ABSTRACT

The principles of using mathematical models to describe processes involved in the movement of water in soils are surveyed from the literature. Various models are considered within a classification system based on the degree of empiricism or mechanism of the approach. Empirical models are compared and contrasted with mechanistic models and the role of these models in agricultural practice is discussed. A new empirical mathematical model to describe the uptake of water by plant roots is developed through a sink term and combined with well established models including the Richards' equation to provide a paradigm for the movement of water throughout the soil/plant system. Methods of solution of the model are considered and a finite difference method is employed to provide a computer implementation of the solutions under a range of initial and boundary conditions. The computer simulation was found to be easily adapted to a variety of field situations. In particular, the introduction of the 'evaporation front' concept and its embodiment in the new sink term, provide insights into the criteria for scheduling irrigations, laying the basis for field verification and investigation. The use of this mathematical model for determining an optimal irrigation regime is discussed in relation to conventional scheduling methods.

IRRIGATION SCHEDULING - A MATHEMATICAL MODEL FOR WATER MOVEMENT IN CROPPED SOILS INCORPORATING SINK TERM AND EVAPORATION FRONT

by

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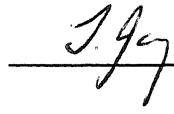
I wish to thank my supervisor, Dr. Russel Stonier of the University of Central Queensland, Department of Mathematics and Computing, for his encouragement, direction and energetic support throughout the course of this study.

DECLARATION

This thesis contains no material which has been accepted for any award at any institution. Furthermore, to the best of my knowledge, these works do not contain any material previously published or written by another author except where duly referenced in the text of this thesis.



Terry Janz.

CHAPTER I

IRRIGATION SCHEDULING

1.1 INTRODUCTION

This chapter provides the rationale for this study. The conventional methods of scheduling irrigation are considered and then the contributions that mathematical modelling of the situation may offer is detailed.

If water supply were limitless and costs associated with irrigating land were negligible, what would be the best policy for irrigation scheduling? Perhaps the soil should be kept constantly wet so that the plants would experience no stress due to lack of water - perhaps this would lead to optimal growth and hence optimal yield? Not so! It is well documented that this 'overwatering' leads to water-logging of soils, (and its subsequent lack of aeration of the soil surrounding the roots), leaching of nutrients, and excessive elevation of the water table.

It is clear then that an irrigation regime be established so that problems of over-irrigation are avoided. This is coupled with the fact that water supply is indeed not without limit and associated cost. So it would seem there is a two-fold incentive even for the unprincipled irrigator (one unconcerned for water conservation) to not overwater.

It is also the case that problems associated with over-irrigation are surpassed only by under-irrigation. Once again crop growth is impaired and yield reduced, particularly

for those crops that have developmental stages where they are extremely sensitive to water deficiency. Furthermore, salinity problems arise with under-irrigation since plants normally extract water leaving soluble salts behind. Unless there is sufficient flow-through drainage, these salts will accumulate in the root zone, becoming detrimental to the proper development of the crop. This is particularly a problem in arid lands.

The process of irrigation scheduling is therefore a matter of optimising the application times and quantities of water to avoid under or over-irrigation and consequently optimise yield. It is to be noted that the term 'optimal' when referring to irrigation has a twofold meaning. Firstly, that it is the 'right' amount of water to achieve maximum yield and secondly that it is optimal in terms of lessening environmental impact of irrigating water. It would, of course, be desirable if the two meanings were coincident. The question remains: "How does one ascertain the optimal irrigation regime"? This question is considered in the following sections, first, in the traditional sense, and then under a contemporary light. These sections will be considered in layman terms without strict definition as this will suffice to highlight the directions of irrigation scheduling. The subject however is inundated with terminology, notation and highly integrated concepts. Such terminology will be detailed in Chapter II and subsequent chapters.

1.2 CONVENTIONAL IRRIGATION SCHEDULING

The conventional view to irrigation scheduling is to recharge the effective rooting zone (i.e. the zone throughout which roots extract water) to field capacity[1] (the water

[1] There is a degree of dissension as to whether field capacity is an intrinsic property of a given soil. Hillel. 1980. pp.67-72.

content of the soil 1-3 days after water has been applied and drainage has largely ceased) after a time of water extraction by the roots and extraction due to evaporation. The maximum allowable deficit is calculated so the water content does not fall under a certain 'critical point' below which was the permanent wilting point of the particular plant. The timing of irrigation was accordingly dependent on meteorological conditions (which influenced the rate of evapotranspiration), soil properties (which influence how easily water is given up for evaporation or drainage), and plant properties (which dictate the 'critical point'). The traditional irrigation cycle consequently consisted of a brief period of infiltration followed by a time of waiting for evapotranspiration to run its course, over which time the soil water status was monitored to determine the time and quantity of the next irrigation event. Various methods are used to determine the soil-water availability to plants.

1.2.1 Soil Water Availability

Soil-water availability may be monitored in-situ by determining soil-water status or plant status or it may be deduced by estimating evapotranspiration and measuring precipitation, thus keeping check on water budgets. Consider firstly, these book-keeping methods:

Book-Keeping Methods.

In the case of book-keeping methods the critical point is predetermined and the root zone is estimated. A book is kept indicating estimated evaporation together with any rainfall thus revealing the accumulated deficit. Once the critical point is reached water is applied in quantities to bring the root zone up to 'field capacity'. Clearly the problem here is the lack of uniformity - the soil conditions and drainage are unlikely to be uniform not only in space but also in time (Van Bavel and Hanks, 1983) and so too

the application of the irrigation may not be homogeneous across the entire area.

