UNIVERSITY OF ALBERTA

SIMULATION OF WATER STATUS IN UNSATURATED SOILS

by

Masoud Parsinejad ©

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IN THE NAME OF GOD THE BENEFICENT THE MERCIFUL

All praises belong to The God, almighty

This thesis is dedicated
to my wife,
Nasrin

and to my daughters
Zahra and Fatemeh

For all that they have been

ABSTRACT

There has been a growing interest in simulation of state and dynamics of soil water in recent decades. Aside from the traditional attention to the unsaturated zone as a source of water supply to plants, recent studies on this zone are motivated by concerns about soil and groundwater pollution from agricultural, industrial and municipal sources. In order to be able to adopt the numerous existing models for various soil management practices with confidence, it is important that the capabilities of these models and the credibility of their results be tested. In this study, the performance of LEACHW and *ecosys* models in predicting dynamics of water in unsaturated soils over time and space under field conditions, was tested against detailed collected data. Overall, performance of the two models were found to be reasonable for prediction of soil-water. A detailed examination of soil water status, during and after intensive precipitation events, showed an under-estimation of drainage fluxes by both models, especially by LEACHW. Such events would contribute most in the production of drainage fluxes. Both models predicted the drying process at a higher rate than actual. However, *ecosys* predictions were found to be more accurate. In addition, a sensitivity analysis on the importance of accurate estimation of the parameters used in hydraulic functions for simulation of transient soil water changes showed that relatively similar soil water storage estimation could result from a wide combination of hydraulic parameter values. This suggests that such estimation is not particularly sensitive to variable soil physical condition. And finally, SIMPLE model for predicting soil water storage, based on the concept of water balance was

developed. The main advantage of this model is that it requires a small data set. The new model was capable of reproducing field-measured soil water contents at three different sites with reasonable accuracy. The SIMPLE model predicted values of soil water content compared with predicted values by the more complex LEACHW model. Even though LEACHW requires more information on physical and hydraulic properties of soils, simulation results of both models were quite comparable.

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GLOSSARY OF SYMBOLS

A	cross sectional area of soil column
b	slope of ln h versus $\ln\theta$
C	soil-water capacity or $(\frac{\partial\theta}{\partial h})$
Dr	drainage or deep percolation
ET	evapotraspiration
g	gravitational acceleration
H	hydraulic head
h	matric head (m), or potential in unsaturated soils
I	irrigation
w	subscript representing number of tubes not contributing to flow
i	subscript representing the depth of a node
j	subscript representing time
$K(h)$	unsaturated hydraulic conductivity as a function of matric potential
L	latent heat of vaporization
X	length of cylindrical capillary
m	number of increments of θ
ME	mean error between measured and simulated soil water content
n	number of data points
P	precipitation
r	capillary tube radius
R	mean hydraulic radius representative of the pore size distribution of the porous material
RE	relative error between measured and simulated soil water content
RSE	relative standard error of estimate or root mean square error
s	subscript denotes saturated value

SE	root mean square of error between measured and simulated soil water content
t	time
z	depth of soil layer
R_a	aerodynamic resistance
h_e	air entry potential
h_z	gravitational head
θ_{mean}	average measured water content over time
ρ_b	bulk density
κ^2	chi-square
m_c	clay mass fraction
ν	coefficient of viscosity
ρ_w	density of water
β	drainage coefficient
λ_{ave}	hydraulic conductance
m_s	silt mass fractions
E_a	vapor density of air
J_w	water flux in vertical direction
ΔW	change in soil-water content
ΔP	hydrostatic pressure difference
r_w	rate of water uptake by plant per unit lean area
K_s	saturated hydraulic conductivity
θ_{FC}	soil-water content at field capacity
θ_{WP}	soil-water content at permanent wilting point
σ_{θ_m}	standard deviation of replicated soil-water measurement
R_o	surface runoff
Δz	thickness of each compartment
E_s	vapor density at the soil surface

ν	viscosity of water
σ	surface tension
ϕ	total porosity
θ	volumetric water content

Chapter One

INTRODUCTION

There has been a growing interest in simulating the state and dynamics of soil water during the past two decades (Addiscott and Wagenet, 1985; Ammentorp et al., 1991; Govindaraju et al., 1992; Reddi and Danda, 1994; Clemente et al., 1994; Zhang et al., 1994), in response to the need to develop solutions for various agricultural and environmental management problems, such as designing irrigation and drainage systems, and controlling pollution of surface and ground water resources. Models can be used to guide future research efforts (Wagenet and Hutson, 1989) in the sense that they can be used to aid testing of hypotheses and the exposure of areas of incomplete understanding. In general, management-oriented models are simpler and require less field-specific data than research models which are input-intensive but can be more accurate (Jemison et al., 1994).

As model predictions improve, they may be used as regulatory tools for providing recommendations for application of water and agricultural chemicals (Pennell et al., 1990). Ultimately, models may reduce the need for labor-intensive field experimentation. This depends on the validity and applicability of models in varied soils and environment (Hutson et al., 1988). According to Hanks (1985), soil water models could also be used to predict the influence of one factor, or a combination of factors on soil water status. They provide answers to "what if" questions such as "what if the soil was a sand instead of a silt loam?". He cited the possibility of determining the sensitivity of soil factors to end result as another advantage of modeling soil water.

Of those that have been developed, many models have not been evaluated with independent data sets from different soil types or environmental conditions (Addiscott and Wagenet, 1985; Pennell et al., 1990). van Keulen (1974) noted that if independent data are not used for evaluation of a model, the most that can be concluded is that "historical events under a given set of conditions may be described by the generated set of equations." This, however, is not the objective of this study, but rather by evaluation, we intend to judge the value of these models. As Penning de Vries (1977) described, evaluation is used for comparison of model output with real data and for judgment of practical utility. Model evaluation could also provide answers to questions such as how much additional effort should be invested in data collection or modeling in relation to perceived increase in accuracy of model predictions (Rasmussen and Fluher, 1990).

In order to be able to adopt existing models for various soil management practices with confidence, it is important that the capabilities of these models and the credibility of their results be tested. Addiscott and Wagenet (1985) discussed the inherent strength and weaknesses attributed to different approaches to modeling. These factors need to be considered in selection of a model. The increasing availability of user-friendly software allows generation of modeling data that may be unrealistic. Continued field checks of models are therefore important (Bouma et al., 1993).

One of the major problems associated with proper evaluation of existing models is the inadequacy and inaccuracy of input data (Clemente et al., 1994). Addiscott and Wagenet (1985) reviewed and discussed a number of modeling approaches with reference to different purposes, with differing requirements of input data, depth of consideration of basic processes and sensitivity and accuracy of simulations. They cautioned that the adoption of models is limited to the cases in which the basic assumptions and structures of the model are valid. They also noted that adequate field data sets are unavailable for testing a range of models, and they suggest that few attempts have been made to test a model by someone other than the developer. Kool and Huyakorn (1990) undertook an exceptionally detailed trench experiment in Las Cruces, New Mexico to obtain data for validating flow and transport models. Such experiments are rarely, if ever, feasible because of the cost, in addition to the major soil disturbances they cause.

1.1 Theoretical Background

For the simplest case, porous media are assumed as a system with ideal geometry, i.e., water-filled capillary tube. The volume of water flowing per unit time, Q (L^3T^{-1}), is calculated as:

$$Q = \frac{\pi r^4 \Delta P}{8 X \nu} \qquad (1)$$

where

r = capillary tube radius (m),

ΔP = hydrostatic pressure difference (kPa),

X = length of cylindrical capillary (m) and

ν = viscosity of water ($g m^{-1} s^{-1}$).

Equation (1), which describes the flux of water in a single capillary, is called Poiseuille's law (Jury et al., 1991). Capillary tubes can theoretically be interconnected in various ways to represent soil pores. According to this equation, small pores conduct water much less readily than do large pores. The exact geometry of pore sizes and channels through which the water flows, however, is unknown. To overcome this problem, Darcy (1856) was first to use the average flow over many pores to describe movement of water through saturated porous media. Darcy's law is described as:

$$Q = K_s A \frac{\Delta P}{L} \qquad (2)$$

where

K_s = saturated hydraulic conductivity ($m^2\, s^{-1}\, kPa^{-1}$) and

A = cross sectional area of soil column (m^2).

Expressing potential in terms of hydraulic head, H, and if the driving force for water movement consists of hydrostatic pressure head gradient and gravitational head, then

$$P = H = h + h_z \qquad (3)$$

where

H = hydraulic head (m),

h_z = gravitational head (m) and

h = hydrostatic pressure head in saturated and matric head in unsaturated soils (m).

This is true for rigid soils, in which h is a function of soil water content (θ). The relationship between h and θ can be used to develop soil water characteristic curves.

When the soil is not saturated, flow paths are represented by narrower and more tortuous channels. The driving force for water movement is due to interactions between soil matrix and water (matric potential) and gravitational force. The value of hydraulic conductivity is highly dependent upon the amount of water in the soil. In 1907, Buckingham modified Darcy's law to describe flow through unsaturated soils, as follows:

$$J_w = -K(h)\frac{\partial H}{\partial z} = -K(h)\frac{\partial}{\partial z}(h+z) = -K(h)(\frac{\partial h}{\partial z}+1) \qquad (4)$$

where

J_w = water flux in vertical direction ($m\ s^{-1}$) and

$K(h)$ = unsaturated hydraulic conductivity as a function of matric potential ($m^2\ s^{-1} kPa^{-1}$).

Two important soil characteristics determine movement of soil water in unsaturated soils, namely the relationship between h and θ (soil water characteristic curves) and the relationship between soil hydraulic conductivity K and θ (unsaturated soil hydraulic conductivity function), which are referred to as soil hydraulic functions.

Mass conservation or continuity equation is used to describe changes in soil water content during a transient water movement. A statement of mass conservation accounts for movement of water in and out of a given soil volume at different rates, as well as plant uptake. For one-dimensional vertical flow process this can been represented as:

$$\frac{\partial J_w}{\partial z} + \frac{\partial \theta}{\partial t} + r_w = 0 \qquad (5)$$

where

r_w = rate of water uptake by plant per unit lean area ($m\ s^{-1}$) and

t = time (s).

If this equation is combined with the Buckingham-Darcy flux relation, an equation may be derived to predict water content or matric potential in during transient flow of water of a non-swelling soil:

$$\frac{\partial}{\partial z}[-K(h)\frac{\partial H}{\partial z}] + \frac{\partial \theta}{\partial t} + r_w = 0 \qquad (6)$$

It should be noted that unsaturated hydraulic conductivity is highly dependent on soil water content (or matric potential). Substituting equation (3) into equation (6) for the case of isotropic, one-dimensional flow, where no plant roots are present (r_w=0), yields:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}[K(h)\frac{\partial(h+z)}{\partial z}] \qquad (7)$$

or:

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}[K(h)(\frac{\partial h}{\partial z}+1)] \qquad (8)$$

These are two forms of Richards' equation that may be used to predict the water content or matric potential in soil during transient unsaturated soils water flow. However, having two unknowns (θ, h), they can only be solved using soil water characteristic curves or matric potential-water content functions $h(\theta)$ to eliminate either θ or h. In order to convert Richards' equation in terms of soil matric potential only, the concept of soil water capacity ($C(h)$) is introduced as:

$$C(h) = \frac{\partial\theta}{\partial h} \qquad (9)$$

Therefore equation (8) can be rewritten as:

$$\frac{\partial h}{\partial t} = \frac{1}{C(h)}\frac{\partial}{\partial z}[K(h)(\frac{\partial h}{\partial z}+1)] \qquad (10)$$

Equation (10) has the advantage of being applicable to the entire flow region, including saturated and partially saturated flow. Using h instead of θ as the dependent variable has the advantage of making the equation applicable in layered soils, where h remains continuous at the boundaries between layers (Feddes et al., 1988).

1.2 Methods of Solution

Water flow in field soils is simulated by application of water flux equations, assuming that soil hydraulic functions, i.e. soil water retention curve and hydraulic conductivity functions ($h(\theta)$ and $K(\theta)$) are constant within a layer but different among layers.

Description of water movement under field conditions could be highly complicated because the boundary and initial conditions are usually not constant throughout the profile, both spatially and temporally. Also spatial and temporal variability of soil properties (retention and hydraulic conductivity functions) must be considered. Heterogeneity of natural soil formations introduces problems in predicting large-scale flow and transport problems. Numerical techniques are possible for complex, compressible, nonhomogeneous and anisotropic flow regions having various initial and boundary configurations.

In the vertical direction, numerical models usually consider heterogeneity in the form of soil layers within a soil profile (Fig. 1.1). The soil layers are subdivided into soil compartments. Halfway within each soil compartment a node is defined, for which state variables are calculated using a finite difference technique. The soil profile is therefore divided into a number of compartments of some specified thickness and the total time period into discrete time increments (time steps). Fluxes through these divisions are calculated to estimate changes in the soil water content. Fluxes are considered to be constant during an individual time step. Thus the choice of an appropriate time step is critical. A compromise must be made between a large time interval, that would produce instability and a poor estimate of water movement, and a small time interval that would result in the practical problem of excessive computer time requirement. A variable time interval method of integration (Speckhart and Green, 1976) may be used as an alternative to a fixed time step.

In the following sections some of the potential problems associated with numerical modeling of soil water flow are discussed.

1.2.1 *Initial and boundary conditions*

When transient soil water flow is modeled, initial conditions (t=0) must be defined. If matric head or soil water content at each nodal point is not available, water contents at field capacity can be considered as the initial conditions. For the case that this value does not represent the initial water content of the soil, imposition of appropriate boundary conditions and redistribution of soil water would lead to the actual water content of the soil after a number of time steps.

The upper boundary condition of a physically based model is controlled by meteorological processes, i.e. rainfall and/or evaporation. Contrary to laboratory conditions where the time and rate of application are controlled, under field conditions a constant rate of rainfall is assumed for the recorded time period (day or hour), depending on the available weather data.

A variety of lower boundary conditions have been used in physically based models. The presence of an impermeable layer indicates no flux at the lower boundary. Free drainage is accomplished by setting this flux equal to the hydraulic conductivity of the lowest compartment. Constant (saturated) water content or matric potential indicates a water table. This condition permits both downward and upward flow at the basal boundary. Most models would provide all the above mentioned options.

1.2.2 *Soil hydraulic functions*

A solution from physically based models can be obtained if the soil water characteristic, $h(\theta)$, and the hydraulic conductivity functions, $K(\theta)$ or $K(h)$, of the soil are known. The unsaturated hydraulic conductivity is a nonlinear function of soil water content or matric potential. The problem in determining the unsaturated hydraulic conductivity is confounded by the expense of experimentally obtaining this relationship and the large number of observations required to adequately characterize its spatial distribution due to commonly occurring field-scale variability (Yates et al., 1992). The inability to characterize such a functional relationship will result in an inaccurate representation of the simulated flow process. Therefore many attempts have been made to estimate these functions from limited data. Childs and Collis-George (1950) predicted hydraulic conductivity of an unsaturated soil as a function of water content, using the ideal representation of a soil column by a model which consists of a bundle of capillary tubes of different sizes. The saturated condition, θ_s, is represented when all of the tubes are full. As soil water decreases from θ_s to ($\theta_s - \Delta\theta$), all tubes of radius $r > R_j$ drain when $h = h_j$ and no longer contribute to the flow. Therefore

$$K(\theta_s - i\Delta\theta) = \frac{\tau\sigma^2\Delta\theta}{2\nu\rho_w g}\sum_{u=w+1}^{m}\frac{1}{h_u^2} \qquad (11)$$

where

w= number of tubes not contributing to flow (unitless),

σ= surface tension ($erg\ m^{-2}$),

ν = coefficient of viscosity ($g\ m^{-1}s^{-1}$),

ρ_w = density of water ($Mg\ m^3$),

m = number of increments of θ (equal intervals from dryness to saturation) (unitless) and

g = gravitational acceleration ($m\ s^{-2}$).

The value of tortuosity, τ, in this equation must be evaluated by fitting the model to measured $K(\theta)$ data. For details on the derivation of the above equation refer to Jury et al. (1991). Scheidegger (1957) developed a model based on Poiseuille's law by integrating the flow over all pore sizes present in the soil. In other words contributions from each pore are summed to get the total flux. The result of this model is

$$K_s = \rho_w \phi R^2 / \nu\tau^2 \qquad (12)$$

where

ϕ = total porosity ($m^3 m^{-3}$),

R = mean hydraulic radius representative of the pore size distribution of the porous material (m).

Although these models produce satisfactory results for coarse soils, they are unreliable for well structured, fine textured soils (de Jong, 1984). Campbell (1974) represented the unsaturated hydraulic conductivity function as:

$$K = K_s(\frac{\theta}{\theta s})^m \qquad (13)$$

where

$m = 2b + 2$.

He suggested that a pore interaction term, equal to 1, be included in m which makes m=2b+3, where the value of b is found by plotting moisture release data on a *ln-ln* scale and fitting a straight line to the data (Campbell, 1985). The slope and intercept of the best-fit line are used to find b and h_e (air entry potential), respectively. Also equation (13) can be written as a function of matric potential:

$$K = K_s(\frac{h_e}{h})^n \quad (14)$$

where

$$n = 2 + \frac{3}{b}.$$

The main advantage of this method is that it can be used to obtain the unsaturated conductivity function directly using K_s and only two points in the moisture retention curve, e.g. saturation and field capacity, which are available in most cases. However, a valid estimate of K could not be expected near saturation (Campbell, 1974), because the water potential approaches the air entry or bubbling pressure value and the water content approaches saturation. Many of the simulation models, such as LEACHW for example, use Campbell's model to represent soil hydraulic functions.

Mualem (1976) developed an extended model for predicting the hydraulic conductivities of different soils. van Genuchten (1980) developed analytical function forms for $K(\theta), h(\theta)$ as follows:

$$\bar{\theta}(h) = [1 + \alpha(-h)^N]^{-M} \quad (15)$$

$$K(\theta) = K_s \bar{\theta}^{\frac{1}{2}}[1 - (1 - \bar{\theta}^{\frac{1}{M}})^M]^2 \quad (16)$$

where

$$\bar{\theta} = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (17)$$

$$M = 1 - \frac{1}{N} \quad (18)$$

N and α are fitted parameters, and θ_r is residual water content, referring to the region of $h(\theta)$ where absorptive forces are dominant and h is increasing rapidly with little change in θ (Jury et al., 1991). This model has been used extensively in numerical modeling.

Yates et al. (1992), by comparing a number of measured, predicted and estimated relative conductivities for a group of soils, analyzed the accuracy of three predictive methods and two simultaneous methods (which include known values of the conductivity). They used a nonlinear least-squares optimization program for the analysis and found that the water-retention curve can be predicted well with minimum data input. But in order to accurately predict hydraulic conductivity relationships, measurement of hydraulic conductivity at least at one soil water content is necessary. Because of natural spatial and temporal variability in soil properties, this requirement can be a limiting factor in large-scale field simulation studies. In addition, various methods for estimation of hydraulic conductivity of soils are often uncertain (Yates et al., 1992).

1.2.3 *Hysteresis*

Another complication in the numerical solution of water flow equations is hysteresis. This problem, along with time-dependency of initial and boundary conditions and nonuniformity in the medium, should be incorporated in the numerical model for complete representation of the physical system. Gilham et al. (1979) used empirical equations to represent the hysteretic $\theta(h)$ and $K(\theta)$ relations. They found a poor agreement between measured and predicted water content values during the wetting phase of the experiment. For the pressure head distribution, however, nonhysteretic simulation was as accurate as the hysteretic simulation. Therefore the authors concluded the adequacy of the predictive model largely depends on the intended use of the model. Kool and Parker (1987) developed and evaluated a closed-form expression for hysteretic soil hydraulic properties. Kool and van Genuchten (1991) adopted hysteresis in their model HYDRUS, which requires that boundary wetting and drying curves be described. Kool and Parker (1987) concluded that inclusion of hysteresis in numerical flow models provides significant improvement in prediction accuracy with "little additional effort and with minimal data requirements".

1.2.4 *Preferential flow*

Macropores are defined as pores that empty at less than 30 mm of water tension head, i.e. pores greater than 1 mm in diameter (Jabro et al. 1994). They are usually described as relatively large and continuous voids through which rapid flow can occur. In soils containing such pores, which would include many agricultural soils (Beven and Germann, 1982), water and agricultural chemicals can move preferentially, through macropores, bypassing much of the soil matrix. Preferential flow thereby contributes significantly to groundwater contamination. Jabro et al. (1994) conducted a field study to evaluate LEACHM to simulate bromide leaching under field conditions. They concluded that although LEACHM does not directly consider preferential flow, it performs well under these conditions if infiltration rate was used as model input for the site. Therefore they had to measure the infiltration rates using double ring infiltrometers. The measured infiltration rates are assumed to be equal to the saturated hydraulic conductivity at the soil surface (Jabro et al., 1994). Inclusion of infiltration rate as an input would actually be an indirect measure of the macropore flow process.

According to Li and Ghodrati (1994) the majority of field soils contain different types of macropores, with their abundance, distribution, and continuity being largely dependent on tillage practices. In a laboratory experiment, isolating root channels from other types of macropores, they conducted leaching experiments in soil columns containing root systems. A wide range of water fluxes were used to simulate unsaturated flow conditions. Large values of saturated hydraulic conductivity (K_{sm}) of the root channel columns (6-7 times greater than K_s of control columns) would indicate the presence of relatively continuous macropores. As a result of preferential flow in most root channel columns, a much earlier NO_3 breakthrough and a greater extent of dispersion was observed in the control columns. This was the case in fluxes as low as 0.042 K_{sm} to 0.358 K_{sm}. Their results indicated that the root channels formed in the column were almost equally effective in inducing preferential flow at the flux of 0.358 K_{sm} as with a flux of 0.042 K_{sm}.

In order to have a complete representation of an actual system, theoretically a model, among others, should consider all of the above factors. Studies of existing models, such as this study, would evaluate the importance of these factors.

1.3 This study

In the study presented in this thesis I consider flow of water in the unsaturated zone only. This zone is an integral part of the hydrological cycle. It plays an important role in various hydrological processes such as soil water storage, infiltration, evaporation, plant water uptake, groundwater recharge, runoff and soil erosion. Besides the traditional interest in the unsaturated zone as a source of water supply for maximum crop production, recent studies on this zone have been focused mainly on soil and groundwater pollution. The unsaturated zone plays an important role in many contamination problems because the contamination source often is located near or at the soil surface (Jensen and Montoglou, 1992).

It is well understood that soil characteristics often show a heterogeneous, anisotropic, spatial, and temporal distribution. Many methods with different degree of sophistication have been developed to describe various soil water processes. Difficulties in utilization of these models are mainly attributed to lack of data rather than to inadequate model formulation. The extra effort in obtaining more input data must be justified by the degree of accuracy required or gained in simulation results (Rasmussen and Fluher, 1990).

This dissertation consists of three main sections. In the first part, the accuracy of two soil water models namely LEACHW (Wagenet and Hutson, 1989) and *ecosys* (Grant, 1992) in predicting dynamics of water in unsaturated soils over time and space under field conditions is evaluated. The evaluations are specifically made during and after intense rain events (intense precipitation periods), and during periods dominated by evaporation with little precipitation (dry-down periods). The models are also tested for their ability to reproduce soil water dynamics during extended part of the growing season (long-term periods). When discrepancies exist between simulated results and collected field data, possible sources of error are discussed. In addition alternative methods, for prediction of soil water storage, with fewer data requirements are suggested.

Many soil water simulation models, such as LEACHW, use Campbell's model (1985) to represent the hydraulic functions. In the second part of this study, a sensitivity analysis is conducted on the importance of accurate estimation of the parameters used in soil hydraulic functions described by Campbell (1985) for simulation of unsaturated soil water dynamics. Such studies can be used as guidelines in justifying the extra effort in obtaining accurate estimation of soil hydraulic parameters as the prerequisite to simulation of various water flux attributes. In addition it is investigated whether simulation of volumetric water content values would constitute a proper evaluation of soil water flow models and if so, for what purpose would these validated models be reliable?

Simulation of soil water storage is necessary in many studies such as design of irrigation systems, prediction of runoff, etc. Results from previous studies have shown that simulation of soil water storage is not particularly sensitive to the accuracy of the parameters used in soil hydraulic functions (Zachmann et al., 1981). Therefore the effort in estimation of these parameters for the sake of simulation of changes in soil water content may not be justifiable. In the third part of this study, an alternate SIMPLE method for prediction water content in soils, based on the concept of water balance, is developed. The basic assumption in this model is that storage of water in soil is mainly controlled by the boundary conditions, i.e. precipitation, evapotranspiration and drainage fluxes. Precipitation and evaporation, as the main elements of water balance equation, are used to estimate the variation in soil water contents. Instead of a well defined soil profile with known physical characteristics, involving numerous parameters and a formulation for hysteresis, which is generally needed for most water flow models (Wagenet and Hutson, 1989, as an example), this model requires only basic soil information, i.e. field capacity and bulk density, in addition to precipitation and potential evaporation, to estimate soil water storage. This model could, therefore, provide satisfactory estimation of the soil water storage that is needed in many irrigation management and hydrological problems. In addition, the model is capable of estimating drainage fluxes which are of importance in environmental management studies.

Fig. 1.1. Concept of the vertical space scale (adopted from Vanclooster et al., 1994)

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Chapter Two

FIELD EVALUATION AND COMPARISON OF TWO SIMULATION MODELS FOR WATER DYNAMICS IN UNSATURATED SOILS

2.1 Introduction

Movement of water in the unsaturated zone is important in many aspects of hydrology, including infiltration, soil water storage, evaporation and runoff. Aside from the traditional attention to the unsaturated zone with respect to storage and supply of water to plants, recent studies on this zone are motivated by concern about soil and groundwater pollution from agricultural, industrial and municipal sources. The unsaturated zone plays an important role in many contamination problems because the contamination source often is located near or at the soil surface (Jensen and Montoglou, 1992).

The growing interest in simulation of water and solute movement in soils (Addiscott and Wagenet, 1985; Ammentorp et al., 1991; Govindaraju et al., 1992; Reddi and Danda, 1994; Clemente R.S. at al., 1994; Zhang and van Genuchten 1994; Noborio et al., 1996, Todini, 1996) is in response to the need for development of solutions for various agricultural and environmental management problems, such as designing irrigation and drainage systems, soil degradation and erosion, and controlling pollution of surface and ground water resources. Models are used to guide our future research efforts (Wagenet and Hutson, 1989), in the sense that models are developed to aid testing of hypotheses and the exposure of areas of incomplete understanding.

Major progress has been made in the conceptual understanding and mathematical description of flow and transport processes in the unsaturated zone. A variety of analytical and numerical models, mostly based on the Richards' equation, are now available that can be used to predict water movement in the unsaturated zone (Montogolou, 1992). A number of deterministic and stochastic models have been proposed to increase our quantitative understanding of heterogeneous field-scale flow processes (Jury and Roth, 1990). Deterministic models are based on the assumption that a system or process operates such that a given set of events leads to a uniquely definable outcome, whereas stochastic models presume that input information and simulation processes can only be estimated within statistical limits, and model predictions therefore have a statistical uncertainty (Addiscott and Wagenet, 1985).

In order to be able to adopt models for simulation of the effects of various soil management practices with confidence, it is important that the capabilities of these models and credibility of their results be tested. Of those that have been developed, many models have not been evaluated with independent data sets from different soil types or environmental conditions (Addiscott and Wagenet, 1985; Pennell et al., 1990). As van Keulen (1974) noted; if independent data are not used for evaluation of a model, the most that can be concluded is that "historical events under a given set of conditions may be described by the generated set of equations".

Penning de Vries (1977) indicated that evaluation is used for comparison of model output with real world data and for judgment of the practical utility of the models. One of the major problems associated with the proper evaluation of existing models is inadequacy and inaccuracy of the input data (Clemente et al., 1994). Model evaluation could provide answers to questions like how much additional effort should be invested in data collection or modeling in relation to perceived increase in accuracy of model predictions (Rasmussen and Fluher, 1990).

The quantity of required input data, depth of consideration of basic processes, is different among various models. Two mechanistic soil water models namely LEACHW, (Hutson and Wagenet, 1992), and *ecosys* (Grant, 1992) with different degrees of complexity and input data requirement are examined in this study. LEACHW is one of the five versions of LEACHM (Leaching Estimation And CHemistry Model) simulation model that describes the water regime in unsaturated soils. LEACHW is a process based model which is organized on a modular basis. Simple, less input data intensive formulations can be used in LEACHW subroutines that deal with calculation of different soil water processes such as evapotranspiration. On the other hand, *ecosys* uses complex, explanatory algorithms based on fundamental scientific principles (Grant, 1995), which requires more and frequent input data. The objectives of this study are to test the accuracy of these two water flow models in predicting soil water status under field conditions.

Specifically the accuracy of the above models in predicting the variation of water storage in the soil profile during and after intense precipitation events is tested against intense field data. In addition performance of these models during dry-down as well as long-term periods during the growing season is tested. Evaluation of specific events such as intense rainy periods could provide justifications for the extra effort in obtaining detailed input information required by the models.

2.2 Site and climatic conditions

2.2.1 *Site Description*

The experimental site is located at the Breton research station of the University of Alberta, 110 km south-west of Edmonton, near Breton, Alberta (53° 07′ N latitude, 114° 28′ W longitude, at an elevation of 850 m). Soils at this site have a 3% slope and they were formed on moderately fine-textured glacial till material. The soils are classified as Orthic Gray Luvisols and Gleyed Gray Luvisols under boreal forest vegetation and mapped as the Breton loam series (Lindsay et al., 1968).

Gray Luvisols, formerly called Gray wooded soils, have distinctive profiles. The names of these soils is taken from a gray colored surface layer of mineral material, which is leached and low in humus content. Because of a rather low organic matter content of most Gray Luvisols, tilth is usually poor (Bentley et al., 1971). Puddling of the surface layer due to showers or rains and subsequent drying may create severe crusting. Surface crusts could hamper entry of water of subsequent rains, which results in lower soil water storage or increased runoff on sloping fields (Bentley et al., 1971). In addition, dynamics of soil water is affected by the presence of the dense subsurface Bt horizon with enriched clay content. During infiltration, the rate of water entering into the soil is first controlled by the coarse layer on top, but when the wetting front reaches and penetrates into the finer-textured layer, the infiltration rate drops and is controlled by the finer sub-horizon (Hillel, 1982).

According to Canadian soil drainage classes, the soils at the experiment site are moderately well drained internally (Crown and Greenlee, 1978). The long-term mean precipitation received at Breton is 547 mm annually, with 89.8 mm, 94.5 mm and 84.4 mm for months of June, July and August, respectively (Juma et al., 1997) as the greatest rainfall months. Precipitation during 1994 and 1995, being at 119.8, 120.0 and 121.6 mm for June, July and August 1994 respectively, and 106.1 mm and 107.3 mm for July and August 1995, were above average.

The general topography at the site is classed as a "very gentle slope" with a slope range 2 to 5% (Canada soil survey committee, 1976). However, the plots for this study are located at a "hill-top" position from which land slopes away in all directions. Therefore the slope at the study plots is minimal. In addition, no signs of runoff were observed within the experimental plots enclosed by raised plot boundaries.

The presence of a dense B horizon in Luvisols generally impedes transmission of water (Juma et al., 1997). However, studies at the Breton plots have provided evidence of drainage fluxes at the site. Howitt (1981) observed a rise in groundwater during the wet growing season of 1980. The water table was observed to be within 4.2 m of the surface throughout that year (Howitt, 1981). Studying the dynamics of Luvisolic soils and clay migration through leachate collections at Breton, Howitt (1981) suggested a possibility of "flush" of colloidal material moving rapidly to lower horizons in response to heavy rainfalls. Izaurralde et al. (1995) observed evidence of nitrate leaching at the Breton plots to a depth of about 4 m. These studies provide signs of water movement to lower soil depths at the site and evidence that intense rainstorms, rather than gradual rainfalls, play an important role in the recharge of groundwater. However, monitoring such events and hence the evaluating of their simulations has not been conducted due to lack of detailed field observations.

Haderlein (1985) calculated evapotranspiration (ET) based on the water balance in a study that accounted for runoff, which was calculated based on the Erosion Productivity Impact Calculator (EPIC) computer model (Sharpley and Williams, 1990) and assumed the subsurface drainage to be negligible. Neither of his assumptions were validated in this study.

2.2.2 Data collection

The soil water measurements were made on "classical" Breton rotation plots, established in 1930. The Breton plots are set out in A-F series, running east to west; and ranges in 1-26 series running north to south. Details of soil map, plot layout and cropping systems are provided by Wani et al. (1994). The experimental plots, for this study, were located in the E-series with a "Two year Wheat-Fallow rotation." The examined plots of E-9 and E-11 were under fallow treatments during this study.

Various soil physical properties (Table 2.1) are available from previous studies (Agriculture Canada, 1989). Izaurralde et al., (1995) compared observed soil bulk densities at different layers with those from previous studies by Maule (1984), Miller (1984) and Agriculture Canada (1989). They found that values obtained within the first meter were in relatively good agreement with those previously published. Bulk density values below 1-m depth was found to have increased as compared to previous studies. However, LEACHW simulated values of soil water content at the top 20-cm of the soil profile, which is evaluated in this study, were similar for either of the two values of bulk density below 1.0-m depth. Hourly averaged climatological data, including net radiation, wind speed, air temperature, relative humidity and rainfall are also available from the weather station located at the site. Soil water content was measured every half hour during the growing season of 1995 at the soil surface, and at 10 and 20-cm depths using buried TDR probes, placed in duplicates in each plot. The probes were placed in a 2x3 grid (within each plot) with a 2-m distance between neighboring probes. To obtain measurements at specified depths probes were inserted horizontally into intact soils from a pit. After installation of the probes, pits were back filled with the original soil and packed. In every plot, an additional 20-cm probe was placed vertically at the surface to determine the average soil water content at top 20-cm of the soil profile. It was assumed that the upper 20-cm is the most active section of the soil profile. Hence this section was chosen for investigation of soil water dynamics. All probes were connected to a central station that was programmed to be activated automatically every half hour to take the measurements.

In addition, direct manual measurements of soil water content were taken during the growing season of 1993, by inserting the TDR probes (vertically) at soil surface. A variable number of measurements (between 10-30 per plot) were taken at weekly intervals. These measurements were used for the analysis of spatial and temporal variability of soil water content.

2.3 Simulation of water flow

2.3.1 *LEACHW*

In this study results from LEACHW simulation model are compared with the measured soil water data. LEACHW requires soil compartments to be defined in equal depth increments only. Complete description of the model is presented by Hutson and Wagenet (1992), however, some of the features of the model that directly pertain to this study are described and compared with *ecosys* in the following sections.

2.3.1.1 *Soil Hydraulic Functions*

Soil water retention and conductivity ($h(\theta)$, $K(h)$) relationships are non-hysteretic in LEACHW and are characterized by the empirical relationships of Campbell (1974). For $h < h_e$, Campbell's water retention equation is given by:

$$h = h_e\left(\frac{\theta}{\theta_s}\right)^{-b} \tag{1}$$

where

h = matric potential (kPa),

h_e = air entry potential (kPa) i.e. potential at which the largest water filled pores start to drain,

θ = volumetric water content ($m^3\ m^{-3}$), where subscript s denotes saturated value and

b = slope of $\ln h$ versus $\ln \theta$.

The slope and intercept of the best-fit line through the moisture release data, plotted on a ln-ln scale, are used to find b and h_e, respectively (Campbell, 1985). All pressure potential values are entered in units of kPa, however during execution of LEACHW they are converted to hydraulic head units (mm) to simplify the summation of pressure and gravitational potential. The exponential equation (1) has a sharp discontinuity near saturation. This equation was, therefore, replaced by a parabolic function at such high potentials, expressed in terms of b and h_e (Clapp and Hornberger, 1978), as follows:

$$h = \frac{h_e(1-\frac{\theta}{\theta_s})^{\frac{1}{2}}(\frac{\theta_c}{\theta_s})^{-b}}{(1-\frac{\theta_c}{\theta_s})^{\frac{1}{2}}} \qquad (2)$$

where subscript c denotes point of intersection of exponential and parabolic curves,

$$h_c = h_e(\frac{2b}{1+2b})^{-b} \qquad (3) \text{ and}$$

$$\theta_c = \frac{2b\theta_s}{1+2b} \qquad (4)$$

The composite water retention curve is sigmoidal, continuous and has a differential water capacity ($\frac{d\theta}{dh}$) of zero at saturation (Hutson and Wagenet, 1992).

LEACHW uses Campbell (1974) model to represent the hydraulic conductivity function as follows:

$$K(\theta) = K_s(\frac{\theta}{\theta_s})^{2b+3} \qquad (5)$$

where

$K(\theta)$ = hydraulic conductivity ($mm\ d^{-1}$) at θ water content and

K_s = hydraulic conductivity at saturation ($mm\ d^{-1}$)

Saturated hydraulic conductivities, which are required as matching factors in this relationship, were estimated from particle size distribution and bulk density using the Campbell model (1985) as follows:

$$K_s = 4\times10^{-3}(1.3/\rho_b)^{1.3b}\exp(-6.9m_c - 3.7m_s) \qquad (6)$$

where

ρ_b = bulk density ($Mg\ m^{-3}$),

m_c = clay mass fraction ($g\ g^{-1}$) and

m_s = silt mass fractions ($g\ g^{-1}$).

Using the above algorithm and the available physical properties of the soil (Table 2.1), the b, h_e and K_s values, which are required as input data to the model, were calculated for each layer (Table 2.2). The b value was calculated by using the soil water content at field capacity (-33 kPa) and at wilting point (-1500 kPa). This value was then used in equation (4) to calculate K_s.

Estimation of hydraulic conductivity of a soil from textural properties, as in Eq. (6), is based on the implicit assumption that soil matrix is randomly dispersed in space. Such assumptions are not valid for prediction of hydraulic conductivity of a soil which contains macropores. Therefore, it is appropriate that estimations to be examined against measured values at the site. Haderlein (1995) was able to establish a least square equation based on a number of actual measurements of Breton soil's hydraulic conductivity at different water contents. With respect to the extent of variability that Haderlein (1995) found among the measured values of hydraulic conductivity, and possible range of variability of about 5 orders of magnitude of hydraulic conductivity values (Hillel, 1982), the estimated K_s values from Campbell equation (Table 2.2) seemed reasonable.

2.3.1.2 *Initial and Boundary Conditions*

To simulate flow and redistribution of water, initial and boundary conditions of the profile have to be defined. Measured soil water contents at the beginning of each simulation period were used as the initial conditions.

Possible lower boundary conditions include a fixed water table depth, a free-draining profile, and a zero water flux. A free-draining lower boundary was used for this study. Surface runoff was assumed to be negligible based on the fact that the plots were enclosed with elevated borders.

LEACHW has an option of using a WEATHER program which uses maximum and minimum daily temperature and daily precipitation to calculate the upper boundary condition. Output from the WEATHER program includes daily values of start time, amount (mm) and rate of precipitation ($mm\ d^{-1}$), weekly total potential ET (mm), depth to water table (mm) (if the lower boundary condition permits), mean weekly temperature

(°C) and mean weekly amplitude (°C) of diurnal temperature cycle. Total rainfall during a day is combined into one event and is assumed to be uniformly distributed over a period starting at time 0.3 day and ending at 0.5 day, lasting for 1/5 of a day (Hutson and Wagenet, 1992). During this period, rainfall intensity is assumed constant. The total daily precipitation is, therefore, distributed uniformly over the period between 0.3 and 0.5 day. As long as the precipitation flux is less than the maximum infiltration rate at atmospheric pressure, defined as infiltration capacity of the soil (Horton, 1940), LEACHW assumes a constant flux is maintained. Otherwise the soil is assumed to be saturated and the remaining water infiltrates at a surface pressure potential of zero, i.e. infiltration rate is reduced to the infiltration capacity of the soil. No runoff is estimated by LEACHW.

The WEATHER program calculates weekly evaporation from free surface of water or pan evaporation (E_{pan}), using the Linacre method (1977). This method, which is an approximation to the physically based Penman formula, requires values for the elevation, latitude, and daily maximum and minimum temperatures. Using a pan factor, potential evapotranspiration is calculated from the pan evaporation. Potential transpiration is then calculated by multiplying the potential evapotranspiration by crop cover. The WEATHER program assumes a constant daily ET_p during the week. It also assumes that evapotranspiration occurs only from 0.3 day to 0.8 day and during this period potential ET_p flux density varies sinusoidally as:

$$ET_p = ET_{\max} \sin\left[2\pi(t - 0.3)\right] \quad (7)$$

where $ET_{\max}$ $(mm\ d^{-1})$ is potential evapotranspiration at $0.55t$ and t varies between 0.3 and 0.8 day (Hutson and Wagenet, 1992). The fraction of the water loss (f) during a time interval is, therefore, calculated by integration of (3) between the start and end of the time interval (Δt). This evaluation is on fallow plots, therefore no crop factors are involved. Potential evaporation (E_p), then, during Δt is calculated by multiplying the daily totals by the calculated fraction (f). The mean potential evaporation flux density during Δt is $\frac{E_p}{\Delta t}$. This is compared to the maximum possible flux density ($q_{\max}$ in $mm\ d^{-1}$), between node 1 (outside of the soil profile) and node 2 (the uppermost soil node), using the current matric potential and conductivity for node 2 and a specified air-dry potential for node 1. The actual evaporation (E_a) is decreased below (E_p) if necessary (Hutson and Wagenet, 1992), or:

$$E_a = Minimum\ (\frac{E_p}{\Delta t}, q_{max}) \qquad (8).$$

The lower boundary is set as free drainage having unit hydraulic potential gradient.

