	A	*	*	*	*	0.42	*	*	0.49	-20.8	*	*	0.50	0.89
		B	*	*	*	*	0.40	*	*	0.29	-31.5	*	*	0.29	0.79
	B4	A	*	*	*	*	0.42	*	*	0.49	-20.8	6.00	6.00	0.50	0.89
		B	*	*	*	*	0.31	*	*	0.40	-22.2	1.38	1.38	0.49	0.92

* = parameter not optimised; $R^2(p)$ = Coef of Determination for matric potentials; $R^2(f)$ = Coef of Determination for bottom inflow

Table VI.17-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for rapid flow event 91119

Simulation	Lys	Optimised parameters												R ² (p)	R ² (f)
		α 1/cm	n -	λ -	ψ_b cm	θ_s^w m ³ /m ³	α^w cm ⁻¹	n ^w -	λ^w -	ψ_b^w cm	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	11.13	11.13	11.13	0.76	-0.5
		B	*	*	*	*	*	*	*	*	14.18	14.18	14.18	0.65	0.87
	V2	A	0.07	1.10	*	*	*	*	*	*	*	*	*	0.87	1.00
		B	0.09	1.10	*	*	*	*	*	*	*	*	*	0.79	0.97
	V3	A	0.11	1.09	*	*	*	*	*	*	16.78	16.78	16.78	0.87	0.99
		B	0.12	1.12	*	*	*	*	*	*	14.64	14.64	14.64	0.81	0.94
	B1	A	*	*	*	*	*	*	*	*	3.00	3.00	3.00	0.80	-0.1
		B	*	*	*	*	*	*	*	*	2.63	2.63	2.63	0.66	0.87
	B1A	A	*	*	0.89	*	*	*	*	*	*	*	*	0.89	-0.2
		B	*	*	0.89	*	*	*	*	*	*	*	*	0.78	0.84
	B2	A	*	*	0.09	*	*	*	*	*	0.15	0.15	0.15	0.87	0.98
		B	*	*	0.87	*	*	*	*	*	6.61	6.61	6.61	0.76	0.88
	B2A	A	*	*	0.08	-1.13	*	*	*	*	*	*	*	0.88	0.99
		B	*	*	0.88	-9.22	*	*	*	*	*	*	*	0.80	0.83
	B3	A	*	*	0.10	-0.52	*	*	*	*	65.78	65.78	65.78	0.89	0.98
		B	*	*	0.53	-4.60	*	*	*	*	10.81	10.81	10.81	0.81	0.88
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	3.42	0.62	0.01	0.88	-2.6
		B	*	*	*	*	*	*	*	*	28.85	12.22	3.45	0.59	0.89
	V5	A	0.09	1.87	*	*	*	*	*	*	12.54	0.64	0.01	0.91	-2.6
		B	0.10	2.53	*	*	*	*	*	*	98.15	24.44	0.17	0.82	0.34
	B3	A	*	*	*	*	*	*	*	*	3.24	3.01	1.15	0.79	-0.1
		B	*	*	*	*	*	*	*	*	3.19	1.94	1.90	0.65	0.86
	B5	A	*	*	0.07	-1.30	*	*	*	*	5.34	5.12	0.80	0.87	0.98
		B	*	*	0.18	-6.96	*	*	*	*	0.84	0.79	0.37	0.77	0.88
HYSTERIC HOMOGENEOUS	V1	A	*	*	*	*	0.28	*	*	*	*	*	*	0.77	0.96
		B	*	*	*	*	0.35	*	*	*	*	*	*	0.75	0.94
	V2	A	*	*	*	*	*	0.23	1.50	*	*	*	*	0.76	0.92
		B	*	*	*	*	*	0.14	1.42	*	*	*	*	0.75	0.92
	V3	A	*	*	*	*	0.23	0.03	1.80	*	*	*	*	0.80	0.97
		B	*	*	*	*	0.35	0.02	1.45	*	*	*	*	0.76	0.99
	V4	A	*	*	*	*	0.39	0.20	1.81	*	*	1.85	1.85	0.88	0.98
		B	*	*	*	*	0.24	0.16	1.62	*	*	0.88	0.88	0.85	0.99
	B1	A	*	*	*	*	0.35	*	*	*	*	*	*	0.62	0.87
		B	*	*	*	*	0.41	*	*	*	*	*	*	0.52	0.78
	B2	A	*	*	*	*	0.37	*	*	0.62	*	*	*	0.59	0.87
		B	*	*	*	*	0.42	*	*	0.42	*	*	*	0.52	0.77
	B2A	A	*	*	*	*	*	*	*	0.55	-6.92	*	*	0.60	0.84
		B	*	*	*	*	*	*	*	0.42	-11.6	*	*	0.52	0.77
	B3	A	*	*	*	*	0.39	*	*	0.58	-8.47	*	*	0.60	0.87
		B	*	*	*	*	0.35	*	*	0.38	-25.0	*	*	0.53	0.77
	B4	A	*	*	*	*	0.33	*	*	0.53	-5.24	0.44	0.44	0.92	0.99
		B	*	*	*	*	0.21	*	*	0.45	-49.7	0.78	0.78	0.78	0.96