The subject of estimating evapotranspiration is indeed broad and many methods are available. Three such methods are briefly outlined below.

(a) Evaporation Pans.

The evaporation pan is a popular method of determining the evaporative demands that the atmosphere places on the soil water. Here an open pan of specified size (of which there are several 'standard' types) is used to measure the loss of water from a free water surface in a particular locality. This may be done by the local Primary Industries Authority. To allow for age and type of crop, the particular crops' estimated water use is calculated by adjusting the pan evaporation by a crop factor, that is, $E_a = kE_0$, where E_a is crop evaporation, E_0 is pan evaporation and k is the crop coefficient.

These crop factors need to be determined for a particular pan, crop and locality over a period of years.

(b) Empirical Approaches.

These include the Thornthwaite method (1948) and the Blaney-Criddle method (1947). These methods have arisen from curve fitting procedures in an attempt to find a functional dependency of evapotranspiration with some easily determined or measurable quantity.

Quite clearly the atmospheric evaporative demands result from a complex combination of temperature, wind humidity and colour and roughness of the evaporative surface (and possibly others). The "Catch 22" in wanting accurate evaporation data is that, to be used in the field it must necessarily be easy to calculate but to be comprehensive in its accurate determination, the

intermingling factors lead to a very complicated system.

Empirical methods try to strike a balance between accuracy and ease-of-use. The Thornthwaite method for example is based only on one atmospheric factor - temperature, that is,

$$E = 16.0\ (10T/I)^a \text{ mm/month},$$

where E = potential evaporation,

T = mean monthly temperature (Celsius),

I = empirical heat index for 12 months (depends on latitude), and

a = empirical parameter based on I.

An example of an application of the Thornthwaite method is found in Withers and Vipond, 1974, pp 93-95.

The Blaney-Criddle method is also dependent on temperature and also relies on long term temperature records for specific locations, that is,

$$U = 0.46\ kp(t + 18),$$

where U = predicted monthly consumptive use (mm),

k = monthly empirical crop-factor.

p = mean monthly percentage of the annual day-time hours (dependent on latitude), and

t = mean monthly air temperature (Celsius).

Consumptive use is another term for actual evapotranspiration in mm/day. A simple example of the use of the Blaney-Criddle equation is found in Benami and Offen (1984) pp 18-20.

(c) Mechanistic Approaches.

The two methods briefly outlined above are strictly empirical and make no claims to fundamentality. They are simple, but not entirely accurate methods

that rely on data accumulated over the years. Penman's method (1963) contrasts strongly with these as it embodies some of the mechanism underlying the process of evapotranspiration. This method is a comprehensive model involving air temperature, humidity, windspeed, radiation rate and reflectivity of the surface. It is physically based in terms of its combination of energy balance considerations and aerodynamic transport factors. Penman's method is used to calculate the potential evapotranspiration and is then adjusted to obtain actual evapotranspiration. Due to the mechanistic base of this method, it has inherent appeal for general application as opposed to the locality dependent empirical formulae and subsequently is considered in greater detail in Chapter II.

In-Situ Methods.

Water availability may be monitored using a variety of tools such as gypsum blocks, neutron probes, pressure bombs, tensiometers and infrared thermometers. These direct measurement methods may be classified according to the aspect of the Soil-Plant-Atmosphere system they are designed to measure. The monitoring methods are summarised in Figure 1.1. Some of the common methods are outlined briefly below.

(a) Soil Moisture Methods - Water Content Evaluation.

The moisture level of the soil is an obvious indicator of water availability to plants. There are various methods available for its determination - some destructive, some non-destructive and all requiring a number of samples to overcome the spatial variability problem.

(i) 'Feel' method.

The appearance and 'feel' method is a 'rule of thumb' method that requires no other equipment other than experience. One question that

arises concerns the farmer with much experience in irrigating his sandy-loam soil by this method, whereupon the farmer sells that farm and buys another on more clayey soil. The water contents may be the same and this may be detected by feel but because of anionic attractions the water is bound more tightly to the clay and whereas this 'feel' was suitable for sandy-loam, it is not equally suitable for the clayey soil.