2.3.1.3 *Flux of water between soil compartments*

Richards' equation, for the transient, one dimensional unsaturated soil water movement is:

$$\frac{\partial h}{\partial t}(C(\theta)) = \frac{\partial}{\partial z}(K(\theta)\frac{\partial(h+z)}{\partial z}) \qquad (9)$$

where

h = matric head (kPa)

t = time (d)

C = soil water capacity or ($\frac{\partial \theta}{\partial h}$)

θ = soil water content ($m^3\ m^{-3}$)

$K(\theta)$ = unsaturated hydraulic conductivity ($mm\ d^{-1}$)

LEACHW is based on a node-centered Crank-Nicolson finite difference solution of Richards' equation that simulates transient vertical water flow in a heterogeneous soil profile. Vertical heterogeneity is represented by a number of uniform horizontal layers of equal thickness. The working numerical equation, then, is represented as (Nimah and Hanks, 1973):

$$(\frac{h_i^j - h_i^{j-1}}{\Delta t})C_i^{j-\frac{1}{2}} = \frac{1}{\Delta z_3}\left[\begin{array}{l}(\frac{h_{i-1}^{j-1} + h_{i-1}^j - h_i^{j-1} - h_i^j + 2\Delta z_1}{2\Delta z_1})K_{i-\frac{1}{2}}^{j-\frac{1}{2}} \\ -(\frac{h_i^{j-1} + h_i^j - h_{i+1}^{j-1} - h_{i+1}^j + 2\Delta z_2}{2\Delta z_2})K_{i+\frac{1}{2}}^{j-\frac{1}{2}}\end{array}\right] \qquad (10)$$

where the subscript i represents the depth of a node (halfway within each soil compartment) and subscript j represents time. Δz is the thickness of each compartment (m) and $\Delta z_1, \Delta z_2, \Delta z_3$ are variable depth increments and are defined by:

$$\Delta z_1 = z_i - z_{i-1}$$
$$\Delta z_2 = z_{i+1} - z_i$$
$$\Delta z_3 = (z_{i+1} - z_{i-1})$$

LEACHW assumes equal compartment depths, therefore $\Delta z_1 = \Delta z_2 = 0.5\Delta z_3$. $K_{i-\frac{1}{2}}^{j-\frac{1}{2}}$, for example, is the hydraulic conductivity for the flux between the two adjacent layers of i and i-1 for the time step j-1 to j. The value of $K_{i-\frac{1}{2}}^{j-\frac{1}{2}}$ is, therefore, calculated by an iterative process from the average water content of the two adjacent layers at start and end of time step, or:

$$K_{i-\frac{1}{2}}^{j-\frac{1}{2}} = \frac{K^{j-1}_{(\frac{\theta_i+\theta_{i-1}}{2})} + K^{j}_{(\frac{\theta_i+\theta_{i-1}}{2})}}{2} \tag{11}$$

An equation similar to (6) can be written for all nodes. Soil water pressure heads at the start of a time interval (h^{j-1}) are known, and the set of equations is then solved iteratively for the unknown pressure heads at the end of time period (h^j).

2.3.1.3.1 *The upper and lower boundary flux of water*

The surface pressure head, h_{i-1}, is computed to give the estimated water flux (evaporation or infiltration) according to the boundary conditions for the given time interval. $K_{i-\frac{1}{2}}^{j-\frac{1}{2}}$ is the hydraulic conductivity representing the soil layer between the surface and $z = z_1$. The surface pressure heads, h_{i-1}, can be changed to simulate ponded or non-ponded infiltration, evaporation or zero flux. During the ponded infiltration, the pressure heads of the upper node is set to zero (Hutson and Wagenet, 1992). During the non-ponded infiltration, an iterative procedure is used to obtain the correct value of h_{i-1}^{j} and

$K_{i-\frac{1}{2}}^{j-\frac{1}{2}}$ to satisfy the surface flux condition, provided the surface pressure is between limits (i.e., saturation or air dry). Between such limits the computed water flux at the surface will equal the potential flux. Constant infiltration rate is maintained providing that the infiltration capacity of the soil is greater than the specified infiltration rate. Infiltration of the specified depth of water is calculated as the water depth per application rate, or for ponded infiltration, the time to the start of the next infiltration event. Water which has not infiltrated at the end of the given time for infiltration is assigned as "excess water" in the mass balance calculation (Hutson and Wagenet, 1992). The actual precipitation for the hour is reduced by the amount of excess water to prevent inconsistencies in soil water balance. This is a limitation on the part of LEACHW algorithm.

The lower boundary condition is maintained by adjusting the potential of the bottom node in order to satisfy the specified boundary condition. In a freely draining profile, as in this study, the hydraulic potential gradient is maintained at unity (Hutson and Wagenet, 1992):

$$\left(\frac{h_{i-1}^{j-1} + h_{i-1}^{j} - h_i^{j-1} - h_i^{j} + 2\Delta z}{2\Delta z}\right) = 1 \qquad (12)$$

since h_{k-1}^{j} is calculated before a value for h_i^{j} is required and h_{i-1}^{j-1} and h_i^{j-1} are known according to the initial condition for each time interval, h_k^{j} may be calculated to satisfy the unit hydraulic potential gradient condition.

2.3.2 *Ecosys*

Ecosys (Grant, 1992) is a comprehensive model that simulates various processes taking place between the soil, plant and atmosphere. In this study, however, only the soil water movement is examined. *Ecosys* uses the forward or explicit finite difference method to solve Richards' equation. It requires a constant time step which is defined by the user. As in LEACHW, vertical heterogeneity is represented by a number of homogeneous horizontal layers, which can have different user-selected thickness in *ecosys*.

2.3.2.1 *Soil hydraulic Functions*

Campbell's soil water retention and hydraulic conductivity relationships can be used in *ecosys*. Saturated hydraulic conductivity values, if not known, are calculated from bulk density and texture using Campbell's model (eq. 2), as in LEACHW. Unsaturated hydraulic conductivity is calculated from saturated hydraulic conductivity and water retention characteristics according to Jackson (1972) based on the algorithm of Millington and Quirk (1960).

2.3.2.2 *Initial and Boundary Conditions*

The initial condition is based on the measured water content at the beginning of simulation period. Boundary conditions are assumed to remain constant for each hour. Surface fluxes are determined from hourly averaged meteorological variables.

Evaporation rate, E (LT^{-1}), is calculated from:

$$E = \frac{LE}{L} \qquad (13)$$

where LE is rate of latent heat transfer by water from soil to atmosphere as in van Bavel and Hillel (1976):

$$LE = \frac{(E_s - E_a)}{R_a} \qquad (14)$$

where

L = latent heat of vaporization ($MJ\ m^{-3}$),

E_s = vapor density at the soil surface ($kg\ m^{-3}$),

E_a = vapor density of air ($kg\ m^{-3}$) and

R_a = aerodynamic resistance ($s\ m^{-1}$).

Vapor density at the soil surface, E_s, is calculated from the temperature and water potential of the soil surface derived from a general solution for the surface energy balance. As in LEACHW, the lower boundary for *ecosys* is set as a freely draining profile for this study.

2.3.2.3 *Flux of water between soil compartments*

Flux between two adjoining compartments (i) and (i-1) is calculated based on Darcy's law as in:

$$q_L = \lambda_{ave}(h_{i-1} - h_i) \tag{15}$$

where λ_{ave} (in $m\ s^{-1} MPa^{-1}$) is hydraulic conductance calculated from the geometric mean of K_i and K_{i-1} as follows:

$$\lambda_{ave} = \frac{1}{\frac{\frac{\Delta z_1}{2}}{K_{i-1}} + \frac{\frac{\Delta z_2}{2}}{K_i}} = \frac{2K_{i-1}K_i}{\Delta z_1 K_i + \Delta z_2 K_{i-1}} \tag{16}$$

This value is then multiplied by the water potential difference between the two compartments. Infiltration is also calculated based on the above algorithm. As soon as the upper layer reaches the air entry potential, i.e. $h_{i-1} = h_e$, instead of a flux calculated at λ_{ave}, a saturated flux is assumed, or (15) and (16) are modified using the following values:

$$K_1 = K_{e_1}$$

$$K_2 = K_{e_2}$$

where K_e is hydraulic conductivity at air entry potential i.e. saturated flow. However, the value of h_2, matric potential of the lower layer (in eq. (15)), does not change and remains at its original value. Above changes are made to successive layers as the wetting front advances i.e. $h_1 > h_{e_1}$ (Grant et al., 1993). However, when $h_1 < h_{e_1}$, the actual values of K_1 and K_2 is used again i.e. unsaturated flow occurs. Conditional calculation of K_1 allows *ecosys* to simulate infiltration between adjacent layers at a higher conductivity if one element is close to saturation.

2.4 Model evaluation

Models for simulation of water and solute transport have been published and used extensively in the last three decades, but still statistical methods for evaluation of these models are limited and subject to debate (Jemison et al., 1994).

Model performance is often qualitatively evaluated by visual comparison of the simulated values produced by the model with actual values from field experiments. Such methods provide an immediate qualitative description of the differences and highlight trends of predicted and measured values. However, model evaluation should ideally incorporate both qualitative and quantitative appraisal. Both qualitative (graphical) and quantitative (statistical) methods are used in this study to compare the observed and predicted water contents over time and space.

The quantitative procedures for evaluation model predictions were adopted from Ambrose and Roesch (1982), in this study. The mean error between measured and simulated values (*ME*) is calculated as:

$$ME = \sum_{i=1}^{n} (\theta_{pi} - \theta_{mi}) / n \tag{17}$$

where n is the number of data points and θ_p and θ_m are the predicted and measured volumetric soil water content. *ME* gives an indication of the bias or consistent error in the model. If *ME* is positive, the model is overestimating the observed value, and vice versa. Ideally, no difference is expected between the predicted and measured values. Lower values of mean error, *ME*, show a satisfactory degree of coincidence between predicted and measured values.

The significance of the absolute mean error (*ME*) would be different depending on the average water content of the soil for the simulated period. Therefore, it would be valuable to represent *ME* as relative error (*RE*) which is defined as the difference or error between measurement and simulation as a proportion of the measurement (Clemente et al., 1994, Smith et al., 1996), as follows:

$$RE = \frac{ME}{\theta_{mean}} \tag{18}$$

where θ_{mean} is average measured water content over time.

Standard error of estimate, *SE*, the root mean square of the difference between the predicted and the observed values, is often proportioned against the mean observed value as relative standard error of estimate or root mean square error, *RSE* (Clemente et al., 1994; Smith et al., 1996), as follows:

$$SE = \left(\sum_{i=1}^{n} (\theta_{mi} - \theta_{pi})^2 / n\right)^{0.5} \tag{19}$$

$$RSE = \frac{SE}{\theta_{mean}} \tag{20}$$

These error terms are used to quantify the degree of systematic deviation of predicted in relation to observed values.

In addition, the statistical significance of the difference between the simulated and measured values, was compared with the variability among measured values using κ^2 (chi-square) for test of goodness of fit as follows:

$$\kappa^2 = \sum_{i=1}^{n} \frac{(\overline{\theta}_{mi} - \theta_{pi})^2}{\sigma_{\theta_m}^{\ 2}} \tag{21}$$

where

$\overline{\theta}_{mi}$ = average of replicated soil water measurements ($m^3\,m^{-3}$) at time i.

θ_{pi} = predicted soil water content ($m^3\,m^{-3}$) at time i.

σ_{θ_m} = standard deviation of $\overline{\theta}_{mi}$ ($m^3\,m^{-3}$).

2.5 Results and discussion

2.5.1. Discretization intensity

Soil water simulation models are generally based on Richards' equation, which describes flow of water in unsaturated soils. The differences, however, between various models could be due to different numerical schemes and variable intensity of discretizations (Haverkamp et al., 1977).

LEACHW (Wagenet and Hutson, 1989) uses an iterative implicit finite difference scheme for numerical simulation of Richards' equation. LEACHW requires the soil profile be divided into uniform size soil compartments. The size of time steps are automatically reduced during periods of high water flux density. A maximum time step length and the maximum allowable water flux during a time step is defined by the user. *Ecosys*, however, uses an explicit forward finite difference method. A constant, user-defined, time step is assigned as input for the entire simulation period. Different sizes of soil compartments can be assigned in *ecosys*.

Prior to evaluation of simulation models against field data, numerical accuracy of the models should be established. Numerical errors in models are affected by intensity of discretization. Theoretically, as the size of node spacing and time steps become smaller, the numerical solution would approach to the true solution of differential equation being simulated. With this respect, the analytical results of the infiltration study on Yolo light clay by Philip (1957) were used as a test for stability and convergence of the numerical schemes in the models. Because of the rapid changes in soil water content and the existence of sharp hydraulic gradient at the wetting front during a continuous ponded infiltration process, stability of the numerical schemes are rigorously tested during this process. However, soil water processes in the field, e.g. infiltration during rainfall, evaporation and redistribution produce much less rapid changes in soil water content and more gradual hydraulic gradients. Therefore, if a numerical scheme is stable and accurate for ponded infiltration process, one could expect that numerical error would not be a problem for the simulation of soil water dynamics in the field.

Theoretical calculation of infiltration into a vertical semi-infinite column of Yolo light clay with an initial volumetric water content of 0.238 m^3m^{-3}, when soil surface was maintained at saturation, was given by Philip (1957). This process with similar boundary conditions was simulated and compared by LEACHW and *ecosys* with separate runs having variable combinations of time steps and soil compartment sizes. The upper boundary condition for LEACHW and *ecosys* were represented with a continuous application of water at a rate higher than infiltration capacity, so that soil surface remained saturated. Excess water was assigned as runoff and was not accounted for by the models. By this scheme a saturated boundary condition was established for the simulations. The output was set to be produced at specific times which corresponded to the results given by Philip.

When the soil profile was divided with compartment size of 10 cm and greater, LEACHW predicted infiltration of water to be faster than what was described by Philip's theory (1957), with the wetting front having a sharp slope (Fig. 2.1). However, simulation of soil water movement, when the soil profile was divided into compartment sizes of 5 cm and lower, was closer to predictions by Philip's theory (Fig.2.2). As the size of soil compartments decreased, predictions of wetting front converged to a stable solution, to the point that no notable differences were observed between predictions with compartment sizes of 2.5 and 2 cm (Fig. 2.2). Prediction of soil water movement was also examined during an infiltration process at a lower rate of water application (5 mm/day), which is more likely to occur in field conditions. Under this condition, no major differences were observed when the soil profile was divided into compartments of 5 or 2 cm (Fig. 2.3). As a result, it was concluded that soil compartments of 5 cm would be a reasonable option for simulation of soil water at field condition. Using a combination of maximum time steps of 1-min. and 5-cm soil compartment LEACHW was able to satisfactorily simulate Philip's results (Fig. 2.4). The position and shape of LEACHW predicted water fronts closely corresponds with the results from the Philip study.

The above infiltration process was also simulated with *ecosys*. A predetermined time step can be assigned in *ecosys*. No difference was observed in the simulation results with either of 1-min or 30-sec time steps. A time step of 1 min was, then, used for all simulation runs by *ecosys*. Predicted water fronts using a 10-cm soil compartment were unstable with abruptly varying slope (Fig. 2.5). Under this condition water was predicted to infiltrate faster than Philip's predictions. *Ecosys* over-prediction of the position of water fronts was similar to the results obtained by LEACHW, but the shape of water fronts predicted by *ecosys* was more erratic and unstable. Predictions from using smaller sizes of soil compartments resulted in a more smooth water front with gradually changing slope, but the instability of wetting fronts persisted. As it was expected, with a decrease in sizes of soil compartments prediction results were converging to a stable position, to such degree that no notable differences were observed between the predictions using 2.5- or 2-cm soil compartments (Fig. 2.6). Infiltration was also simulated by *ecosys*, with a continuous water application at a lower rate of 5 mm/day, using different sizes of soil compartments (Fig. 2.7). A small difference was observed in the predicted results using 5- and 2-cm soil compartments, which indicates that selection of a 5-cm soil compartment for field studies, as it was done for LEACHW, is reasonable.

Using the 5-cm soil compartment Philip infiltration process was simulated by *ecosys*. The average position of the *ecosys* predicted wetting fronts corresponded with the predicted results by Philip. However, the shape of the wetting fronts were slightly unstable (Fig. 2.8), resulting in wetting fronts with abruptly varying slope. This problem appears to be related to mass balance and numerical oscillation. In addition, the general shape of the wetting fronts predicted by *ecosys* had a steep slope which predicts a more gradual change of water front than Phillip's results. This problem was not corrected when a smaller size of soil compartment was used. However, the instability problem, resulting in predictions of irregular wetting fronts reduced with a decrease in the size of soil compartments (Fig. 2.6). Such instability is not likely to happen in field conditions for which a smaller hydraulic gradient occurs during infiltration, evaporation and redistribution as compared to the continuous ponded infiltration as described by Philip's experiment.

As a result of above analysis, a uniform compartment size of 5 cm was selected, in all simulation runs by both models, in order to remove the differences attributed to discretization intensity. In addition, since maximum number of soil compartments are limited in LEACHW and *ecosys*, selection of soil compartments lower than 5 cm would result in a shallow depth of soil profile.

LEACHW requires soil compartments to be defined in equal depth increments only. The soil profile from the surface to the lower boundary was, therefore, divided into 5-cm increments in this study, for a total of 15 compartments. The output was set to be produced for the 0-5, 5-15, and 15-25 cm intervals to correspond with the depth of the actual measurements at the surface, 10- and 20-cm depths. In *ecosys* soil compartments can have different user-selected thicknesses. However to be consistent with representation of vertical heterogeneity in LEACHW, the soil profile was divided into 5-cm increments for *ecosys* simulations. In addition, *ecosys* requires a thin layer at the surface to represent the boundary condition, therefore the first 5-cm was divided into two compartments of 1- and 4-cm, respectively. In this study, a constant time-step of 1 min. was used for *ecosys* simulations. The output of the model at midpoint of the 2nd, average of 3rd and 4th layers and average of 5th and 6th layers would produce predicted soil water values corresponding to the observed values at surface, 10- and 20-cm depths, respectively.

2.5.2 Field evaluation of models

One of the major obstacles in evaluation of simulation models is lack of sufficient and detailed field data. The extensive, continuous and accurate soil water data collected in this study permits evaluation of models during periods of intense precipitation. Because these events contribute most to drainage and preferential movement of water, it is important for the models to be able to adequately simulate such events. In addition, performance of models during dry-down periods dominated by evaporation, as well as over long-term periods (2 month) during the growing season is examined.

Weather was generally rainy during the two months of July and August 1995, with rainfalls of as high as 30 mm during one day. Runoff was insignificant within the enclosed plots under investigation. In the WEATHER program embedded in LEACHW daily precipitation is accumulated and distributed uniformly over the period of 0.3 to 0.5 day. With this assumption, however, infiltration and water distribution during intense storms of short duration, would not be adequately represented. To eliminate this problem, using the actual hourly rainfall readings, the input data file was modified to account for each precipitation separately, using the actual precipitation readings. The recorded hourly precipitation, is assumed to have a uniform rate for the hour.

The following time periods were selected for evaluation of the performance of the models:

A. **Period of 1-6 July 1995**: There were two intense rainfalls during this period. It was chosen to test performance of the models in "intense precipitation events".

B. **Period of 20-27 August 1995**: For the most part no rain occurred during this period. It was chosen to test performance of the models in "Dry-down periods".

C. **Period of 1 July-31 August 1995**: This period was chosen to test performance of the models in "long-term periods".

2.5.2.1 *Variability among soil water content measurements*

During the 1993 growing season, a large number of soil water measurements at the top 20 cm of soil were made using TDR probes inserted vertically, to determine the extent of spatial variability of soil water content within individual plots. As an example, in Table 2.3, statistics of 25 readings within each of four separate plots on May 3rd are presented.

The water content values, for the 25 readings within a single plot, vary over an average range of 0.09 m^3m^{-3}, with an average standard deviation of 0.025 m^3m^{-3}.

Measurements of soil water content with the TDR technique are made with an accuracy of ±0.02 m^3m^{-3}, therefore the accuracy is sufficient for using the technique without having to carry out a calibration for each soil or field (Topp and Davis, 1985). The overall variation of field measurements result from both soil heterogeneity and instrument variation. In order to obtain mean soil water measurements within the ±0.02 m^3m^{-3} instrument accuracy with 95% confidence interval, standard deviation of mean measurements should be about 0.01 m^3m^{-3}. Such an accuracy could be obtained with average of 6 measurements ($\frac{0.025}{\sqrt{6}} \cong 0.01$). In this study field measurements are replicated between 2-4 times. For an average of 3 measurements, the standard deviation can be expected to be $\frac{0.025}{\sqrt{3}} = 0.014$, which is less than the limits of instrument accuracy. Such variations should be put in perspective in comparison of simulated and observed results, for example. Simulation of soil water status in many one dimensional soil water models is based on the assumption of a constant and uniform soil layering. Our observations show that neither of these assumptions are necessarily valid. Such assumptions may result in over- and/or under-prediction of soil water storage, which is directly translated into under- and/or over-prediction of drainage. For example in Fig. 2.9, four sets of soil water measurements at a 10-cm depth within two adjacent fallow plots (E-9 and E-11) for the period of July 1-6, 1995 are presented. This period is selected because of the extent of highly intense rainfalls. An average difference of 0.04 to 0.05 m^3m^{-3} is found between the water content measurements at two points 2-m apart within a plot. This difference is almost identically repeated in both plots. It is interesting to note that in response to the 14.3-mm rain on July 1, volumetric soil water content at one point (triangle symbols) increased from about 18% to about 30% (or 12% absolute) in a few hours. Whereas, for the same event, water content at an adjacent position (asterisk symbols) increased from about 0.027 to 0.033 m^3m^{-3}. If the measurements by each probe represents the average water content of a 10-cm thickness, a difference of 0.06 m^3m^{-3} (0.012-0.06) in storage can only be accounted as 6 mm of excess drainage from the layer in response to 14.3-mm rainfall, i.e. if there is a 0.06 m^3m^{-3} less storage there should be 6 mm more drainage from the 10 cm layer. Evaporation for this short period immediately after the intense precipitation was assumed to be negligible. Runoff was insignificant within the plots. This calculation shows the significance of heterogeneity of soils and precautions that must be taken in the interpretation of limited data. This problem is confounded by the expenses involved in collecting more measurements. An adequate number of measurements depends on the purpose. To establish a representative average of field soil water content, as described above, 3 measurements would produce an standard deviation of 0.014 m^3m^{-3}. However, if similar number of measurements are used to estimate drainage fluxes from soil water changes, an unacceptable results may be produced. The observed difference in our measurements (0.04-0.05) is still within the 95% confidence interval of measurements. But, when same measurements are applied for estimation of recharge of lower soil layer as a result of 14-mm rain, as described above, the error can be unacceptably high.

In most studies such detailed information is not available. As a result models are usually evaluated based solely on the prediction of soil water content. Such evaluations, however, do not validate simulation of drainage flux, which is the main focus of most environmental studies.

2.5.2.2 *Evaluation of models*

The average of replicated soil water measurements are compared with the predicted values for the three selected periods. In our experiment, water content measurements were made at 0.5-hour intervals, whereas LEACHW produces predicted values at 0.1 day, for its most frequent output interval. Therefore, measured values were directly selected or interpolated to the 0.1-day intervals for comparison purposes. *Ecosys* produces hourly predicted values. Therefore, every other measurement was used for comparison with *ecosys* predicted values.

2.5.2.2.1 *Qualitative comparison*

Variability among replicated measurements are represented by an envelop of ± one standard deviation of mean measured values. Both models predicted greater fluctuations in soil water contents than observed values.

Water contents simulated by LEACHW (Figs. 2.10 to 2.12) and *ecosys* (Figs. 2.13 to 2.15) were compared with observed values for the selected period of 1-6 July 1995, during which two intense rainfalls occurred. At the soil surface, where maximum fluctuation in soil water occurs, following the initial rain, both models predicted an immediate increase in water content in response to the rainfall on 1st of July, but according to measured data a lower increase took place several hours later (Figs. 2.10 and 2.13). This observation could be related to the presence of surface crusts which prevented the water from entering the soil, or to the cracks which flushed the water through the macropores with no interaction with the soil matrix. Inspection of individual TDR probes responses at the 10-cm depth (Fig. 2.9) indicates that 3 out of 4 probes immediately responded to the initial rainfall, which supports either of the above assumptions, depending on the location of the probes. It should be noted that the probes at different depths were not stacked above one another, therefore responses of surface probes could not directly be related to 10-cm probes. Both models, therefore, predicted a higher soil water (Figs. 2.11 and 2.14). Such a discrepancy between simulated and observed results would amount to a difference in drainage flux to lower depths, as a result of a single intense precipitation event.

At the 10-cm depth, both models generally over predicted the measured values (Figs. 2.11 and 2.14). LEACHW and *ecosys* were both capable of simulating the transient water content at 20-cm depth (Figs. 2.12 and 2.15). Contrary to the trend for upper layers, water content at this depth remained essentially constant.

In Figs. 2.16-2.18 and also in Figs. 2.19-2.21 LEACHW and *ecosys* predicted values, are compared with measured water contents for the period of 20-27 August 1995, during which, for the most part, no rainfall occurred. Soil water content for this period was simulated with a separate initial condition based on observed values. This period was selected to test predictive capability of the models in a soil water depletion period. Predicted surface soil water contents by LEACHW (Fig. 2.16) and *ecosys* (Fig. 2.19) exhibit distinct diurnal cycles which were not evident for the measured values. Both models reproduced surface water increase in response to rainfalls on 20th August. LEACHW reproduced fast drying immediately after rain but afterward predicted much more rapid drying than observed results. *Ecosys* did not reproduce the initial rapid drying. Instead it predicted a more gradual constant rate drying over the entire period. Both models predicted that evaporation losses decreased the soil water content through 20-cm depth, whereas measurements showed that soil water content was essentially not affected at the 20-cm depth.

In addition, LEACHW and *ecosys* predicted water loss of about $0.17 m^3 m^{-3}$ (0.40-0.23) from the surface layer for the 7-day period following the rain (Figs. 2.16 and 2.19). These predictions were higher than the actual water loss from the same layer, based on the observed values. Predicted water losses from the lower layers for both models were also higher than the observed results.

The algorithm used in *ecosys* for simulation of evaporation more closely represents the dynamic condition of the drying processes at soil surface than that adopted by LEACHW. *Ecosys* calculates the rate of evaporation separately for each hourly time step, which reflects changing surface properties and atmospheric stability. In contrast, a weekly value of potential evaporation, E_p, is used in LEACHW with the assumption that it is evenly proportioned for the seven days. Therefore, the LEACHW approach is less data intensive and hence more feasible in most cases.

Comparison of the predicted values for the long-term period (Figs. 2.21-2.24 for LEACHW, and Figs. 2.25-2.27 for *ecosys*) indicates that both models performed similarly. *Ecosys* was able to reproduce the observed values at the surface more accurately, whereas the LEACHW predicted values were more erratic. LEACHW predicted soil water content is consistently lower than observed values during drying periods. The high soil water contents after rainfalls are simulated satisfactorily. However, because of faster drying predictions, as discussed above, simulated soil water contents during drying period were much lower than the measured values. As a result significant fluctuation in predicted soil water content was produced. The difference is expected to be statistically significant.

At the 10-cm depth LEACHW was able to closely predict the observations, best match among all soil depths. Agreement between model and observation results at 20-cm, although poor compared to that at 10-cm depth, was better than results at the surface and was generally within the bounds of variability of observed values.

Ecosys simulated results at the soil surface were similar to those from LEACHW simulations, although with fewer fluctuations. At the 10-cm depth, *ecosys* reasonably predicted the observed results. At the 20-cm depth *ecosys'* predictions were poorer than with LEACHW and they were lower than observed results, especially during periods of drying.

Measured soil water contents at 20 cm was higher than those at 10 cm during drying periods and were approximately equal when the soil was wet. This is intuitively correct, because when the soil is recharged, profile water contents become uniform with depth, approximately at field capacity. During drying, water is lost at the surface and is subsequently supplied from the lower layers. The predicted values by *ecosys* produced opposite results, i.e. predicted water content at the 10-cm depth was always higher than those at 20 cm.

2.5.2.2.2 ***Quantitative comparison***

Most water drainage is produced during and after precipitation events. Hence, capability of simulation models in reproducing the observed water content values during and after such dynamic events is essential. Generally previous model evaluations are based on weekly or at most daily measurements of soil water content (Clemente et al., 1994, for example). It is obvious that much water movement could take place between such observations.

Because of natural heterogeneity of soil, replicate measurements at the same depths within a plot were not identical. Therefore the average of the observed values was used for the quantitative comparison of the models.

Mean errors between observed and predicted values (*ME*) for the period July 1-6, 1995 (Table 2.4) indicate that both models were slightly over-estimating the observed values. Agreement between *ME* and *SE* values is an indication that the over-prediction was systematic. In addition, standard error of estimates (*SE*) and standard error of measurements (*SM*) (Table 2.4) were comparable, indicating that predicted results by both models were within the range of measurement variability. Chi-square (κ^2) values (Table 2.4) for a randomly selected sub-sample from the population of measurements were calculated. Based on this test, performance of both models during the wet period of 1-6 July 1995 were identical. Simulated result at soil surface were found to be significantly different (at 95% probability, designated by ♣ symbol in the Tables 2.5-2.7) from the measured values as compared with the variability among measured values. At the 10- and 20-cm depths, simulated and measured values were similar.

For the dry-down period, mean error and relative error values (*ME* and *SE*) indicate that LEACHW systematically under-estimated the averaged observed values (Table 2.5). However, values of standard error of estimate range only between 2-5%, which is more reasonable than the standard error of the observed values (*SE*) for the three layers. According to the chi-square tests only, simulations by both models were not different than the measurements for other soil depths. Qualitative rather than statistical evaluations of the results, as above, are more descriptive of the performance of models in this case.

Selected daily measurements were used for comparison with predicted values for the period of 1 July to 31 August 1995. The simulated results for the surface layer, by both models (Tables 2.7), indicate an under-estimation of measurements, which is attributed to underestimation of measured results during drying periods, as described above. At soil surface the difference between the simulated and measured results were significantly different than the standard deviation of the replicated measured results (as expressed by the chi-square value). At 10- and 20-cm depths LEACHW predicted results were in close agreement with observations. *Ecosys* reasonably estimated the observed results at 10-cm depth and the differences between the simulated and measured results were not significantly different as they were compared with the standard deviation of the replicated measured results (expressed by the chi-square value). *Ecosys* slightly under-estimated the measured results at the 20-cm depth. Detailed analysis of selected periods, as was presented above, is generally more descriptive of simulation models' performance.

2.5.2.3 Analysis of prediction of water balance

2.5.2.3.1. Infiltration

In Table 2.7 various components of the soil water balance for the top 20 cm, predicted by the two models are presented. In addition, Fig. 2.28 shows cumulative predictions of evaporation and net drainage fluxes. General inspection of these results indicates that performance of both models for the two months of July and August 1995 was very similar. Evaluation of each model during shorter periods would highlight their capabilities on specific processes.

For the intense precipitation period of 1-6 July, 1995 evaporation loss predicted by both models are similar. However, LEACHW predicted a lower drainage flux compared to *ecosys*. A detailed description of the algorithm used by the two models for prediction of water flux at the surface, i.e. infiltration, and in the soil is presented previously. The main difference between the two models is that in *ecosys*, as soon as the water potential of the upper layer exceeds the air entry potential, the hydraulic conductivity value for the lower layer is calculated at the water potential of the upper layer, keeping the water potential gradient at the original value. This modification allows the model to simulate infiltration between adjacent layers under higher hydraulic conductivity, if one layer is close to saturation (Grant et al., 1995). Therefore a higher water flux between layers is produced, especially for cases where a steep hydraulic gradient exists between the layers, e.g. infiltration of water into an initially dry soil. In LEACHW, however, such an alteration is not made, and the value of hydraulic conductivity for the flux of water between the two adjacent layers is calculated based on the average value of their water contents.

The difference between the two algorithms adopted by LEACHW and *ecosys* is further examined in the following example.

To calculate the flux between two points at the soil surface, 5 cm vertically apart, for the case when the point in the upper layer is saturated and the lower layer is at pressure a potential equal to -500 cm.

$$K_s = 12.3\ cm\ d^{-1}$$

$$\theta_{sat} = 0.49$$

$$\theta_{(h=-500cm)} = 0.22$$

1. LEACHW:

$$K_{ave} = K_{(\frac{0.49+0.22}{2})} = K_{(0.358)} = 0.40 \ cm \ d^{-1}$$

$$J_w = 0.40 \times (\frac{0-500}{5}) = -40 \ cm \ d^{-1}$$

2. *ecosys*

$$K_{sat} = 12.3 \ cm \ d^{-1}$$

$$J_w = 12.3 \times (\frac{0-500}{5}) = -1230 \ cm \ d^{-1}$$

It is, therefore, clear that *ecosys* would produce more infiltration at the surface, or larger flux between adjacent layers with the advancement of the wetting front. This assumption seems reasonable because *ecosys* predictions for water status at the surface layer (Fig. 2.25) are smoother compared with the LEACHW predicted results (Fig. 2.22), which are more erratic. Although short-term differences in simulated infiltration fluxes are observed between the two models, they are offset by their differences in evaporation simulation. Therefore, the net seasonal results are similar for the two models (Table 2.7).

2.5.2.3.2 Evaporation losses

Predicted evaporation losses for the period of 1-6 July are similar for the two models (Table 2.7). During this period, soil surface was generally wet, therefore evaporation was at the potential rate. However, for the drying period of 20-27 August, LEACHW prediction of evaporation was higher than by *ecosys*. In LEACHW weekly potential evaporation losses are divided into uniform daily rates. The daily rates are, then, assumed to be distributed sinusoidally for a period of 12 hours (0.3-0.8 day). The mean potential evaporation rate during every time step is limited by the maximum possible flux density, calculated from soil surface water status (Hutson and Wagenet, 1989). In contrast, the evaporation algorithm used in *ecosys* closely reflects continuous changes of climatological variables, i.e. net solar radiation rate, air humidity, temperature etc. The latter approach better represents the actual process. Comparison of soil water status during the period of 20-27 August (Figs. 2.16-2.21) also shows that *ecosys* predictions are closer to measured results than are LEACHW predictions. No measured evaporation losses are available in this study. However, measured water contents during the period of 20-27 August, or the "dry-down" period indicate that the rate and degree of water loss from the three layers is lower than that predicted by both models.

Overall, cumulative evaporation predictions for the two month period of July and August (Fig 2.28) by both models are very similar, which indicates that the less data intensive approach adopted by LEACHW would produce similar results as *ecosys* in long-term periods, therefore is more feasible.

2.5.2.3.3 Drainage fluxes

Based on the water balance, and with the assumption that runoff was negligible in this study, the following points are discussed.

During the wet period of 1-6 July, 1995, a higher drainage flux, from the top 25 cm of soil is predicted by *ecosys* than LEACHW (Table 2.7). The main reason for the difference is attributed to the difference in formulation of inter-layer water fluxes between the two models, which results in a higher predicted rate of water flux by *ecosys* during the advancement of wetting front. A lower water storage is, thus, predicted by *ecosys*.

No notable differences in the predicted drainage fluxes were observed during the period of 20-27 August, 1995, as it was mostly a dry period and evaporation was the dominant process.

For the long-term period, the net drainage fluxes predicted by the two models were similar. These predictions include water flux through the lower boundary, both in upward and downward directions. This observation is clear from the net flux results depicted in Fig. 2.28. Following the rainy periods of early July which resulted in production of significant amount of drainage, cumulative drainage flux is shown to deplete, which is an indication of some capillary flux from the lower boundary. For example, during rain periods *ecosys* could allow more water to drain, while during the drying period it allows more water to move up to the surface layer, which leads to similar total net flux for a long term period as compared with LEACHW. This assumption is based on the algorithm used to calculate the average hydraulic conductivity. However, because only net drainage fluxes are calculated, the difference between the two models is not detected here.

2.6 Summary and Conclusions

In this study, predicted water contents by LEACHW and *ecosys* are compared against observed results. By providing information on the spatial variability of natural soils, it was shown that simulation of soil water, which is commonly based on the simplifying assumptions of steady and uniform soil layering on both models, is not necessarily valid. These simplifications could result in over- and/or under-estimation of drainage fluxes. The common approach, in many studies, for evaluation of water flow models, which is based on weekly or even daily water content values, are not sufficient to highlight such observations.

Prior to the evaluation of models, the importance of discretization intensity for proper representation of soil profile and time-steps was examined. For this reason, performance of these models, with variable sizes of depth increments and time-steps, for prediction of Philip's infiltration experiment (1957) was studied. As a result, 5-cm depth increments were found to adequately simulate Philip's results. LEACHW requires the soil profile to be divided into uniform depth increments. In order to remove discrepancies resulted from variable discretization intensity, a common 5-cm depth interval was used for both models.

Three time periods were selected for the evaluation of the models representing intense precipitation, dry-down and long-term periods. A detailed examination of soil water status, during and after intense precipitation events showed an under-estimation of drainage fluxes by LEACHW. Such events contribute most in the production of drainage fluxes. Differences in algorithm adopted by the two models are presented and discussed. *Ecosys*' algorithm resulted in more dynamic water fluxes between layers, which has resulted in better predicted results than LEACHW, especially at soil surface.

Both models use the Campbell's method for prediction of saturated hydraulic conductivity (K_s) and soil hydraulic functions, namely moisture retention curve ($h(\theta)$) and hydraulic conductivity functions ($K(\theta)$). These functions that are related to soil texture are derived based the assumption that soil matrix is randomly dispersed in space (Campbell, 1985). Due to the natural heterogeneity of field soils and presence of cracks and/or root channels such assumptions are often not valid. Therefore, prediction of K_s, as a matching factor in the $K(\theta)$ function, cannot be correct. Such problems are expected to be more evident in the simulation of selected periods such as a dominantly wetting period. Such predictions can be improved if measured K_s was used instead (Grant, 1995). Adequate representation of highly variable K_s value can be a limiting factor in fulfilling such requirement. In the meantime, estimation of hydraulic functions based on empirical relationships remains to be the most viable alternative. Importance of accurate representation of hydraulic functions in simulation models is further examined in the following chapter.

Discussion of different approaches adopted by the two models for calculation of evaporation process, in addition to the predictions of the two models during the dry-down period, were used to evaluate the capabilities of these models for simulating the evaporation processes. The predicted water status during this period indicates that both models were predicting that the soil profile would dry at a higher rate than observed results. However, predictions by *ecosys* were found to be closer to measurements for this period. Cumulative predictions of evaporation losses for the long-term period of 1 July - 31 August, 1995, were very similar. For general purposes, therefore the lower intensive input data approach adopted by LEACHW for calculation of evaporation was found to be more feasible than *ecosys*.

Overall, performance of the two models were found to be reasonable for prediction of soil water. This evaluation, however, cannot readily be extended as assessment of the performance of models for prediction of drainage flux.

Table 2.1. Soil properties of the Breton loam series (Agriculture Canada, 1989)

	Depth increments (cm)					
	0-15	15-30	30-76	76-112	112-150	150-170
Bulk Density($Mg\ m^{-3}$)	1.35	1.40	1.50	1.50	1.50	1.50
$^{*}\theta_{FC}$ (at 33 kPa) ($m^3 m^{-3}$)	0.251	0.286	0.317	0.296	0.268	0.272
$^{\dagger}\theta_{WP}$ (at 1500 Kpa) ($m^3 m^{-3}$)	0.095	0.158	0.208	0.19	0.154	0.159
Silt ($g\ g^{-1}$)	0.62	0.37	0.35	0.36	0.38	0.40
Clay ($g\ g^{-1}$)	0.12	0.29	0.33	0.33	0.27	0.28
Organic C ($g\ g^{-1}$)	0.027	0.006	0.01	0.006	0.004	0.003

* Water content at field capacity

† Water content at wilting point

Table 2.2. Calculated hydraulic parameters of soil layers using Campbell equations

	Depth increments (cm)					
	0-15	15-30	30-76	76-112	112-150	150-170
b	3.93	6.43	9.06	8.61	6.89	7.11
$h_e\,(kPa)$	-2.37	-1.32	-1.92	-1.22	-1.19	-1.19
$K_s\,(mm\ d^{-1})$	123	62.7	17.7	18.5	35.8	29.8

Table 2.3. Statistics on top 20-cm soil water measurements ($m^3/100\,m^3$) on May 3rd, 1993, for four adjacent plots.

‡Plot	E-1	E-3	F-1	F-3
Mean	26.3	22.0	24.2	24.6
Standard Deviation	2.4	2.6	2.2	2.5
Range	10.2	9.0	8.1	9.2
Number	25	25	25	25
Largest	28.7	26.2	28.5	28.6
Smallest	18.5	17.2	20.4	19.4

‡ Plot designations are based on different tillage and fertilizer treatments. For details refer to Wani et al. (1994).

Table 2.4. Statistics on top 20-cm soil water measurements ($m^3/100\,m^3$) on July 30^{th}, 1993, for four adjacent plots.

Plot	E-1	E-3	F-1	F-3
Mean	29.9	31.4	31.3	32.6
Standard Deviation	1.4	1.3	0.9	1.0
Range	4.5	4.3	3.0	3.0
Number	9	9	9	9
Largest	31.9	33.2	32.2	33.7
Smallest	27.4	28.9	29.2	30.7

Table 2.5. Statistical analysis of simulated soil water contents by ecosys and LEACHW against measured data ($m^3 m^{-3}$), at soil surface, 10- and 20-cm depths, for period of July 1-6 1995 (Intense precipitation events).

	LEACHW			ecosys		
Depth	Surface	10-cm	20-cm	Surface	10-cm	20-cm
§ME	0.02	0.02	0.00	0.02	0.02	-0.01
⁎⁎RE	0.07	0.07	0.00	0.08	0.07	-0.03
††SE	0.04	0.03	0.01	0.04	0.03	0.02
‡‡RSE	0.11	0.09	0.05	0.12	0.08	0.06
§§SM	0.02	0.03	0.04	0.02	0.03	0.04
⁎⁎⁎ κ^2	♣ 148	10	1	♣123	9	0

§ mean error of estimate

⁎⁎ Relative error of estimate

†† Standard error of estimate

‡‡ Relative standard error of estimate

§§ standard error for the replicated measurements

⁎⁎⁎ chi-square

♣ significantly different at 95% probability level

Table 2.6. Statistical analysis of simulated soil water content by ecosys and LEACHW against measured data (m^3m^{-3}), at the soil surface, 10- and 20-cm depths, for period of August 20-27 1995 (dry-down period).