* = parameter not optimised; R²(p) = Coef of Determination for matric potentials; R²(f) = Coef of Determination for bottom inflow

**Table VI.18-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for rapid flow event 91136**

Simulation		Lys	Optimised parameters													R ² (p)	R ² (f)
			α l/cm	n -	λ -	ψ_b cm	θ_s^w m ³ /m ³	α^w cm ⁻¹	n ^w -	λ^w -	ψ_b^w cm	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h			
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	*	0.08	0.08	0.08	0.80	-22	
		B	*	*	*	*	*	*	*	*	*	1.31	1.31	1.31	0.81	-2.0	
	V2	A	0.37	1.18	*	*	*	*	*	*	*	*	*	*	0.63	-12	
		B	0.12	1.12	*	*	*	*	*	*	*	*	*	*	0.84	0.01	
	V3	A	0.23	1.18	*	*	*	*	*	*	*	1.06	1.06	1.06	0.67	-15	
		B	0.11	1.19	*	*	*	*	*	*	*	4.61	4.61	4.61	0.84	-1.4	
	B1	A	*	*	*	*	*	*	*	*	*	0.01	0.01	0.01	0.75	-39	
		B	*	*	*	*	*	*	*	*	*	0.23	0.23	0.23	0.79	-9.0	
	B1A	A	*	*	0.90	*	*	*	*	*	*	*	*	*	0.99	-496	
		B	*	*	0.90	*	*	*	*	*	*	*	*	*	0.97	-102	
	B2	A	*	*	0.19	*	*	*	*	*	*	0.09	0.09	0.09	0.92	-32	
		B	*	*	0.90	*	*	*	*	*	*	1.15	1.15	1.15	0.67	-2.6	
B2A	A	*	*	0.46	-1.20	*	*	*	*	*	*	*	*	0.30	-63		
	B	*	*	0.10	-1.32	*	*	*	*	*	*	*	*	0.94	-2.6		
B3	A	*	*	0.71	-5.94	*	*	*	*	*	0.01	0.01	0.01	0.63	-41		
	B	*	*	0.62	-7.97	*	*	*	*	*	1.29	1.29	1.29	0.80	-1.7		
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	*	4.53	0.34	0.09	0.96	-23	
		B	*	*	*	*	*	*	*	*	*	5.06	0.14	0.10	0.92	-2.9	
	V5	A	0.11	1.24	*	*	*	*	*	*	*	37.42	2.70	0.11	0.90	-18	
		B	0.08	1.31	*	*	*	*	*	*	*	20.83	0.34	0.18	0.90	-2.2	
	B3	A	*	*	*	*	*	*	*	*	*	46.45	0.01	0.01	0.84	-39	
		B	*	*	*	*	*	*	*	*	*	0.18	0.18	0.18	0.76	-9.0	
	B5	A	*	*	0.07	-3.08	*	*	*	*	*	31.18	0.68	0.07	0.82	-20	
		B	*	*	0.35	-6.68	*	*	*	*	*	2.95	0.55	0.43	0.95	-2.5	
HYSTERIC HOMOGENEOUS	V1	A	*	*	*	*	0.24	*	*	*	*	*	*	*	0.88	-120	
		B	*	*	*	*	0.42	*	*	*	*	*	*	*	0.97	-98	
	V2	A	*	*	*	*	*	0.32	2.77	*	*	*	*	*	0.64	-72	
		B	*	*	*	*	*	0.42	2.97	*	*	*	*	*	0.77	-3.9	
	V3	A	*	*	*	*	0.29	0.45	1.93	*	*	*	*	*	0.65	-15	
		B	*	*	*	*	0.23	0.42	2.07	*	*	*	*	*	0.69	-4.6	
	V4	A	*	*	*	*	0.40	0.39	1.90	*	*	0.76	0.76	0.76	0.93	-1.8	
		B	*	*	*	*	0.41	0.45	1.81	*	*	4.29	4.29	4.29	0.84	-2.2	
	B1	A	*	*	*	*	0.20	*	*	*	*	*	*	*	0.69	-166	
		B	*	*	*	*	0.20	*	*	*	*	*	*	*	0.68	-90	
	B2	A	*	*	*	*	0.20	*	*	0.49	*	*	*	*	0.68	-198	
		B	*	*	*	*	0.20	*	*	0.54	*	*	*	*	0.68	-69	
	B2A	A	*	*	*	*	*	*	*	0.54	-0.59	*	*	*	0.63	-4.9	
		B	*	*	*	*	*	*	*	0.84	-10.0	*	*	*	0.68	-662	
	B3	A	*	*	*	*	0.21	*	*	0.50	-10.9	*	*	*	0.70	-182	
		B	*	*	*	*	0.20	*	*	0.57	-9.96	*	*	*	0.68	-63	
B4	A	*	*	*	*	0.21	*	*	0.49	-8.08	12.85	12.85	12.85	0.63	-105		
	B	*	*	*	*	0.20	*	*	0.42	-10.0	12.00	12.00	12.00	0.66	-6.8		