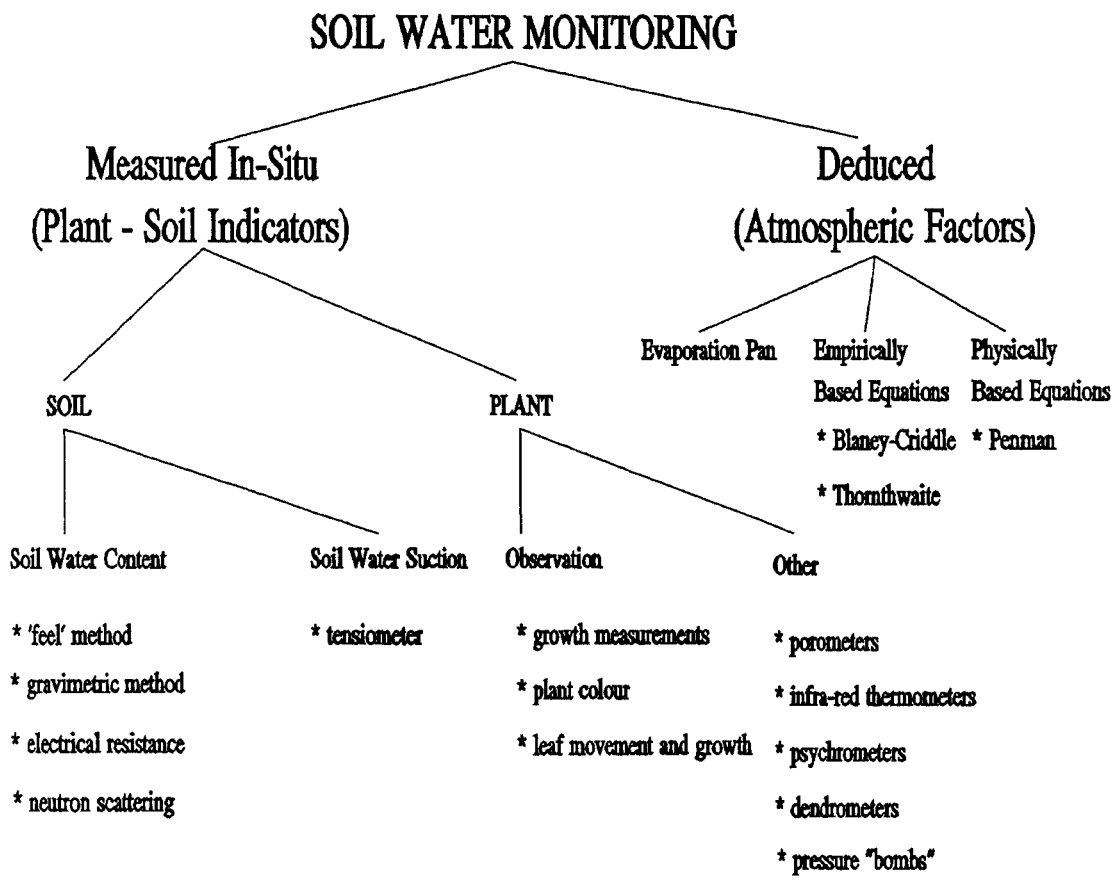


FIGURE 1.1 Summary of methods of assessing water availability to plants.

(ii) Gravimetric Determination.

The 'wetness' of the soil in its most traditionally simple yet impractical sense may be measured "gravimetrically". That is, to sample soil, weigh it, dry it, reweigh it and express the result as a percentage of water mass to dry soil mass. This water content on a mass basis may be converted

to volumetric wetness if the bulk density of the soil is known by using the relation

$$\theta = \theta_m(\rho_b / \rho_w),$$

where θ_m = wetness by mass (kg/kg),

ρ_b = dry bulk density of soil (kg m^{-3}), and

ρ_w = density of water (kg m^{-3}).

Time and labour costs as well as inaccuracy lead to the impractical nature of this method (Hillel, 1971; Marshall and Holmes, 1988). This method is destructive.

(iii) Indirect Methods.

The preceding two methods directly monitored the wetness of the soil. Several indirect methods are available which have the advantage that frequent or continuous monitoring may take place at the same points. One such method is that of determining the electrical resistance of a volume of soil. This method is considered in Hillel, 1971 and in Campbell and Campbell, 1982 and uses a gypsum block to measure electrical resistance and to infer water content. This method suffers from a problem with uncertainty of calibration. Another method that is considered most satisfactory (Hillel, 1980) at the present time, is that of neutron gauging. Indeed, Campbell and Campbell (1982), state that the neutron probe offers the best combination of features for irrigation scheduling. Neutron gauging is a non-destructive method that functions by effectively counting the hydrogen atoms in the soil. The probe emits fast neutrons which lose maximal energy upon collision with hydrogen nuclei. In practise, it is found that the loss of energy of the fast neutrons

is proportional to the hydrogen atom content of the soil. Since water is the only variable source of hydrogen in the soil, the probe readings correspond to soil wetness changes. Dr. Peter Cull, as reported in the 4th National Conference of the National Association of Teachers of Agriculture, 1986, evaluated all of the tools available and used in other countries for irrigation scheduling. He concluded in his PhD thesis that the neutron probe was found to be the most appropriate tool in order to accurately schedule irrigations. These finding are given support by the fact that in 1986 there were 26 neutron probe consultants in eastern Australia and that 45% of the national cotton crop (180,000 acres) was irrigation scheduled by using the neutron probe.

(b) Soil Water Potential.

So far the state of water in soils has been discussed only in terms of the amount of water in a given volume, with no consideration given to the energy state of the water in the soil. The fundamental question here is "just how 'available' is the available soil water?" The water content or wetness is only part of the story. Water molecules in one type of soil may be bound more or less tightly than in another soil type. Therefore some method is required to determine how easily that water may be extracted rather than determine how much is present. The use of a tensiometer is such a method. Tensiometers are practical instruments and are commercially produced and as such, a great deal of information is available about them. The Queensland Department of Primary Industries has information pamphlets and has produced a video on their correct installation and use.

The preceding section provided only a brief outline of some of the methods available to

determine soil water availability. A more detailed description may be found in Soil Physics and Irrigation texts. A useful summary of methods was found in the report of the 1987 seminar of the Irrigation Association of Australia in a session conducted by R.A. Stephenson. A copy has been reproduced below in Table 1.1.