	LEACHW			*ecosys*		
Depth	Surface	10-cm	20-cm	Surface	10-cm	20-cm
ME	-0.04	-0.00	-0.02	0.00	0.00	-0.01
RE	-0.13	-0.00	-0.05	0.00	0.00	0.03
SE	0.05	0.02	0.03	0.02	0.02	0.02
RSE	0.15	0.06	0.07	0.07	0.07	0.06
SM	0.04	0.03	0.06	0.04	0.04	0.04
κ^2	15	4	2	2	4	3

Table 2.6. Statistical analysis of simulated soil water content by ecosys and LEACHW against measured data ($m^3 m^{-3}$) at soil surface, 10 and 20-cm depths, for the months of July and August 1995 (long-term periods).

	LEACHW			ecosys		
Depth	Surface	10-cm	20-cm	Surface	10-cm	20-cm
ME	-0.03	0.00	0.00	-0.03	0.00	-0.02
RE	-0.09	0.02	0.00	-0.10	-0.02	-0.06
SE	0.05	0.03	0.02	0.05	0.03	0.05
RSE	0.17	0.10	0.06	0.15	0.11	0.15
SM	0.03	0.04	0.06	0.03	0.04	0.06
κ^2	♣138	12	1	♣73	23	3

Table 2.7. Comparison of various components of soil water balance predicted by LEACHW and ecosys for the three selected periods.

	LEACHW			ecosys	
Period	†††Cum Rain (mm)	‡‡‡CEVAP (mm)	§§§Net Flux (mm)	CEVAP (mm)	Net Flux (mm)
1-6 July	54.2	21.6	17.1	22.0	21.7
20-27 Aug	18.0	28.4	5.3	22.0	7.2
1July-31Aug	234.0	196.6	40.4	200.6	44.9

††† Cumulative rainfall

‡‡‡ Cumulative evaporation

§§§ Net flux from the lower boundary (at 25-cm depth)

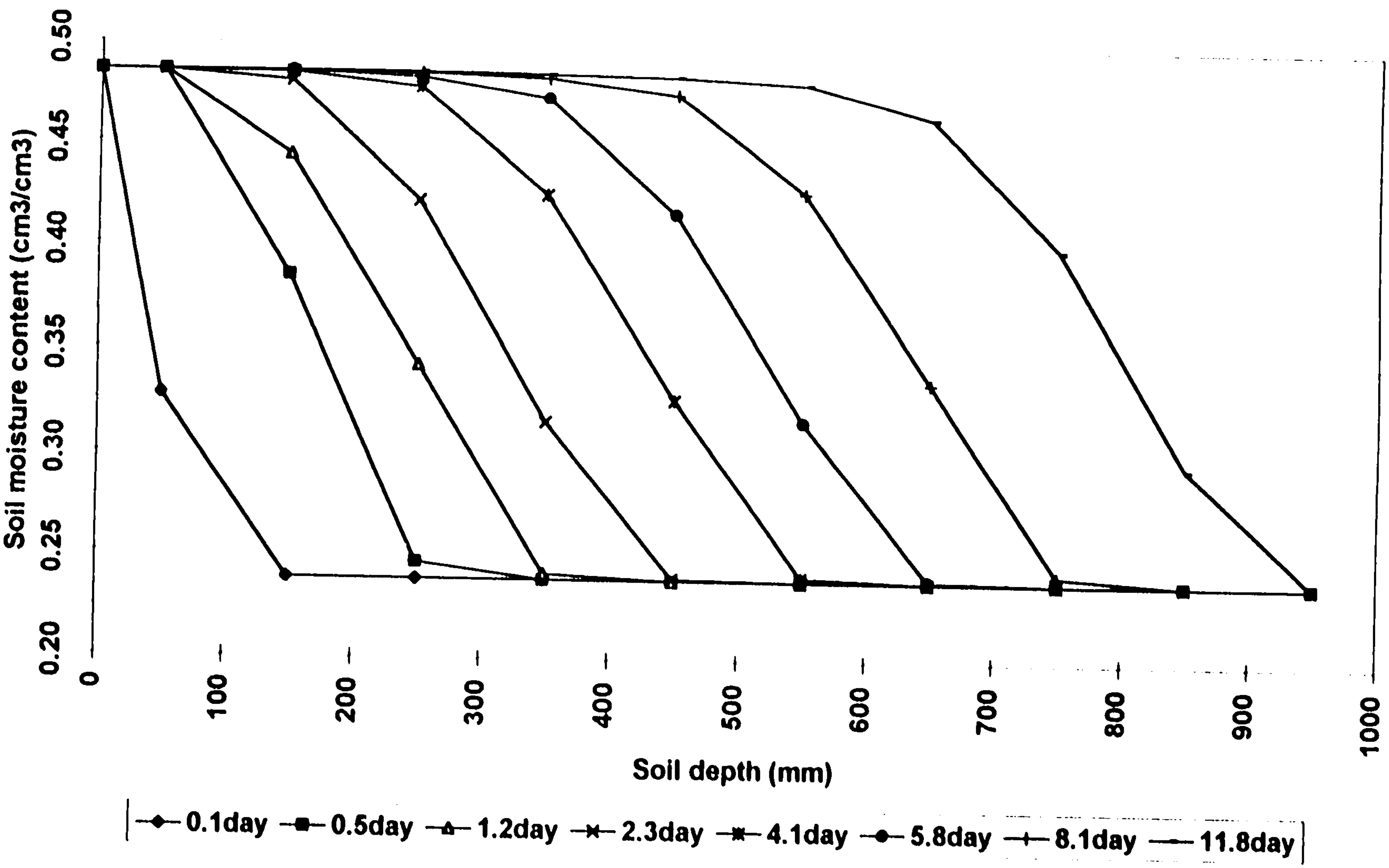

Fig. 2.1 LEACHW prediction of soil water profile during a continuous water infiltration into Yolo light clay (with 10-cm soil depth increments and time steps of 1 min).

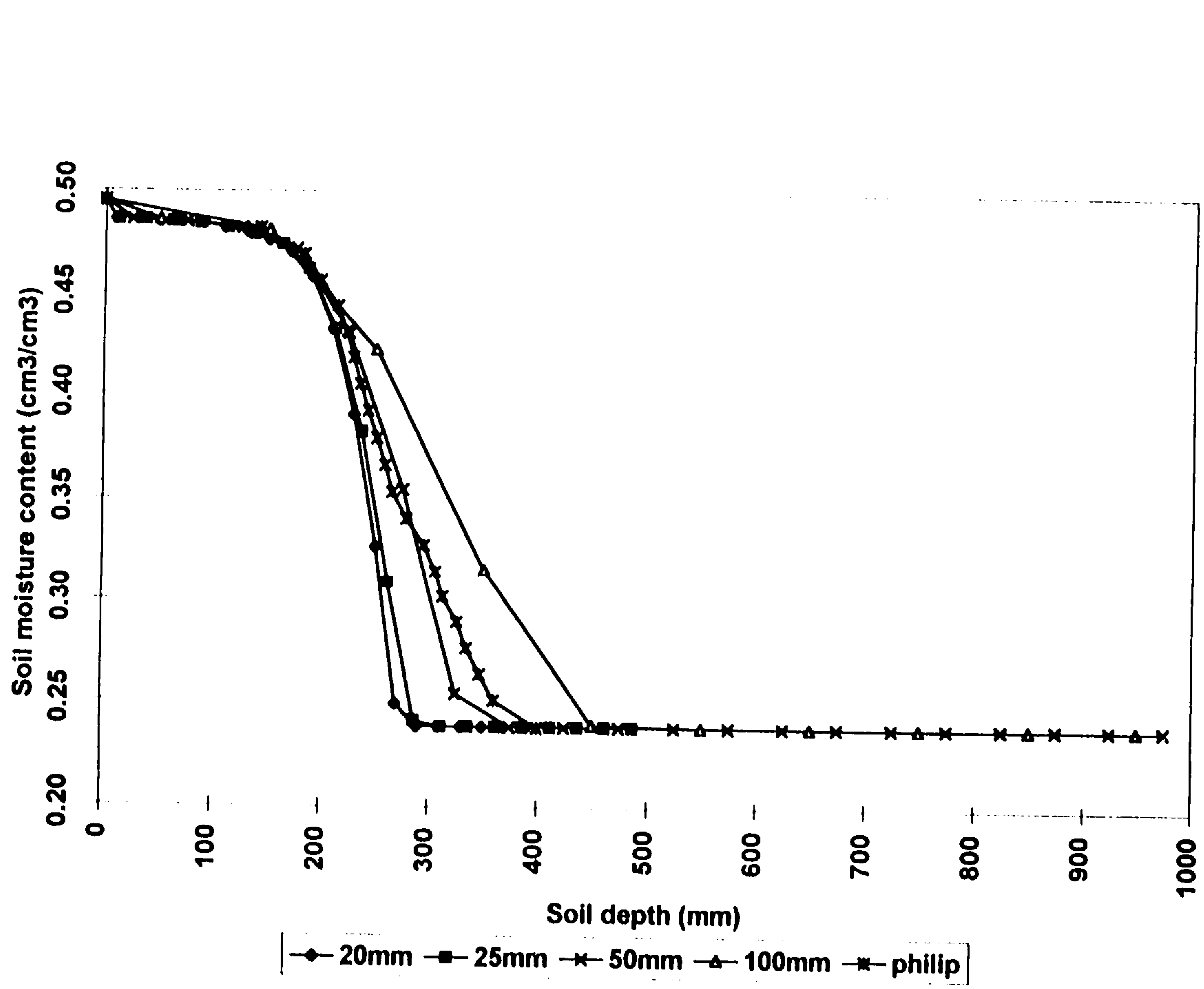

Fig. 2.2 LEACHW prediction of soil water profile during a continuous water infiltration into Yolo light clay with 2-, 2.5-, 5- and 10-cm soil depth increments as compared with results fronm Philip.

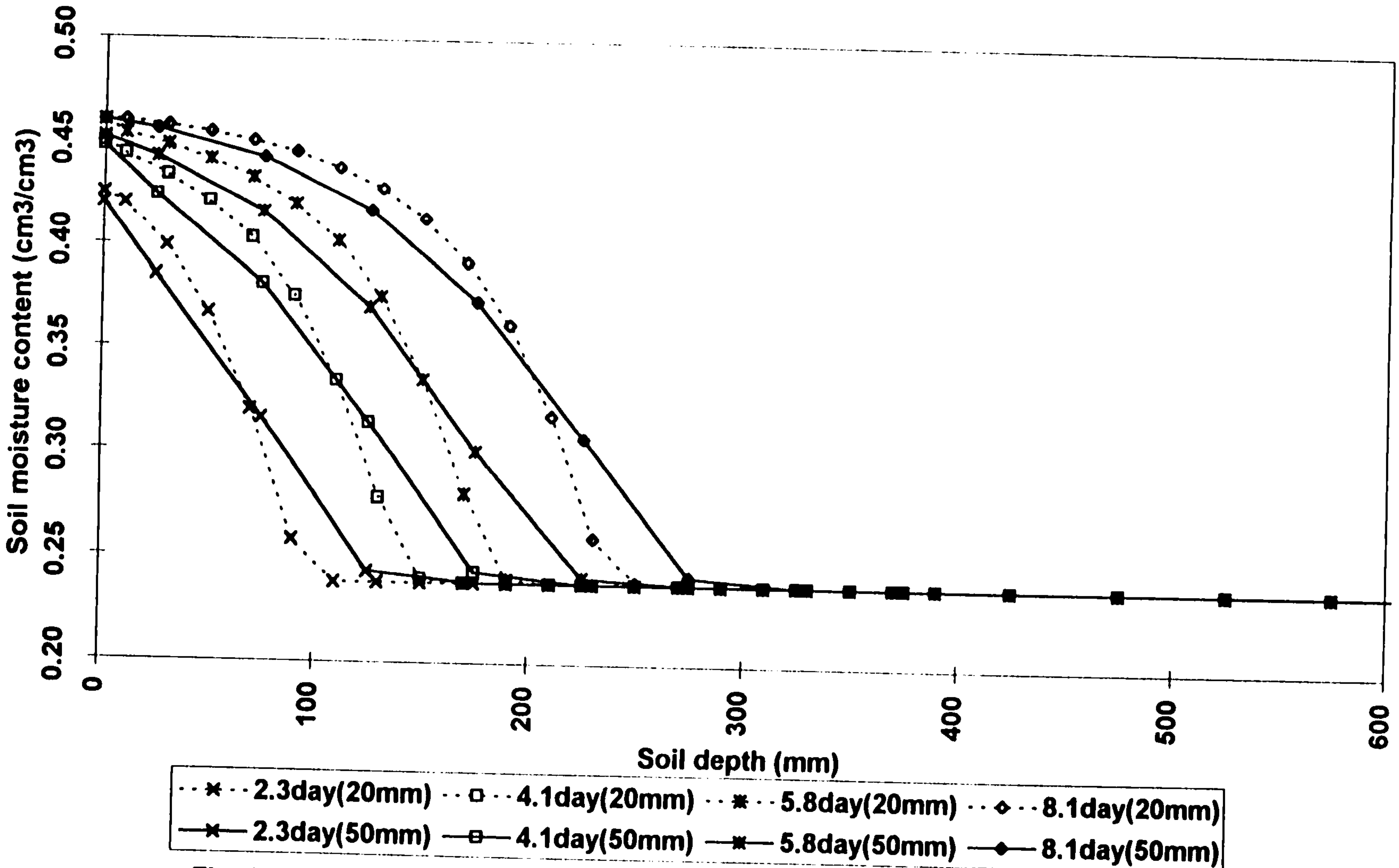

Fig. 2.3 Comparison of LEACHW prediction of soil water profile during a continuous water infiltration into Yolo light clay for 2- and 5-cm soil depth increments (low water application).

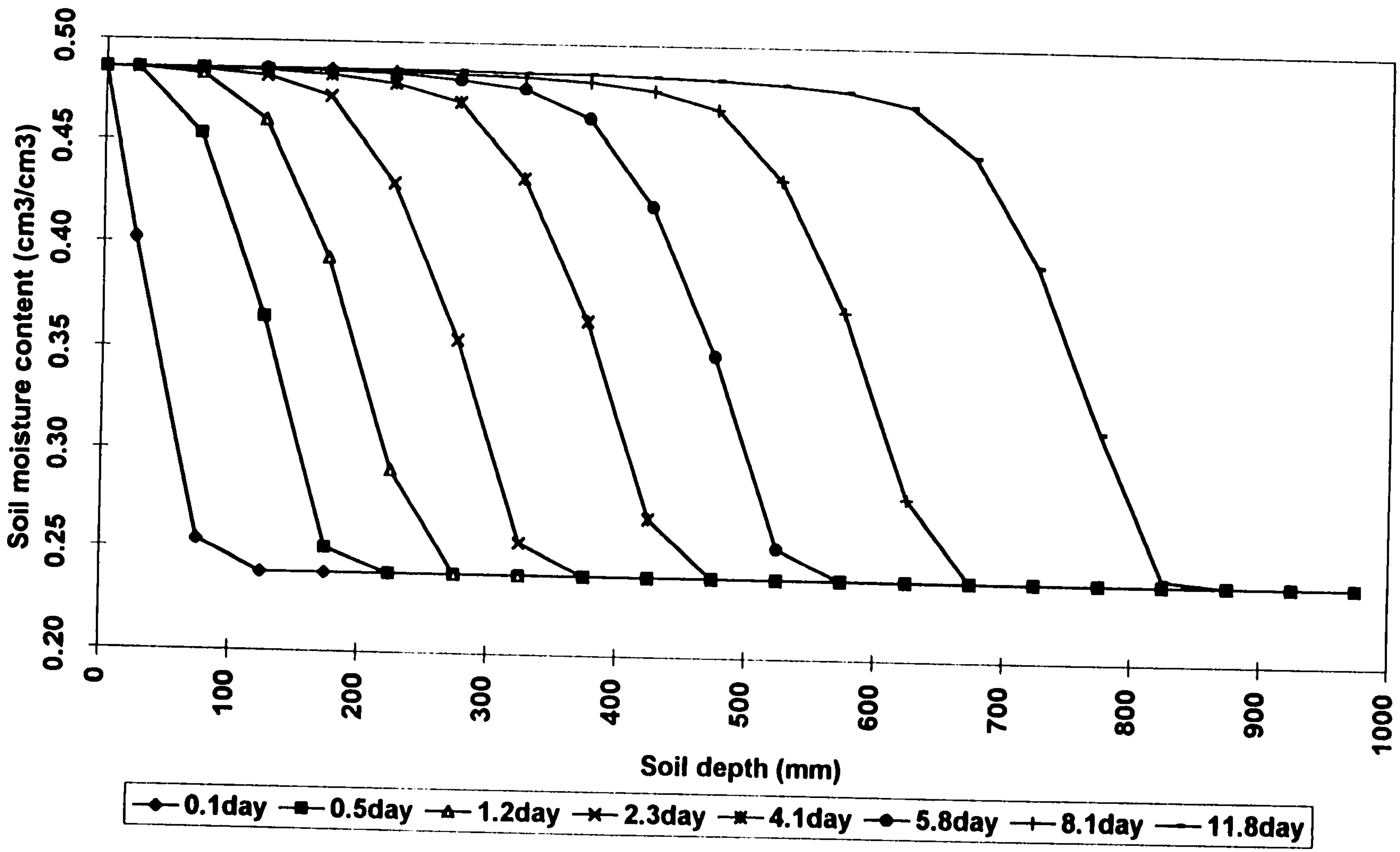

Fig. 2.4 LEACHW prediction of soil water profile during a continuous water infiltration into Yolo light clay (with 5-cm soil depth increments and time steps of 1 min).

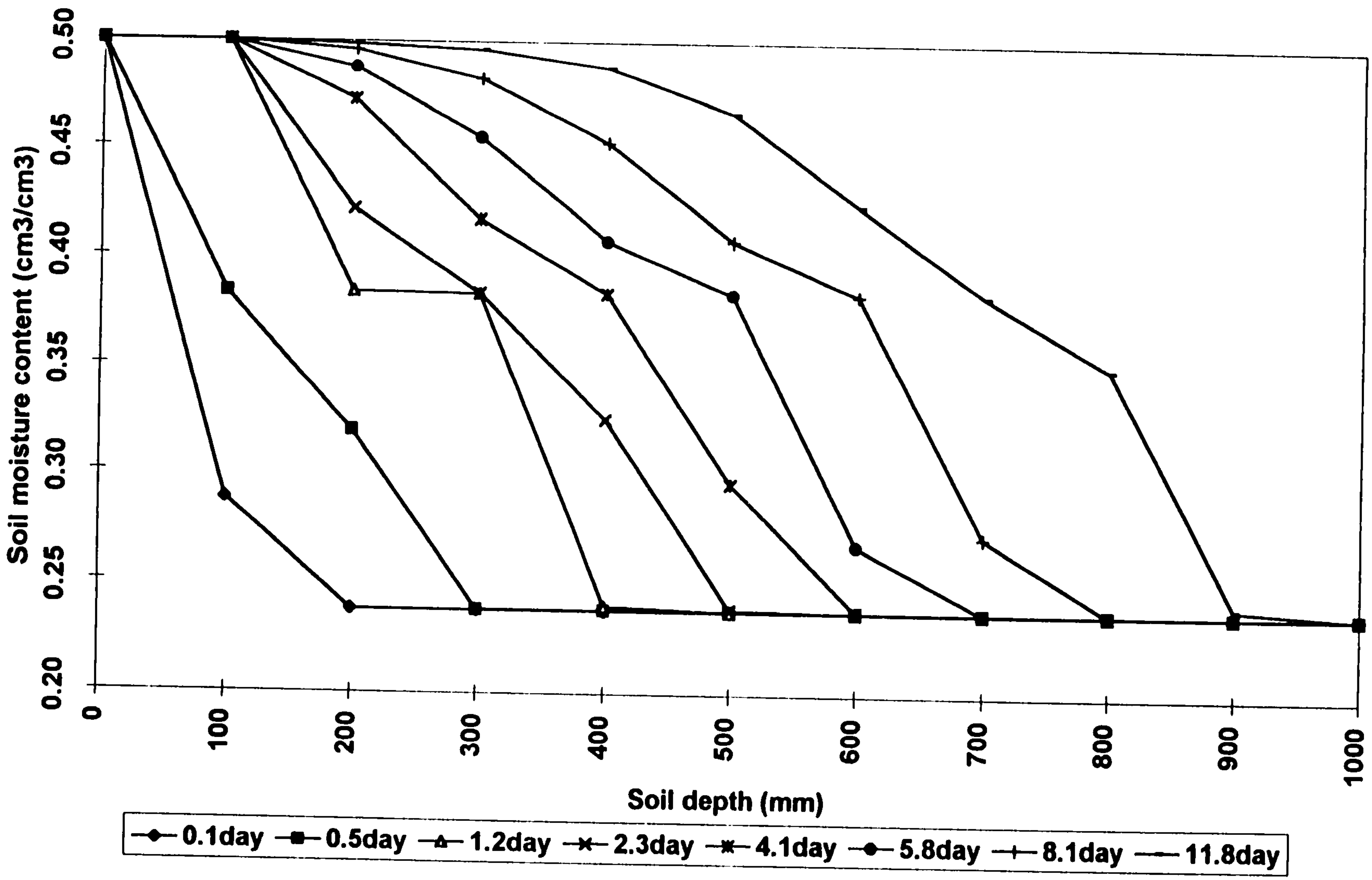

Fig. 2.5 ecosys prediction of soil water profile during a continuous water infiltration into Yolo light clay (with 10-cm soil depth increments and time steps of 1 min).

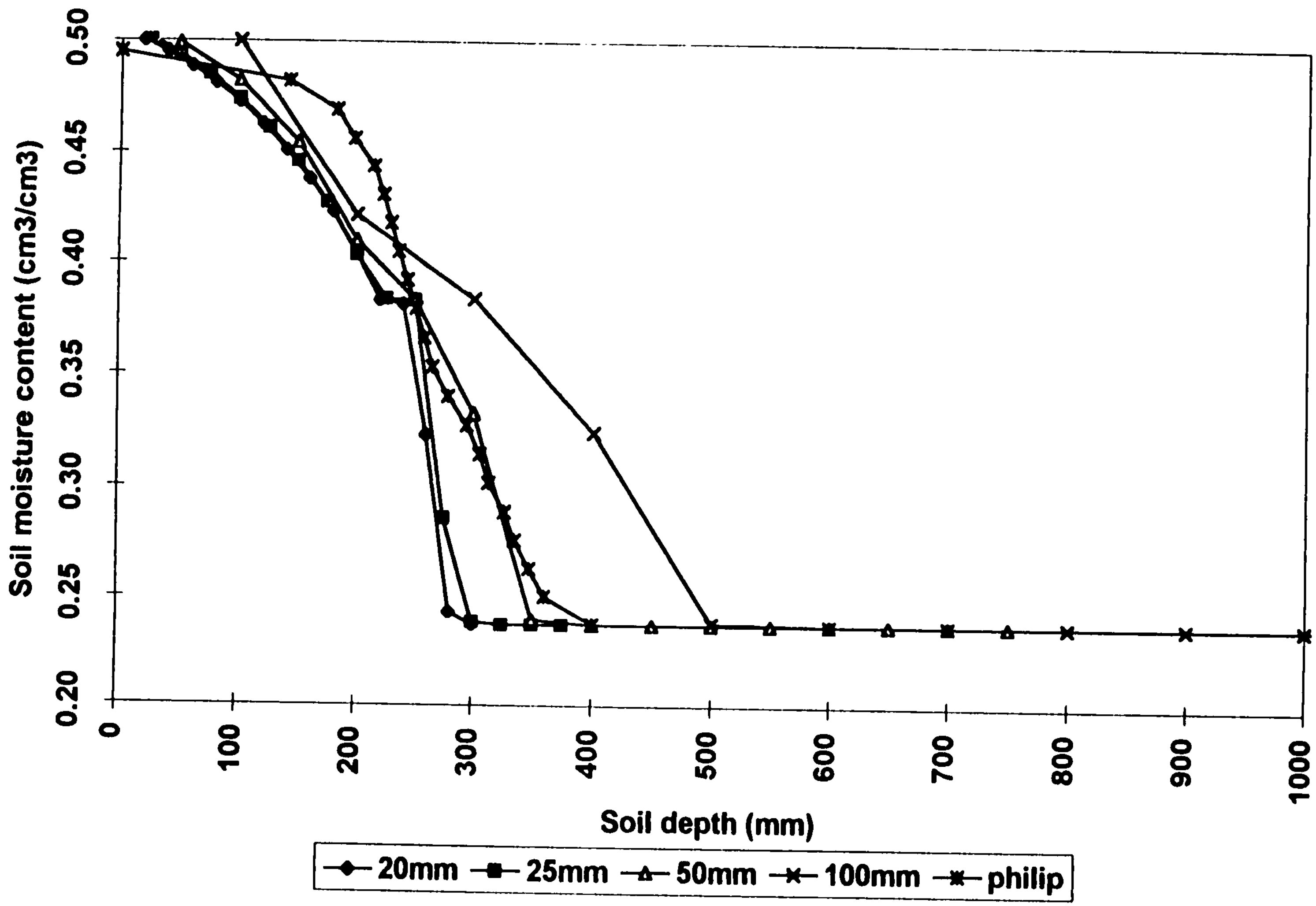

Fig. 2.6 *Ecosys* prediction of soil water profile during a continuous water infiltration into Yolo light clay with 2-, 2.5-, 5- and 10-cm soil depth increments as compared with results fronm Philip.

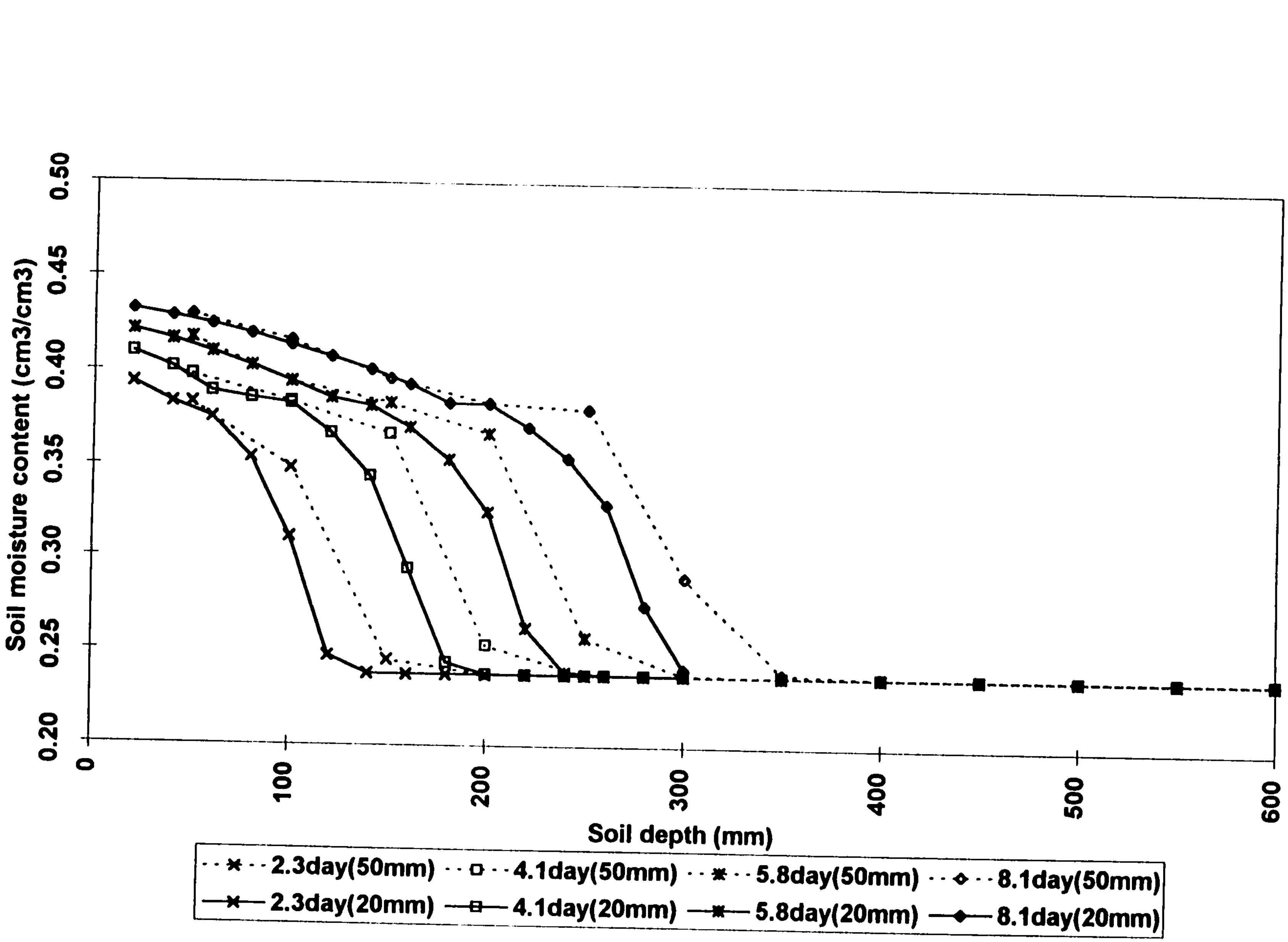

Fig. 2.7 Comparison of ecosys prediction of soil water profile during a continuous water infiltration into Yolo light clay for 2- and 5-cm soil depth increments (low water application).

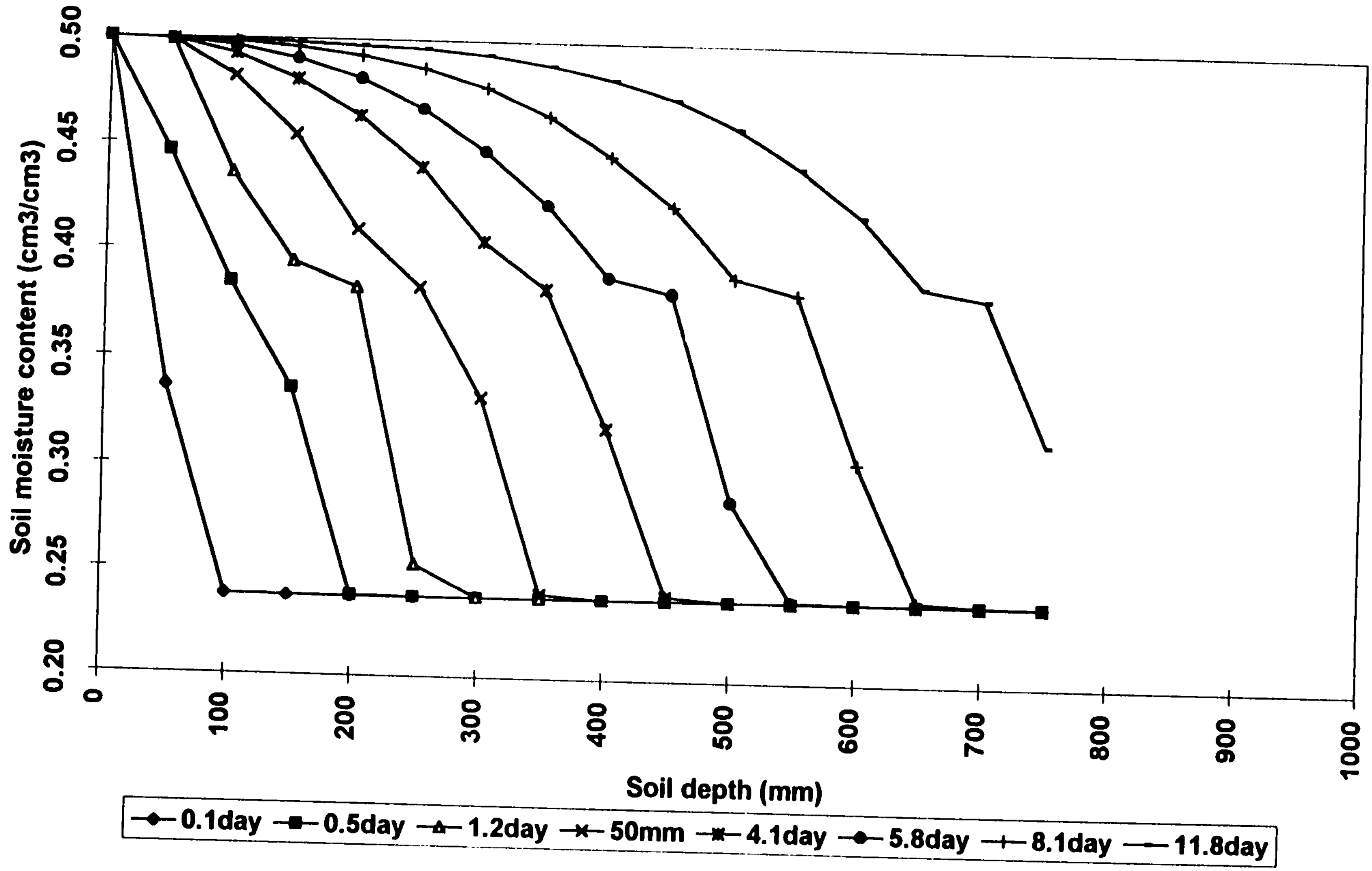

Fig. 2.8 ecosys prediction of soil water profile during a continuous water infiltration into Yolo light clay (with 5-cm soil depth increments and time steps of 1 min).

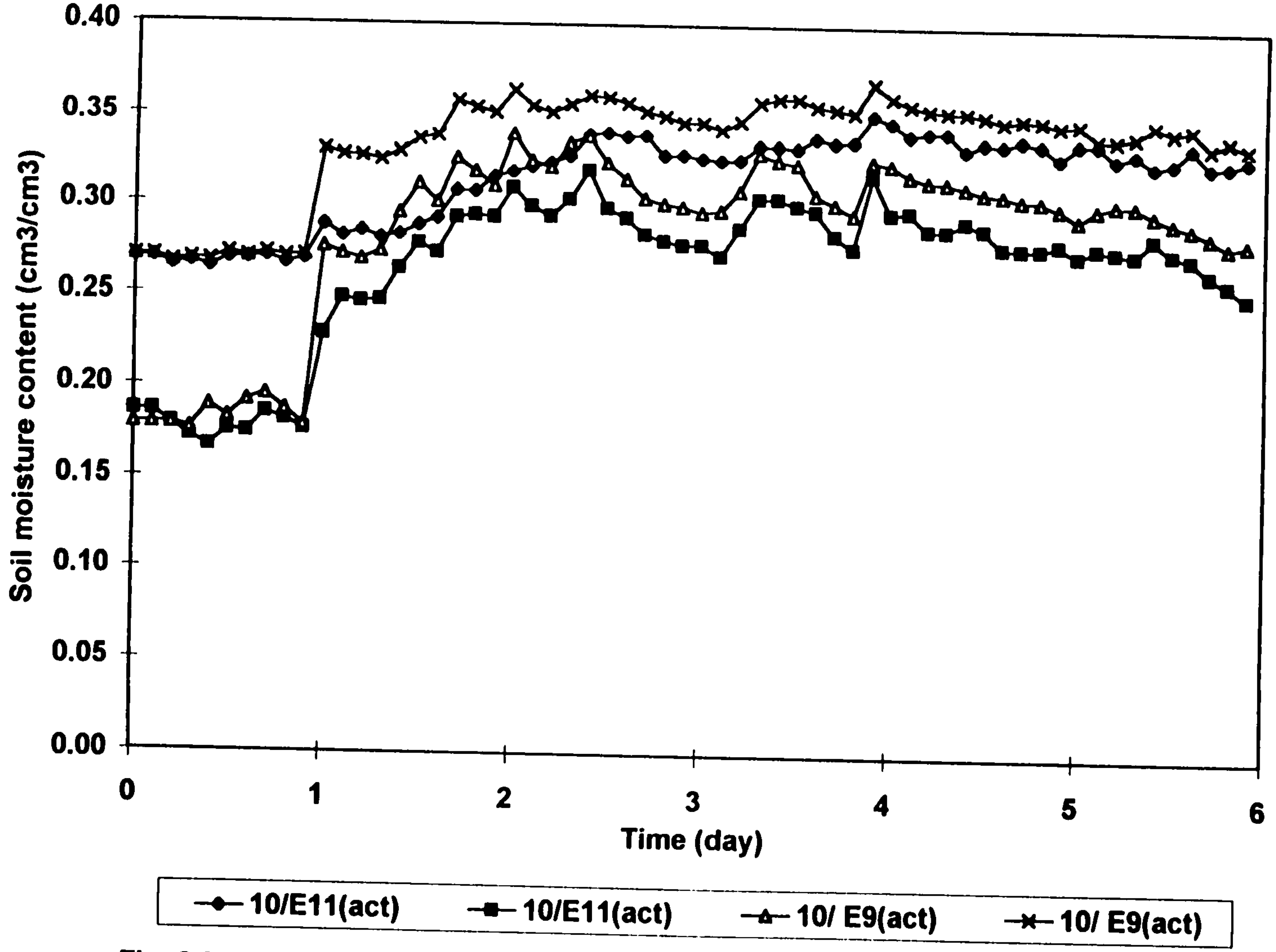

Fig. 2.9 Measured soil-water content at 10-cm depth, in two adjacent plots of E-9 and E-11, for the period of 1-6 July 1995.

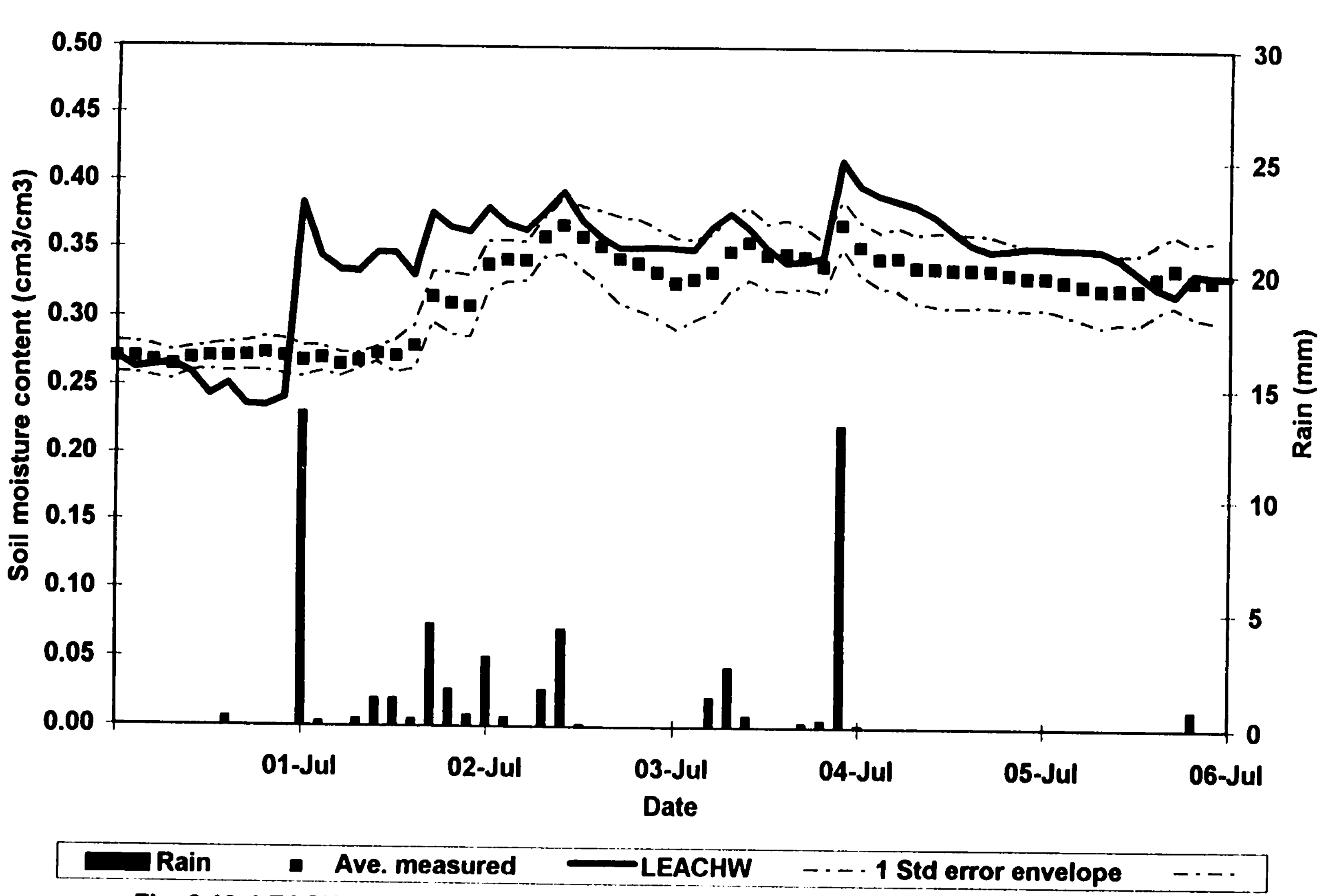

Fig. 2.10. LEACHW simulated water content as compared with the observed values at surface for the period of 1-6 July 1995 (Intense precipitation period).