* = parameter not optimised; R²(p) = Coef of Determination for matric potentials; R²(f) = Coef of Determination for bottom inflow

**Table VI.19-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for rapid flow event 91198**

Simulation		Lys	Optimised parameters												R ² (p)	R ² (f)
			α 1/cm	n	λ	ψ_b cm	θ_s^w m ³ /m ³	α^w cm ⁻¹	n ^w	λ^w	ψ_b^w cm	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	*	0.11	0.11	0.11	0.41	-11
		B	*	*	*	*	*	*	*	*	*	0.28	0.28	0.28	0.61	-1.2
	V2	A	0.10	1.10	*	*	*	*	*	*	*	*	*	*	0.92	-0.7
		B	0.21	1.08	*	*	*	*	*	*	*	*	*	*	0.65	-0.7
	V3	A	0.40	1.10	*	*	*	*	*	*	*	2.48	2.48	2.48	0.54	-0.7
		B	0.18	1.08	*	*	*	*	*	*	*	4.11	4.11	4.11	0.65	-0.7
	B1	A	*	*	*	*	*	*	*	*	*	0.01	0.01	0.01	-0.1	-1.1
		B	*	*	*	*	*	*	*	*	*	1.69	1.69	1.69	0.90	-41
	B1A	A	*	*	0.90	*	*	*	*	*	*	*	*	*	0.97	-238
		B	*	*	0.90	*	*	*	*	*	*	*	*	*	0.94	-13
	B2	A	*	*	0.11	*	*	*	*	*	*	0.11	0.11	0.11	0.96	-2.2
		B	*	*	0.90	*	*	*	*	*	*	8.20	8.20	8.20	0.92	-12
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	*	7.49	0.01	0.01	0.84	-0.5
		B	*	*	*	*	*	*	*	*	*	3.26	3.20	0.05	0.92	-0.8
	V5	A	0.20	1.23	*	*	*	*	*	*	*	38.73	0.72	0.01	0.93	-0.3
		B	0.04	1.21	*	*	*	*	*	*	*	35.69	0.12	0.07	0.84	-0.5
	B3	A	*	*	*	*	*	*	*	*	*	15.45	0.01	0.01	0.74	-1.1
		B	*	*	*	*	*	*	*	*	*	30.52	0.14	0.01	0.82	-0.3
	B5	A	*	*	0.10	-1.11	*	*	*	*	*	11.98	4.87	0.02	0.93	-0.3
		B	*	*	0.90	-10.6	*	*	*	*	*	10.38	0.35	0.01	0.91	-0.4
HYSTERIC HOMOGENEOUS	V1	A	*	*	*	*	0.26	*	*	*	*	*	*	*	0.82	-29
		B	*	*	*	*	0.35	*	*	*	*	*	*	*	0.92	-2.8
	V2	A	*	*	*	*	*	0.19	1.71	*	*	*	*	*	0.78	-44
		B	*	*	*	*	*	0.12	1.56	*	*	*	*	*	0.92	-4.4
	V3	A	*	*	*	*	0.24	0.05	1.80	*	*	*	*	*	0.82	-27
		B	*	*	*	*	0.32	0.05	1.66	*	*	*	*	*	0.92	-3.4
	V4	A	*	*	*	*	0.29	0.08	1.67	*	*	3.58	3.58	3.58	0.91	-8.9
		B	*	*	*	*	0.29	0.05	1.86	*	*	2.66	2.66	2.66	0.95	-1.2
	B1	A	*	*	*	*	0.28	*	*	*	*	*	*	*	0.60	-107
		B	*	*	*	*	0.38	*	*	*	*	*	*	*	0.72	-49
	B2	A	*	*	*	*	0.28	*	*	0.51	*	*	*	*	0.60	-108
		B	*	*	*	*	0.41	*	*	0.66	*	*	*	*	0.68	-47
	B2A	A	*	*	*	*	*	*	*	0.60	-4.65	*	*	*	0.59	-109
		B	*	*	*	*	*	*	*	0.87	-11.7	*	*	*	0.67	-47
HOMOGENEOUS	B3	A	*	*	*	*	0.40	*	*	0.58	-5.24	*	*	*	0.60	-94
		B	*	*	*	*	0.40	*	*	0.66	-11.0	*	*	*	0.69	-46
	B4	A	*	*	*	*	0.27	*	*	0.65	-10.8	0.74	0.74	0.74	0.95	-14
		B	*	*	*	*	0.21	*	*	0.68	-45.5	0.86	0.86	0.86	0.93	-2.2

* = parameter not optimised; R²(p) = Coef of Determination for matric potentials; R²(f) = Coef of Determination for bottom inflow