Component of the system measured	Type of Measurement	Instrument(s) used	Comments
Soil	"total" water content	weighing (gravimetric)	simple,very time consuming difficult to characterise all root zone, research technique only
		neutron moisture probe	expensive, accurate, needs careful calibration to each soil and crop
	"available" water	tensiometer	simple, cheap, convenient, good for farm use
	soil conductivity	meter	soil solution concentrates with drying, complex and prone to errors
Stem	water flow up stem	dendrometer	research technique, measures stem expansion and contraction
		heat pulse	for research, measures rate of flow in xylem
Leaf	water content	weight (relative water content)	research, simple, meaningful in terms of plant function
	water potential	pressure "bomb"	simple, accurate, robust
		psychrometers	complex, for research, prone to contamination errors
	stomatal potential	porometer	stomata close when tree is stressed
		infra red thermometer	water stress: stomata close, leaf temperature rises (no cooling by transpiration) - needs careful calibration
Atmosphere	rainfall, evaporation, humidity, wind	weather stations	construct models on potential water use eg. Penman, Bowen Ratio, complex, must calibrate to soil, crop
Whole System	actual water use (evapotranspiration)	lysimeters (weighing or through draining)	research, measure weight or volume of water used

TABLE 1.1 Monitoring Water Status for Irrigation Scheduling.

1.3 RECENT CONTRIBUTIONS TO IRRIGATION MANAGEMENT

The classical questions in irrigation management are: 'When does one irrigate?' and 'How much water does one apply?'. The conventional answers, as stated by Hillel, 1980, are: Irrigate when the available moisture is nearly depleted by using the appropriate instrument or observation and apply sufficient moisture to bring the moisture reserve of the soil root zone to field capacity, plus a "leaching fraction" for salinity control. However, as Hillel points out, recent contributions have shed a new light on this area. The focal change is a movement away from the view of soil water as a static entity. Terms such as "Field Capacity", "Wilting Point" and even "Rooting Zone" give a sense of unchangingness and of being well defined. Figures put to these, like 15 bars for permanent wilting point reinforce this notion. Technology has opened the way for the realisation that soil water is far from static and indeed is extremely dynamic.

It is little wonder that the focus is changing. With the massive experimentation that has taken place in this area and the subsequent empirical relationships that rose out of them, it was only a matter of time that the emphasis would change to that of 'what forces cause this flow of soil water?' and 'how does the plant regulate uptake?', that is, a shift to **mechanism.** The physical basis of the movement of water through soils was considered in the late 1950's and 1960's. This paralleled the development of the thermocouple psychrometer (1951) and the pressure bomb (1965), thus allowing more accurate and detailed measurement of soil and plant attributes. Thornley and Johnson (1986), state that traditional empirical approaches "have little further to contribute" to our quantitative understanding of plants and how they function. This move towards a mechanistic paradigm was, and still is, not without problems. Powell and Thorpe,

(1975) highlighted this by stating that there was a "scant understanding by many workers of the physics involved, as the plethora of inexact terminology in the literature bears witness". Furthermore, the broad knowledge base required by workers in diverse areas such as soil physics, plant physiology, statistics and mathematical modelling inhibits speedy and reliable progress. Presently, mechanistic approaches still suffer from a lack of physical understanding of some of the processes involved.

By the very nature of the processes involved, any truly mechanistic mathematical model will be necessarily complex. Clearly, the major process that drives the soil-plant-atmosphere system is evapotranspiration. Evapotranspiration firstly depends on meteorological conditions such as radiation, wind, humidity, etc. This places a demand on the plant to maintain sufficient flow of water from the soil, through the roots so that it may be sufficiently hydrated for normal functioning. This in turn depends on the soil properties such as its pore size, tortuosity and the charge of the individual soil particles, to name obvious properties. Plant properties are important here also. Rooting depth, 'ability' of the individual roots to draw water from the soil matrix, rooting density and the rate of root extension all play their part in the uptake of water from the soil to maintain the evaporative demand. Thus, irrigation policy based on a comprehensive set of parameters such as described above would require a suitable vehicle to put them into perspective. Such a vehicle could be **mechanistic mathematical models.**

In summary, traditional methods are concerned with soil-water budgets and static characteristics of the soil water. It is evident that whilst both conventional and more modern scheduling are based on conservation of matter, conventional scheduling is concerned with the volume of water required to restore the root zone to field capacity

and not to allow the wetness to drop below some critical point. There is little regard given to the actual movement of the water in relation to the root system. Mathematical modelling can take this rather finer view of water movement and takes into account what happens to water after it disappears from view beneath the soil surface. In the chapters that follow, mathematical models and their solutions will be considered with the aim of using such models to aid in decision making with regards to irrigation scheduling and other related agricultural problems.

About 200 million hectares of land are irrigated through the world, half of which is in China and India. To these countries in particular, savings in the form of water, leached applied nutrients and irrigation expenses in return for an economically optimal yield would be valuable savings indeed. The 1000 km^3 of water required annually for irrigated land effectively can be translated into lives. By optimising its use in terms of increased yield can therefore improve quality of life for many people, it may well represent a saving of life, particularly in the third world countries.

CHAPTER II

THE STATE OF WATER IN SOILS - SOME BACKGROUND

2.1 AN OVERVIEW OF THE PROCESSES

The terminology and concepts in this area are extensive. The aim of this chapter is to elucidate on the various processes involving water movement, principally through soil, but also through the atmosphere and plant. Further to this it is intended to provide definitions where appropriate and to introduce the various models and notation and therefore provide the necessary background to underpin later chapters. This is done by surveying the literature dealing with the mathematical modelling of the various processes.

The system under consideration is extremely dynamic with energy of the water in a continual state of flux. The varying processes are highly interrelated but for clarity of description they will first be considered as individual and independent and then in a holistic sense in Chapter III.

The interdependence of these processes were acknowledged by J.R. Philip (1966), calling the whole system SPAC (Soil-Plant-Atmosphere Continuum). The underlying principle of SPAC is the same as that of the Universe, and that is (a) Matter and Energy are conserved and (b) water flow moves according to the direction of the lowest potential energy.