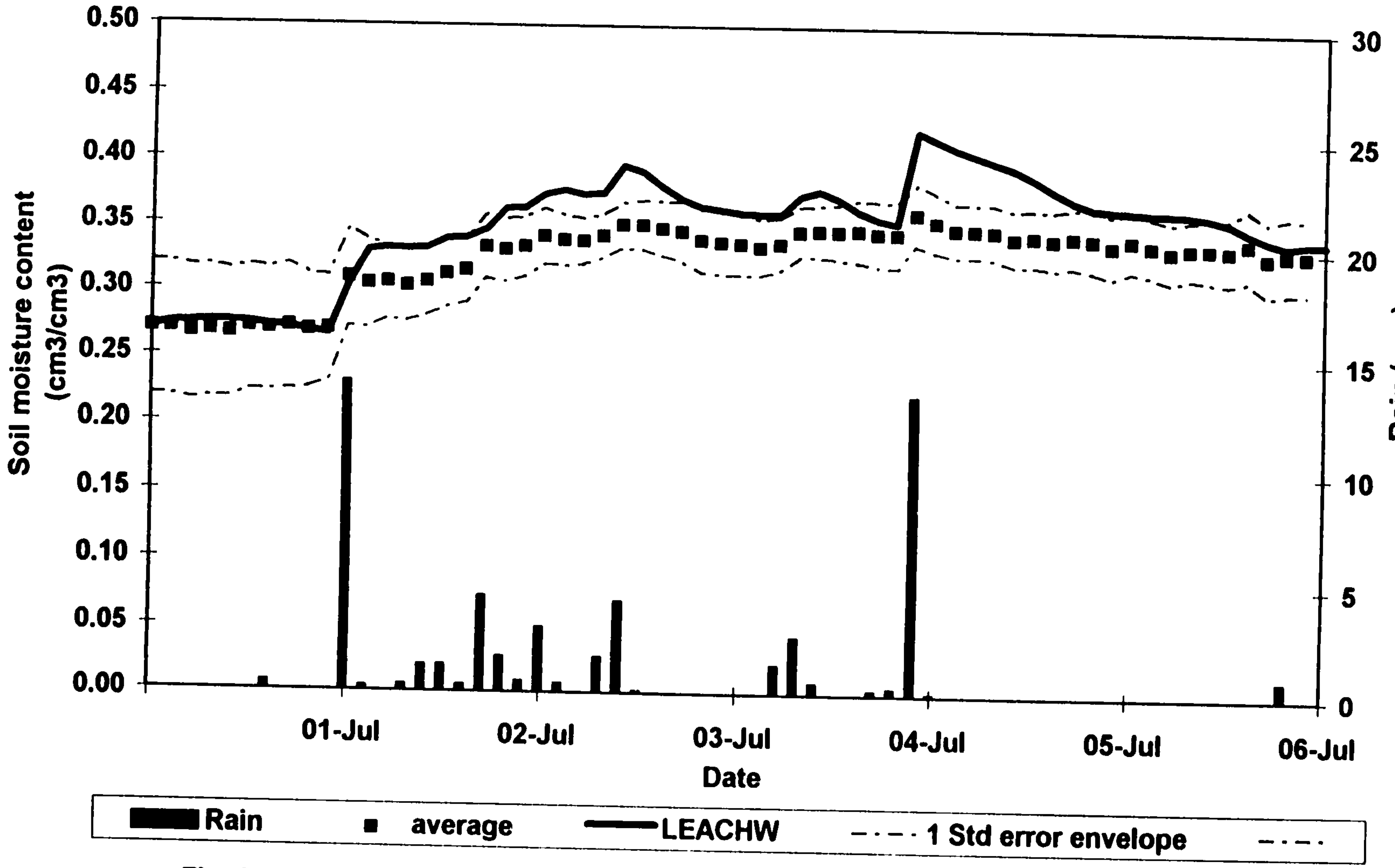

Fig. 2.11. Fig. 2.6. LEACHW simulated water content as compared with the observed values at 10 cm depth, for the period of 1-6 July 1995 (Intense precipitation period).

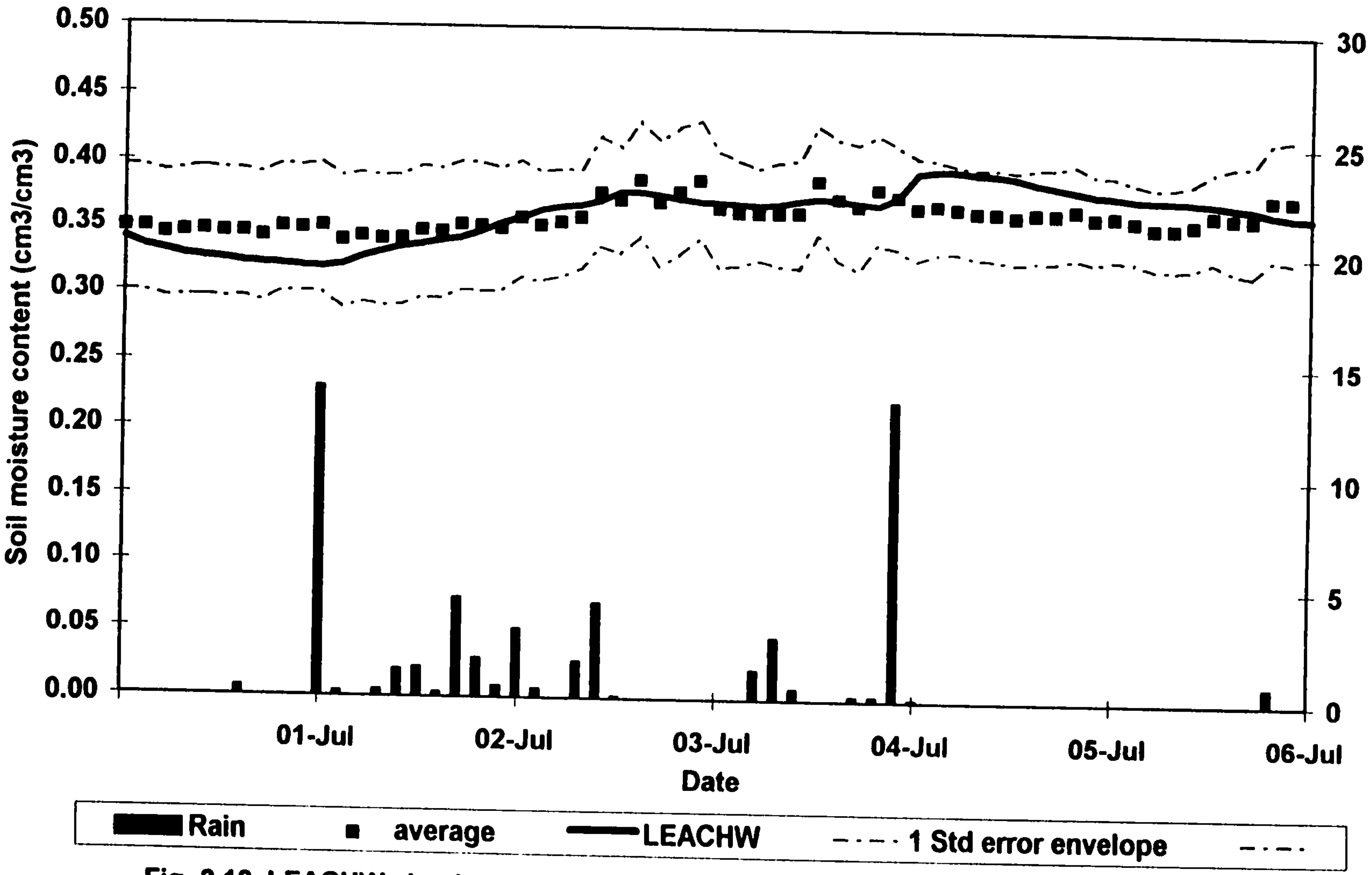

Fig. 2.12. LEACHW simulated water content as compared with the observed values at 20-cm depth, for the period of 1-6 July 1995 (Intense precipitation period).

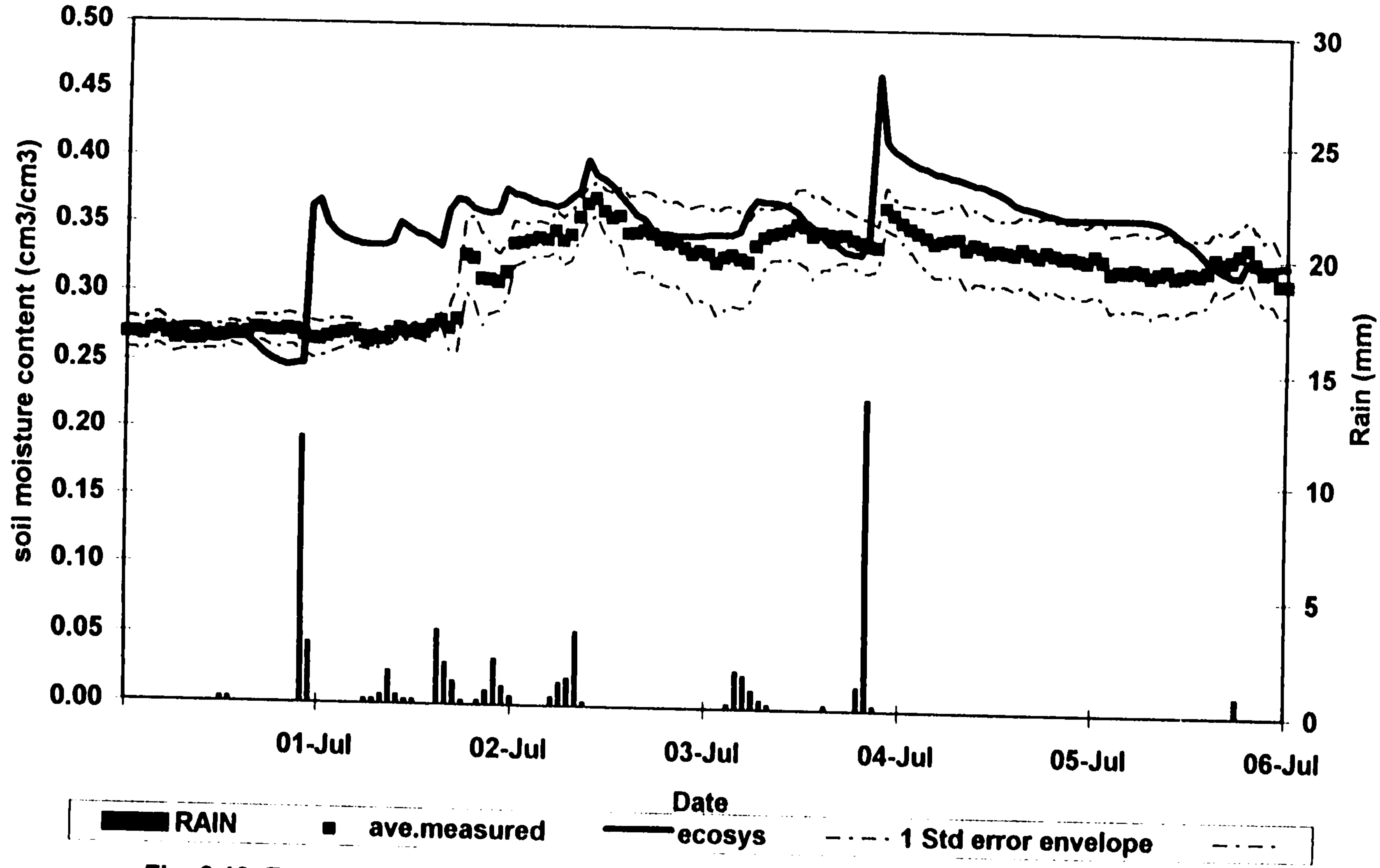

Fig. 2.13. Ecosys simulated water content as compared with the observed values at soil surface for the period of 1-6 July 1995 (Intense precipitation period).

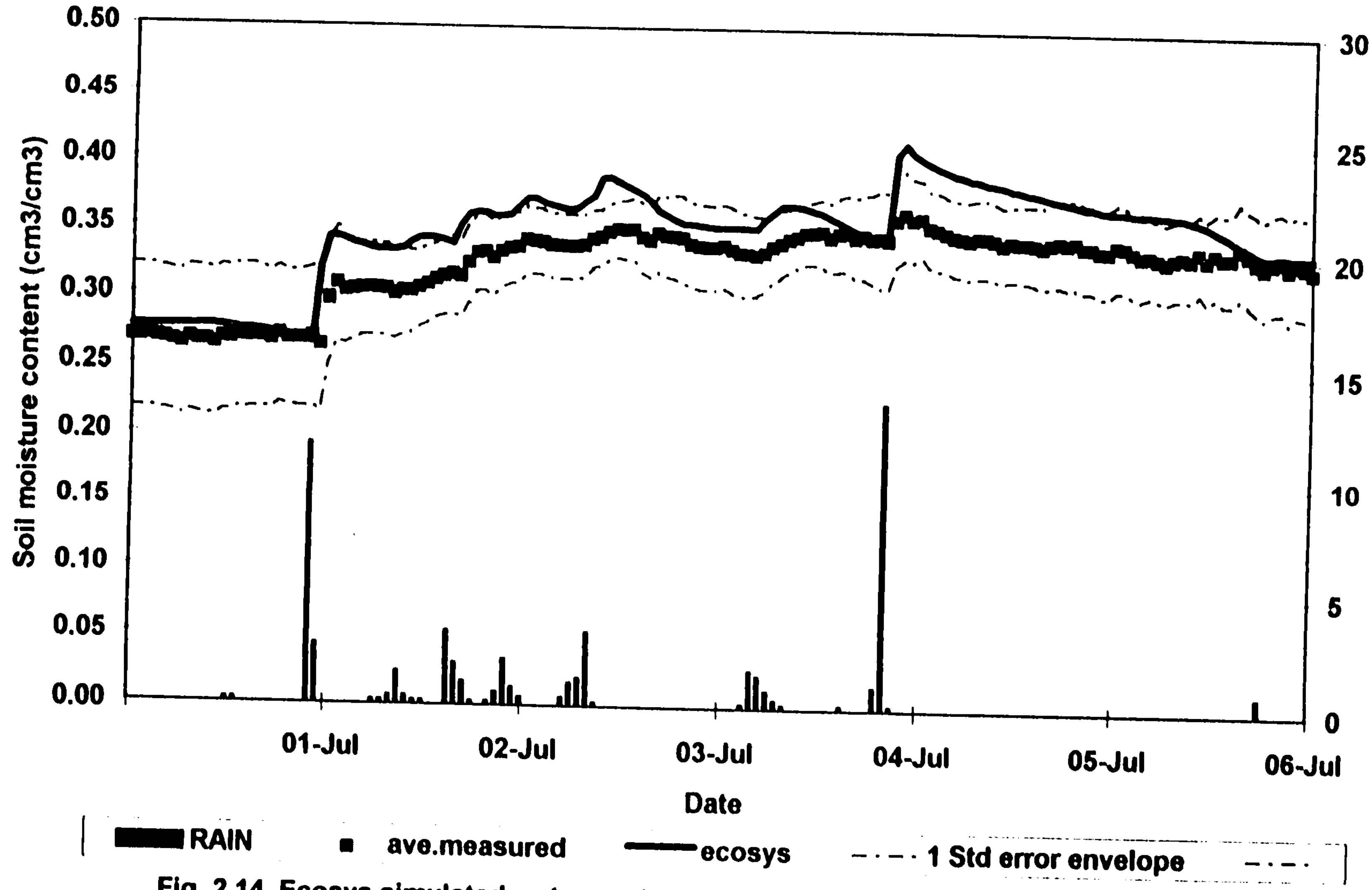

Fig. 2.14. Ecosys simulated water content as compared with the observed values at 10-cm depth for the period of 1-6 July 1995 (Intense precipitation period).

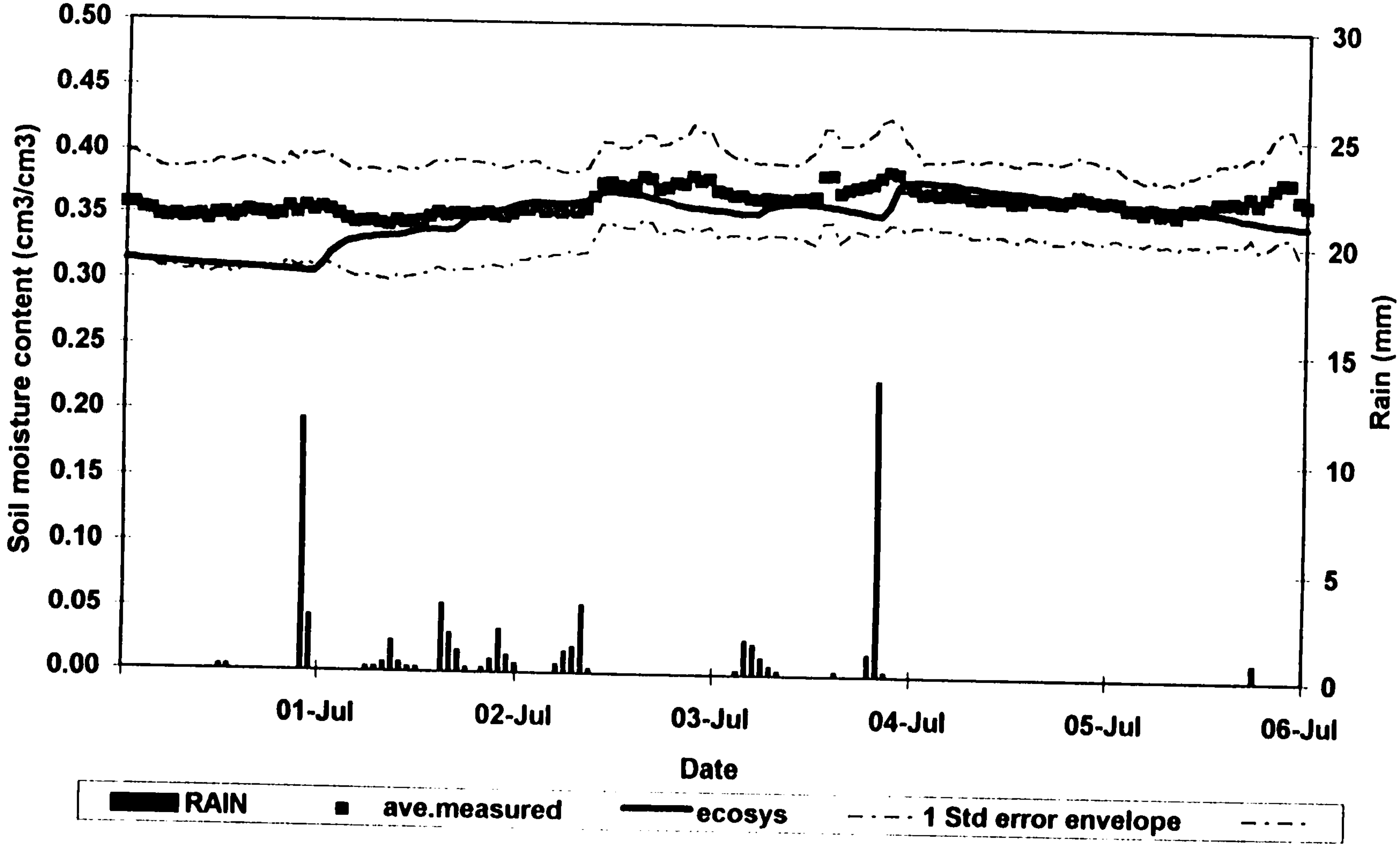

Fig. 2.15. Ecosys simulated water content as compared with the observed values at 20-cm depth for the period of 1-6 July 1995 (Intense precipitation period).

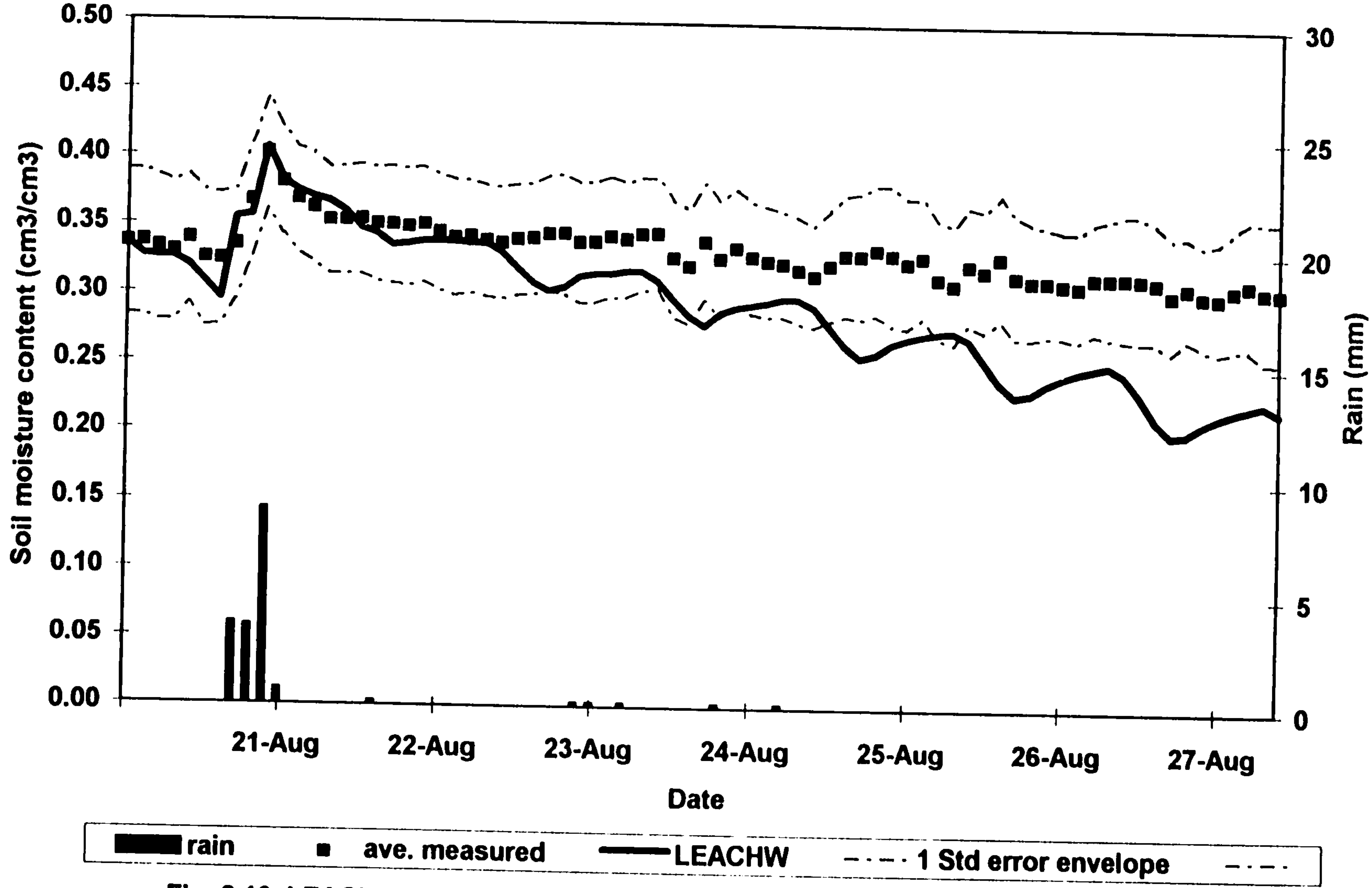

Fig. 2.16. LEACHW simulated water content as compared with the observed values at soil surface for the period of 20-27 Aug. 1995 (dry-down period)

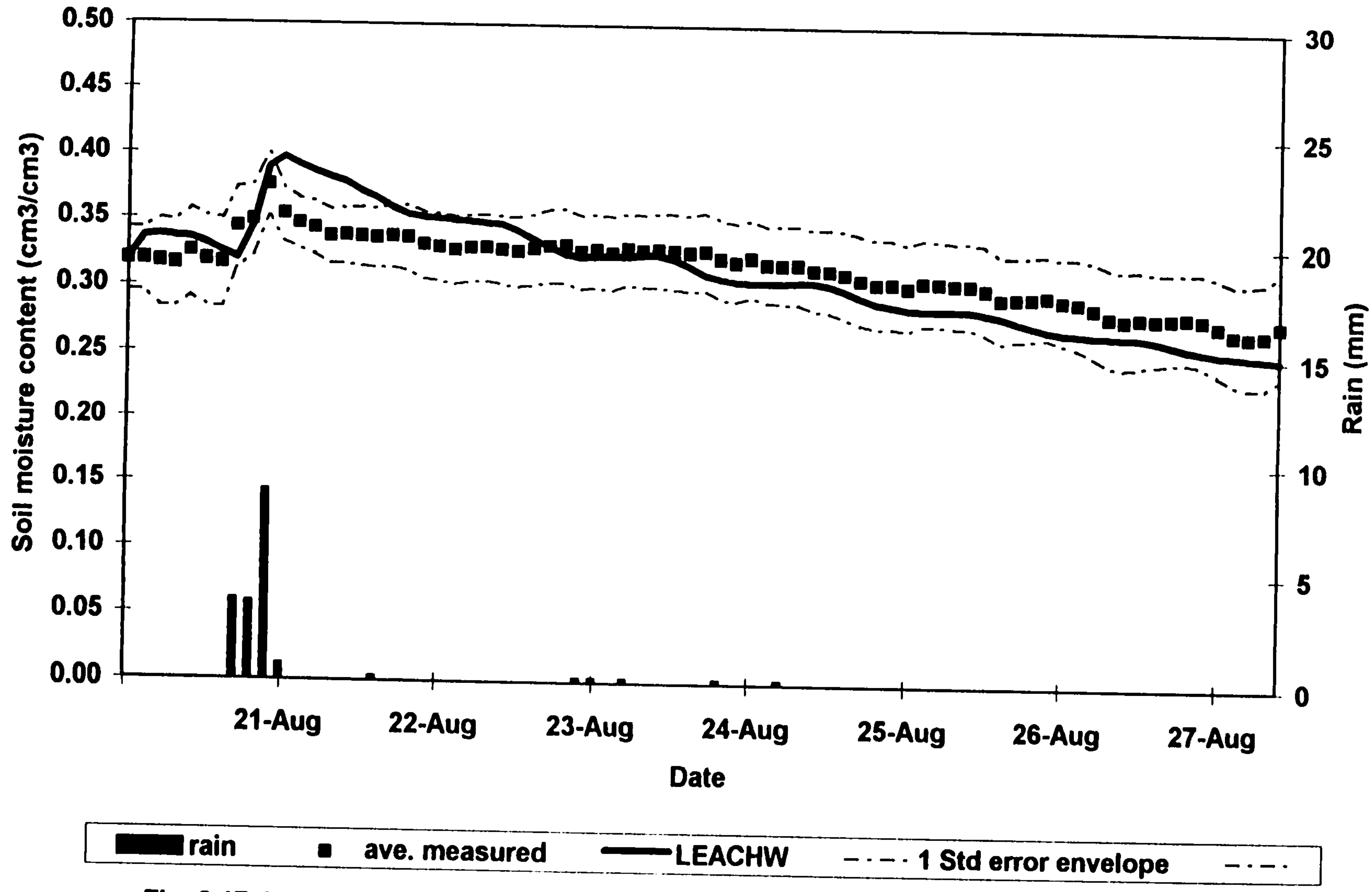

Fig. 2.17. LEACHW simulated water content as compared with the observed values at10-cm depth for the period of 20-27 Aug. 1995 (dry-down period).

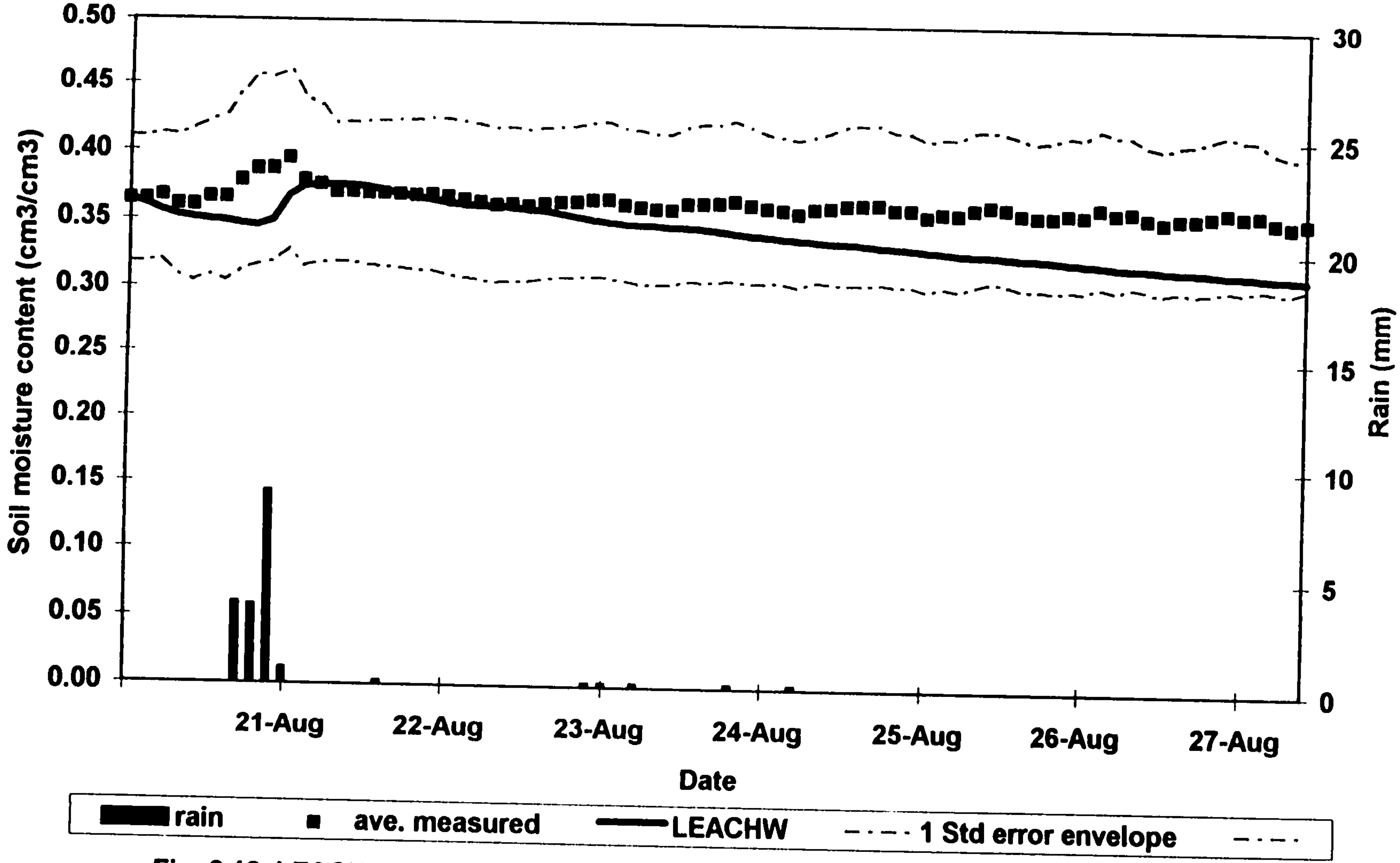

Fig. 2.18. LEACHW simulated water content as compared with the observed values at 20-cm depth for the period of 20-27 Aug. 1995 (dry-down period).

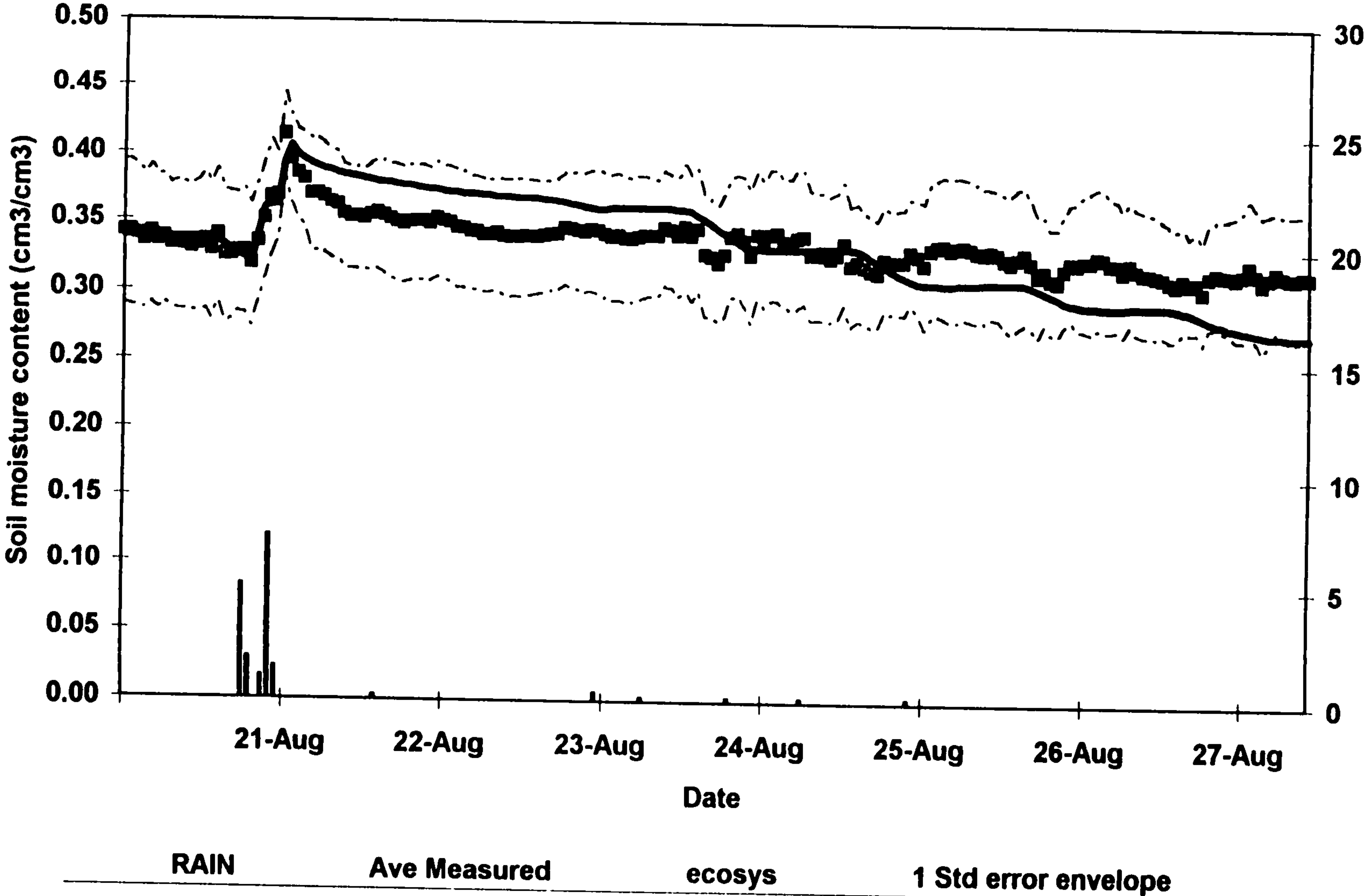

Fig. 2.19. Ecosys simulated water content as compared with the observed values at soil surface for the period of 20-27 Aug. 1995 (dry-down period).

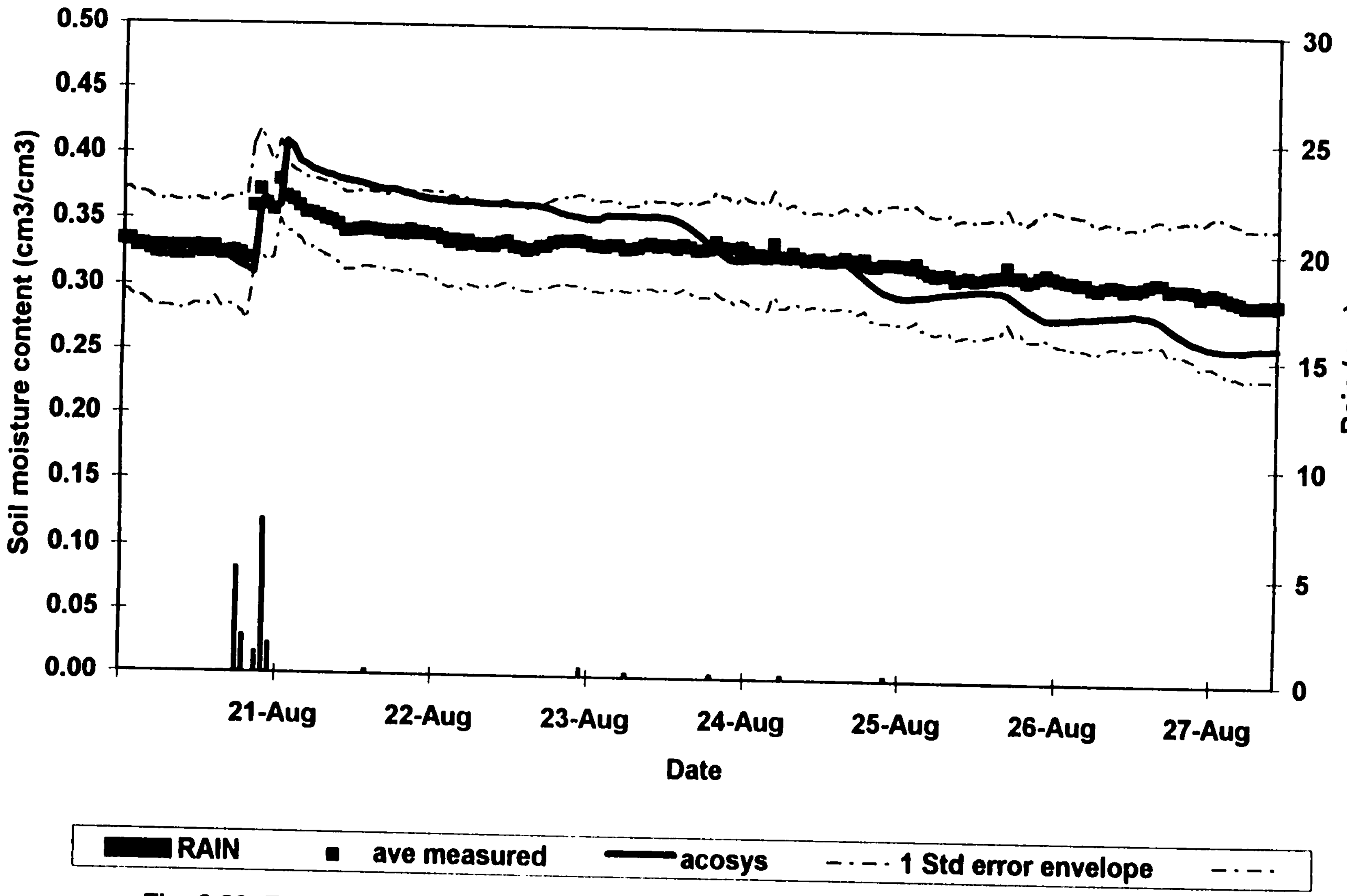

Fig. 2.20. Ecosys simulated water content as compared with the observed values at 10-cm depth for the period of 20-27 Aug. 1995 (dry-down period)

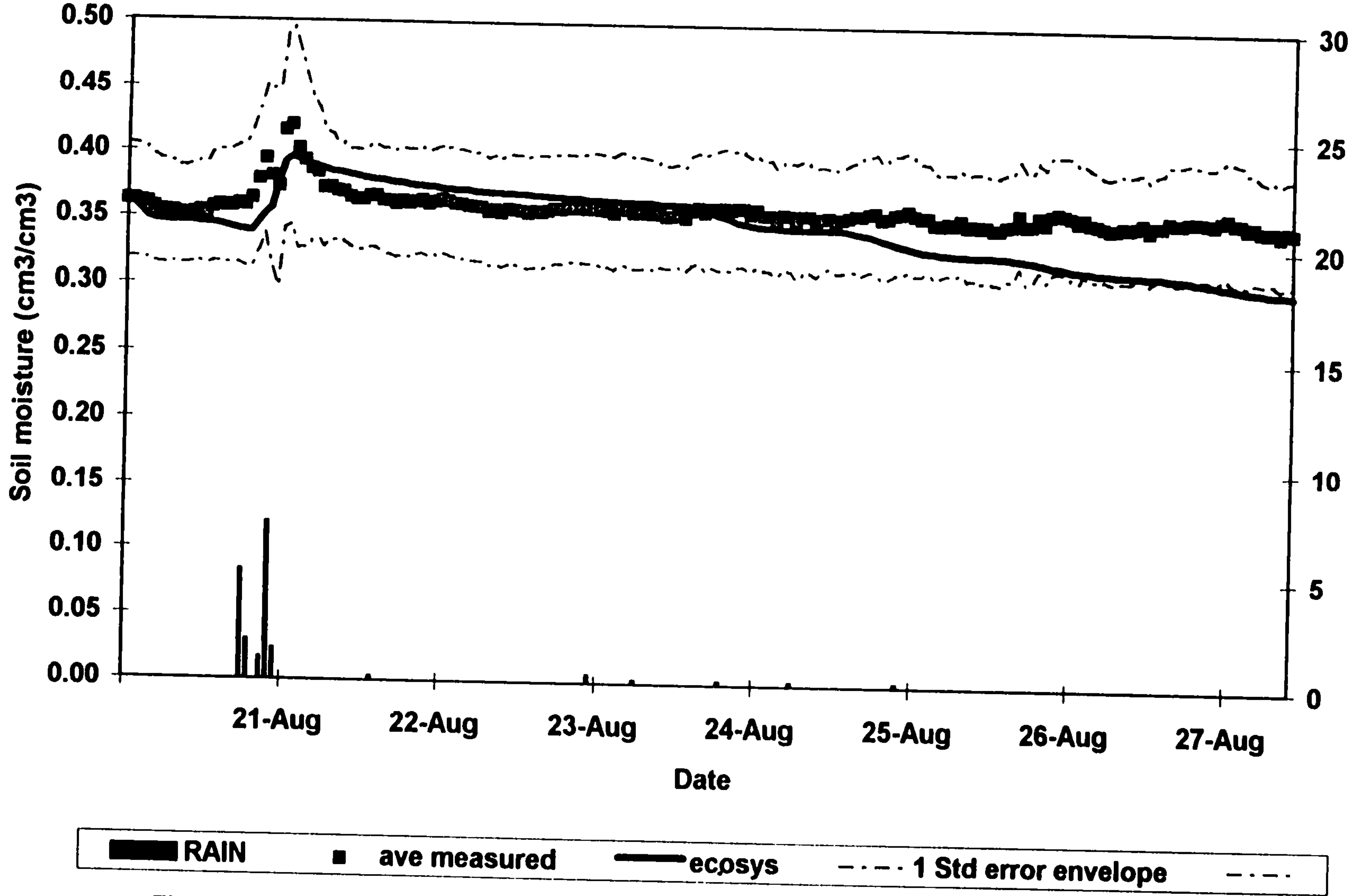

Fig. 2.21. ecosyssimulated water content as compared with the observed values at 20-cm depth for the period of 20-27 Aug. 1995 (dry-down period).