Table VI.20-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for rapid flow event 91211

Simulation		Lys	Optimised parameters													R ² (p)	R ² (f)
			α 1/cm	n -	λ -	ψ_b cm	θ_s^w m ³ /m ³	α^w cm ⁻¹	n ^w -	λ^w -	ψ_b^w cm	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h			
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	*	11.63	11.63	11.63	0.82	-3.8	
		B	*	*	*	*	*	*	*	*	*	14.10	14.10	14.10	0.86	-0.5	
	V2	A	0.07	1.13	*	*	*	*	*	*	*	*	*	*	0.89	0.95	
		B	0.07	1.16	*	*	*	*	*	*	*	*	*	*	0.96	0.78	
	V3	A	0.11	1.12	*	*	*	*	*	*	*	16.6	16.6	16.6	0.90	0.94	
		B	0.09	1.16	*	*	*	*	*	*	*	10.7	10.7	10.7	0.96	0.77	
	B1	A	*	*	*	*	*	*	*	*	*	3.75	3.75	3.75	0.82	-2.0	
		B	*	*	*	*	*	*	*	*	*	2.25	2.25	2.25	0.88	-0.3	
	B1A	A	*	*	0.20	*	*	*	*	*	*	*	*	*	0.62	-1.2	
		B	*	*	0.89	*	*	*	*	*	*	*	*	*	0.93	0.31	
	B2	A	*	*	0.13	*	*	*	*	*	*	0.24	0.24	0.24	0.92	0.88	
		B	*	*	0.14	*	*	*	*	*	*	0.20	0.20	0.20	0.96	0.71	
B2A	A	*	*	0.11	-1.5	*	*	*	*	*	*	*	*	0.89	0.90		
	B	*	*	0.25	-3.1	*	*	*	*	*	*	*	*	0.96	0.75		
B3	A	*	*	0.13	-0.83	*	*	*	*	*	35.63	35.63	35.63	0.88	0.86		
	B	*	*	0.43	-3.49	*	*	*	*	*	13.56	13.56	13.56	0.96	0.75		
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	*	6.87	6.67	0.01	0.85	-2.8	
		B	*	*	*	*	*	*	*	*	*	67.69	4.84	2.69	0.82	0.45	
	V5	A	0.12	1.21	*	*	*	*	*	*	*	17.93	7.71	0.01	0.91	-2.4	
		B	0.05	1.19	*	*	*	*	*	*	*	4.81	4.80	0.76	0.93	0.79	
	B3	A	*	*	*	*	*	*	*	*	*	37.98	3.22	0.22	0.72	-1.1	
		B	*	*	*	*	*	*	*	*	*	59.84	1.06	0.43	0.79	0.32	
	B5	A	*	*	0.16	-10.5	*	*	*	*	*	98.58	2.99	0.04	0.73	0.93	
		B	*	*	0.18	-5.56	*	*	*	*	*	29.51	0.44	0.21	0.87	0.77	
HYSTERIC HOMOGENEOUS	V1	A	*	*	*	*	0.30	*	*	*	*	*	*	*	0.85	0.53	
		B	*	*	*	*	0.35	*	*	*	*	*	*	*	0.93	0.70	
	V2	A	*	*	*	*	*	0.21	1.62	*	*	*	*	*	0.81	0.38	
		B	*	*	*	*	*	0.17	1.36	*	*	*	*	*	0.93	0.71	
	V3	A	*	*	*	*	0.30	0.06	1.70	*	*	*	*	*	0.85	0.56	
		B	*	*	*	*	0.35	0.07	1.77	*	*	*	*	*	0.92	0.70	
	V4	A	*	*	*	*	0.38	0.17	1.49	*	*	2.86	2.86	2.86	0.92	0.81	
		B	*	*	*	*	0.29	0.07	1.61	*	*	2.49	2.49	2.49	0.97	0.82	
	B1	A	*	*	*	*	0.33	*	*	*	*	*	*	*	0.72	-0.4	
		B	*	*	*	*	0.40	*	*	*	*	*	*	*	0.75	-0.9	
	B2	A	*	*	*	*	0.33	*	*	0.49	*	*	*	*	0.71	-0.6	
		B	*	*	*	*	0.42	*	*	0.51	*	*	*	*	0.75	-0.8	
	B2A	A	*	*	*	*	*	*	*	0.59	-5.47	*	*	*	0.69	-0.5	
		B	*	*	*	*	*	*	*	0.65	-10.7	*	*	*	0.74	-0.7	
	B3	A	*	*	*	*	0.33	*	*	0.57	-10.8	*	*	*	0.71	-0.5	
		B	*	*	*	*	0.37	*	*	0.44	-12.4	*	*	*	0.75	-0.8	
B4	A	*	*	*	*	0.27	*	*	0.54	-11.5	0.62	0.62	0.62	0.96	0.78		
	B	*	*	*	*	0.33	*	*	0.75	-10.0	0.49	0.49	0.49	0.95	0.84		