Consider the "continuum" for a single plant and a volume of soil in its immediate vicinity.

The source of water may be rainfall, irrigation or the often underestimated upward capillary flow. The rainfall or irrigation may be applied at a rate whereby the entire quantity of water infiltrates the soil. If the rate of input however, is greater than the penchant of the soil to absorb it then runoff may occur to an adjacent surface and similarly, water may flow into the area under consideration. If the surface contains pits, then ponding may occur, the ponded water later to be subjected to evaporation or infiltration. The infiltrated water then redistributes itself through the soil profile, some being taken up by the roots of which less than 1% plays its part in photosynthesis and thus becomes assimilated as part of the plant, whilst the greater remainder is transpired up the stem and out the stomata of the leaf and into the atmosphere. The remainder of the redistributed water is directed towards two fates - to be stored in the soil profile (later to either move up to the soil surface and evaporated to the atmosphere or drawn into the roots) or to drain further down the soil profile away from the root zone either to later be drawn upward by capillary flow or further downward to join the underground water. This latter flow may constitute 10% or more of the total water input (Rose and Stern, 1967).

Consider these various processes affecting the state of water in soils as depicted in Figure 2.1. These processes are driven by:

- the evaporative power of the atmosphere,
- gravity,
- matric potential of the soil and
- regulatory powers of the plant.

This section considers each of the processes illustrated here and outlines modelling approaches. For simplicity, they are considered as independent processes first, then they are treated in an integrated fashion.

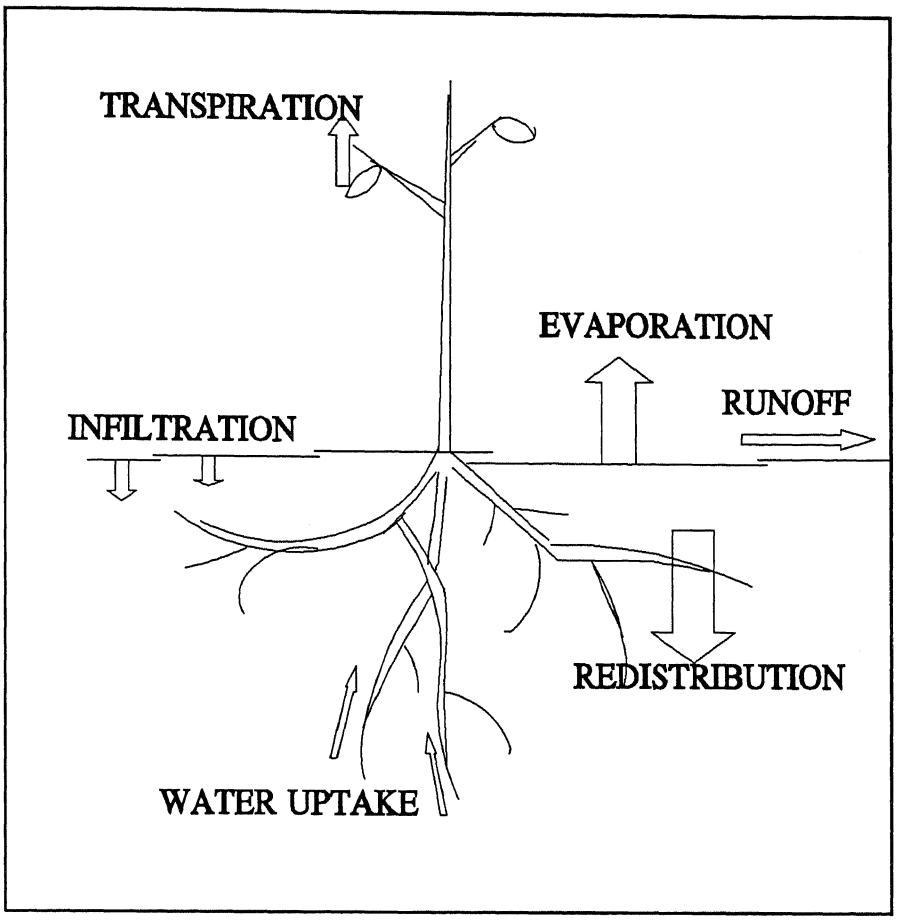


FIGURE 2.1 Processes affecting the state of water in soils.

2.2 THE SPECIFIC PROCESSES

2.2.1 Redistribution

The process whereby water, after its entry into the soil, moves through the soil profile is called redistribution. This process will be considered first because within the development of models relating to it, many broader concepts of water flow in soils can be introduced, as these are necessary for the analysis of the other processes.

The discussion that follows will be based on a homogeneous soil profile with a sufficient degree of uniformity of individual pores to neglect processes such as preferential movements of water along cracks and fissures and to avoid the complication of *hysteresis*. The hysteresis effect is considered in detail in Hillel (1980) and will not be considered

here, other than the following brief description. Hysteresis involves the relationship between water content and matric suction. As the soil wets (sorption) the suction is reduced, as the soil dries (desorption) the suction increases. Hysteresis is the phenomenon whereby this relationship is not single-valued and there is no unique relation between water content and matric suction. The curve describing the water content (θ) / matric suction (ψ) relation in desorption does not superimpose the sorption curve as shown in Figure 2.2.