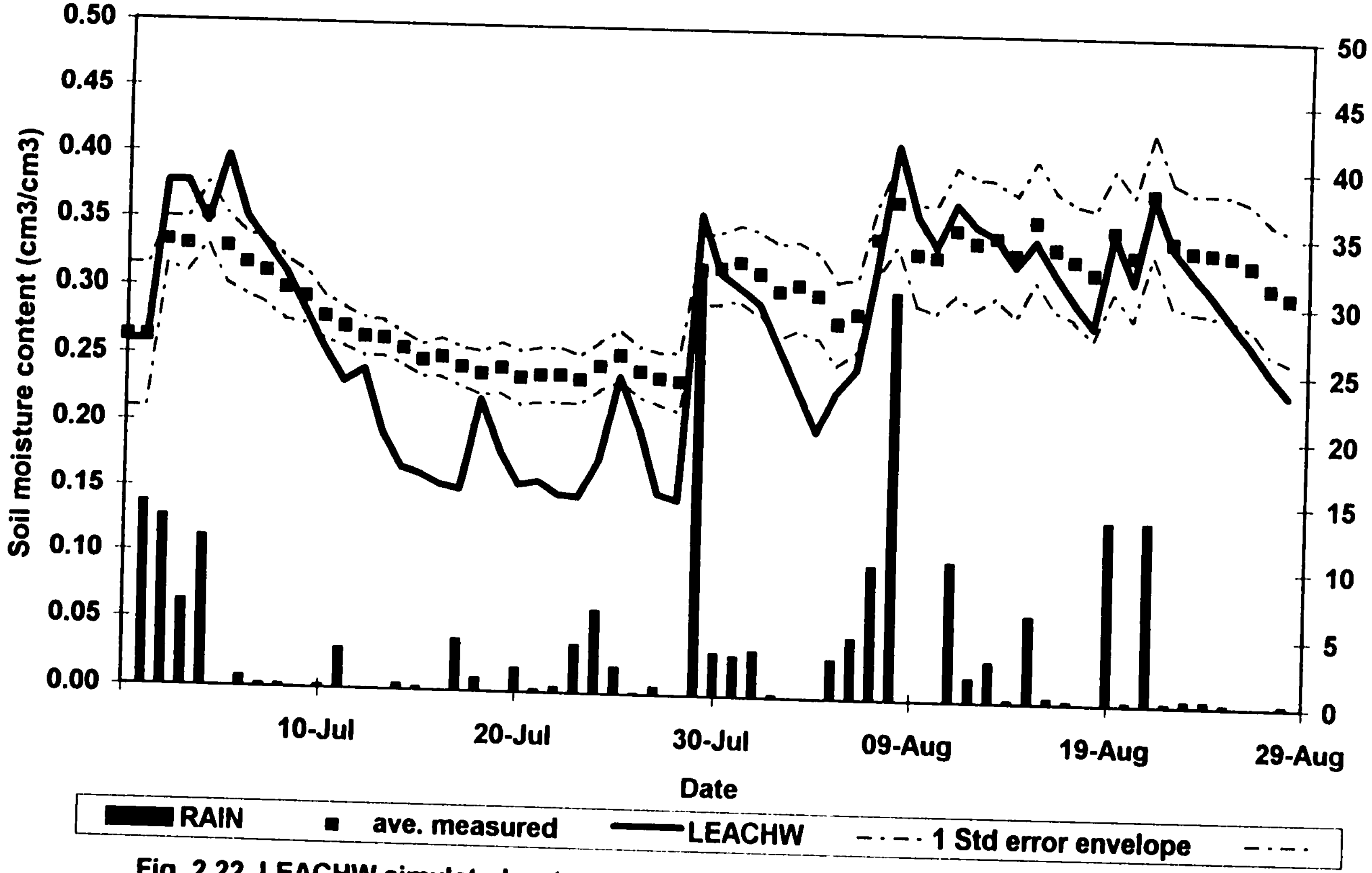

Fig. 2.22. LEACHW simulated water content as compared with the observed values at soil surface for the period of months of July and August 1995 (Long-term period).

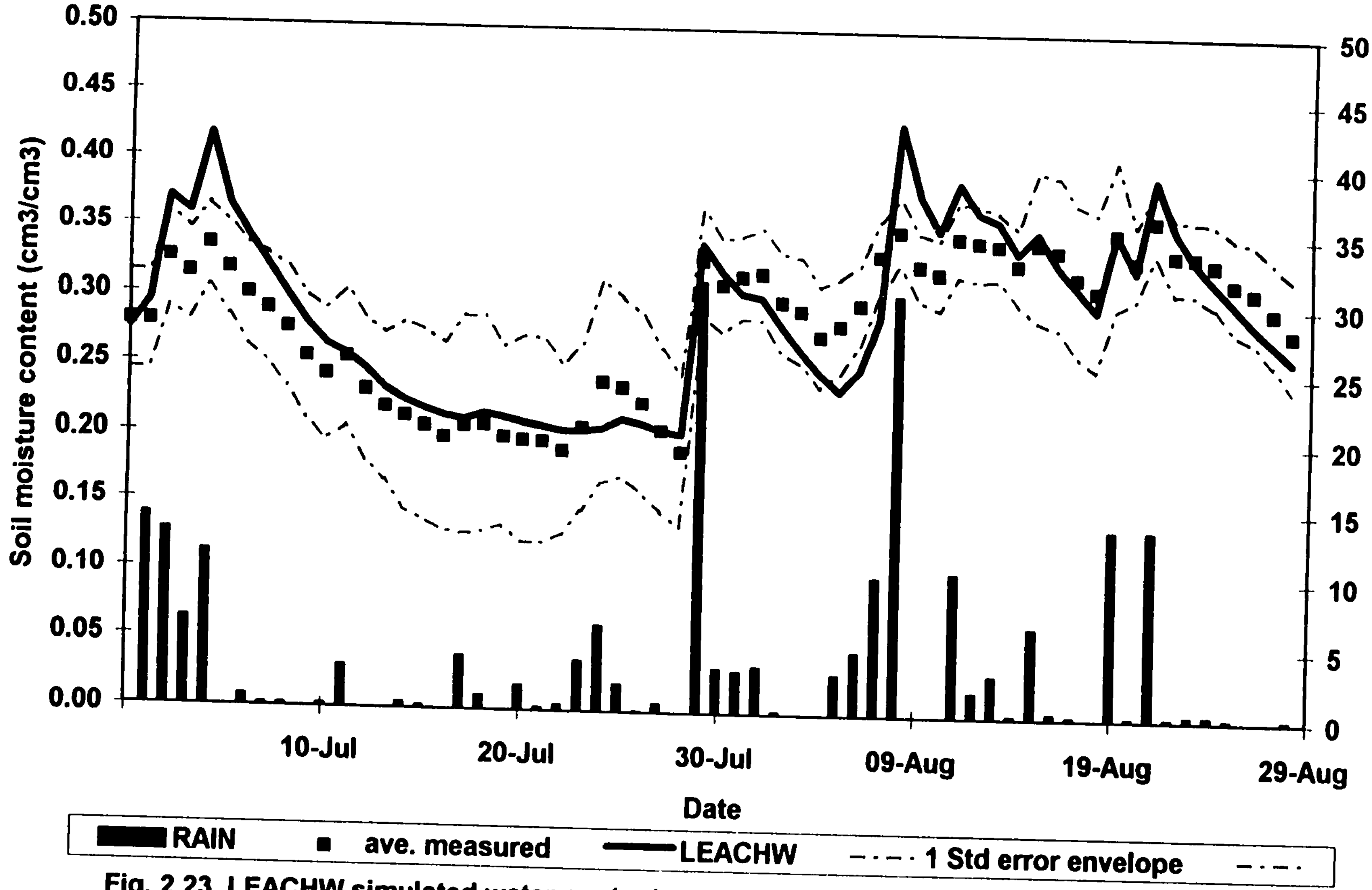

Fig. 2.23. LEACHW simulated water content as compared with the observed values at10-cm depth for the period of months of July and August 1995 (Long-term period).

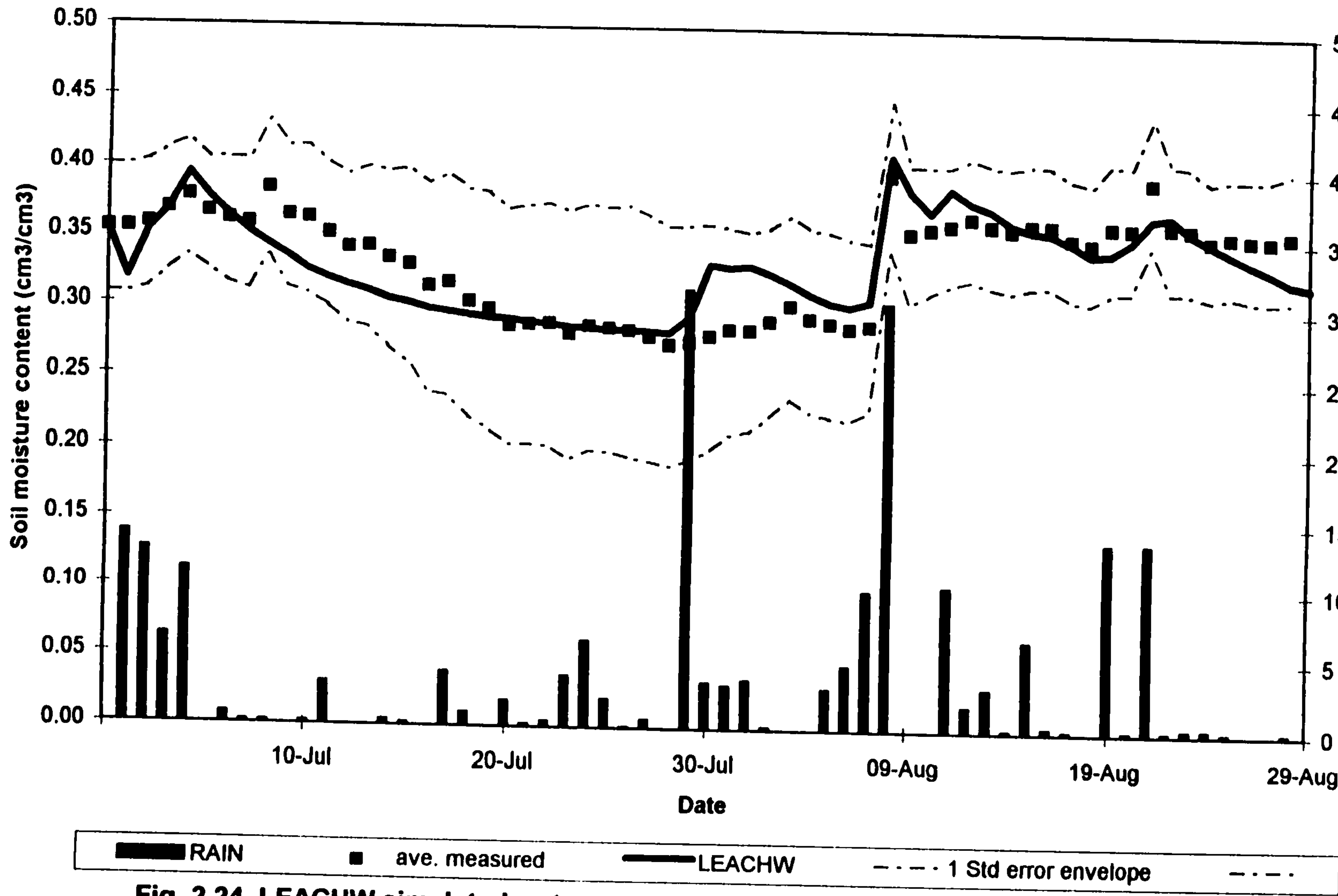

Fig. 2.24. LEACHW simulated water content as compared with the observed values at 20-cm depth for the period of months of July and August 1995 (Long-term period).

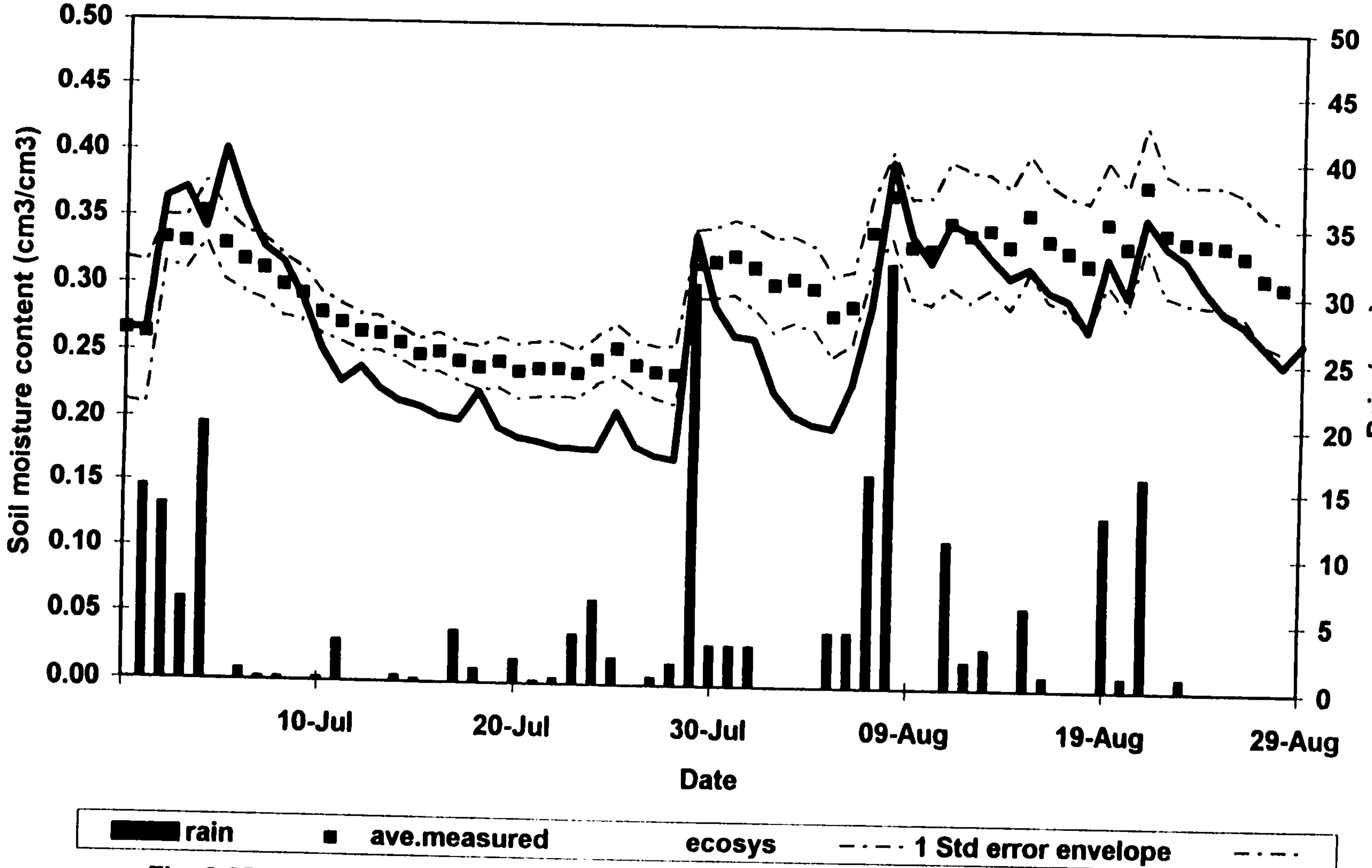

Fig. 2.25. Ecosys simulated water content as compared with the observed values at soil surface for the period of months of July and August 1995 (Long-term period).

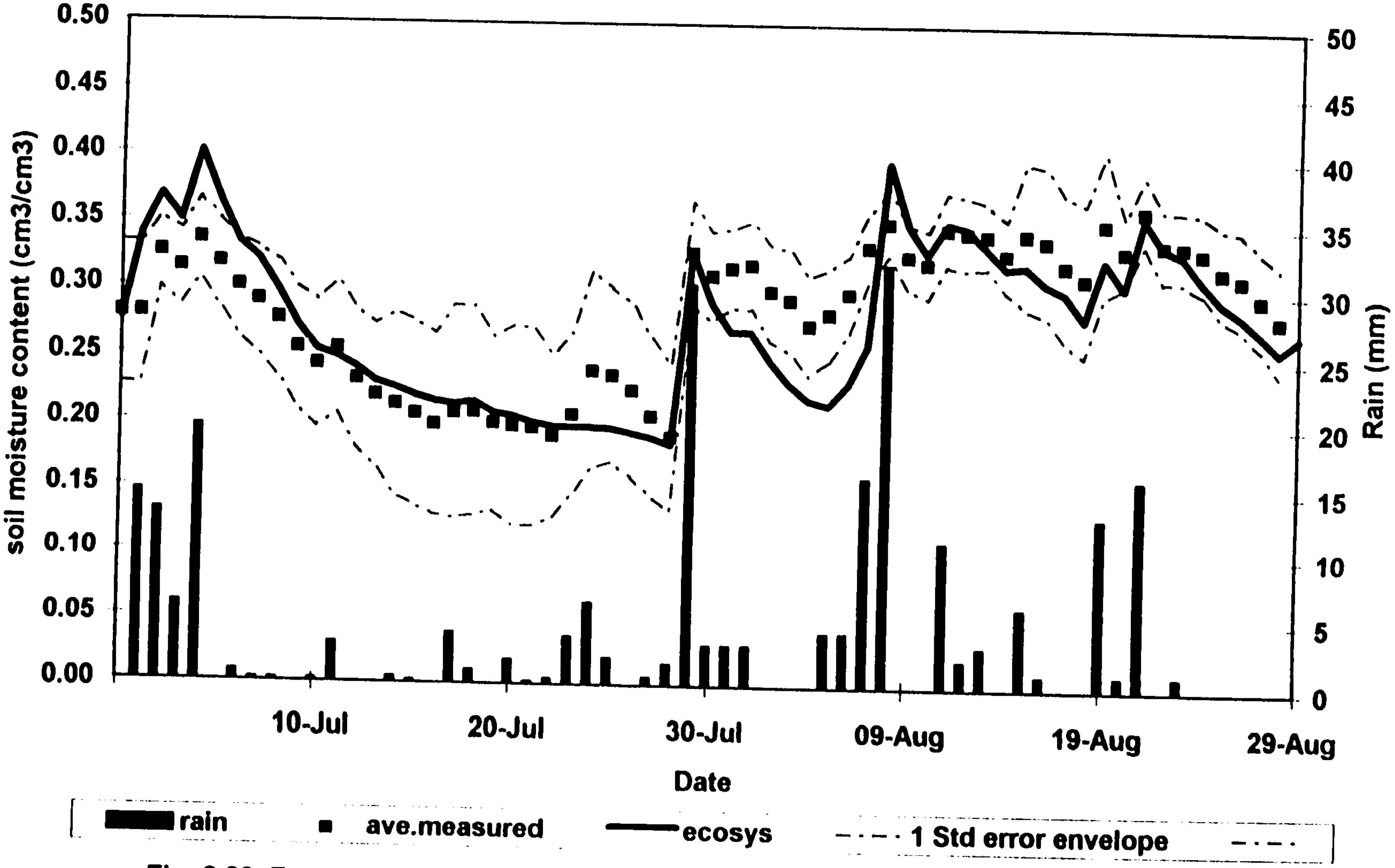

Fig. 2.26. Ecosys simulated water content as compared with the observed values at10-cm depth for the period of months of July and August 1995 (Long-term period).

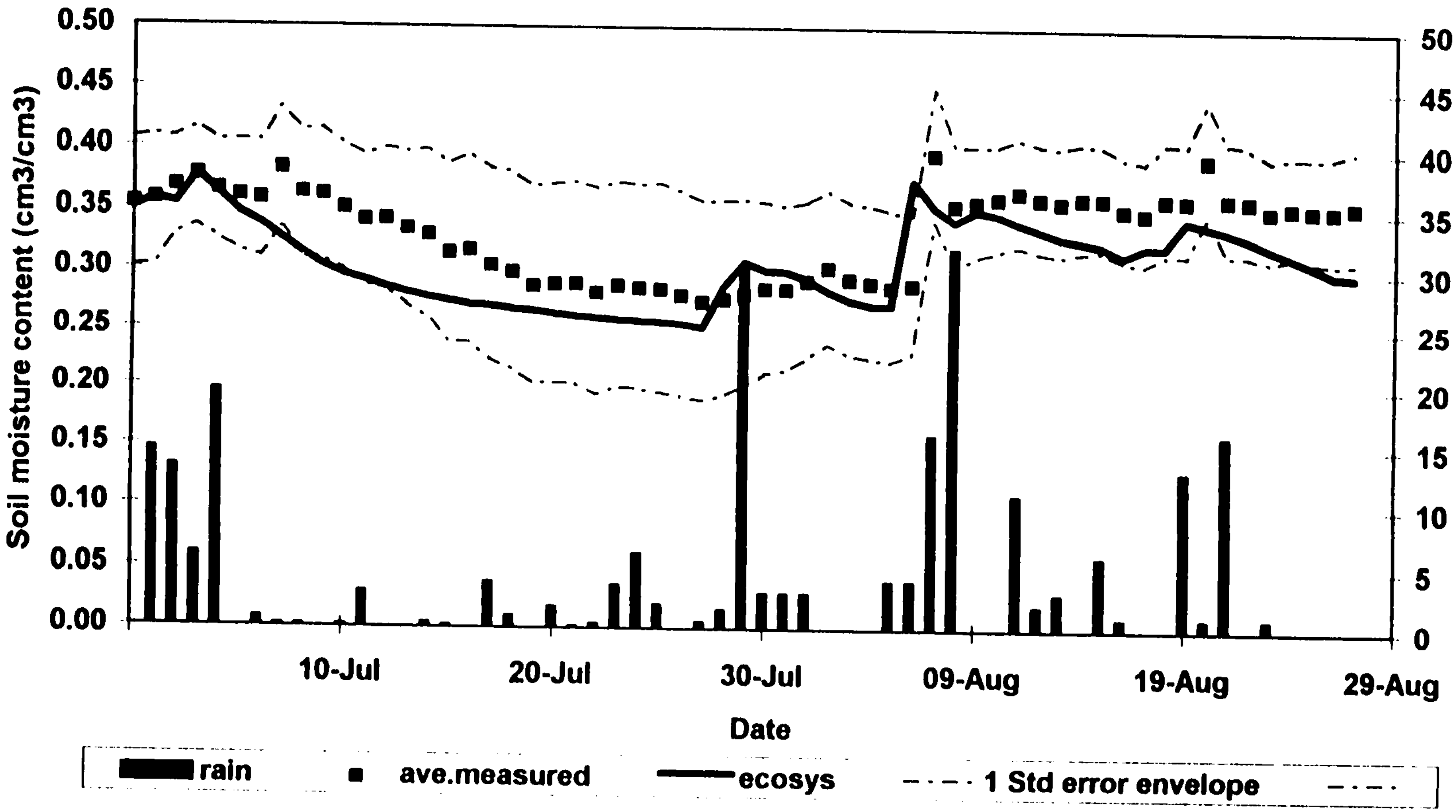

Fig. 2.27. Ecosys simulated water content as compared with the observed values at20-cm depth for the period of months of July and August 1995 (Long-term period).

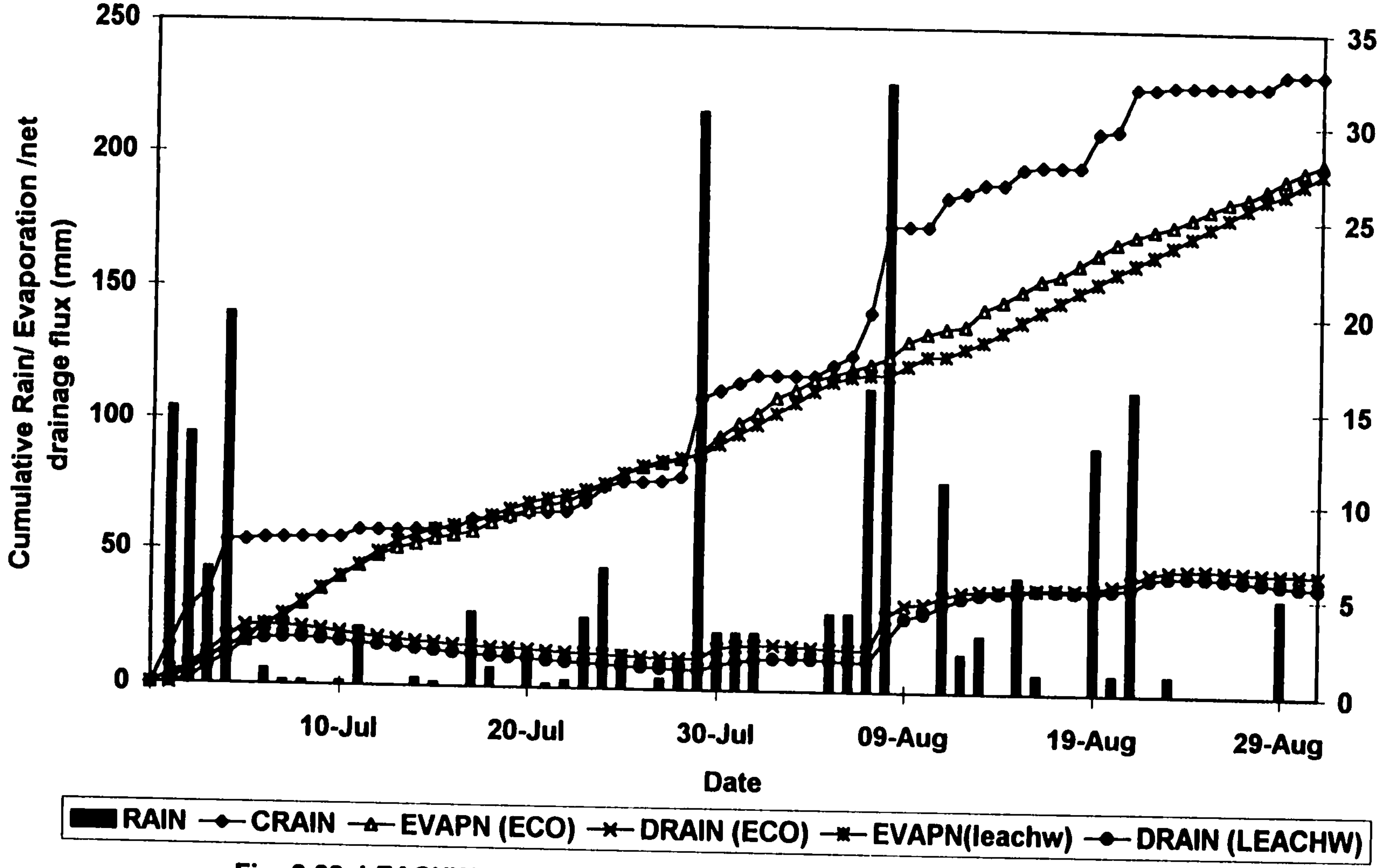

Fig. 2.28. LEACHW and ecosys simulated cumulative evaporation demand for the months of July and August 1995.

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Chapter Three

SENSITIVITY ANALYSIS OF HYDRAULIC PARAMETERS IN SIMULATION OF UNSATURATED SOIL WATER DYNAMICS

3.1 Introduction

Soil water simulation models are used to provide guidance for agricultural and environmental management, such as the design of irrigation and drainage systems, and control of surface and ground water pollution (Wagenet and Hutson, 1989).

Soil hydraulic characteristics, including the soil water characteristic($h(\theta)$) and soil hydraulic conductivity ($K(\theta)$) functions, play critical roles in transport and retention of water in soils. These soil properties often exhibit significant spatial and temporal variation. Many models with different degrees of sophistication have been developed to describe soil water processes, which are complicated by hysteresis (Kool and van Genuchten, 1991), preferential flow (Li and Ghodrati, 1994), and temporal / spatial variability of soil properties (Warrick, 1990). Difficulties in utilization of these models are mainly attributed to a lack of detailed information on soil characteristics. In many cases these functions are not adequately defined for the soil being considered. Direct measurement of the nonlinear functions of $\theta(h)$ and $K(h)$ is time consuming and expensive. In addition, several measurements are required to accurately represent field soil conditions. Instead, soil hydraulic functions are often estimated from other more easily obtainable soil properties such as texture, bulk density and organic matter content (Campbell, 1974; Mualem, 1976 and van Genuchten, 1980). However, these predictions can have high degrees of uncertainty and error, especially for the estimation of soil hydraulic conductivity (Yates et al., 1992, Stolte, et al., 1994).

Complex simulation models, such as LEACHW (Wagenet and Hutson, 1989) and *ecosys* (Grant, 1995) attempt to present a theoretically rigorous representation of soil water processes. They require many input parameters that describe the properties of soil water system. At the same time they provide many predictions on the soil water process, including evaporation, transpiration, infiltration, drainage, soil water distribution, etc.

In practice it is far from clear how much input would be sufficient and what is the required accuracy of soil characteristics in model input for a reasonable prediction of soil water conditions in the field. Although model predictions will theoretically improve with increased accuracy of input soil properties, the extra effort must be justified by the degree of prediction accuracy required or gained (Rasmussen and Fluher 1990). Theoretically there is a unique relation between model inputs and model predictions. This has two implications:

First, the proximity between model predictions and the physical reality of the soil water system will improve as more and more accurate input information is provided. This relates to importance of inputs in model predictions. It must be considered when one attempts to validate the model by comparing model predictions with corresponding measured values. Also it must be taken into account when considering the requirement for the accuracy of input parameters for different applications with various requirements for model predictions. Secondly, if the desired output i.e. various attributes of soil water processes are known, the unique relation between model input and output can be used to determine the values of input parameters.

Inverse parameter estimation methods have been used to determine soil hydraulic properties from transient flow measurements (refer to Kool et al., 1987 for a review). In this approach hydraulic functions are assumed to be described by deterministic expressions that contain a small number of unknown parameters. The problem of determining hydraulic functions thus becomes a problem of determining values of the unknown parameters. Estimates of these parameters are made from minimizing deviations between observed and predicted values of some soil water flux-controlled attributes, such as transient soil water contents or drainage fluxes. Zachmann et al. (1981) compared four parameter identification or indirect methods and one direct simulation method used for estimation of soil hydraulic properties of a draining column. For the indirect approaches, some easily measured auxiliary data, such as volumetric water content or capillary pressure head at some fixed location as a function of time, or cumulative discharge from a draining column, were obtained. The parameters were then adjusted until the calculated output of the mathematical model simulating the experimental flow systems agreed with the measured auxiliary data. "For the sample problem considered", they concluded, "the method that used cumulative discharge data to estimate hydraulic functions performed the best". Kool et al. (1987) set a number of conditions for obtaining accurate solutions of the parameter estimation problems. These conditions mostly include knowledge of outflow volumes with time, but such information is not generally available in field studies.

Interestingly, Zachmann et al. (1981) determined that the method that used water content as measured auxiliary information to estimate hydraulic parameters ranked last, which means that different sets of hydraulic parameters could lead to prediction of similar water content values. Thus water content fails to distinguish among different soil hydraulic properties. Wopereis et al. (1993) used three different direct and calibration methods to generate hydraulic conductivity functions. Despite large differences obtained in hydraulic conductivity functions, simulated soil water contents were found to be comparable. Similarly, Wosten et al. (1990) did not find significant differences between the soil water storage simulated using four different methods to generate soil hydraulic functions.

One may argue that these studies imply that prediction of soil water is not uniquely related to soil hydraulic properties, or different combinations of hydraulic parameters could result in similar predicted water contents. In other words, in the application of soil water simulation models, if the objective is to predict soil water, accurate information on soil hydraulic functions may not be necessary. Further, solutions based on Richards' equation may not be necessary because of the insensitivity of their results to specific soil properties. In the same context, one could conclude that it is not appropriate to validate performance of water flow models based on water content simulation only. In spite of above observations, many evaluation studies have been performed on this basis (Clemente et al., 1994, for example).

Simulation models, however complicated, are still a simplified version of the physical reality. For example, many natural properties of soil such as heterogeneity and hysteresis are often ignored or greatly simplified in soil water models. Such simplifications make models less perfect, therefore, the models need to be validated. In many cases, required input parameters are estimated, which may result in errors in model predictions. The effect of such prediction errors and the importance of increased accuracy in predictions from improved estimation of input parameters, if available, need to be assessed. These depend on the particular process of interest.

I evaluated (chapter 2) the performance of both LEACHW and *ecosys* models in simulating $\theta(t, z)$, i.e. change in water content with respect to time and space. Despite the fact that these models require different intensities of input-data, both models predicted similar soil water storage. Results from this study, in addition to other evidences in literature (Zachmann et al., 1981; Wosten et al., 1990; Wopereis et al., 1993) indicate that prediction of soil water content is not particularly sensitive to soil hydraulic parameters.

Many water flow simulation models, such as LEACHW and *ecosys*, use Campbell's model (1985) to represent the hydraulic functions. In this study a sensitivity analysis is conducted on the importance of accurate estimation of the parameters used in soil hydraulic functions described by Campbell for simulation of soil water storage. Such study can provide guidelines on the level of accuracy necessary in obtaining measurements of soil hydraulic parameters prior to simulation of various soil water attributes. In addition, it is discussed (i) whether simulation of volumetric water content would constitute proper evaluation of soil water flow models, and (ii) the limitations for the use of models such as LEACHW and *ecosys*.

3.2 Theory and Methods

3.2.1 *Simulation model*

LEACHW is one of the five versions of the LEACHM model that simulates the water regime in unsaturated or partially saturated soils (Hutson and Wagenet, 1992). LEACHW is based on a node-centered Crank-Nicholson finite difference solution of Richards' equation that simulates transient vertical flow in a heterogeneous soil profile. Vertical soil heterogeneity is represented by a number of horizontal layers of equal thickness, each with different hydraulic properties. This model was used in this study for simulation of water flow for a range of hydraulic function parameters. Since many of water simulation models (*ecosys*, for example) use similar hydraulic functions, results of this study would be typical of other models.

Campbell's empirical hydraulic functions (1985) that represent the transient conditions of both soil water characteristic function and soil hydraulic conductivity function for $h < h_e$ are as follows:

$$h(\theta) = h_e(\frac{\theta}{\theta_s})^{-b} \tag{1}$$

$$K(\theta) = K_s(\frac{\theta}{\theta_s})^{m} \tag{2}$$

where

$m = 2b + 3$,

h = matric potential (m),

h_e = air entry water potential (potential at which the largest water filled pores drain, or intercept of $ln\ h$ versus $ln\ \theta$) (m),

b = the slope of $ln\ h$ versus $ln\ \theta$,

θ = volumetric water content ($m^3 m^{-3}$),

K = hydraulic conductivity (ms^{-1}) and

the subscript s denotes respective saturated values. Campbell's hydraulic functions can, therefore, be characterized as:

$$h(\theta) = f(h_e, b, \theta_s) \tag{3}$$

$$K(\theta) = g(h_e, b, \theta_s, K_s) \tag{4}$$

Although h_e and b are both empirical parameters obtained by fitting a straight line to the $ln(h)$ versus $ln(\theta)$ relation, they also have some physical significance (Campbell, 1985). Simulation models using Campbell's hydraulic functions thus require h_e, b and K_s as inputs.

3.2.2 *Field experiment*

Soil water was monitored continuously throughout the growing season of 1995. Using buried TDR probes, volumetric soil water content, in two adjacent fallow plots, was measured every half an hour. The probes were installed vertically to represent average water content of the uppermost 20 cm of soil surface. Further details on the field experiment are discussed in Chapter 2.

Measured water contents for the "wet" period of 1-6 July and the "dry" period of 20-29 August 1995 were used for this sensitivity analysis. Because of the intense rainfalls during 1-6 July 1995, this period was selected to represent the dynamic state of soil water content in the upper 20 cm of the soil profile. In addition, the period of 20-29 August 1995 was used to represent the gradual drying of the soil.

In addition, consecutive multiple measurements of water content were made in the top 15 cm, during the growing season of 1993. These measurements were made at weekly intervals, by manual insertion of the probes at different locations of a plot. Variability among these measurements gives an indication to the extent of spatial variation of soil water contents.

3.2.3 *Data Analysis*

A sensitivity analysis on importance of accurate hydraulic parameters for simulation of soil water contents was conducted by comparing measured water contents with simulated ones, produced by LEACHW, using a range of values for h_e, b, and K_s parameters.

A quantitative procedure adopted from Smith et al. (1996) was used for this analysis. The procedure involved calculation of the average difference between the measured and simulated values (*ME*), the relative error (*RE*) as a proportion of the measurement and standard error of estimate (*SE*) root mean square of the difference between the predicted and the observed values, which is often proportioned against the mean observed value as relative standard error of estimate, *RSE* (Clemente et al., 1994, Smith et al., 1996). Details about and implications of these parameters have been presented previously (Chapter 2) and are not repeated here.

Simulation models generally divide the soils into a number of horizontal layers, having uniform physical characteristics throughout each layer. According to this assumption, predictions of water contents within a plot at a common depth would, then, be the same throughout the layer. Significance of variations among a number of observed water contents at common depths is used to examine the validity of this assumption. Furthermore, variability in the range of values of soil water measurements within a plot, at different times, are used to explore the temporal variability of soil condition during a growing season.

3.3 Results and Discussion

3.3.1 *Estimated soil hydraulic parameters*

LEACHW represents the vertical heterogeneity of soils by a number of uniform horizontal layers. The soil profile from the surface to the lower boundary was divided into 5-cm increments in this study. Physical properties of soil, available from previous studies (Agriculture Canada, 1989), were used in Campbell's equations to calculate the "estimated" values of h_e, b and K_s for each layer (Table 3.1).

3.3.2 *Sensitivity of soil hydraulic parameters*

3.3.2.1 *Air entry value, h_e*

To test for the sensitivity of variability in h_e values to the simulation of water content profiles, two possible extreme values of -0.6 kPa and -8.0 kPa (Campbell,1985), corresponding to maximum pore sizes of 500 μm and 38 μm respectively, were used for simulation of soil water during the "wet" period. The less negative values of h_e correspond to the larger pore size, which is assumed to be correlated to particle size. The simulated moisture contents were then compared with observed values (Table 3.2). Similar results were obtained for the two extreme values, which indicate that simulated water content results are little sensitive to the values of air entry potential. The calculated h_e values ranged between -1.22 and -2.37 kPa for different depths (Table 3.1) and were used for the different scenarios throughout this study.

3.3.2.2 *Slope of ln h versus ln θ, or b value and saturated hydraulic conductivity*

Campbell (1985) stated that the expected range of b values would be from 2 to 24 in typical soils. The higher values of b represent soils with more widely distributed particle sizes. The expected values of hydraulic parameters, calculated from physical properties of distinct soil layers are presented in Table 3.1.

From a number of measurements using undisturbed soil samples from the surface layer, Haderlein (1995) developed least square equations of $K(\theta)$ for the Breton site with different tillage treatments. The general equation (not considering surface tillage treatments) for the site was:

$$-\log(K) = 14.7 - 15.7(\theta) \qquad R^2 = 0.72 \qquad (5)$$

where K is the hydraulic conductivity in $m\ s^{-1}$. Using this equation and the saturation water content of θ_s = 0.49 (Agriculture Canada, 1989), the saturated hydraulic conductivity of $K_s \cong 10\ mm\ d^{-1}$ is found. Considering the fact that hydraulic conductivity values are highly variable and many samples are required for a reliable estimate (Warrick and Nielsen, 1980), in addition to the extent of variability was found among hydraulic conductivity data in Breton site, particularly near saturation (Haderlein, 1995), the "estimated" value of $K_s \cong 123\ mm\ d^{-1}$ from Campbell equation seems to be reasonable. The calculated values of b and h_e, from the best fit line through measured $h(\theta)$ results for the Breton site (Haderlein, 1995), were 18.2 and -4.3 kPa, respectively. These values are within the range of b and h_e used in this study.

Saturated hydraulic conductivity (K_s) values of one order of magnitude smaller and also one and two orders of magnitude greater than the "estimated" value ($K_{s(est)}$), i.e. $0.1\,K_{s(est)}$, $10\,K_{s(est)}$ and $100\,K_{s(est)}$, were used in the analysis, to represent an extensive range of soils with variable range of physical and hydraulic characteristics. The $0.1\,K_{s(est)}$ value used in this analysis closely corresponds to the K_s value obtained by Haderlein (1995). Each of these hydraulic conductivity values was combined with b values ranging between 2 to 24. The extent of input parameters that were used in this analysis represent a wide range soils with different pore size distribution and hydraulic properties. These representations are expected to result in highly variable soil water retention and transmission characteristics. Because of the fact that accurate measurement of these soil properties is not feasible and estimation methods have high degrees of uncertainty, this sensitivity analysis could highlight the importance of obtaining accurate soil parameters for the purpose of prediction of soil water contents.

Simulated and observed results were compared graphically in figs. 3.1-3.8 for the "wet" period and the "dry" period respectively. Despite the large range of values of hydraulic parameters used for simulations, the results indicate that, aside from "extreme" cases where saturated hydraulic conductivity values of 10 or 100 times greater than estimated value were combined with b=2, corresponding to a soil with extreme particle size uniformity, for any combinations of hydraulic parameters the predicted results were similar, i.e. their responses to intense rainfalls and/or during drying periods were similar. In addition, predicted soil water contents deviated systematically from observed values, i.e. result in nearly parallel lines. The overall shapes of the prediction and measured curves are similar. Water retention increases with b and decrease with K_s. Lower b values represent soils with higher pore size uniformity, i.e. most of soil moisture is held within a smaller range of suction (close to h_e) and therefore drains easily. Similarly higher values of K_s correspond to soils with higher hydraulic conductivity, therefore, lower retention capacity. As a result predictions of soil water retention with b = 2, especially when combined with higher hydraulic K_s, were consistently lower than the measured results. Other combinations of hydraulic parameters resulted in overestimation of measured results, but at a lesser extent. Such deviation were observed for both "wet" and "dry" simulation periods.

Based on the measured results, no immediate response was observed to the major rainfall (13.8 mm) on 1st of July. Interestingly, prediction results using $\frac{K_s}{K_{s(est)}}=0.1$ reproduced such a lag of response (Fig. 3.2). This observation could be attributed to the presence of surface crusts, which is likely in Luvisolic soils.