* = parameter not optimised; $R^2(p)$ = Coef of Determination for matric potentials; $R^2(f)$ = Coef of Determination for bottom inflow

Table VI.21-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for slow flow event 90129

Simulation		Lys	Optimised parameters												R ² (p)	R ² (f)
			α 1/cm	n -	λ -	ψ_b cm	θ_b^w m ³ /m ³	α^w cm ⁻¹	n ^w -	λ^w -	ψ_b^w cm	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h		
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	*	1.01	1.01	1.01	0.92	0.97
		B	*	*	*	*	*	*	*	*	*	2.81	2.81	2.81	0.71	-1.3
	V2	A	0.12	1.49	*	*	*	*	*	*	*	*	*	*	0.85	0.97
		B	0.05	1.07	*	*	*	*	*	*	*	*	*	*	0.36	0.91
	V3	A	0.06	1.69	*	*	*	*	*	*	*	0.89	0.89	0.89	0.92	0.97
		B	0.02	2.18	*	*	*	*	*	*	*	0.05	0.05	0.05	0.96	0.71
	B1	A	*	*	*	*	*	*	*	*	*	0.40	0.40	0.40	0.88	0.87
		B	*	*	*	*	*	*	*	*	*	0.49	0.49	0.49	0.72	-0.6
	B1A	A	*	*	0.90	*	*	*	*	*	*	*	*	*	0.54	-9.0
		B	*	*	0.89	*	*	*	*	*	*	*	*	*	0.31	-2.3
	B2	A	*	*	0.59	*	*	*	*	*	*	0.47	0.47	0.47	0.88	0.97
		B	*	*	0.26	*	*	*	*	*	*	0.24	0.24	0.24	0.68	0.21
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	*	1.14	1.11	0.65	0.91	0.96
		B	*	*	*	*	*	*	*	*	*	0.69	0.68	0.01	0.96	-6.3
	V5	A	0.04	1.60	*	*	*	*	*	*	*	0.33	0.33	0.31	0.92	0.89
		B	0.36	1.12	*	*	*	*	*	*	*	7.55	0.72	0.01	0.90	-5.0
	B3	A	*	*	*	*	*	*	*	*	*	0.39	0.39	0.38	0.88	0.96
		B	*	*	*	*	*	*	*	*	*	3.95	3.85	0.03	0.14	0.78
	B5	A	*	*	0.53	-10.5	*	*	*	*	*	0.38	0.38	0.17	0.89	0.80
		B	*	*	0.42	-10.7	*	*	*	*	*	21.82	1.94	0.02	0.16	0.79
HYST HOMOGENEOUS	V1	A	*	*	*	*	0.20	*	*	*	*	*	*	*	0.23	0.45
		B	*	*	*	*	0.40	*	*	*	*	*	*	*	0.43	-7.9
	V2	A	*	*	*	*	*	0.40	1.82	*	*	*	*	*	0.13	-0.3
		B	*	*	*	*	*	0.42	1.49	*	*	*	*	*	0.16	0.19
	V3	A	*	*	*	*	0.20	0.06	1.70	*	*	*	*	*	0.23	0.45
		B	*	*	*	*	0.42	0.42	1.48	*	*	*	*	*	0.16	0.16
	V4	A	*	*	*	*	0.20	0.06	1.70	*	*	6.00	6.00	6.00	0.23	0.45
		B	*	*	*	*	0.22	0.08	1.52	*	*	6.22	6.22	6.22	0.13	0.48
	B1	A	*	*	*	*	0.21	*	*	*	*	*	*	*	0.08	-1.3
		B	*	*	*	*	0.22	*	*	*	*	*	*	*	-0.1	-1.4
	B2	A	*	*	*	*	0.20	*	*	0.54	*	*	*	*	0.07	-1.1
		B	*	*	*	*	0.21	*	*	0.54	*	*	*	*	-0.1	-0.8
	B2A	A	*	*	*	*	*	*	*	0.66	-1.25	*	*	*	0.05	-1.0
		B	*	*	*	*	*	*	*	0.82	-4.30	*	*	*	-0.1	-1.0
	B3	A	*	*	*	*	0.29	*	*	0.68	-0.82	*	*	*	0.04	-0.6
		B	*	*	*	*	0.40	*	*	0.81	-4.00	*	*	*	-0.1	-0.6
	B4	A	*	*	*	*	0.20	*	*	0.53	-10.3	6.10	6.10	6.10	0.07	-1.0
		B	*	*	*	*	0.20	*	*	0.44	-10.1	9.37	9.37	9.37	-0.1	-0.6

* = parameter not optimised; R²(p) = Coef of Determination for matric potentials; R²(f) = Coef of Determination for bottom inflow

Table VI.22-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for slow flow event 91108