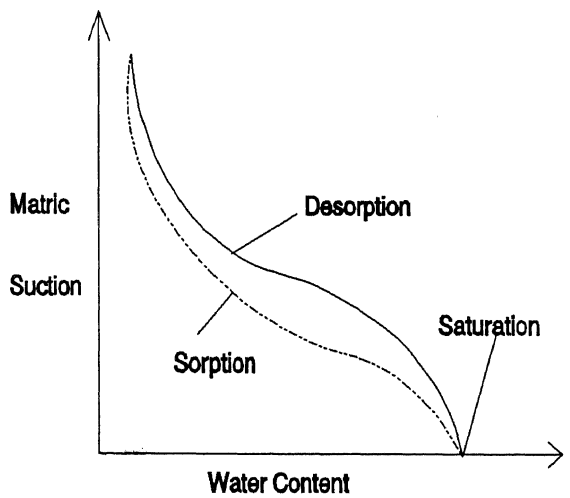


FIGURE 2.2 The dual valued suction/water content curve under Hysteresis.

To describe the physical basis of redistribution one must consider the energy status of water and soil. The following discussion takes this perspective with the aim of laying a physical foundation for the subsequent mathematical discussion.

The entropy of the earth increases or in other words, the direction of change for an isolated system is always towards equilibrium. From the moment water strikes the ground it begins its inevitable movement in accordance with the unavoidable rules of nature. Consider its movement from an energy state viewpoint. Soil water movement is under the influence of kinetic and potential energy. Since the magnitude of kinetic energy depends on the magnitude of the velocity and that soil water movement is slow, then its kinetic

energy is small. Hence the first of the many simplifying assumptions in the effort of describing water movement through soil - that kinetic energy is negligible. For this reason potential energy becomes of primary importance. This potential is called soil-water potential.

This energy is due to:

- the effects of gravity (gravitational potential),
- the effect of the attraction by the soil matrix (this is called matric potential, matric suction or soil-water suction) and
- the effect of dissolved salts (osmotic potential).

There are other potentials here such as submergence and pneumatic (Rose, 1966) and these together with matric potential comprise *pressure potential.* Pressure potential is the larger category and subsumes the others, however, the terms 'matric' and 'pressure' will be used interchangeably here, since in the zone of interest (soil above the water table, in the root zone) matric potential is dominant.

When hydrostatic pressure of the soil-water is above atmospheric pressure, the pressure potential is considered positive (this will become evident from the definition which follows). This is the case when considering water under a free-water surface since the surface of the water would be subject to one atmosphere and a hydrostatic pressure of zero and subsequently a pressure potential of zero. Beneath this surface, the single atmosphere would be compounded with the pressure due to the depth of water leading to a positive pressure potential. A negative pressure potential is commonplace within the zone of interest since water can rise above a free-water surface due to capillary rise (and adhesive forces with the soil matrix) and this would lead to sub-atmospheric potentials. Negative

pressure potentials are called suctions or tensions.

Pressure potentials are grouped with gravity potentials in a category called hydraulic potentials (Rose, 1966). Osmotic pressure is placed outside this group probably because it does not directly cause movement of soil-water in the soil matrix other than when water is in the vicinity of a semi-permeable membrane, the plant root being such a membrane.

As indicated in Rose 1966, the International Soil Science Society defined the total potential of soil water as "the amount of work that must be done per unit quantity of pure water in order to transport reversibly and isothermally an infinitesimal quantity of water from a pool of pure water at a specified elevation at atmospheric pressure to the soil water." In ascertainment of total potential energy however, water is **not** transported and its work done **not** calculated, but rather these ideas form the basis of a rather theoretical definition where in fact, total potential is obtained from other directly measurable quantities.

Therefore, the potential gradient constitutes the driving force of the soil-water by virtue of the position of the soil water in relation to some reference state. To illustrate this, consider the movement of water in one dimension, that of the direction perpendicular to the direction of gravity. The change in total potential (ϕ), is the product of the driving force (F), and the change in distance (Δx). That is,

$$\Delta\phi = F\Delta x \quad \text{or} \quad F = \Delta\phi/\Delta x \, .$$

Here, total potential is the sum of gravitational potential (ϕ_{grav}), pressure potential ($\phi_{pressure}$), and osmotic potential ($\phi_{osmotic}$).

It is appropriate at this point to clarify what is meant by the term 'a quantity of water' in the above definition of total potential of soil water. The 'quantity' could either be mass, weight or volume which, of course are related by the functions: weight equals the product

of mass and gravitational acceleration and mass equals the product of density and volume. As such, water content may be determined on a volumetric basis or on a mass basis. Similarly, as will become evident, potentials may be expressed per unit mass, per unit weight or per unit volume.

In much of the literature concerned with the movement of water in the root zone the term 'hydraulic head' is frequently used in describing potentials due to gravity and pressure combined. To provide some background, consider the gravitational component of the total soil water potential. From the definition, work is done in elevating a quantity of water (z metres, say) from a reference level (z=0). Consider the work done (W) on an infinitesimal mass of water (dm): $W = (dm)gz = (dv)\rho gz = (dw)z$,

where m, v, ρ, w, g are mass, volume, density, weight and gravity respectively. Therefore,

Pot. energy/unit mass = gz (J kg^{-1}),

Pot. energy/unit volume = $\rho.gz$ (N m^{-2}),

Pot. energy/unit weight = z (m).

It can be seen from the latter equation that potential energy **per unit weight** has units metres and a magnitude equal to that distance that the infinitesimal weight of water must have been transported from the reference level. A similar analysis conducted on the other components of the pressure potentials clearly gives the same units for energy per unit weight. Thus it is found that hydraulic potential (gravity plus pressure) per unit weight can be expressed in terms of an equivalent height of a liquid column corresponding to the particular pressure. This column of water may be termed **hydraulic head**. Of course each of the ways of expressing the energy state of soil-water are easily converted to one another and are basically equivalent.