During the "dry" period, simulation of soil water content using lower values of b, indicate a higher rate and degree of water loss from the upper soil layer as compared with observed results. Since the slope of water depletion is fairly linear following the rainfalls, indicating a constant rate of water loss, this deviation could be attributed to high prediction of evaporation, rather than drainage losses. The latter would have resulted in a higher rate of water loss immediately after rain.

Statistical comparisons of the estimated and observed results for the "wet" and the "dry" periods are presented in Tables 3.4 and 3.5, respectively. According to the values for *ME*, for the "extreme" cases, the model greatly underestimated the observed soil water contents (Tables 3.3 and 3.4). For all other combinations of hydraulic parameters, predicted results showed overestimation of 0 to 4% (*ME*) of the observed water contents. In addition, similarity between absolute values of standard error (*SE*) and error of estimate values (*ME*), for every scenario, is an indication of a systematic under or over estimation of observed results for any individual scenario. This is in agreement with the generally parallel positions of the observed and predicted lines in Figs. (3.1-3.8).

Excluding the extreme cases described above, average values of *ME* and *SE* obtained for any combination of $\frac{K_s}{K_{s(est)}}$ with b were 0.025 and 0.035 for the "wet" period, and 0.02 and 0.04 for the "dry" period. These results are comparable with those obtained using the expected values of b and K_s (Table 3.3).

Theoretically, values of b and K_s, using the physical properties of soil for every discrete soil layer (Campbell, 1985), should be used for simulation. Due to the natural heterogeneity of soils, collection of such information is both expensive and time consuming. Still, our results using inaccurate values of these parameters were not substantially less accurate than the results obtained from "estimated" hydraulic parameters using actual physical properties of each soil layer. These results suggest that factors other than b and K_s are more important in controlling the change in water content of upper soil horizons.

As depicted in Figs. 3.1-3.8, the predicted soil water contents for any combinations of hydraulic parameters are generally parallel with, i.e. systematically deviate from the observed values. In effect, any set of predicted results can be corrected to closely represent observed soil water content. Using only a few observations, the correction can be made by drawing a line through the observed values in a general trend with any set of predicted results.

For example, predicted results using $b = 24$ and $\frac{K_s}{K_{s(est)}} = 100$ were systematically decreased by 0.03 m^3m^{-3} (Fig. 3.9), keeping the initial condition the same. The "corrected" results are in close agreement with observed values. Considering natural variability of field soils, and uncertainty involved in estimation methods, in many cases this calibration procedure is simpler than collection of detailed information on physical properties of soils for estimation of hydraulic properties.

However, as we have described in the previous chapter, replicate observations of soil water contents within a plot are often quite different. For example, four sets of measurements at a 10-cm depth taken within close proximity resulted in relatively different soil water contents (Fig. 3.10). Interestingly, the spatial variation of these measurements resulted in lines approximately parallel to each other, similar to the behavior of the predicted soil water contents for different combinations of b and K_s. The fact that separate measurements are in parallel over time indicates that a point having high soil water content at one time is likely to have high values throughout the season. Thus factors that control soil spatial variability in the field were not disturbed during the season, leading to a persistent spatial variability pattern that was not time dependent. This observation, an indication of soils heterogeneity, is further examined in the following section.

3.3.3 Heterogeneity analysis

In many simulation models, soil profile is represented by a series of horizontal layers with different properties to represent the variability of soil between horizons. Soil properties within each layer are assumed to be uniform, and no allowance is made possible variation in the horizontal direction. The soil water content simulated by these models is thought to represent the mean conditions within each of the soil layer. However, field observations have shown repeated significant variations in soil water content in the horizontal direction, which is not represented in these models. Measured soil water variations across the horizontal direction, at a common depth and time, can be used to reflect the heterogeneity of the soil and the adequacy of the models.

For the earlier part of the growing season of 1993 (month of May) the average standard deviation of observed soil water contents was 0.024 m^3m^{-3}, whereas later in the season (months of July and August) the standard deviation dropped to 0.013 m^3m^{-3} (Table, 3.7). Such variation in soil water measurements, resulting from spatial heterogeneity of soils, are comparable in magnitude to variations (*SE*) among simulated results, using widely different soil hydraulic parameters. In addition, variability in observed water contents is larger during the earlier parts of the season. Settlement of soil as a result of the first few rains following tillage probably creates a uniform soil condition.

The fact that replicate soil water measurements within close proximity resulted in parallel $\theta(t)$ curves (e.g. Fig. 3.10), and the fact that simulation of soil water contents for different combinations of hydraulic parameters are also parallel (Figs. 3.1-3.8), indicates that different set of measurements could be closely simulated with widely different parameters. There are cases where variability of b and K_s within a field must be known as an assessment of soil heterogeneity. This assessment, however, is both time consuming and expensive. For example, Warrick and Nielsen (1980) suggested that 1300 samples are required for estimation of the mean value of hydraulic conductivity, which is generally not feasible.

Based on our results such variability can be represented by different but limited sets of soil water measurements. Intensive readings at limited locations would provide a detailed temporal representation, but poor spatial representation of the variability. On the other hand, a large number of measurements throughout the field, at selected times, would provide a good representation of spatial variability and average field condition, with no detailed temporal representation. Combination of these two options would be ideal, because of the fact that different points are likely to produce parallel $\theta(t)$ lines. The actual number of measurements depends on the required accuracy of estimation (Warrick and Nielsen, 1980), which could vary according to the specific purpose.

Validation of simulation models based on one or two sets of measurements would not be very valuable because one set of simulation results could be in agreement with a set of measurements and in difference with another set of measurements. Therefore, contrary to the common approach, evidence of proper soil water simulations, based on their comparison with limited measurements of water contents, are not sufficient for complete evaluation of water flow models. In addition, although proper simulation of soil water would be valuable for studies such as design of irrigation systems, it should not directly be translated as the model being applicable for environmental studies, for which the prime objective would be prediction of discharge fluxes.

3.4 Summary and Conclusions

In this study various combinations of hydraulic parameters were used to simulate the transient status of soil water content during a six-day wet period and a nine-day dry period. The simulated results were then compared with the observed values. For the entire range of possible b and h_e values, and a range of three orders of magnitudes of K_s values (similar to the range of possible values for K_s), the predicted water contents systematically deviated from the observed results i.e. variation of predicted values over time resulted in generally parallel lines with respect to the observed values. Similarly, replicate measurements of soil water content were parallel over time. In many cases, pedotransfer estimation of hydraulic parameters have shown to be uncertain, which has led to calibration of the predictions based on such methods. Alternatively it is proposed that the predicted results using any combination of hydraulic parameters could be easily "corrected" using a few observed values. This procedure resulted in close reproduction of measured results. The correction procedure is much simpler than alternative methods which require parametric representation of the heterogeneous physical properties of soils.

The results obtained in this study are limited to the simulation of soil water content, and should not be expanded to simulation of other components of water balance equation. In the same context we propose that evaluation of models based on proper simulation of soil water contents alone should not be interpreted as validation of the model for simulation of other components of water balance equation, such as drainage fluxes.

The importance of accurate predictions of soil water contents is not to be minimized here. Systematic deviation of predicted water content from actual conditions which results in consistently higher or lower soil water content predictions, even by a few percent, could have extensive implications to growth of plants or may lead into huge amount of water in large scales. Therefore, irrigation designs, for example, based on such predictions could result in over- or under-application of water.

Lastly, the results of this study showed that soil water simulation is not particularly sensitive to hydraulic properties. Large variation in hydraulic properties resulted in relatively small changes in simulated soil water contents. The deviations between predictions from observed results were systematic.

Differences in soil water fluxes, e.g. evaporation and drainage fluxes, resulted from variability in hydraulic parameters could be substantial. This was not examined in this analysis. However, for the purpose of predictions of soil water changes, the extra effort in obtaining more accurate hydraulic properties of soils may be expected to result in only minor improvements. Therefore, because of insensitivity of simulated soil water content to hydraulic properties, it may be possible to substantially simplify the representation of storage of water in soils without a detrimental effect on prediction accuracy. This option is further explored in next chapter.

Table 3.1 Expected values of hydraulic parameters using the physical properties of the soil.

Soil depth (cm)	0-15	15-30	30-110	110-150
h_e (kPa)	-2.4	-1.3	-1.9	-1.2
b	3.9	6.4	9.1	8.6
ρ_b (Mgm^{-3})	1.35	1.4	1.5	1.5
K_s (mmd^{-1})	123	62.7	17.7	18.5

Table 3.2 Statistical analysis of estimated vs. observed water contents($m^3 m^{-3}$) using two possible extreme values of h_e as compared with observed results, for the wet period of 1-6 July 1995.

h_e (kPa)	-0.6	-8.0
ME	0.05	0.04
RE	0.17	0.14
SE	0.05	0.04
RSE	0.18	0.15

Table 3.3 Statistical analysis of estimated vs. observed water contents ($m^3 m^{-3}$), using estimated values of b and K_s values obtained from available physical properties of soil, as compared with observed results, for the wet period of 1-6 July and the dry period of 20-29 August1995.

	1-6 July	20-29 August
ME	0.04	0.01
RE	0.13	0.04
SE	0.04	0.02
RSE	0.14	0.06

Table 3.4 Statistical analysis of estimated water contents ($m^3 m^{-3}$), using different combinations of b and K_s values as compared with observed results, for the wet period of 1-6 July 1995.

b	2	4	8	12	16	20	24
				$K_s / K_{s(exp)}$ =100			
ME	-0.11	-0.03	0.02	0.03	0.03	0.03	0.03
RE	-0.59	-0.12	0.05	0.09	0.10	0.10	0.10
SE	0.12	0.05	0.03	0.04	0.04	0.04	0.04
RSE	0.63	0.18	0.09	0.11	0.11	0.12	0.12
				$K_s / K_{s(exp)}$ =10			
ME	-0.06	0.01	0.02	0.03	0.03	0.03	0.04
RE	-0.24	0.02	0.07	0.10	0.10	0.11	0.11
SE	0.07	0.02	0.03	0.04	0.04	0.04	0.04
RSE	0.28	0.07	0.09	0.11	0.12	0.12	0.13
				$K_s / K_{s(exp)}$ =1			
ME	-0.01	0.01	0.03	0.03	0.04	0.04	0.04
RE	-0.04	0.04	0.10	0.12	0.12	0.12	0.13
SE	0.02	0.02	0.04	0.04	0.04	0.05	0.05
RSE	0.07	0.07	0.12	0.14	0.15	0.15	0.16
				$K_s / K_{s(exp)}$ =0.1			
ME	0.00	0.01	0.02	0.03	0.03	0.03	0.03
RE	-0.01	0.02	0.07	0.08	0.08	0.08	0.09
SE	0.03	0.02	0.03	0.04	0.04	0.04	0.04
RSE	0.09	0.07	0.10	0.11	0.12	0.12	0.13

Table 3.5 Statistical analysis of estimated water contents ($m^3 m^{-3}$), using different combinations of b and K_s values as compared with observed results, for the dry period of 20-29 August 1995.

b	2	4	8	12	16	20	24
				$K_s / K_{s(exp)}$ =100			
ME	-0.14	-0.06	0.00	0.01	0.01	0.03	0.04
RE	-0.47	-0.19	0.00	0.03	0.04	0.09	0.12
SE	0.14	0.06	0.01	0.01	0.02	0.03	0.04
RSE	0.48	0.19	0.03	0.04	0.06	0.10	0.13
				$K_s / K_{s(exp)}$ =10			
ME	-0.10	-0.03	0.00	0.01	0.02	0.03	0.04
RE	-0.33	-0.11	0.00	0.02	0.07	0.11	0.13
SE	0.10	0.04	0.01	0.02	0.03	0.04	0.05
RSE	0.34	0.12	0.04	0.05	0.09	0.13	0.15
				$K_s / K_{s(exp)}$ =1			
ME	-0.04	-0.02	0.01	0.03	0.04	0.05	0.05
RE	-0.14	-0.06	0.02	0.09	0.13	0.16	0.18
SE	0.06	0.04	0.03	0.04	0.05	0.06	0.07
RSE	0.18	0.13	0.11	0.15	0.18	0.21	0.23
				$K_s / K_{s(exp)}$ =0.1			
ME	-0.03	-0.01	0.02	0.03	0.04	0.05	0.05
RE	-0.08	-0.02	0.06	0.11	0.14	0.15	0.16
SE	0.04	0.03	0.04	0.05	0.06	0.06	0.07
RSE	0.13	0.11	0.14	0.18	0.20	0.22	0.22

Table 3.6. Standard deviation of water content measurements within four plots during the growing season of 1993.

Date	Plot	Standard Deviation (%)	Average Standard Deviation (%)
May 3	E-1	2.4	2.4
	E-3	2.6	
	F-1	2.2	
	F-3	2.5	
May 14	E-1	3.1	2.3
	E-3	2.5	
	F-1	2.3	
	F-3	1.4	
May 30	E-1	2.1	2.4
	E-3	2.2	
	F-1	3.0	
	F-3	2.3	
July 16	E-1	1.5	1.3
	E-3	1.7	
	F-1	1.4	
	F-3	0.8	
July 30	E-1	0.9	1.15
	E-3	0.9	
	F-1	1.4	
	F-3	1.3	
Aug. 17	E-1	2.7	1.4
	E-3	1.7	
	F-1	0.8	
	F-3	1.4	

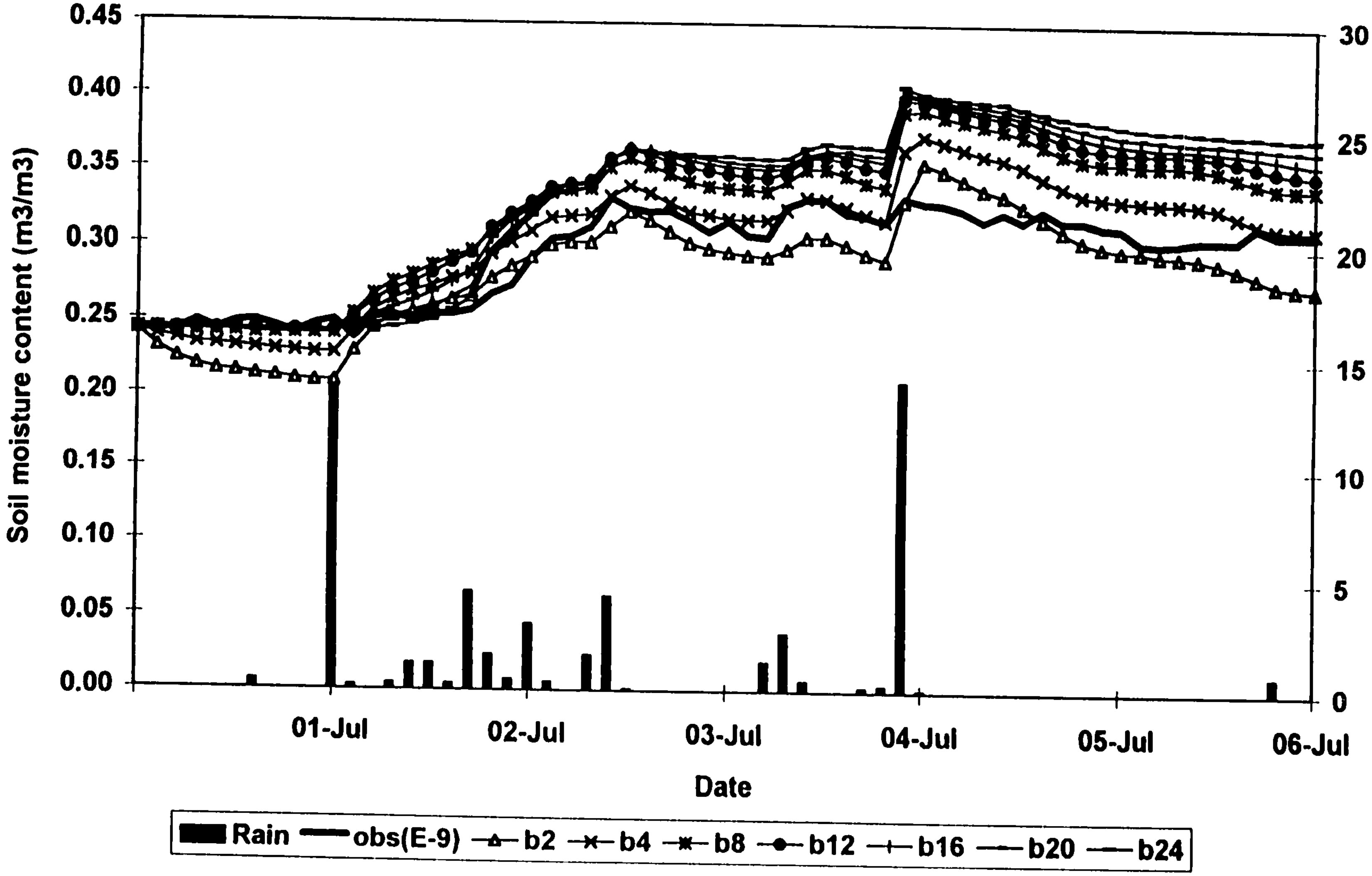

Fig. 3.1. Observed soil-water contents as compared with simulated results using a range of b values between 2-24 and K/K(est)=1 for the period of 1-6 July 1995.

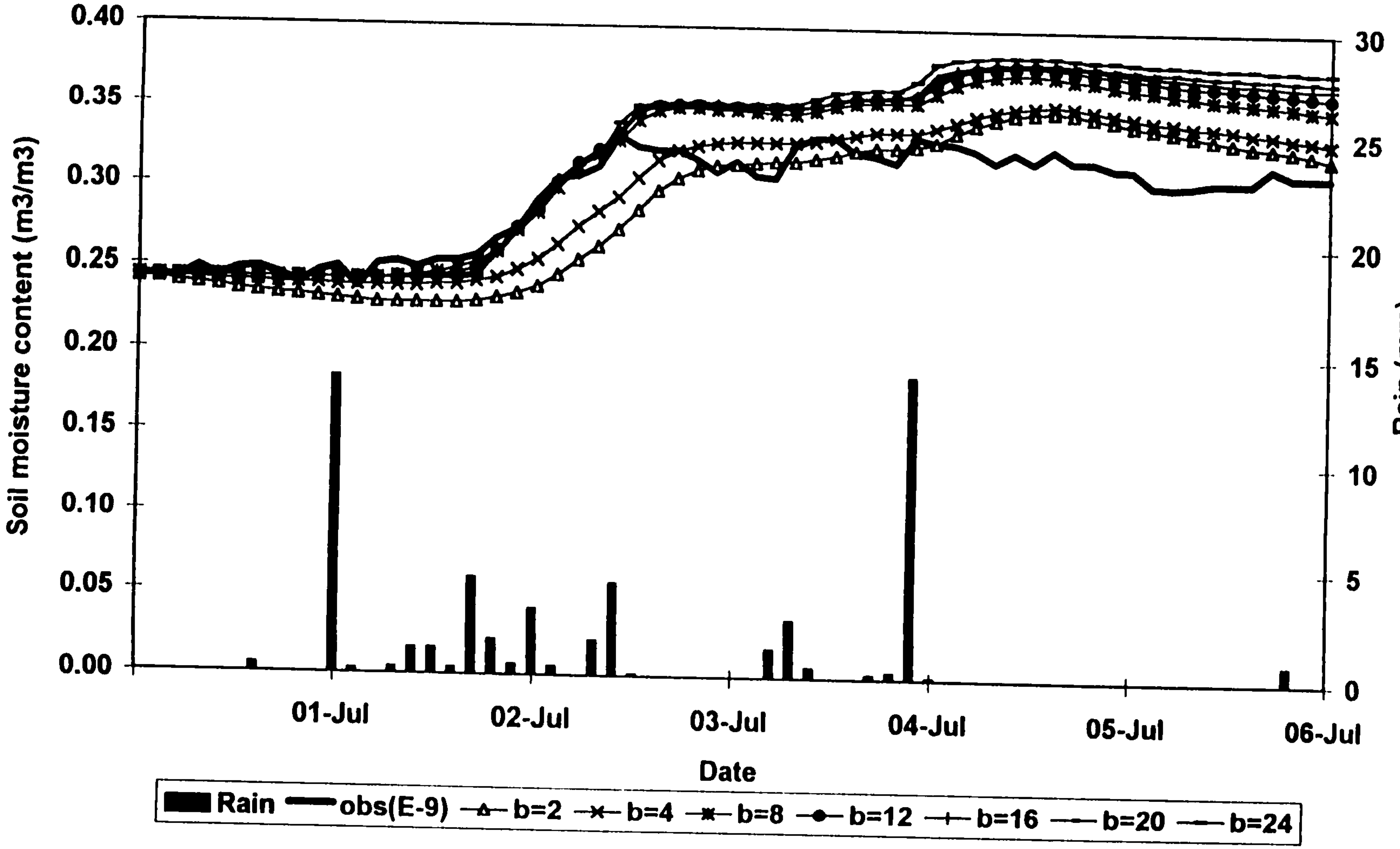

Fig. 3.2. Observed soil-water contents as compared with simulated results using a range of b values between 2-24 and K/K(est)=0,1 for the period of 1-6 July 1995.

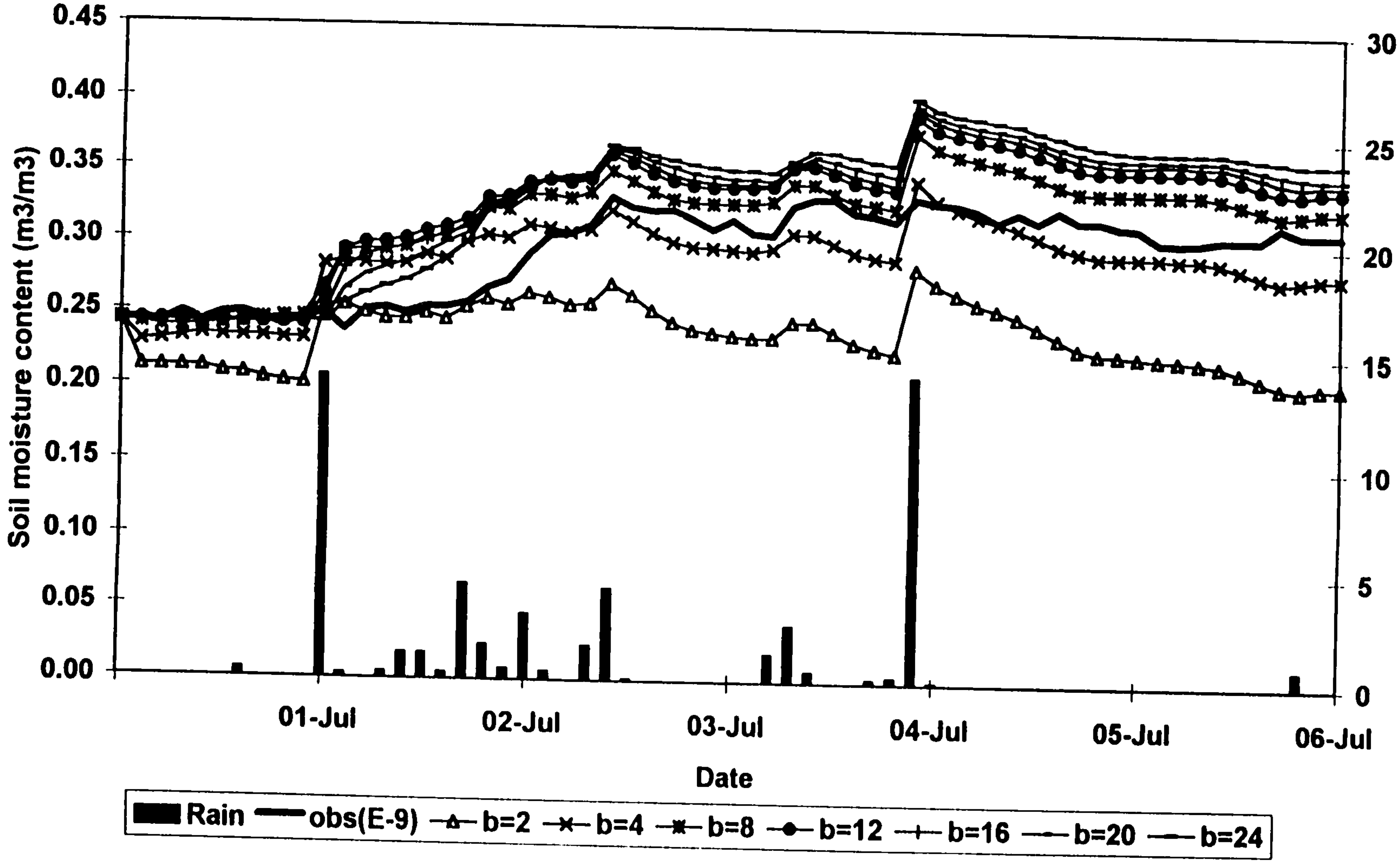

Fig. 3.3. Observed soil-water contents as compared with simulated results using a range of b values between 2-24 and K/K(est)=10 for the period of 1-6 July 1995.

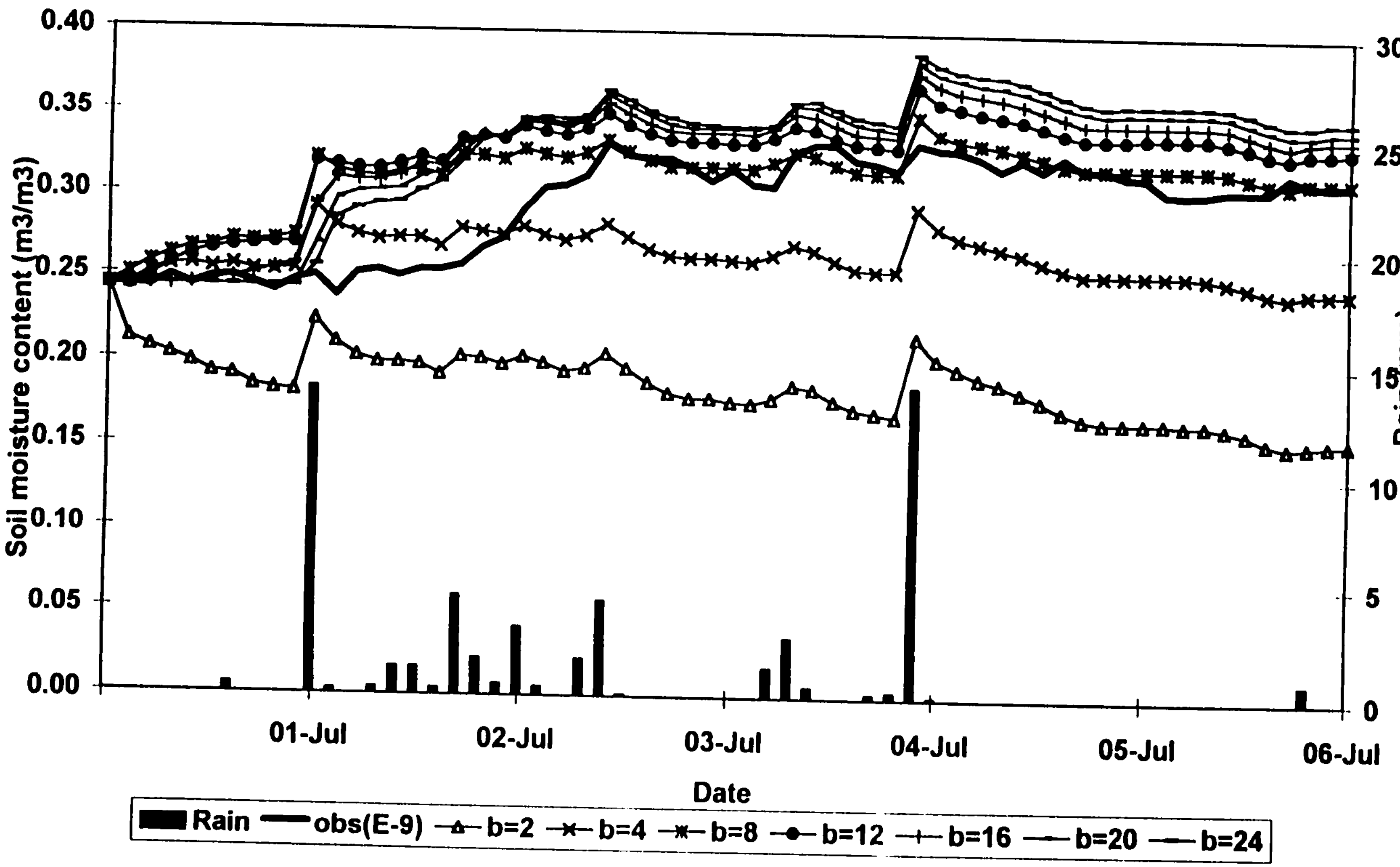

Fig. 3.4. Observed soil-water contents as compared with simulated results using a range of b values between 2-24 and K/K(est)=100 for the period of 1-6 July 1995.

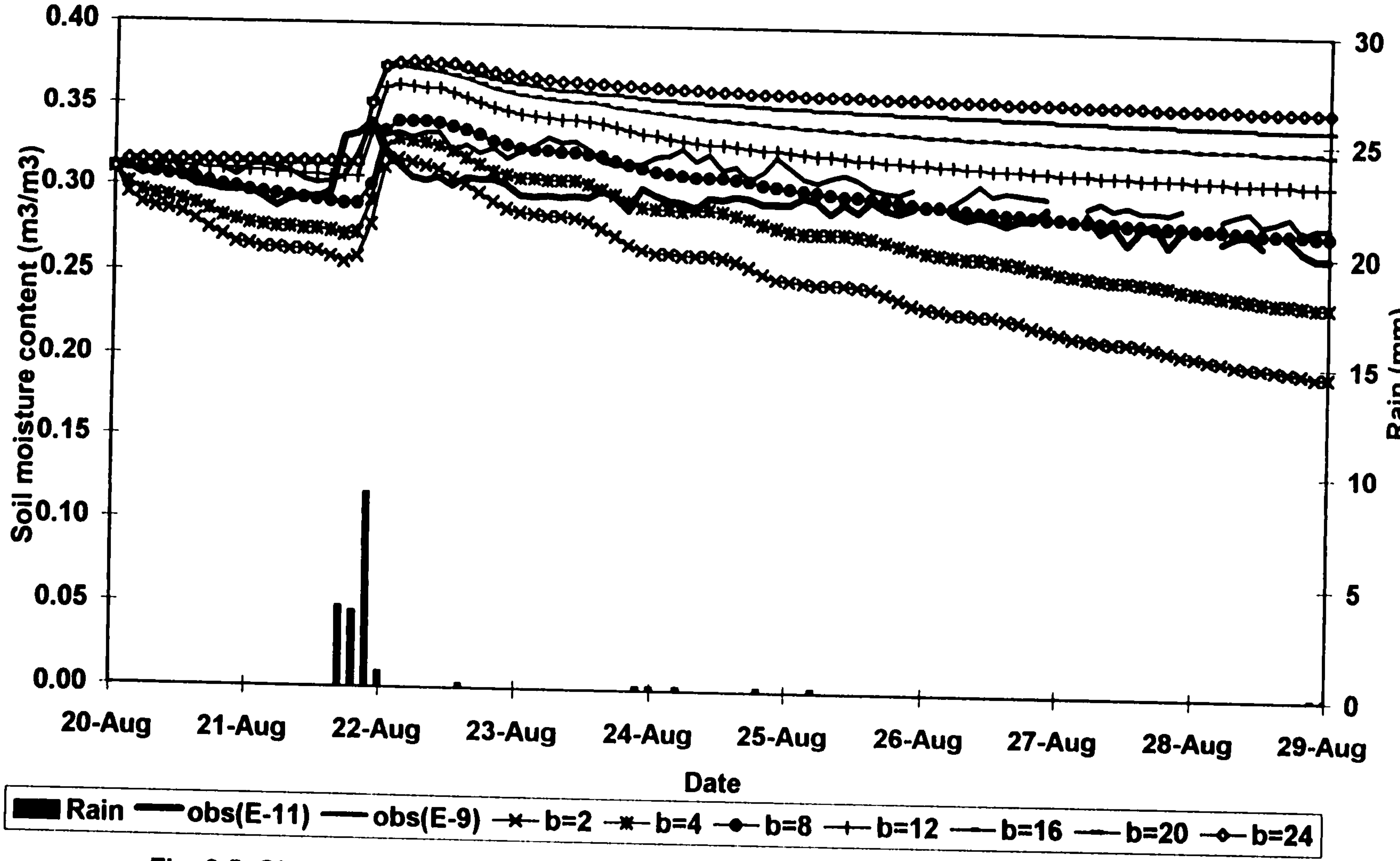

Fig. 3.5. Observed soil-water contents as compared with simulated results using a range of b values between 2-24 and K/K(est)=1 for the period of 20-29 Aug 1995.

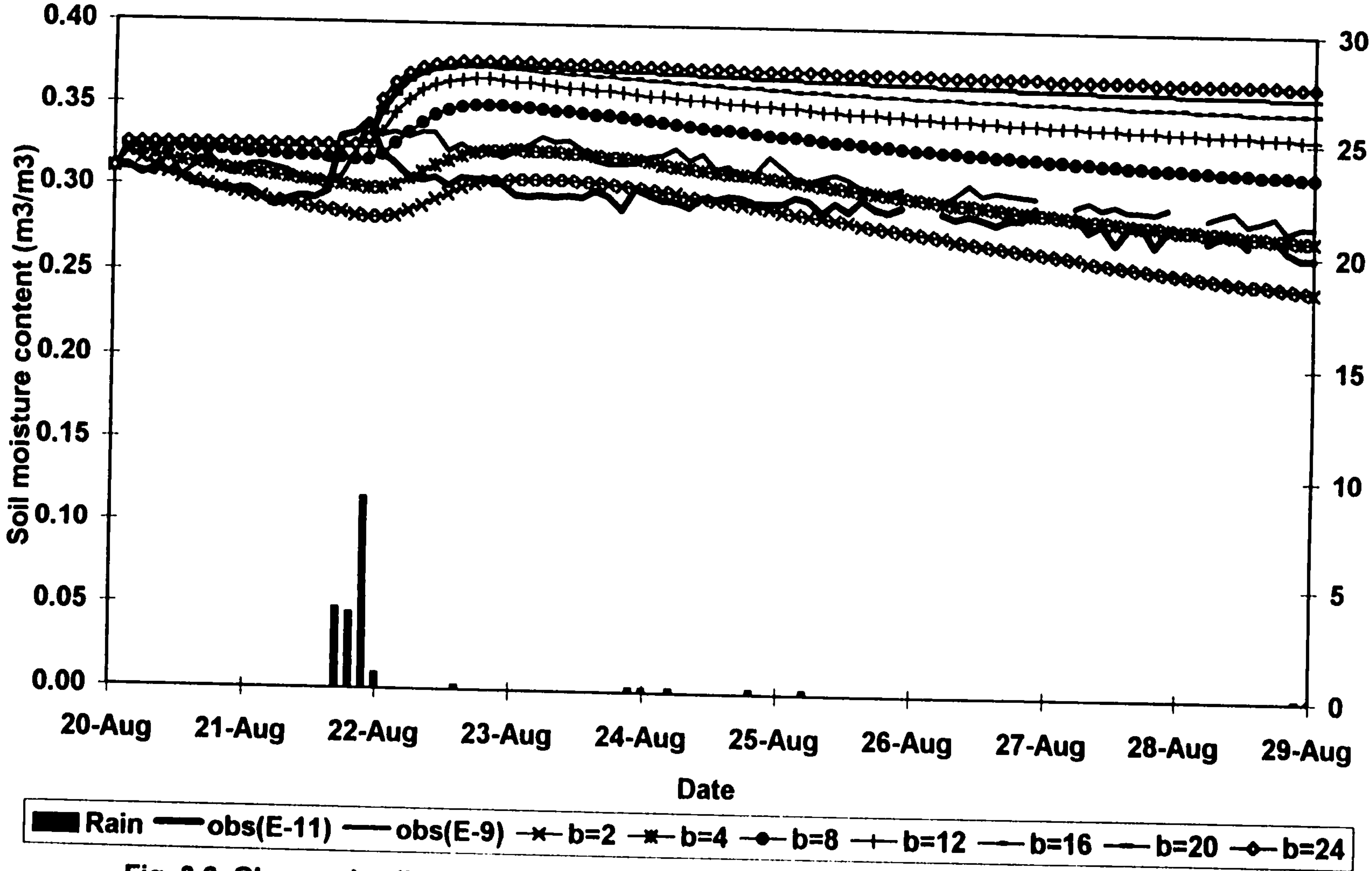

Fig. 3.6. Observed soil-water contents as compared with simulated results using a range of b values between 2-24 and K/K(est)=0.1 for the period of 20-29 Aug 1995.

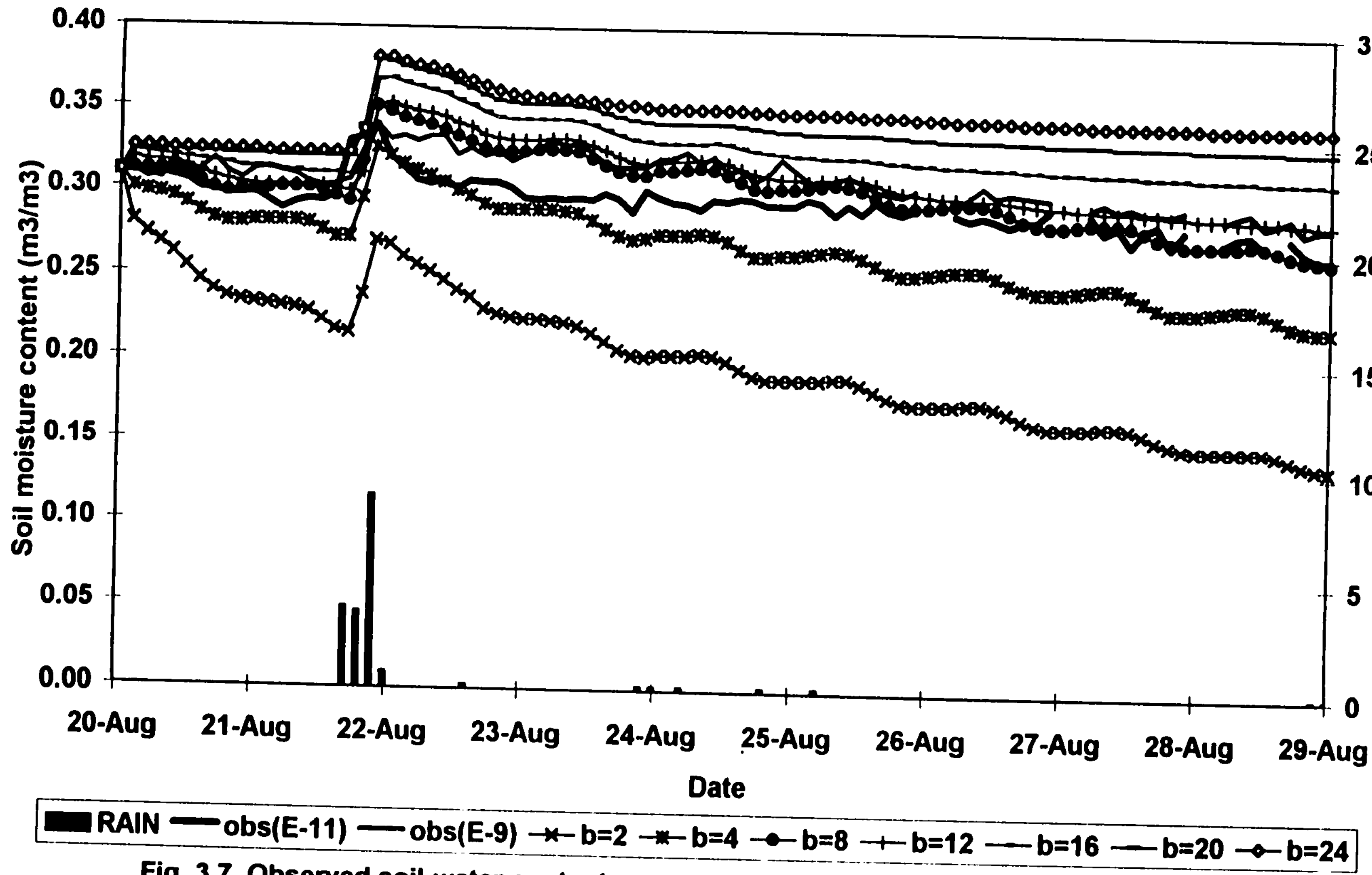

Fig. 3.7. Observed soil-water contents as compared with simulated results using a range of b values between 2-24 and K/K(est)=10 for the period of 20-29 Aug 1995.