Simulation		Lys	Optimised parameters												$R^2(p)$	$R^2(f)$
			α 1/cm	n -	λ -	ψ_b cm	θ_s^w m ³ /m ³	α^w cm ⁻¹	n^w -	λ^w -	ψ_b^w cm	K_{s1} cm/h	K_{s2} cm/h	K_{s3} cm/h		
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	*	0.12	0.12	0.12	-0.3	0.74
		B	*	*	*	*	*	*	*	*	*	0.42	0.42	0.42	0.77	0.98
	V2	A	0.13	1.11	*	*	*	*	*	*	*	*	*	*	0.85	0.96
		B	0.20	1.40	*	*	*	*	*	*	*	*	*	*	0.77	0.99
	V3	A	0.09	1.12	*	*	*	*	*	*	*	2.51	2.51	2.51	0.87	0.97
		B	0.20	1.47	*	*	*	*	*	*	*	5.94	5.94	5.94	0.76	0.99
	B1	A	*	*	*	*	*	*	*	*	*	0.04	0.04	0.04	-0.2	0.96
		B	*	*	*	*	*	*	*	*	*	0.07	0.07	0.07	0.76	0.99
	B1A	A	*	*	0.90	*	*	*	*	*	*	*	*	*	0.83	-84
		B	*	*	0.90	*	*	*	*	*	*	*	*	*	0.64	-66
	B2	A	*	*	0.15	*	*	*	*	*	*	0.04	0.04	0.04	0.90	0.99
		B	*	*	0.33	*	*	*	*	*	*	0.06	0.06	0.06	0.79	0.99
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	*	2.78	1.53	0.03	0.91	0.99
		B	*	*	*	*	*	*	*	*	*	1.39	0.44	0.30	0.81	0.97
	V5	A	0.07	1.72	*	*	*	*	*	*	*	19.46	1.24	0.04	0.82	0.98
		B	0.09	1.45	*	*	*	*	*	*	*	1.75	1.70	0.20	0.81	0.93
	B3	A	*	*	*	*	*	*	*	*	*	1.24	1.22	0.01	0.88	0.95
		B	*	*	*	*	*	*	*	*	*	25.93	0.43	0.01	0.60	0.93
	B5	A	*	*	0.51	-7.65	*	*	*	*	*	24.90	0.34	0.03	0.79	0.99
		B	*	*	0.51	-8.62	*	*	*	*	*	21.29	0.41	0.03	0.64	0.95
HYSTERIC HOMOGENEOUS	V1	A	*	*	*	*	0.22	*	*	*	*	*	*	*	0.69	-4.7
		B	*	*	*	*	0.21	*	*	*	*	*	*	*	0.53	-1.4
	V2	A	*	*	*	*	*	0.37	1.86	*	*	*	*	*	0.62	-1.6
		B	*	*	*	*	*	0.20	1.82	*	*	*	*	*	0.52	-1.4
	V3	A	*	*	*	*	0.23	0.08	1.67	*	*	*	*	*	0.67	-1.5
		B	*	*	*	*	0.22	0.09	1.17	*	*	*	*	*	0.55	-1.0
	V4	A	*	*	*	*	0.22	0.07	1.55	*	*	6.52	6.52	6.52	0.69	-2.8
		B	*	*	*	*	0.25	0.08	1.86	*	*	3.24	3.24	3.24	0.57	-0.2
	B1	A	*	*	*	*	0.26	*	*	*	*	*	*	*	0.61	-3.1
		B	*	*	*	*	0.25	*	*	*	*	*	*	*	0.44	-3.4
	B2	A	*	*	*	*	0.25	*	*	0.62	*	*	*	*	0.60	-2.1
		B	*	*	*	*	0.25	*	*	0.87	*	*	*	*	0.42	-4.0
	B2A	A	*	*	*	*	*	*	*	0.56	-2.01	*	*	*	0.59	-2.2
		B	*	*	*	*	*	*	*	0.75	-2.64	*	*	*	0.42	-4.1
	B3	A	*	*	*	*	0.20	*	*	0.48	-14.8	*	*	*	0.60	-2.0
		B	*	*	*	*	0.42	*	*	0.78	-3.64	*	*	*	0.42	-3.6
	B4	A	*	*	*	*	0.20	*	*	0.48	-21.2	1.88	1.88	1.88	0.69	-1.0
		B	*	*	*	*	0.40	*	*	0.88	-3.46	4.97	4.97	4.97	0.43	-3.7

* = parameter not optimised; $R^2(p)$ = Coef of Determination for matric potentials; $R^2(f)$ = Coef of Determination for bottom inflow

Table VI.23-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for slow flow event 91165