Hydraulic head (H), as is hydraulic potential, is made up of the two components,

gravitational head (H_g) and pressure head (H_p),

$$H = H_g + H_p .$$

The mathematical model that embodies the principles of potential gradients and the subsequent flow of water through the soil matrix i.e. redistribution, is the **flow equation.** A derivation of the flow equation is given in Appendix A. For vertical flow,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} K(\psi) \left[\frac{\partial \psi}{\partial z} \right] - \frac{\partial K}{\partial z} = \frac{\partial}{\partial z} \left[K(\psi) \frac{\partial \psi}{\partial z} - K(\psi) \right] \qquad (2.1)$$

where t is time (s),

θ is the volumetric water content (m^3/m^3),

ψ is the matric potential (N m^{-2}),

K is called the hydraulic conductivity (kg^{-1} m^3 s) and

z is depth, positve in the direction of gravity (m).

This is one of the two major forms of the **flow equation and is commonly called the potential form of the Richard's Equation.**

The other form to be described below is called the 'Diffusivity' form and is so named since it parallels the equations of diffusion for which solutions are available. The term diffusion is not the most appropriate name since the water does not move by diffusion at all but rather by mass flow. This form is simply a device to tap into already solved differential equation types.

Recognising a dependence of ψ upon θ, and assuming a single-valued relation (no hysteresis), the following form of the flow equation is obtained

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K \frac{\partial \psi}{\partial z} - K \right] = \frac{\partial}{\partial z} \left[K \frac{\partial \psi}{\partial \theta} \cdot \frac{\partial \theta}{\partial z} - K \right] .$$

Defining parameters

$$c(\theta) = \frac{\partial \theta}{\partial \psi} ,$$

and

$$D(\theta) = \frac{K(\theta)}{c(\theta)} ,$$

the **diffusivity** form or water content form of Richard's equation is obtained.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[D(\theta)\frac{\partial \theta}{\partial z} - K(\theta)] \qquad (2.2)$$

The parameter c is termed the specific water capacity and is the slope of the soil-moisture characteristic curve, this being a plot of soil-water suction versus soil-water content. D is called the soil-water diffusivity function.

Since the water content under consideration here is the volumetric water content, then a volumetric water uptake term (these will be considered in detail later in this chapter) by roots may be included to model the water movement in cropped soils. Introducing this term the flow equation becomes:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[D(\theta)\frac{\partial \theta}{\partial z} - K(\theta)] - S(\theta, t) , \qquad (2.3)$$

where $S(\theta,t)$ is the water uptake function.

The flow equation states that the time rate of change of volumetric water content in a profile of soil is dependent not only upon the hydraulic head drop with depth into the profile but also upon the ease with which water can pass through the soil pores as effected by size and tortuosity of capillaries. Furthermore, the head drop is not usually constant and neither is the effect of size and tortuosity of the capillaries (hydraulic conductivity).

2.2.2 Infiltration and Runoff

For the water to become part of the redistribution process, the water must first penetrate the soil surface. Infiltration is the name of this passage of the water through the surface

and occurs as a result of rainfall, irrigation or the flow of water across the surface. The **infiltration** rate is the maximum rate that water can enter the soil through the soil surface. In the case of irrigation, it would be preferable if the rate of applied water did not exceed the infiltration rate, in which case water would be lost to the local soil profile due to the **surface runoff**. Depending on the depressions on the soil surface, some water may accrue in a ponded fashion whereupon it will be acted upon by evaporative forces or in time may infiltrate the soil surface.

It has been found that as wetting time increases, the infiltration rate decreases usually until some limit is reached. Suppose the infiltration is into an initially dry soil. The water enters the soil as a result of matric suction and gravity. As the upper layers wet, the matric gradient becomes less steep and the subsequent force drawing water into the soil reduces and consequently the infiltration rate decreases until it approaches its limiting value (due to the constant effect of the gravitational gradient). It is clear from the preceding information that the infiltration rate depends on the initial wetness of the soil surface layers and the time since infiltration began. These factors may be coupled with the soil structure and its subsequent hydraulic conductivity.

Infiltration Equations.

Bodman and Coleman (1944), described a typical moisture profile during infiltration which provides a useful foundation for the forthcoming discussion. The profile is illustrated in Figure 2.3.

As previously stated, infiltration rate reduces to some asymptotic value as time increases. This is reflected in the early empirical formulae, that is, $i = Bt^{n}$ where B and n are empirical constants and i is the infiltration flux (the volume of water entering a unit area

of soil per unit time). In this equation of Kostiakov (1932) in Aoda *et al.* 1988, the asymptotic value is zero rather than the constant infiltration rate that is known to occur. Further empirical formulae adjusted for this fact, Horton,1940 and Holtan, 1961 (in Aoda *et al.* 1988).