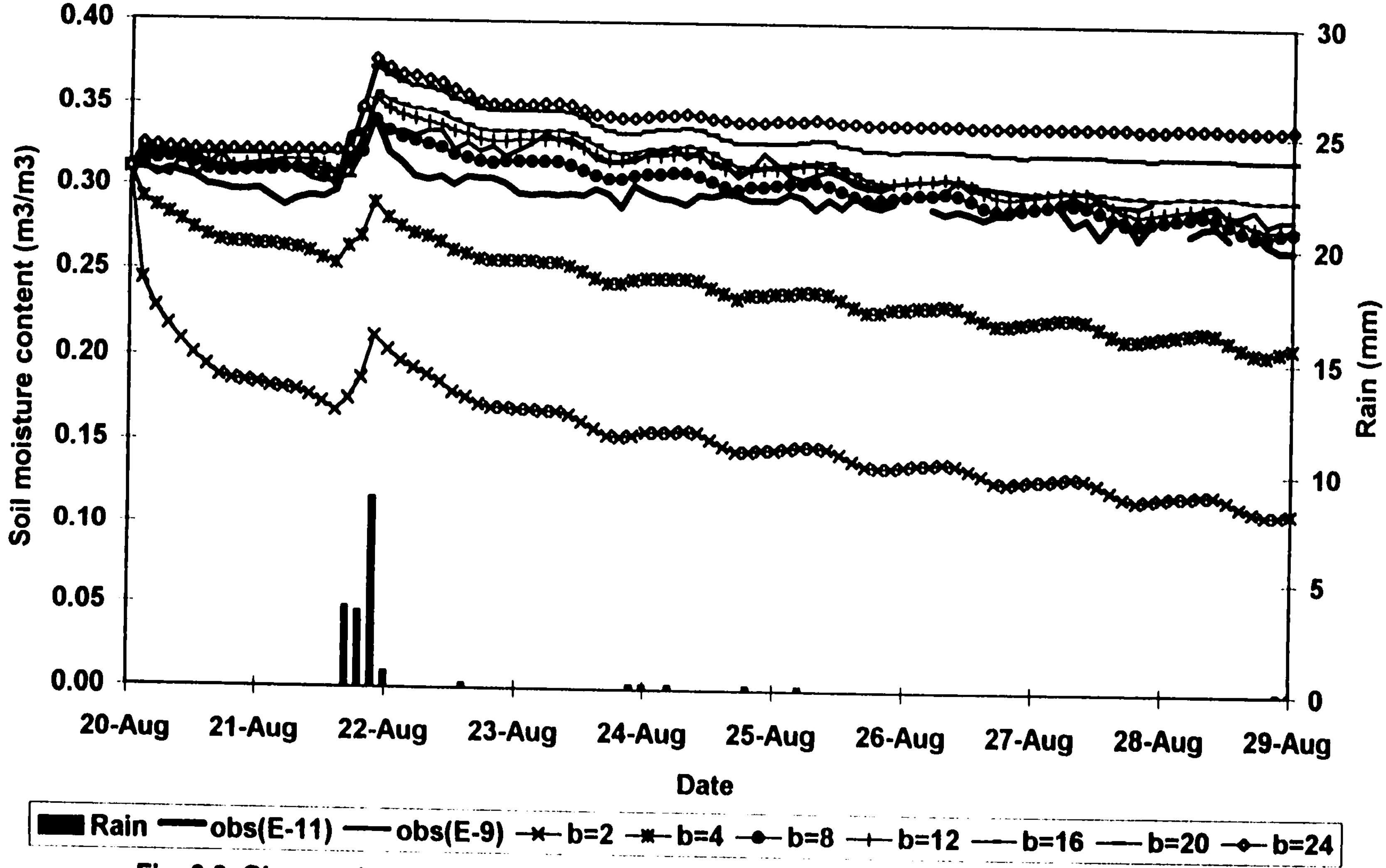

Fig. 3.8. Observed soil-water contents as compared with simulated results using a range of b values between 2-24 and K/K(est)=100 for the period of 20-29 Aug 1995.

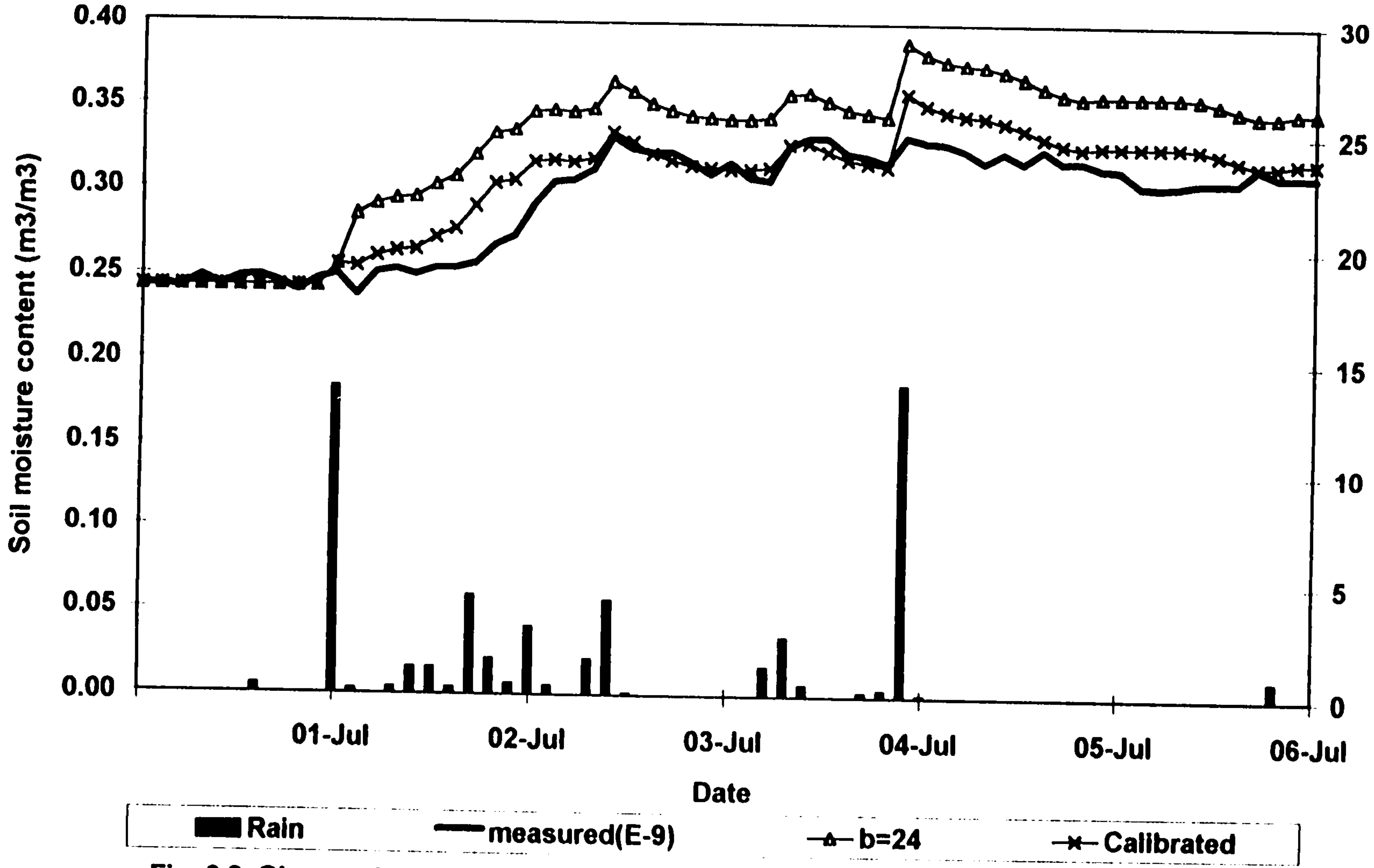

Fig. 3.9. Observed soil-water contents as compared with simulated results using a range of b values between 2-24 and K/K(est)=0,1 for the period of 1-6 July 1995.

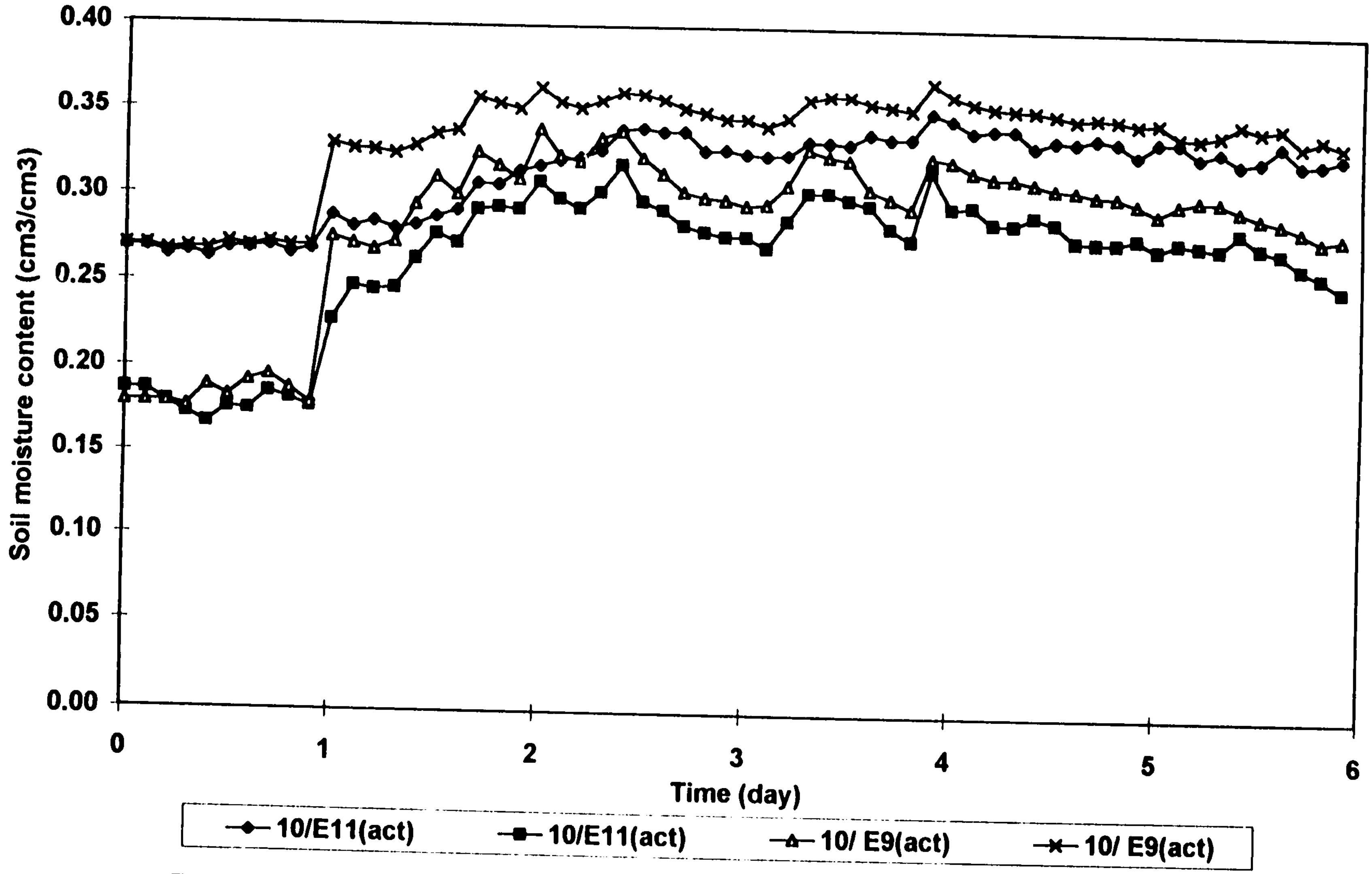

Fig. 3.10. Measured soil-water content at 10-cm depth, in two adjacent plots of E-9 and E 11, for the period of 1-6 July 1995.

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Chapter Four

A SIMPLE METHOD FOR PREDICTION OF TRANSIENT CHANGES OF SOIL WATER CONTENT

4.1 Introduction

Simulation of soil water dynamics and storage has received much attention in the past two decades (Addiscott and Wagenet, 1985; Clemente et al., 1994). These models are used for both agronomic and environmental management purposes. Storage and percolation of water in the soil is a primary concern in many regions of the world where agriculture is important (Ritchie, 1985). The main purpose of using soil water models is to asses the effect of water management schemes such as irrigation, drainage and soil improvement plans on the soil water balance of agricultural areas. Simulation of water status of the near-surface soil horizons is especially important because of its direct effect on plant growth and crop development, mass and energy transport processes between soil-plant ecosystem and atmosphere. In addition, environmental impacts of agricultural activities, such as nitrogen losses from soil-crop systems, are dependent on soil water status (Gabrielle et al., 1995).

Complex simulation models based on physical principles have been used to predict soil water status. Most of these models are based on Richards' equation that describes transient water movement in unsaturated soils (Jury et al., 1991). Numerical methods commonly used to solve these models require data on the relationship between soil water potential and soil water content $h(\theta)$, commonly referred to as the soil water retention curve, and the relationship between hydraulic conductivity and either the soil water potential or the soil water content $K(\theta)$ or $K(h)$. Measurement of these often highly variable unsaturated soil properties is expensive, time consuming, and labor intensive. As an alternative parametric functions using easily attainable soil properties such as particle size distribution and bulk density have been used to estimate soil hydraulic functions (Campbell, 1974; Mualem, 1976; van Genuchten, 1980). These models, however, are often associated with high degrees of uncertainty (Yates et al., 1992). This is especially true for prediction of hydraulic conductivity under field conditions. For instance, when van Genuchten's (1980) empirical relationship for describing the water-retention curve is coupled to the model of Mualem (1976) to predict unsaturated hydraulic conductivities, it was found that the method worked well for a sand and two silt loams but not for a clay (Yates et al., 1992). Such estimations can be improved by using measured conductivity values at some water content (Yates et al., 1991). Due to natural heterogeneity of soils, complete representation of soils would require a large number of observations to adequately characterize the spatial and temporal distributions of hydraulic parameters.

My study in Chapter three confirmed that simulation of transient soil water content is not particularly sensitive to the accuracy of the parameters used in soil hydraulic functions (Wopereis et al., 1993; Wosten et al., 1990; Kool and Parker, 1988; Zachmann et al., 1981). As a result, one may wonder whether soil parameters are essential for the purpose of soil water estimation, and whether it is possible to significantly simplify models such that they would only require parameters that soil water content is sensitive to.

Several soil water budget models have been developed to estimate the daily soil water balance. These models, which are generally based on meteorological observations, have the advantage of being applicable at large scales. A soil water budget involves calculation of the soil water as affected by the input and withdrawal of water in a soil profile for a given period of time. Variations of the soil water content are in response to the conditions at the boundaries of the system e.g. precipitation, evapotranspiration and drainage. These models are designed specifically for estimating changes in soil water. They are less input-data intensive as compared to process-oriented models, such as LEACHW and *ecosys*.

de Jong (1984) gave a detailed review of these earlier attempts. Baier and Robertson (1966) developed a "versatile" technique for estimation of soil moisture from standard meteorological data. The Versatile Soil Moisture Budget (VSMB) Model, similar to many soil water budget models, assumed potential evapotranspiration (ET_p) as a possible maximum of actual evapotranspiration (ET), and that water is extracted simultaneously from different depths of the soil profile permeated by roots in relation to the rate of ET_p and the available soil water in each zone. The model also assumed that the infiltrating water brought the water content of the top zone to field capacity and that the remainder would drain to the next zone. In this model calculation of ET, however, would require determination of various coefficients accounting for factors such as soil and plant characteristics and for adjustment of different types of soil dryness curves. This model has been modified and coupled into other models to describe specific processes in ecosystem. For example, Stuff and Dale (1978) developed a soil water budget model for describing the influence of a shallow water table and de Jong and Shaykewich (1981) for conditions under which an impermeable layer in the profile existed. Klein et al. (1989) used the VSMB Model to estimate the level of soil moisture stress at different stages of plant growth. The results were then used to estimate the yields of a given crop at a specific location and moisture stress.

The EPIC (Sharpley and Williams, 1990) and Ceres (Jones and Kiniry, 1986) simulation models have been developed for the modeling of various processes in the soil-crop system, and have been extensively tested and used for different scenarios. These models also use an approach similar to many soil water budget models for prediction of soil water content of the upper horizon. But these models still require parameters which are not readily available in many cases. For example, requirement of saturated hydraulic conductivity (K_s) can be a limiting factor by itself. Estimation of K_s based on pedotransfer functions have shown to be uncertain with respect to specific applications (Vereecken et al., 1992) and requires calibration with measured K_s.

In this study, it is assumed that the water status of the upper soil layer is mainly controlled by boundary conditions at the soil surface, and by soil water storage and transmission properties. Detailed soil information, such as hydraulic functions, may not be necessary for satisfactory prediction of soil water content. Simply stated, soil water content could be simulated with minimum consideration of variable nature of soil properties. Based on the above assumptions, a simplified model (SIMPLE) for predicting soil water, using the basic concepts of soil water balance, is developed. The model proposed in this study can be considered as a step toward simplification of existing soil water budget models, for the specific purpose of soil moisture prediction, without compromising the obtained accuracy. The model is validated under different conditions to assess its applicability at varying soil-plant-atmosphere ecosystems.

4.2 Theory and Method

The general equation describing the daily soil water balance can be expressed as:

$$\Delta W = (P + I) - (Dr + ET + R_o) \tag{2}$$

where

ΔW = change in soil water content (cm)

P = precipitation (cm),

I = irrigation (cm),

Dr = drainage or deep percolation (cm),

ET = evapotranspiration (cm) and

R_o = surface runoff (cm).

All quantities in the above equations are expressed in terms of depth units, i.e. volume per unit area, for the specified time period i.e. daily, in this model. Amount of runoff in nearly flat fields can be regarded as negligible in comparison with the major components of water balance. No irrigation is also applied in a dryland situation. The above equation for such conditions would then be reduced to:

$$\Delta W = P - (ET + Dr) \tag{3}$$

The daily change in soil water content for the modeled soil depth can be expressed as:

$$\Delta W = (\theta(t_2) - \theta(t_1))z \tag{4}$$

Combination of (3) and (4) would lead to:

$$(\theta(t_2) - \theta(t_1))z = [\int_{t_1}^{t_2} (P - ET - Dr)dt] \tag{5}$$

According to (5) the change in soil water content over a given depth of soil (z) is directly related to the cumulative difference of precipitation, evaporation and drainage fluxes hereinafter called net boundary flux, over the time period of $(t_2 - t_1)$ i.e. one day in this study. Based on our own earlier results (Chapter 2) and evidence from the literature (Ren, 1997; Haderlein, 1995) soil water changes mainly occurs in the upper soil layers, where the plant roots are active, and remains essentially steady at lower layers. As a result the soil water status of the surface layer is considered in this study.

4.2.1 Input data requirements

4.2.1.1 Soil storage properties

The most widely used storage properties relevant to plant growth is soil water content at field capacity (θ_{FC}), i.e. at 33 kPa matric potential, and soil water content at permanent wilting point (θ_{WP}), i.e. 1500 kPa matric potential. This input information is generally available for most soils.

4.2.1.2 Potential evaporation

Climatological data such as daily air temperature, net radiation, wind speed, relative humidity, and rainfall are used to estimate potential evaporation rate using Penman's equation (1948). Alternative methods, such as Linacre (1977), which require values of elevation, latitude, and daily maximum and minimum temperature for estimation of potential evaporation can also be used, if available data are limited. Actual evapotranspiration (*ET*) is usually estimated by multiplying potential evaporation by empirical factors to account for the effects of crop development and atmospheric demand (Stuff and Dale, 1978).

When the soil is wet, evapotranspiration occurs at the potential rate, which is limited by the amount of energy available at the soil surface, called a weather controlled stage according to Hillel (1982). If the rate of evapotranspiration is higher than the rate at which water is supplied from the soil, the surface layer becomes drier and evapotranspiration then becomes limited by the amount of water available. To adjust for the effect of soil water content on evapotranspiration, this process is assumed to take place in two stages. During the first or constant rate stage, the evapotranspiration takes place at the potential rate and is controlled by external conditions (Jury et al. 1991). During the second stage, or the falling rate stage, the rate of evapotranspiration decreases continuously with time as soil water content decreases. Stuff and Dale (1978), based on a number of reported studies, derived a relationship which showed that during the falling rate stage the ratio of actual to potential evapotranspiration ET / ET_p is linearly related to the total soil moisture deficit. Accordingly, it is assumed that actual evapotranspiration remains at its potential rate as long as the soil water content in the upper horizon is at or above field capacity, and to decrease linearly to zero at permanent wilting point (θ_{WP}), as described below:

$$ET = ET_p \qquad \text{when} \quad \theta > \theta_{FC} \qquad (6)$$

$$ET = ET_p\left(\frac{\theta - \theta_{WP}}{\theta_{FC} - \theta_{WP}}\right) \text{ when} \quad \theta_{WP} \le \theta \le \theta_{FC} \qquad (7)$$

4.2.1.3 Drainage

According to Richards' equation, movement of water is controlled by the hydraulic gradient and hydraulic conductivity in soils. Hydraulic conductivity is a nonlinear function of water content or matric potential. Water which is added to soils redistributes, as a result of induced hydraulic gradient until an equilibrium status is achieved.

The lower boundary condition of most soil water budget models allows deep drainage, during a daily time-step, as the excess amount of water above field capacity. As long as a hydraulic gradient exists between layers, water percolation persists, i.e. it actually does not stop at field capacity. However, as a result of soil water redistribution within a soil profile, the hydraulic gradient is generally small. Therefore we can assume that percolation of soil water is mainly controlled by hydraulic conductivity. When soil water is below field capacity, movement of water is very slow. For example, hydraulic conductivity of the soils at Breton plots at field capacity is approximately 4.4×10^{-4} cm/day (based on Campbell's equation), which is much lower than the rate of evaporation or water use by plants. Therefore at such conditions water in the profile is lost primarily by evapotranspiration, and drainage has little effect on water balance. As a result, drainage flux below field capacity is assumed to be negligible in this study.

Drainage flux, then, is assumed to occur when soil water content is greater than field capacity. Since soil hydraulic conductivity (K) depends on soil water content, drainage flux increases with soil water content, to a maximum value at saturation. Actual drainage rate is expected to depend on, in addition to K, to hydraulic gradient which depends on rainfall intensity, as well as antecedent soil water content before rainfall. Soil water status below the surface horizon change little with time. For simplification, the possible variation with rainfall intensity is ignored. Therefore drainage flux is assumed to depend on soil water content only.

A linear relationship between drainage flux and soil water content, similar to the method in Ceres (Jones and Kiniry, 1986) is used for estimation of drainage flux. The daily drainage is reduced by a constant coefficient, β (daily constant ranging from 0 to 1), which represents the fraction of the drainage volume that percolates from the modeled soil (Gabrielle et al., 1995), and it can be computed by:

$$Dr = \beta(\theta_i - \theta_{FC}) \tag{8}$$

where

θ_i = initial water content for each daily time interval (Δt) and

θ_{FC} = water content at field capacity.

In our model, then, the drainage coefficient (β) has been combined with the depth of soil or:

$$\beta = \beta' z \tag{9}$$

where

β' = drainage coefficient in Ceres model

z = depth of soil layer (cm)

At saturation ($\theta_i = \theta_s$) the rate of drainage flux is close to saturated hydraulic conductivity ($Dr = K_s$), or:

$$\beta_s = \frac{K_s}{\theta_i - \theta_{FC}} \tag{10}$$

However, this is expected to overestimate the drainage flux at $\theta_i < \theta_s$, because hydraulic conductivity and hence drainage flux decreases exponentially with a decrease in soil water content rather than linearly as suggested by Eq (8). The β_s value obtained by Eq (10) can be considered as the upper limit for this parameter, and actual β is expected to be lower and is ideally determined from field data.

In the Ceres Model (Jones and Kiniry, 1986) the drainage parameter β was determined with a procedure based on soil porosity. Gabrielle et al. (1995) for calibration of Ceres against field data changed the resulting β value from 0.37 to 0.05 to remove a bias error in estimation of soil water storage. As a result, they replaced this parameter, with two additional parameters, i.e. saturated hydraulic conductivity of the soil(K_s), and an empirical coefficient (A) related to soil texture and hydrological classification. Similarly, the approach adopted in EPIC Model (Sharpley and Williams, 1990), requires the saturated hydraulic conductivity of soil, K_s, as input. Such information is not available in many cases.

To eliminate the above limitation, in this study the coefficient β is proposed to be a fitting parameter. Simulation could start with an observed initial soil water content (θ_i). Using an arbitrary value of β, simulated soil water content at the end of a specified period (θ_f) is matched with the observed value. The specific value of β that produces $\theta_f = \theta_{observed}$ is then taken as the correct value. The obtained β value can then be used in the model for prediction of transient soil water for any other simulation periods for the specific soil.

Although β is obtained as a fitting parameter, in reality its value depends on the rate of the water loss from the modeled soil, which is a function of $K(\theta)$ and it is used as a gross approximation of the complex soil system. Performance of this model which is based on many simplifying assumptions is examined against collected results at three sites having different climatic and soil conditions. A list of the program codes in BASIC is included in the appendix.

4.3 Evaluation of model

Data from field experiments conducted at three locations namely Breton, Alberta, on Orthic Gray Luvisol (Chapter, 2); Simcoe, Ontario, on Caledon sandy loam (Clemente et al., 1994) and Lethbridge, Alberta, on a Dark Brown Chernozemic (Ren, 1997) are used for evaluation of the SIMPLE Model. Performance of the model in such contrasting soil and climatic conditions will help to establish the validity of the model and its simplifying assumptions.

Both qualitative (graphical) and quantitative (statistical) methods are used to compare the observed and predicted water contents over time. The quantitative procedures, adopted from Ambrose and Roesch (1982) in this study, involved calculation of error or the average difference between the predicted and measured values (*ME*); the relative error (*RE*) representing the error as a proportion of mean measurement and the root mean square of the difference between the predicted and the observed values (*SE*), which is often proportioned against the mean observed value as *MSE*. Definitions and implications of these statistical parameters have been provided previously (Chapter 2) and are not repeated here.

4.4 Site description

4.4.1 Breton site

Soil water content of the top 20 cm of soil, monitored continuously during the growing season of 1994 and 1995, in fallow plots, designated as E-1 and E-3 (in 1994), and as E-9 and E-11 (in 1995), in addition to cropped plots designated as F-1 and F-3 (wheat in 1994), and as F-9 and F-11 (oats in 1995), are used for evaluation of this model. Details on the crop rotation and tillage treatment are discussed by Wani et al. (1994). Measurements were made on hourly basis using vertical TDR probes buried at soil surface. However, since the SIMPLE simulations are on a daily time-step, only selected daily measured values were used in this study. Results from previous studies indicate that the upper 20 cm of soil profile is the most active section of profile in terms of soil water dynamics (Chapter 2 and Haderlein, 1995). Proper simulation of transient soil water content of the upper horizon, then, would provide adequate information for many studies, such as agronomic problems and irrigation system designs.

4.4.2 Simcoe site

The site consisted of a flat 2.6-ha field of Caledon sandy loam cropped to soybeans (Clemente et al., 1994). Soil water content measurements throughout the 1974 growing season for the "free-draining" soil profile on a flat field near Simcoe, Ontario are used for evaluation of SIMPLE. The measurements were made on a daily basis for the 0-25 cm depth interval using the gravimetric method. Daily precipitation and soil water content measurements, in addition to potential evapotranspiration estimations were obtained from R. de Jong (1996, personal communication).

4.4.3 Lethbridge site

The site is located near the Agriculture and Agri-Food Canada Research Center, Lethbridge, Alberta, on a Dark Brown Chernozemic soil. Soil water contents were measured at 5-, 10-, 20- and 40-cm depths using the TDR technique (Ren, 1996). Daily climatological data such as average wind speed, maximum and minimum temperature, relative humidity, net radiation and precipitation collected at the site were obtained from Ren (1996, personal communication). This information was used to estimate daily evapotranspiration using Penman's method.

Input parameters used in SIMPLE for each site are listed in Table 4.1.

4.5 Results and Discussion

4.5.1 Field evaluation of SIMPLE model

Simulation of soil water content by the SIMPLE model is based on the following simplifying assumptions:

SIMPLE algorithm is designed on the assumption that storage of water in the upper part of soil profile is controlled by the net boundary fluxes i.e. drainage, precipitation and evaporation (in fallow plots) or evapotranspiration (in cropped plots). Actual evapotranspiration is calculated from potential evaporation using empirical coefficients, and drainage losses are obtained using β coefficient (Eq. 9). Since the latter coefficient is retrieved through a calibration procedure using actual soil water measurements, the obtained value of β indirectly takes evapotranspiration factors into account. As a result, instead of imposing all these parameters as input requirements, it is proposed that potential evaporation remain as the input requirement and β should be calibrated separately for fallowed and cropped situations.

4.5.1.1 Breton site

The SIMPLE model predictions of soil water content and the actual measurements for the two growing seasons of 1994 and 1995 at Breton are presented in Figs. 4.1 and 4.2 (fallow plots) and in Figs. 4.3 and 4.4 (cropped plots). The significance of these two simulation periods is that they include highly active surface flux periods (31 May- 12 Sep, 1994), as well as periods that are mainly dry (6 July- 28 July, 1995).

The variability among replicated measurements is represented as an envelope of ± one standard error from the mean measurements. Input parameters required by SIMPLE, available from previous studies (Agriculture Canada, 1989), are presented in Table 4.1. Results presented in Fig. 4.1 show that the model adequately reproduced the observed results. The drainage coefficient, β, obtained for the site was 10 $cm\ d^{-1}$. If this value was used in Eq. 10, a saturated hydraulic conductivity value of 2.3 $cm\ d^{-1}$ is obtained for the surface layer at the Breton site. This value agrees closely with the measured values obtained by Haderlein (1995).

The drainage coefficient β was obtained based on the initial and final soil water contents for the simulation period in 1994. The same value was also used to predict the transient changes in soil water for the following year of 1995. It should, however, be noted that the field plots used for the two years of 1994 and 1995 were not the same (plots E-1 and E-3 were used in 1994 and E-9 and E-11 in 1995). Due to the undulating terrain in Breton plots, the field slope at the two sites are not identical, therefore, they have different internal drainage characteristics. Nevertheless, using the same value of β for both years of 1994 and 1995 resulted in reasonable simulation of observed values (Figs. 4.1 and 4.2).

The same approach was adopted for estimation of the β coefficient for the cropped plots. However, since the initial and final soil water contents in the cropped plots were similar to those in the fallowed plots, identical β values were obtained. Simulated results for cropped conditions are compared with the measurements (Figs. 4.3 and 4.4). The SIMPLE Model was able to reasonably reproduce the observed results.

For the second half of the simulation period in 1994, during which water consumption by plants was higher, SIMPLE simulated results were higher than measured results. During this period, plant roots were extracting water from the entire depth of surface layer resulting in a lower average soil water content as compared to fallowed conditions. But, having similar β coefficient for both fallowed and cropped condition, SIMPLE overestimated the observed results. Such a problem was not observed during 1995 growing season.

ME and *RE* values for fallow and cropped plots in Breton during mostly wet 1994 growing season indicated that the model was able to closely estimate the observed results (Table 4.2). During the climatically variable 1995 growing season, the SIMPLE Model generally overestimated the observations, however differences were mostly within one standard error of replicate measurements. Low SE values also indicated that there was no systematic deviation between observed and simulated results.

Simulation results for cropped conditions are represented in Figs. 4.3 and 4.4. The statistical comparison of simulated and observed results, presented in Table 4.2, indicate that SIMPLE over-estimated soil water during 1994 growing season, but performed satisfactorily during 1995 growing season.

4.5.1.2 Simcoe site

Soil water content measurements and SIMPLE simulated results are compared in Fig 4.5. The soil on this site is fairly coarse. The measured results obtained for the Simcoe site are extremely variable during the growing season of 1978 (Fig. 4.5). During the latter part of the growing season measured results indicated that the average soil water content for the upper 25-cm depth fell below 0.03 cm^3cm^{-3}, which is even lower than the reported soil water content at wilting point (de Jong, personal commucications). If the measurements were accurate, and plants were to survive the water content at wilting point should be lower, therefore it was assumed to be at 0.01 cm^3cm^{-3}. Overall, SIMPLE was able to reasonably reproduce the general variation of measured results. For the earlier parts of season when more rainfall occurred, SIMPLE under-estimated the observed results, however, it performed satisfactorily for the rest of season. This problem may be resulted from over-estimation of the β coefficient.

Simulated results generally fell within 2% (absolute) of the measured values (Table 4.1). However, similarity between *ME* and *SE* values shows a systematic under-estimation of measured results. Simulated results following major rainfalls, as compared with observations, showed that the actual water loss from the soil layer was at a higher rate than that predicted by SIMPLE. For the most part, average soil water content at the surface layer was below field capacity, therefore, this problem is attributed to an under-estimation of evaporation rather than drainage.

4.5.1.3 Lethbridge site

Soil water measurements for the two growing seasons of 1994 and 1995 are compared with the SIMPLE simulations in Figs 4.6 and 4.7. Measurements are made for various surface tillage treatments and crop patterns (Ren, 1996). An envelope of ±

one standard deviation from mean measurements represent the variability of measurements. The SIMPLE Model was able to closely reproduce the measurements during the mostly dry 1994 growing season. Using the same drainage coefficient (β) for the following year SIMPLE slightly overestimated the observations. Similarity of *ME* and *SE* values for the period indicates that overestimation was systematic. Simulation errors fell within one standard deviation of mean measurements. Estimation of the β coefficient from the 1994 growing season, which had infrequent rainfalls, may have resulted in a low prediction of drainage fluxes for the rainy growing season in 1995.

Agreement between model predictions and observations indicate the model is acceptable for the purpose of predictions of soil water. However, the simulated results for prediction of dynamic variables such as evaporation and drainage fluxes, which were made based on many simplified assumptions, may not be certain.

4.4.2 Comparison of SIMPLE with LEACHW

Details on the LEACHW algorithm (Hutson and Wagenet, 1992) and data requirements are presented previously (Chapter 2) and are not repeated here. For this study, measurements made by vertical TDR probes measuring average soil water content of the upper 20-cm depth are used, and therefore are different than the set of data used in Chapter 2. SIMPLE is a soil water budget model that requires minimum amount of input data. It benefits from the calibration procedure for estimation of drainage coefficient, whereas LEACHW is a physically based model that requires detail representation of hydraulic properties of soil.

The SIMPLE Model's predicted values of soil water content, for the fallowed plots in Breton site, are graphically compared with predicted values by the more complex LEACHW Model in Figs. 4.8 and 4.9. Results from LEACHW and SIMPLE simulations are quantitatively compared with the observed data in Table 4.3. These results indicate that both models are quite comparable in reproducing the observed values. In fact, for the drier year of 1995, the predicted soil water values by SIMPLE model are closer to the observed results, as compared to the LEACHW simulations.

During this period LEACHW predictions were consistently higher than the observed water contents. This could be related to an under-estimation of evaporation and/or drainage fluxes from the top 20 cm of soil.

Even though LEACHW requires more information on the physical and hydraulic properties of soil, simulation of soil water by both models are comparable. LEACHW, which is a physically based model, however, is expected to be able to reproduce other soil water processes such as the drainage fluxes. LEACHW therefore can be used as basis for other simulation studies such as prediction of fate and transport of solute in soils. This is a task that SIMPLE has not been designed to perform.

4.5 Conclusions

A functional soil water budget model, SIMPLE, is developed for estimation of transient soil water. The main advantage of this model is its simplicity. Perhaps this model could be considered as the model with least input-data requirement for simulation of soil water content. This model requires only commonly available soil information i.e. water content at field capacity and wilting point, soil bulk density, and basic information on precipitation and potential evaporation. In addition, the fitting factor, β, is required as the drainage coefficient. This factor can be estimated by matching the predicted and measured water contents at the two ends of a time period. The β coefficient should be calibrated separately for fallowed or cropped fields. This value can then be used for simulation of water contents for any other time periods, for the particular soil.

The SIMPLE Model was tested against observed results for both fallowed and cropped fields for three different locations with contrasting soil and climate conditions. The model was capable of reproducing the measured water contents with reasonable accuracy. Such results are required in many studies, such as agronomic problems and irrigation system designs.

Table 4.1. Parameter values used in SIMPLE for three different sites.

Site	Breton	Lethbridge	Simcoe
[1] θ_{sat}	0.49	0.51	0.36
[2] θ_{FC}	0.26	0.32	0.16
[3] θ_{WP}	0.11	0.22	0.01
[4] β	10	30	25

[1] Water content at saturation ($m^3 m^{-3}$)

[2] Water content at field capacity or 33 kPa ($m^3 m^{-3}$)

[3] Water content at permanent wilting point or 1500 kPa ($m^3 m^{-3}$)

[4] Drainage flux coefficient ($mm\, d^{-1}$)

Table 4.2. Quantitative comparison predictions from the SIMPLE Model with observed results at three different sites.

Site	Year	Crop	[1]ME	[2]RE	[3]SE	[4]RSE
Breton	1994	Fallow	0.00	-0.01	0.02	0.07
	1995	Fallow	0.02	0.07	0.03	0.10
	1994	Wheat	0.02	0.06	0.03	0.12
	1995	Wheat	0.01	0.02	0.01	0.08
Lethbridge	1994	Wheat	0.00	0.02	0.03	0.12
	1995	Wheat	0.02	0.08	0.02	0.08
Simcoe	1978	Soybean	-0.02	-0.14	0.02	0.24

[1] Mean error

[2] Relative error

[3] Standard error

[4] Relative standard error

Table 4.3. Quantitative comparison of the SIMPLE and LEACHW simulated water content values compared to observed values during 1994 and 1995 growing seasons.

	SIMPLE	LEACHW	SIMPLE	LEACHW
	1994		**1995**	
ME	0.00	0.02	0.02	0.05
RE	0.01	0.08	0.08	0.21
SE	0.02	0.03	0.03	0.06
MSE	0.06	0.11	0.12	0.23

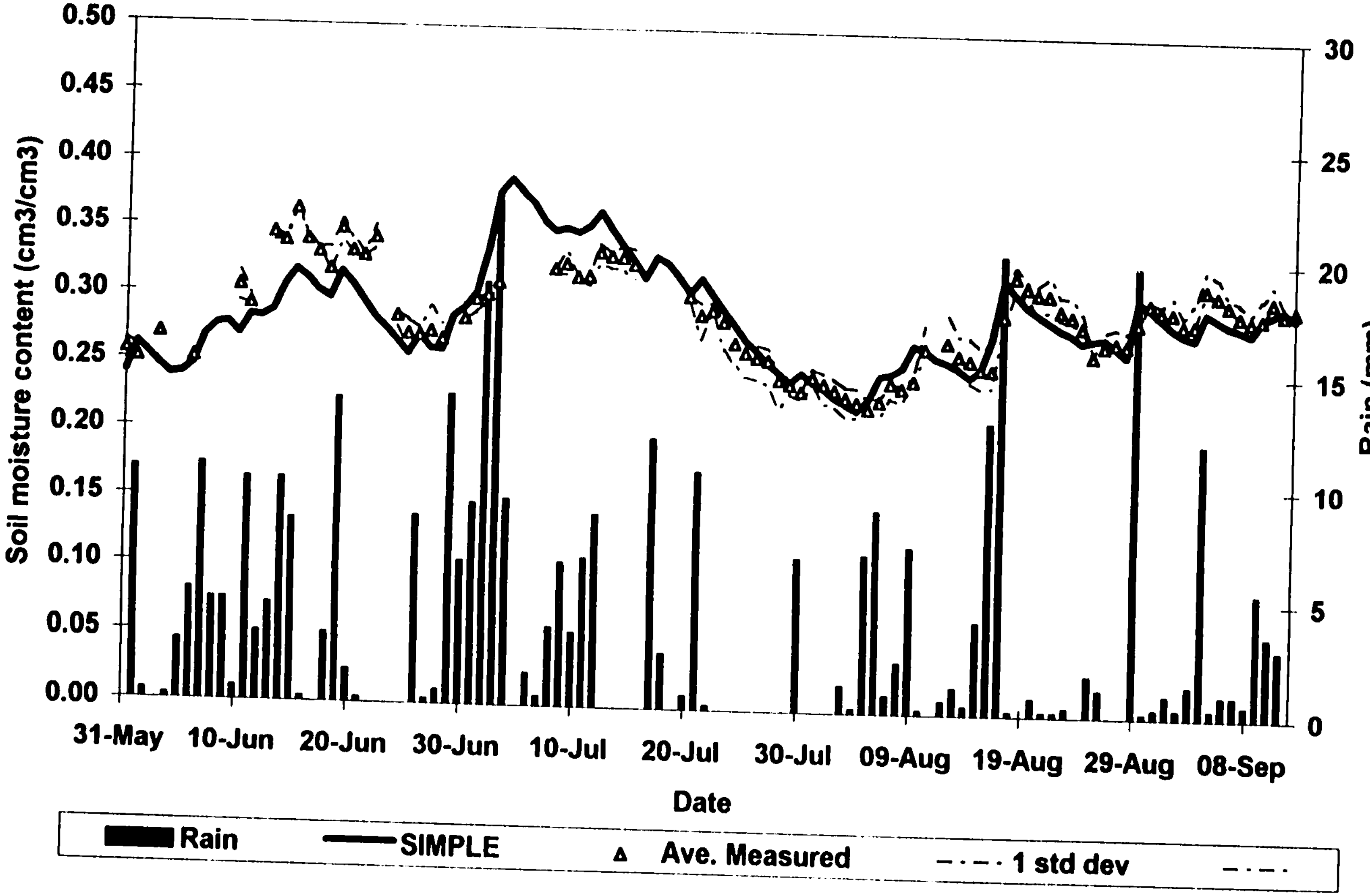

Fig. 4.1. SIMPLE simulated water contents compared to observed values in fallowed plots at Breton during the growing season of 1994.