Simulation		Lys	Optimised parameters													R ² (p)	R ² (f)
			α 1/cm	n	λ -	ψ_b cm	θ_b^w m ³ /m ³	α^w cm ⁻¹	n ^w -	λ^w -	ψ_b^w cm	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h			
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	*	0.27	0.27	0.27	0.65	0.97	
		B	*	*	*	*	*	*	*	*	*	0.68	0.68	0.68	0.79	0.99	
	V2	A	0.11	1.14	*	*	*	*	*	*	*	*	*	*	0.96	0.97	
		B	0.14	1.20	*	*	*	*	*	*	*	*	*	*	0.91	0.99	
	V3	A	0.10	1.14	*	*	*	*	*	*	*	6.65	6.65	6.65	0.96	0.97	
		B	0.12	1.16	*	*	*	*	*	*	*	6.71	6.71	6.71	0.94	0.99	
	B1	A	*	*	*	*	*	*	*	*	*	0.10	0.10	0.10	0.67	0.98	
		B	*	*	*	*	*	*	*	*	*	0.12	0.12	0.12	0.77	0.98	
	B1A	A	*	*	0.08	*	*	*	*	*	*	*	*	*	0.79	-0.2	
		B	*	*	0.06	*	*	*	*	*	*	*	*	*	0.68	0.09	
	B2	A	*	*	0.14	*	*	*	*	*	*	0.08	0.08	0.08	0.96	0.98	
		B	*	*	0.10	*	*	*	*	*	*	0.14	0.14	0.14	0.91	0.93	
	B2A	A	*	*	0.10	-1.00	*	*	*	*	*	*	*	*	0.93	0.91	
		B	*	*	0.13	-1.23	*	*	*	*	*	*	*	*	0.93	0.96	
	B3	A	*	*	0.13	-5.00	*	*	*	*	*	0.25	0.25	0.25	0.95	0.98	
		B	*	*	0.16	-4.17	*	*	*	*	*	0.46	0.46	0.46	0.93	0.98	
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	*	3.28	1.16	0.09	0.91	0.98	
		B	*	*	*	*	*	*	*	*	*	12.05	1.59	0.21	0.87	0.98	
	V5	A	0.07	2.59	*	*	*	*	*	*	*	18.94	5.12	0.07	0.95	0.99	
		B	0.08	1.95	*	*	*	*	*	*	*	7.53	1.51	0.18	0.92	0.98	
	B3	A	*	*	*	*	*	*	*	*	*	23.49	0.76	0.03	0.87	0.97	
		B	*	*	*	*	*	*	*	*	*	21.98	0.39	0.04	0.84	0.96	
	B5	A	*	*	0.19	-2.82	*	*	*	*	*	2.12	1.93	0.31	0.96	0.96	
		B	*	*	0.43	-9.61	*	*	*	*	*	18.67	0.42	0.04	0.84	0.96	
HYSTERIC HOMOGENEOUS	V1	A	*	*	*	*	0.23	*	*	*	*	*	*	*	0.87	0.50	
		B	*	*	*	*	0.29	*	*	*	*	*	*	*	0.85	0.52	
	V2	A	*	*	*	*	*	0.50	1.10	*	*	*	*	*	0.84	0.36	
		B	*	*	*	*	*	0.48	1.94	*	*	*	*	*	0.78	0.71	
	V3	A	*	*	*	*	0.23	0.09	1.63	*	*	*	*	*	0.86	0.52	
		B	*	*	*	*	0.22	0.15	1.58	*	*	*	*	*	0.80	0.76	
	V4	A	*	*	*	*	0.38	0.32	1.74	*	*	0.70	0.70	0.70	0.92	0.98	
		B	*	*	*	*	0.37	0.25	1.66	*	*	5.16	5.16	5.16	0.83	0.87	
	B1	A	*	*	*	*	0.22	*	*	*	*	*	*	*	0.80	0.15	
		B	*	*	*	*	0.24	*	*	*	*	*	*	*	0.70	0.34	
	B2	A	*	*	*	*	0.20	*	*	0.49	*	*	*	*	0.79	-0.03	
		B	*	*	*	*	0.23	*	*	0.81	*	*	*	*	0.68	0.30	
	B2A	A	*	*	*	*	*	*	*	0.54	-1.10	*	*	*	0.79	-0.1	
		B	*	*	*	*	*	*	*	0.76	-3.05	*	*	*	0.69	0.30	
	B3	A	*	*	*	*	0.20	*	*	0.49	-10.0	*	*	*	0.79	-0.03	
		B	*	*	*	*	0.20	*	*	0.42	-15.0	*	*	*	0.69	0.21	
B4	A	*	*	*	*	0.20	*	*	0.49	-10.0	6.00	6.00	6.00	0.79	-0.1		
	B	*	*	*	*	0.20	*	*	0.42	-15.0	6.00	6.00	6.00	0.69	0.21		

* = parameter not optimised; R²(p) = Coef of Determination for matric potentials; R²(f) = Coef of Determination for bottom inflow

Table VI.24-SPW1hyst simultaneous optimisation of matric potential and bottom inflow
Results for slow flow event 91204