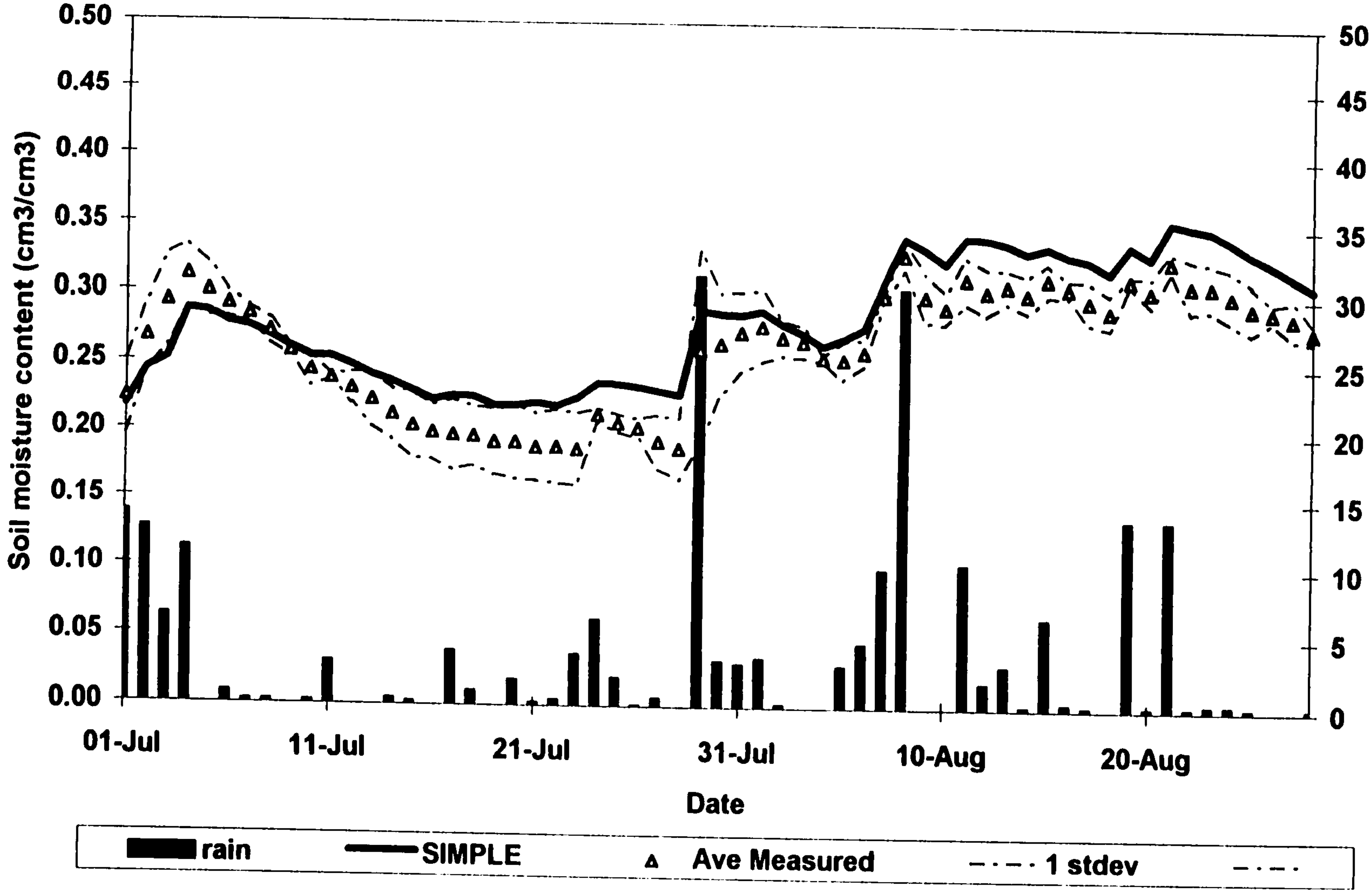

Fig. 4.2. SIMPLE simulated water contents compared to observed values in fallowed plots at Breton during the growing season of 1995.

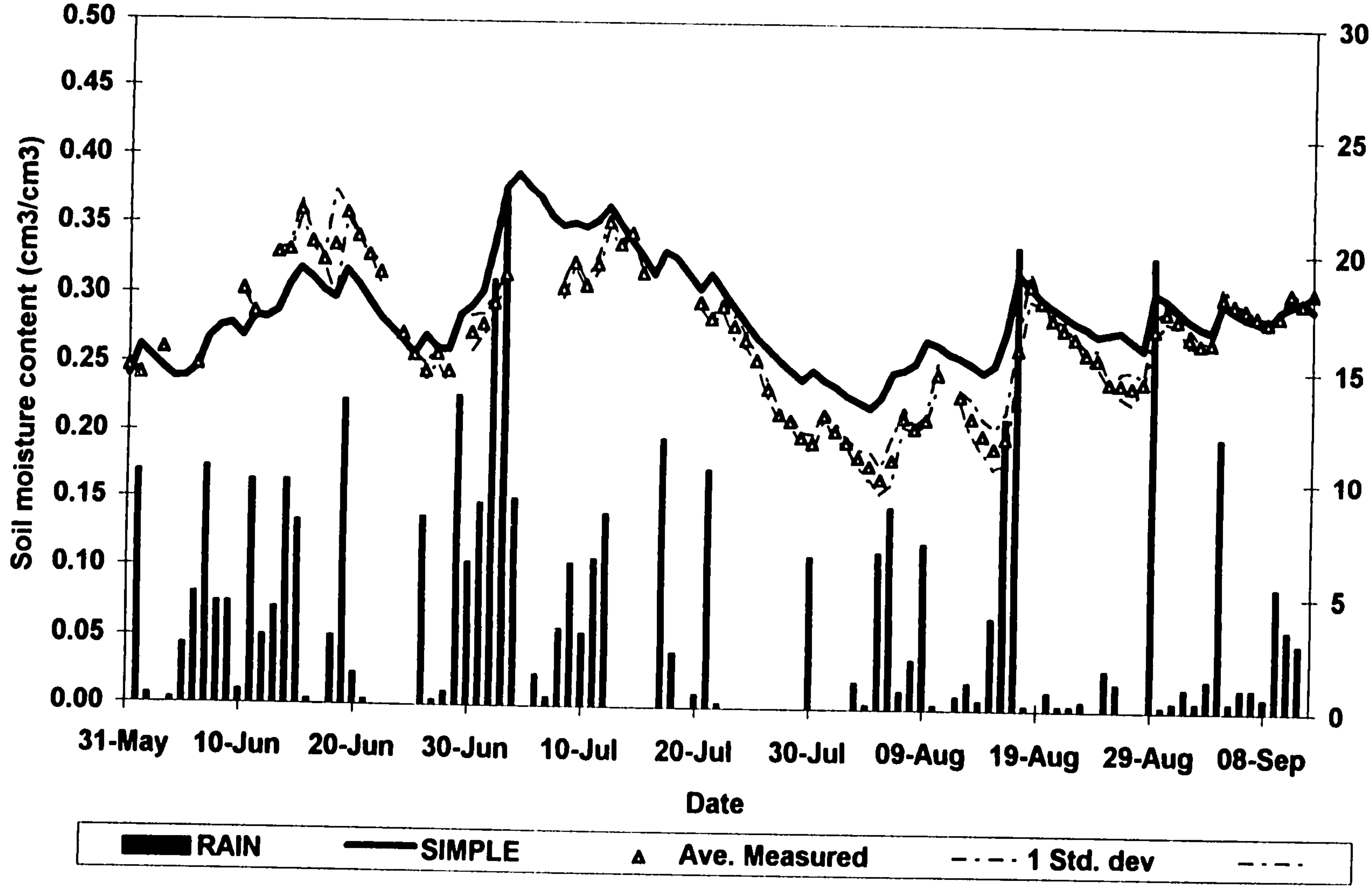

Fig. 4.3. SIMPLE simulated water contents compared to observed values in cropped plots at Breton during the growing season of 1994.

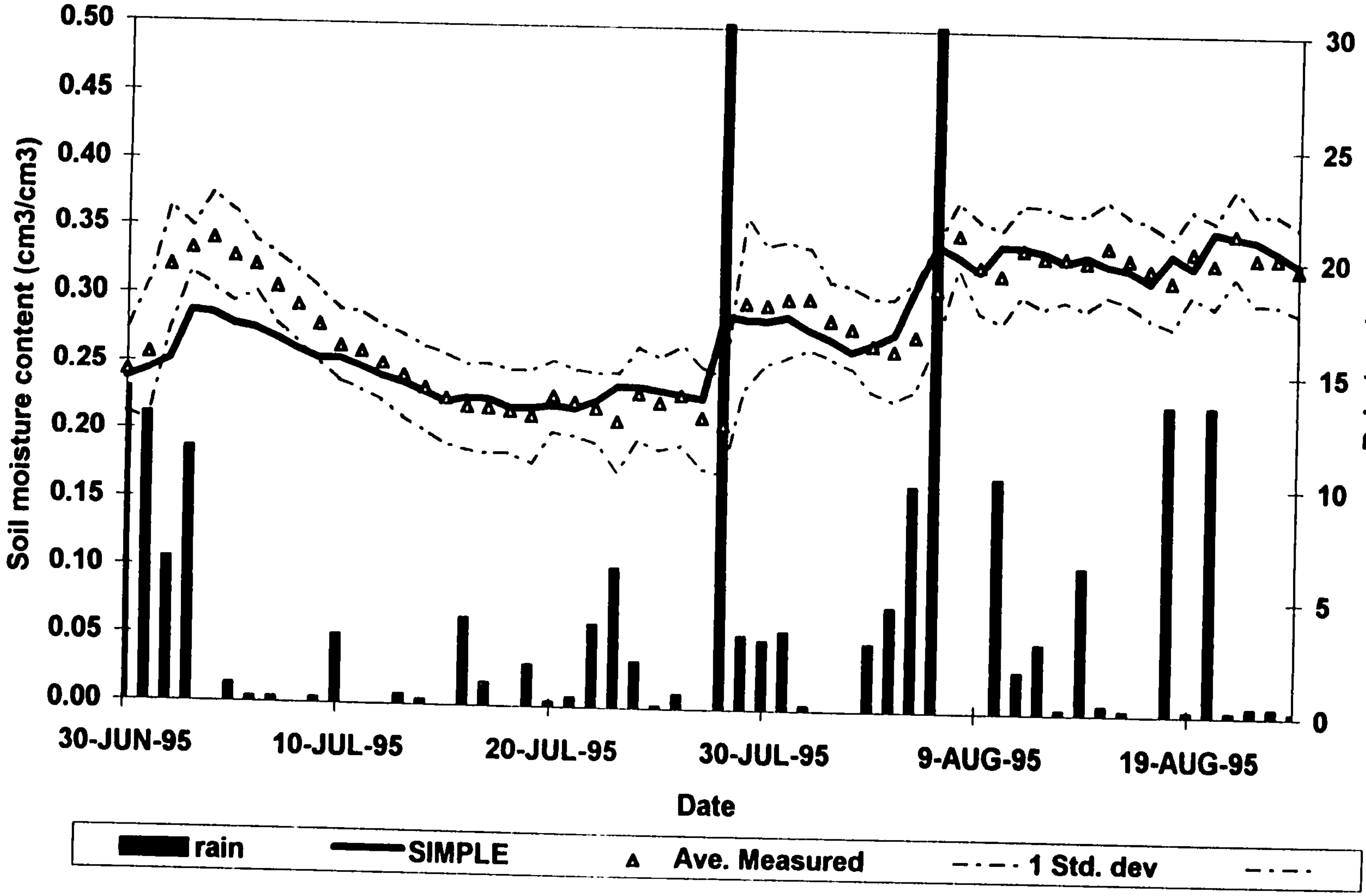

Fig. 4.4. SIMPLE simulated water contents compared to observed values in cropped plots at Breton during the growing season of 1995.

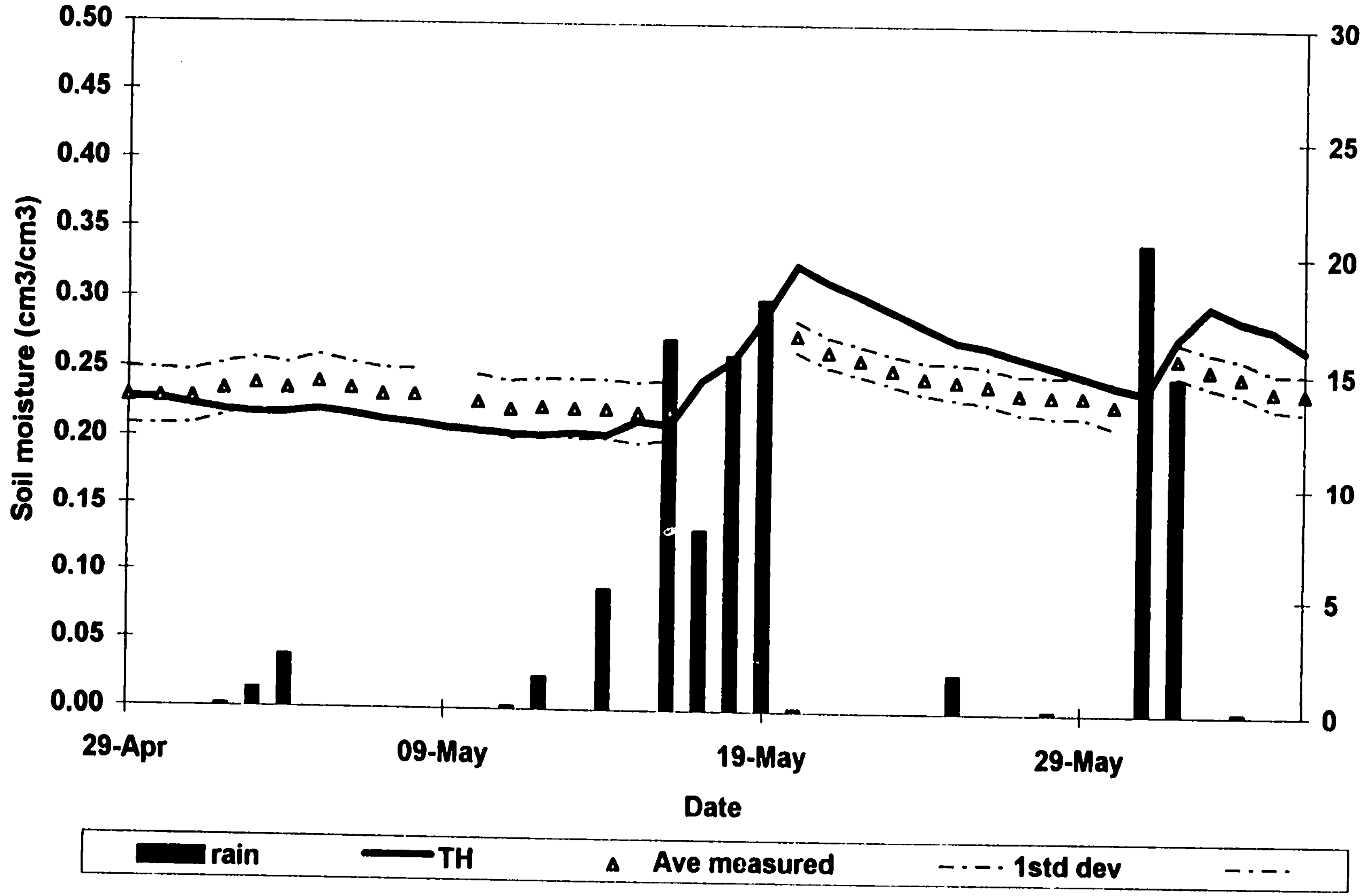

Fig. 4.5. SIMPLE simulated water contents compared with observed values in cropped plots at Lethbridge during the growing season of 1994.

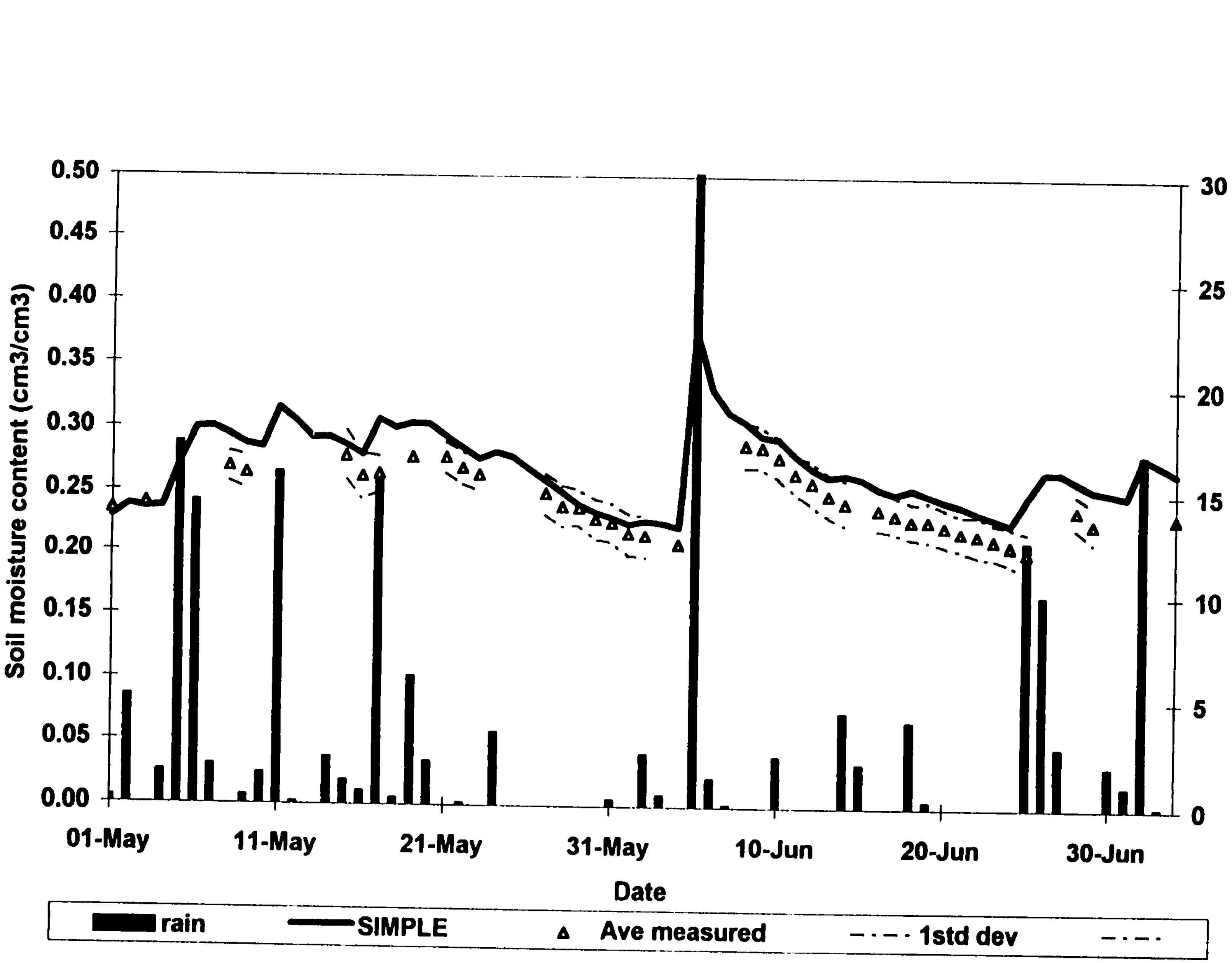

Fig. 4.6. SIMPLE simulated water contents compared to observed values in cropped plots at Lethbridge during the growing season of 1995.

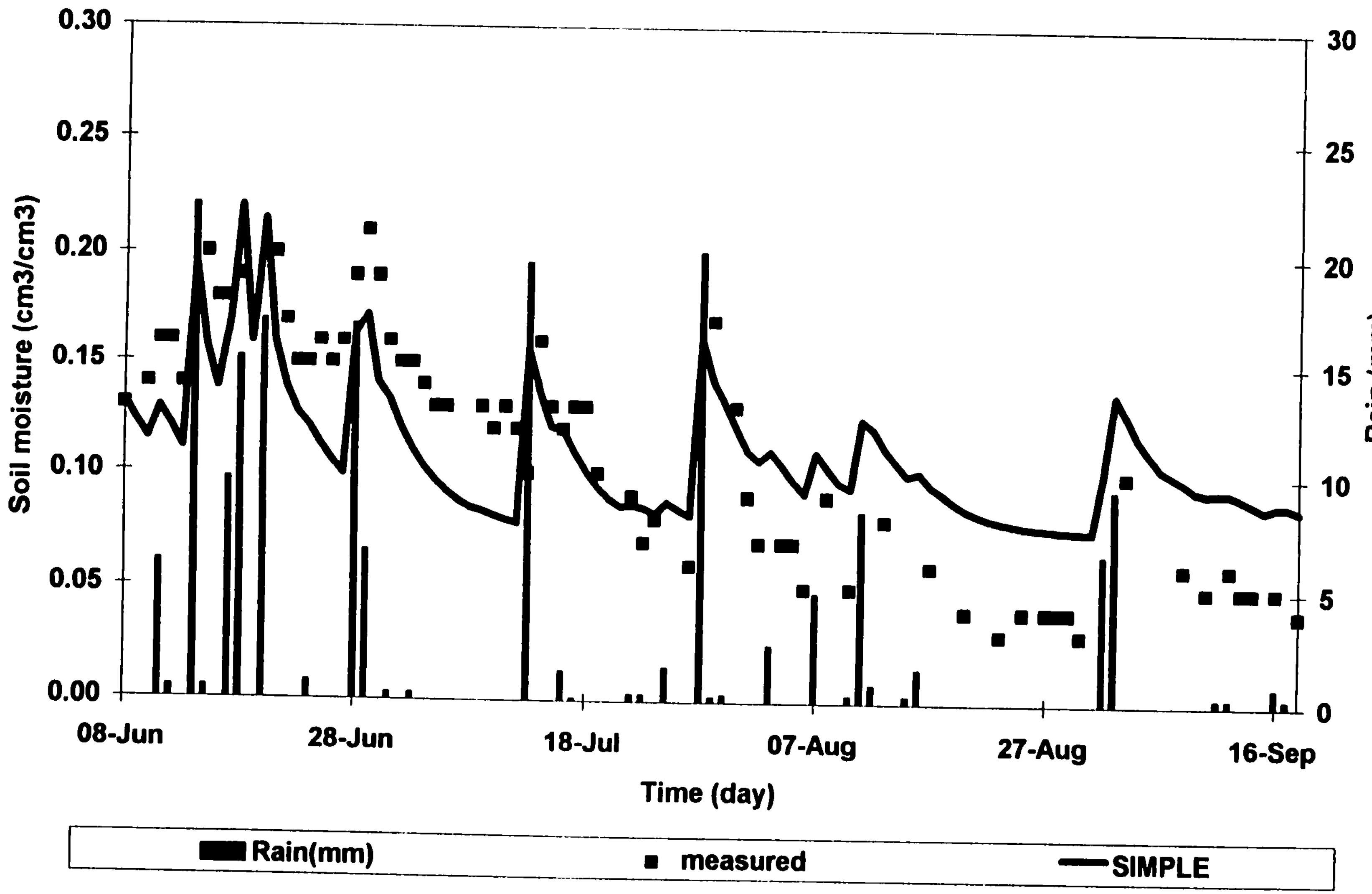

Fig. 4.7. SIMPLE simulated water contents compared to observed values in cropped plots at Simcoe during the growing season of 1978.

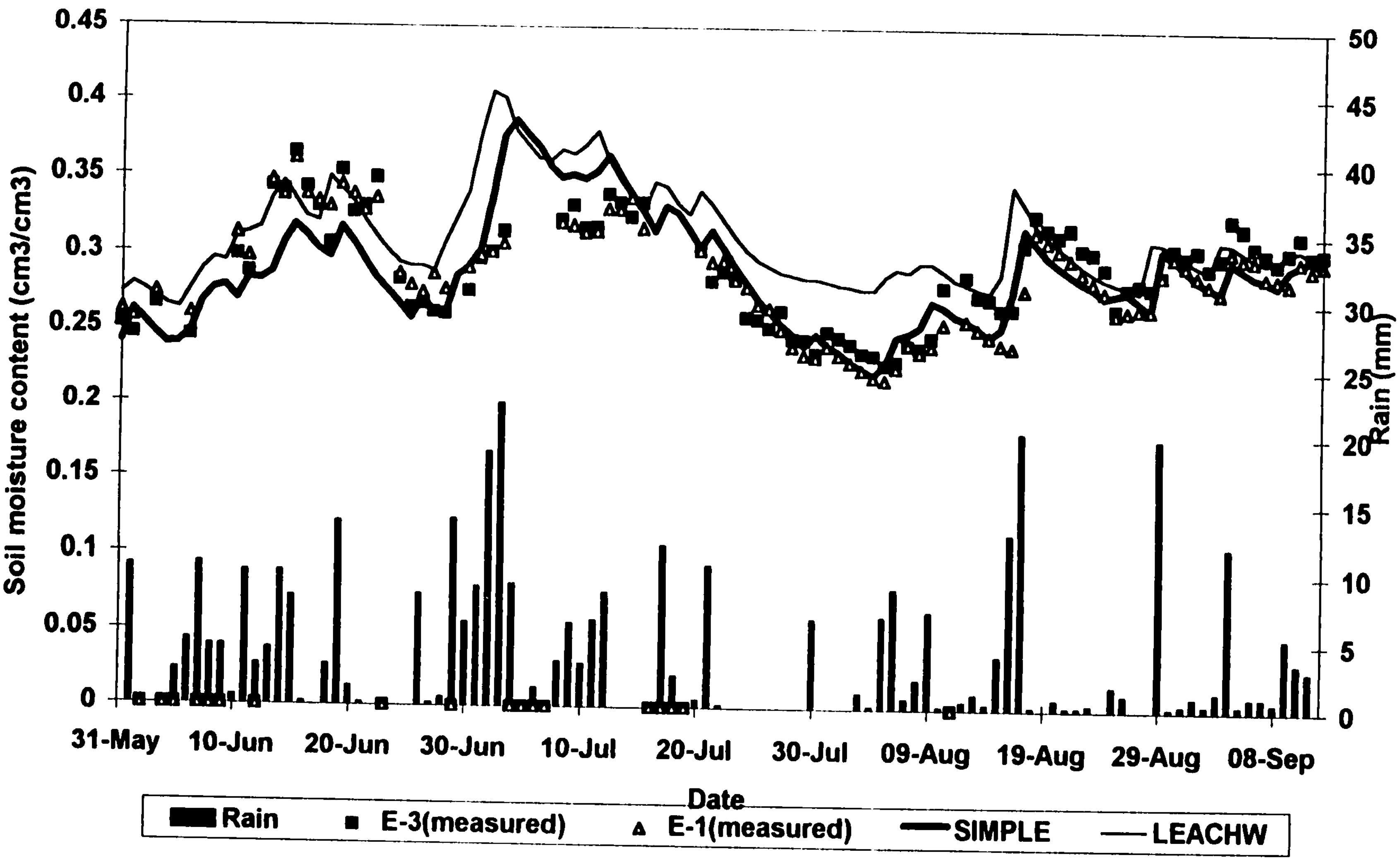

Fig. 4.8. SIMPLE and LEACHW simulated water contents compared to observed values in fallowed plots at Breton during the growing season of 1994.

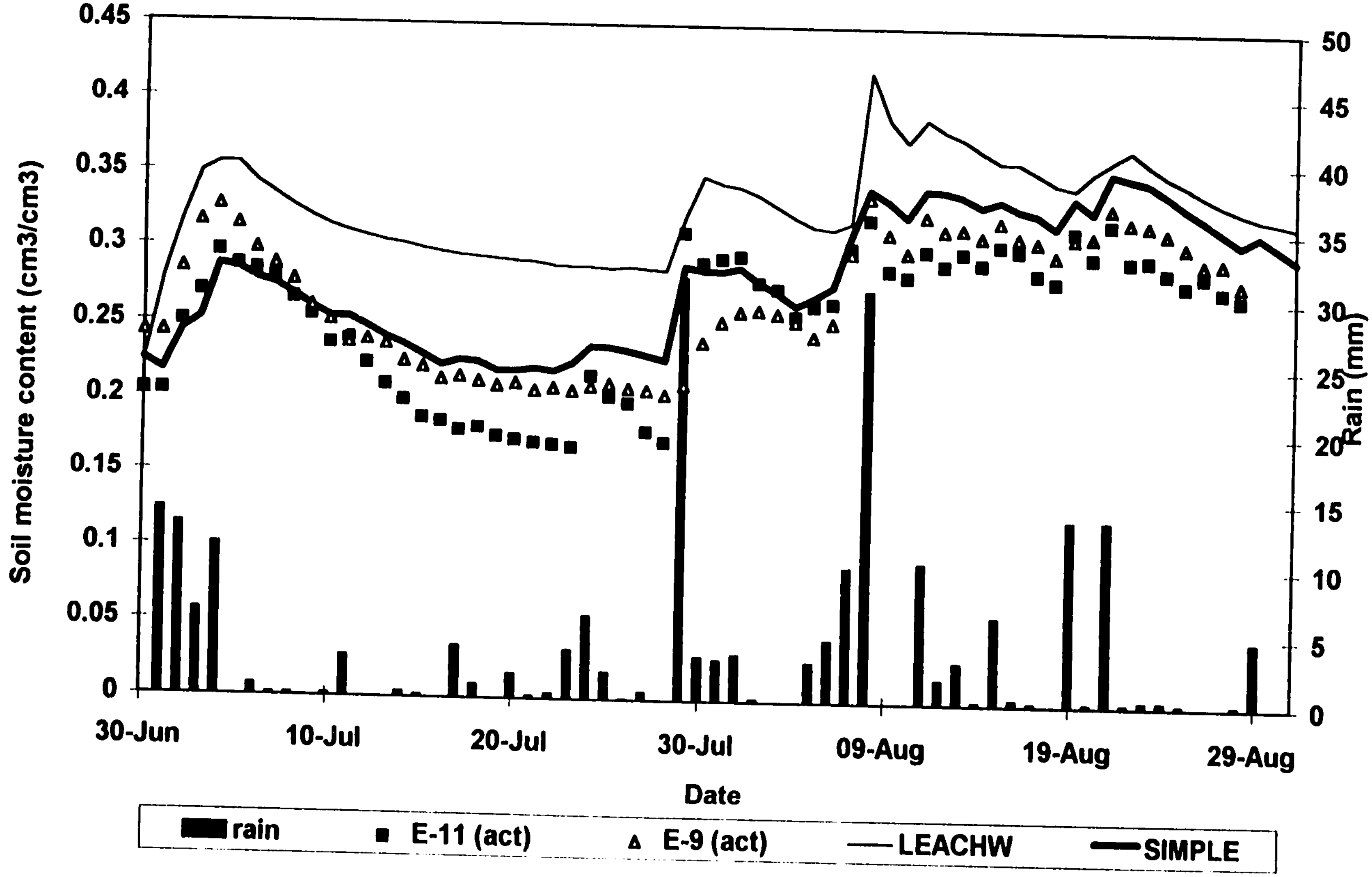

Fig. 4.9. SIMPLE and LEACHW simulated water contents compared to observed values in fallowed plots at Breton during the growing season of 1995.

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APPENDIX

Program codes in BASIC for the SIMPLE model[1].

```
INPUT "TH1=", TH1                         "initial water content"
INPUT "FC =", FC                          "water content at field capacity"
INPUT "SAT=", SAT                         "water content at saturation"
INPUT "THR =", WP                         "water content at wilting point"
INPUT "SD =", SD                          "soil depth"
INPUT "BETA =", BETA                      "drainage coefficient"
TH = TH1
NF = 0
DR = 0
INPUT "ENTER NAME OF INPUT DATA FILE:", FILEIN$
INPUT "ENTER NAME OF OUTPUT FILE:", FILEOUT$
OPEN FILEIN$ FOR INPUT AS #1
OPEN FILEOUT$ FOR OUTPUT AS #2
PRINT #2, "D", " R", "E", "TH", "DRN"          "DRN = drainage flux"
10 IF EOF(1) THEN STOP
INPUT #1, D, R, EP
     IF TH > FC THEN
          DRN = BETA * (TH - FC)
          E = EP
     ELSE
          DRN = 0
          E = EP * (TH - WP) / (FC - WP)
     END IF
NF = R - E - DRN                               "NF = net boundary flux"
TH = TH + NF / SD
PRINT #2, D, R, E, TH, DRN
GOTO 10
END
```

[1] Definition of each symbol is given between " ".

Chapter Five

SYNTHESIS

During the past two decades mathematical models have been used extensively to predict both the state and dynamics of soil water. In addition to the traditional importance of soil water status in agronomic studies, simulation of soil water has been accepted as a tool for solving various practical management problems such as groundwater recharge, leaching of nutrients and pollutants (Zepp and Belz, 1992) and assessment of soil erosion and degradation (Sharpley and Williams, 1990). Research efforts continue to improve modeling of the fate and transport of water in complex and variable soils and ecosystems. Such explanatory algorithms, based on fundamental scientific principles, are used to reproduce water fluxes through soil-plant atmosphere systems and the processes by which they are controlled (Grant, 1995). Therefore, these models are used as tools to apply scientific knowledge in practice (Penning de Vries, 1983). The use of comprehensive models for research purposes is increasing, however simpler functional, management-oriented models with minimum requirements for field specific data are also needed (Jemison et al., 1994). In order to be able to adopt existing models for various soil management practices with confidence, it is important that the capabilities of these models and the credibility of their results be tested.

Attempts to validate simulations of soil water status against field observations have largely been based on periodic (e.g. weekly or biweekly) measurements of soil water content. Such observations are not sufficient for examination of highly dynamic processes such as flux of water during intense precipitation events which contribute to soil water drainage and groundwater recharge. Monitoring of water fluxes requires frequent observations of the dynamic changes of soil water during precipitation events. Evaluation of models for such events could provide justification for the extra effort in obtaining additional input data and in improving data accuracy required for comprehensive models. Otherwise simpler functional soil water models could be adequate for the prediction of general behavior of soil water status.

The LEACHW and *ecosys* models were able to reasonably simulate the general variation of soil water content. However, their performance during heavy rainfall events that generally lead to drainage fluxes was not satisfactory. High rate of drainage fluxes have already been reported at the same site (Howitt 1981; Izaurralde et al., 1995), however, both models especially LEACHW, were not able to adequately reproduce such observations. Preferential water fluxes through macropores were not considered in this study. This could be the reason for the shortcomings of the predictions by the two models. Prediction of preferential fluxes is possible by *ecosys*, however it would require additional input data.

In spite of the fact that LEACHW and *ecosys* require different degrees of input data, they were both able to adequately reproduce the general status of soil water, i.e. transient soil water content changes for a long-term period. Such predictions, however, have also been obtained using simpler functional water budget models that do not require representation of water flux using Richards' equation which in turn requires representation of hydraulic properties of soils. Therefore the question was raised whether soil water content changes are sensitive to the variability of hydraulic parameters of soils.

This question was examined in the second part of this study, through a sensitivity analysis on the importance of accurate estimation of the parameters used in the hydraulic functions described by Campbell (1985) for simulation of soil water content changes. Soil water predictions by LEACHW, as one of many simulation models using Campbell's hydraulic functions, were not particularly sensitive to the variations in soil hydraulic properties. In fact, the variation among observed soil water content, as a result of soil heterogeneity, was similar to the range of soil water contents predicted using a wide range of hydraulic parameter values. It is, therefore, concluded that simulation of soil water could be achieved without detailed consideration of the hydraulic properties of soils. This conclusion, however, should not readily be extended to simulation of soil water fluxes, such as drainage fluxes. It is also disclosed that evaluation of water flow simulation models based only on proper predictions of changes of soil water content is not sufficient for other purposes such as prediction of soil water fluxes.

As a result in the third part of this study, a SIMPLE model was developed for simulation of water content. The basic assumption in this model is that water content of the upper layer of the soil profile is mainly controlled by the boundary conditions. Therefore, it can be simulated with minimal knowledge of the hydraulic properties of the soil. In a sense, this model could be considered as an extension of the existing soil water budget models to the point that requires the least input data. Through a one-time calibration procedure, a net boundary flux parameter is found which could then be used for any other time periods for the particular soil. In turn, no detailed soil information is required by the model. Examination of SIMPLE in different soil and climatic conditions showed that the model is universally applicable for prediction of soil water content, using the basic information on soils and climate. Such predictions are adequate in many studies, such as agronomic problems and irrigation system designs.

5.1 Conclusions of our study

The results of this study indicate that, in as much as water flow modeling is a strong tool in agronomic and environmental studies, it must not be used without evaluation. In addition, the evaluation must be purpose specific. Therefore, the results of an evaluation study for a specific process (e.g. prediction of changes in soil water content) should not be extrapolated to another process (e.g. prediction of water fluxes). Furthermore, it is evident that the common problem of insufficient available input data (as prerequisite for comprehensive soil water simulation models) may not be avoidable for simulation of specific processes, such as prediction of changes in soil water content which is essential in agronomic problems and irrigation system designs.

Although complex simulation models are useful research tools for investigation of various processes taking place in heterogeneous soils, they remain of limited use in management-oriented problems. Therefore, simple models with minimum data requirements could be a feasible alternative to complex models in many cases. Lack of sophistication in development of new models, however, should not be translated as compromising accuracy.

5.2 Implications of this study

First, we take the advice of Philip (1991) in recognizing the difference or "dichotomy" between natural science and professional practice, and the fact that one should not take one for the other. There are always cases in which decisions must be made with a limited source of data. In this respect, models are used as a convenient tool to apply scientific knowledge in practice, but not as a replacement for the "real thing."

Models are simplified representations of reality. The degree of their simplification depends on what is needed of the model. One could emphasize on "representing reality" so that underlying fundamental physical processes are represented with best information available (complex models). Or, one may give emphasis to "simplification", so much it is not compromised with accuracy. The objectives of complex or explanatory models is that by representation of all or most fundamental processes the models would work in wide range of conditions. As long as the fundamental physical laws are deemed valid; the trade off is intense input-data requirement. Vast simplifications of the underlying physical processes could be considered as a viable alternative in management-oriented problems. There may be situations where such simplifications may lead to serious errors. The range of applicability of simplified, functional models is far from what can be expected of complex models; the trade off is simplicity.

5.3 A note on spatial variability

Spatial variability in soils presents a significant challenge in soil water simulation models. In addition to the already large number of soil properties required by such models, spatial variation and correlation of these properties are also required for simulation of soil water movement in field soils.

Recently, there have been attempts to represent the heterogeneity of soils. Tseng and Jury (1993) generated a hypothetical random field to describe unsaturated hydraulic conductivity in heterogeneous soils. Young (1995) suggested that complicating factors such as the effect of soil heterogeneity should be addressed in order to provide a better "physical understanding" of infiltration behavior in the field. However, because of the limitations in availability of such intensive data required in these representations, they could be used as research tools, but remain of limited practical use.

In many simulation models soil heterogeneity is represented in the vertical direction only. Soil layers are assumed to be uniform. However, our observations indicate that such assumptions are not necessarily valid. In fact, due to the variability of soil properties significant differences were observed in simultaneous measurements of soil water contents at common depths within close proximity. Interestingly, the differences observed between any sets of such measurements were persistent throughout the season, resulting in parallel $\theta(t)$ curves between different locations. These observations were similar to the results obtained from simulation of water contents using variable soil hydraulic parameters.

The observation that soil water contents at different locations in the same field follow essentially parallel $\theta(t)$ curves throughout the season and the fact that different combinations of soil hydraulic parameters in simulation models predict parallel $\theta(t)$ curves similar to those observed between different locations in the field suggest a potentially efficient means of characterizing soil water movement in the presence of spatial soil variability. Spatial and temporal variability of soil water content can be represented by a family of essentially parallel $\theta(t)$ curves. Measurements at small time intervals in a few locations would produce representative members in the family of $\theta(t)$ curves with detailed information on the temporal variation of soil water content. However, these observations lack spatial resolution, and from these observations, it could not be established whether measurements at these few locations represent the average condition of the field. On the other hand, a relatively large number of measurements at specific times during the season could be made. These measurements provide detailed information on field average and variability at specific times but little information on the temporal dynamics of the soil water. A combination of the two types of measurements would then yield information on the dynamics of soil water with sufficient resolution both spatially and temporally.

To predict the average soil water dynamic in the field, computer simulations could be conducted with estimated soil hydraulic parameters, e.g. Campbell's model. This would produce a predicted $\theta(t)$ typical of the family of many such curves for the particular field. A relatively large number of soil water content measurements at selected times can be used to establish the range and variation of soil water content at these times to establish the relative position of the predicted $\theta(t)$ curve within the population similar curves. The predicted curve can then be adjusted to predict the average water contents at these specific times resulting in a prediction of average field water dynamics. Because of the insensitivity of predicted soil water content to specific soil water hydraulic parameters, the specific model used for such an exercise is not important. The more complicated models such as LEACHW and *ecosys*, and the simpler models, such as SIMPLE, are expected to produce similar results.

5.4 Future research

First a general comment: The intense effort in developing and refining comprehensive models is continuing. This effort will contribute to our understanding of the real world. As the objectives of a model broaden, the size of the model increases. In this case the number of parameters required by such comprehensive models increases. In turn, the sensitivity of the model to each parameter decreases (Penning de Vries, 1983). I suggest that more attention should be paid to development and evaluation of models that would simulate specific processes representing the behavior of a part of the complex systems. The less detailed the desired results are, the simpler the predictive model can be. These models would be of great value especially in management oriented studies.

More specifically and in direct regards to this study, our SIMPLE model should be tested in different environments with different soil properties and climatic conditions. The model can be modified so that it would be able to simulate potential evaporation, which is now an input requirement, with minimum weather data.

Alternative approaches for representation of spatial / temporal variability of soils, as suggested in above section, using different values of hydraulic parameters for example, requires further research.

Dominant parameters and factors controlling specific processes in an ecosystem should be identified. Different processes require different subsets of parameters. It would also be valuable to find out to what extent simplifications of a specific process can be extended without compromising accuracy. Further simplification of these processes could provide means for universal application of models, where lack of detailed information is commonly a limiting factor.

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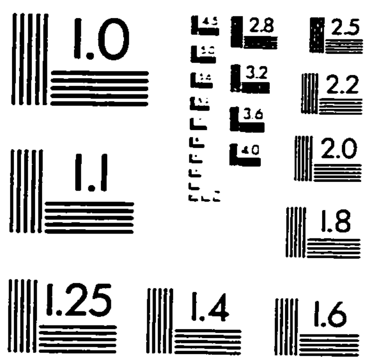
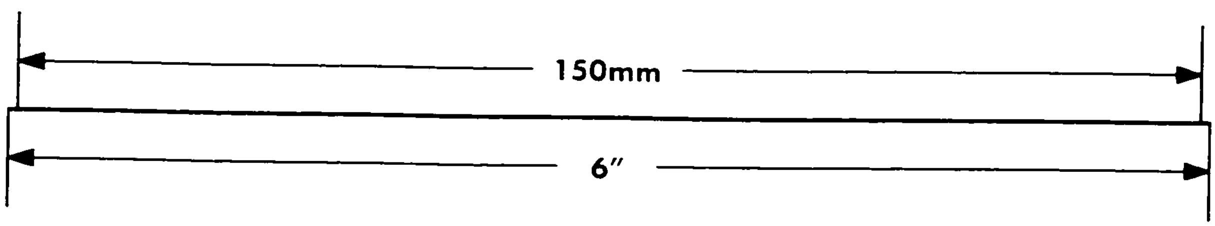
IMAGE EVALUATION TEST TARGET (QA-3)





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