Simulation		Lys	Optimised parameters													R ² (p)	R ² (f)
			α 1/cm	n -	λ -	ψ_b cm	θ_b^w m ³ /m ³	α^w cm ⁻¹	n ^w -	λ^w -	ψ_b^w cm	Ks ₁ cm/h	Ks ₂ cm/h	Ks ₃ cm/h			
NON-HYST HOMOGENEOUS	V1	A	*	*	*	*	*	*	*	*	*	0.12	0.12	0.12	0.75	0.76	
		B	*	*	*	*	*	*	*	*	*	0.70	0.70	0.70	0.87	0.96	
	V2	A	0.21	1.14	*	*	*	*	*	*	*	*	*	*	0.68	0.70	
		B	0.16	1.32	*	*	*	*	*	*	*	*	*	*	0.87	0.97	
	V3	A	0.10	1.28	*	*	*	*	*	*	*	0.57	0.57	0.57	0.75	0.77	
		B	0.19	1.32	*	*	*	*	*	*	*	8.39	8.39	8.39	0.85	0.98	
	B1	A	*	*	*	*	*	*	*	*	*	0.05	0.05	0.05	0.75	0.73	
		B	*	*	*	*	*	*	*	*	*	0.12	0.12	0.12	0.88	0.94	
	B1A	A	*	*	0.004	*	*	*	*	*	*	*	*	*	0.78	-22	
		B	*	*	0.90	*	*	*	*	*	*	*	*	*	0.90	-27	
	B2	A	*	*	0.60	*	*	*	*	*	*	0.05	0.05	0.05	0.70	0.76	
		B	*	*	0.81	*	*	*	*	*	*	0.27	0.27	0.27	0.77	0.97	
	B2A	A	*	*	0.11	-0.58	*	*	*	*	*	*	*	*	0.49	0.70	
		B	*	*	0.16	-1.27	*	*	*	*	*	*	*	*	0.86	0.97	
	B3	A	*	*	0.26	-4.00	*	*	*	*	*	0.12	0.12	0.12	0.63	0.84	
		B	*	*	0.17	-1.10	*	*	*	*	*	8.99	8.99	8.99	0.85	0.97	
NON-HYST HET	V3	A	*	*	*	*	*	*	*	*	*	16.04	0.17	0.07	0.90	0.67	
		B	*	*	*	*	*	*	*	*	*	25.88	0.65	0.59	0.92	0.95	
	V5	A	0.10	1.73	*	*	*	*	*	*	*	10.98	0.20	0.19	0.93	0.84	
		B	0.06	1.59	*	*	*	*	*	*	*	11.11	1.23	0.12	0.92	0.87	
	B3	A	*	*	*	*	*	*	*	*	*	42.58	0.55	0.02	0.88	0.50	
		B	*	*	*	*	*	*	*	*	*	20.56	0.82	0.03	0.87	0.92	
	B5	A	*	*	0.64	-5.83	*	*	*	*	*	7.48	0.08	0.08	0.93	0.88	
		B	*	*	0.43	-10.3	*	*	*	*	*	29.52	0.69	0.03	0.87	0.92	
HYSTERIC HOMOGENEOUS	V1	A	*	*	*	*	0.30	*	*	*	*	*	*	*	0.88	-58	
		B	*	*	*	*	0.21	*	*	*	*	*	*	*	0.86	-1.5	
	V2	A	*	*	*	*	*	0.39	1.81	*	*	*	*	*	0.82	-21	
		B	*	*	*	*	*	0.33	1.71	*	*	*	*	*	0.86	-1.5	
	V3	A	*	*	*	*	0.21	0.18	1.55	*	*	*	*	*	0.81	-18	
		B	*	*	*	*	0.20	0.07	1.85	*	*	*	*	*	0.85	-1.7	
	V4	A	*	*	*	*	0.28	0.15	1.63	*	*	0.11	0.11	0.11	0.87	0.78	
		B	*	*	*	*	0.40	0.43	1.79	*	*	0.74	0.74	0.74	0.91	0.97	
	B1	A	*	*	*	*	0.20	*	*	*	*	*	*	*	0.79	-26	
		B	*	*	*	*	0.21	*	*	*	*	*	*	*	0.75	-3.4	
	B2	A	*	*	*	*	0.21	*	*	0.48	*	*	*	*	0.79	-25	
		B	*	*	*	*	0.20	*	*	0.53	*	*	*	*	0.74	-3.2	
	B2A	A	*	*	*	*	*	*	*	0.58	-2.50	*	*	*	0.80	-36	
		B	*	*	*	*	*	*	*	0.72	-0.63	*	*	*	0.74	-3.2	
	B3	A	*	*	*	*	0.20	*	*	0.49	-12.1	*	*	*	0.79	-25	
		B	*	*	*	*	0.22	*	*	0.56	-1.63	*	*	*	0.74	-2.9	
B4	A	*	*	*	*	0.22	*	*	0.50	-10.7	6.37	6.37	6.37	0.79	-25		
	B	*	*	*	*	0.39	*	*	0.85	-1.08	7.27	7.27	7.27	0.74	-3.0		

* = parameter not optimised; R²(p) = Coef of Determination for matric potentials; R²(f) = Coef of Determination for bottom inflow