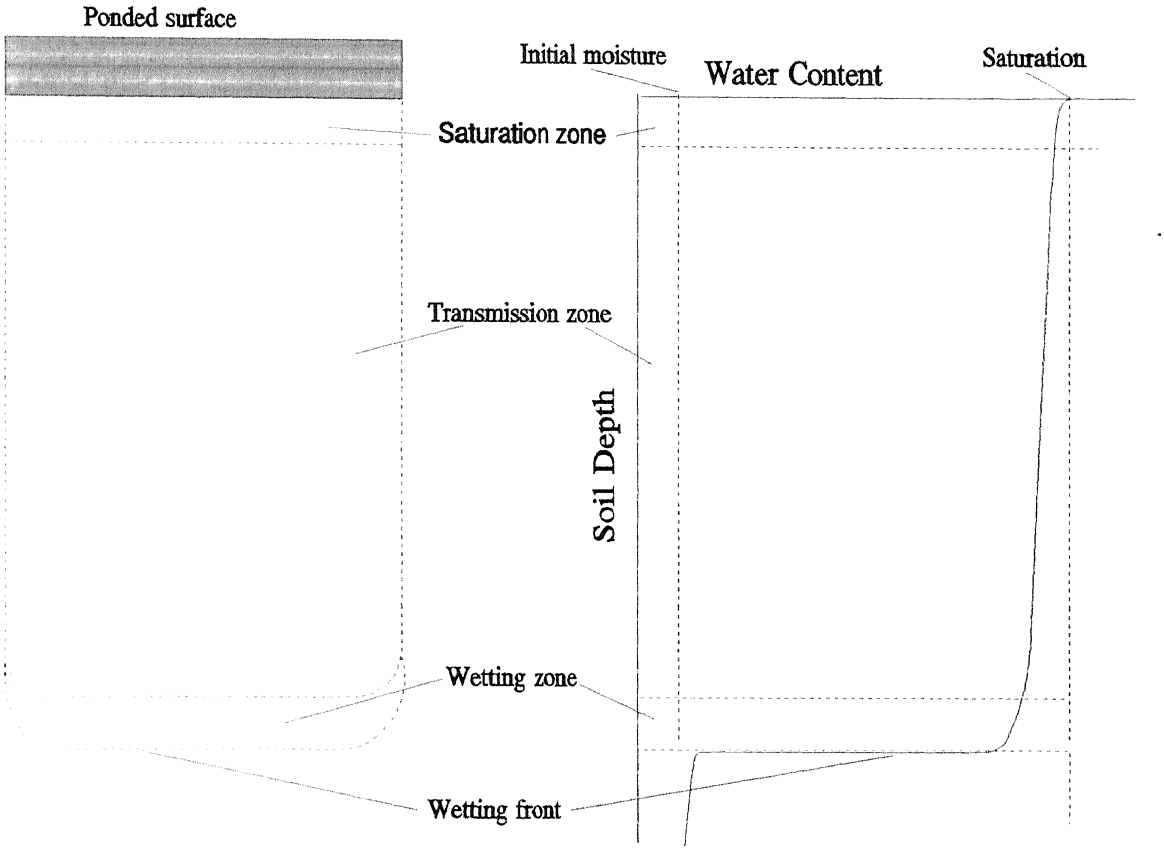


Figure 2.3. The moisture profile in an infiltration event as described by Bodman and Coleman (1944). The diagram on the left is a typical profile, on the right, the water content versus depth curve.

Theoretically derived formulae where the equations are based on the mechanisms of infiltration were developed by Green and Ampt (1911) and Philip (1957). Aoda et al (1988), stated that the Green and Ampt model is most widely used.

Philip (1957) predicted vertical infiltration by solving the flow equation with the following boundary conditions; at $t = 0$ and $z > 0$, $\theta = \theta_i$ and for $t > 0$ and $z = 0$, $\theta = \theta_0$.

Philip (1957) found that the cumulative amount of infiltration water entering a porous media follows a power series in the square root of time ($t^{½}$). In practice, this infinite, converging power series may be approximately be described by the first two terms as follows:

$$I(t) = St^{½} + At. \qquad (2.4)$$

where I is the cumulative infiltration, S was termed the sorptivity of the soil and A is a constant reflecting an 'essentially steady rate at long time' (Aoda *et al.* (1988)). It is to be noted that the derivative of (2.4) yields the infiltration rate, that is,

$$i(t) = ½St^{-½} + A.$$

The two term equation is inappropriate as time approaches infinity. This is because, as was pointed out by Philip (1957), at large t, $i(t) \approx A$. However, it is known that the infiltration rate approaches the value of the saturated conductivity of the soil (K_s), but A does not equal K_s at small values of time. Aoda *et al.* (1988) indicate that the adopting the first three terms of the Philip solution would remedy this. This equation is as follows:

$$I = St^{½} + At + Bt^{3/2}, \quad \text{where } B \text{ is another constant.}$$

Infiltration Approaches Compared.

The Green and Ampt approach has been found accurate when considering infiltration into an initially dry soil that has characteristics that lead to a sharply defined wetting front (Hillel (1980)). Green and Ampt made several assumptions such as the existence of a definite plane behind which was uniformly wet and the zone in front of this plane was totally uninfiltrated. These assumptions simplified the flow equation so that it may be solved analytically. Aoda *et al.* (1988) conducted an experiment to test the goodness of fit of predictions made by the equations of the Philip two term equation, the Philip three term equation, the equations of Green and Ampt and that of Knight (1976), as reported in Aoda *et al.* 1988, with those obtained in laboratory experiment.

In this comparative study, it was found that, whilst all were generally a good fit,

the Philip three term was the best, followed by that of Green and Ampt.

Whilst Philip was the first to provide a mathematically rigorous solution to the flow equation as applied to vertical infiltration, other workers have since produced physically based infiltration equations from the solution of the flow equation. Parlange (1971) introduced a quasi-analytical technique to solve the flow equation under gravity and Parlange *et al.* (1985) presented a general analytical solution to the water content form of the flow equation which approximated the surface water content and the time to surface saturation. Several workers have continued developments in these areas, Broadbridge and Knight (1988), Broadbridge *et al.* (1988), Hogarth *et al.* (1989a), Hogarth *et al.* (1989b), Philip (1990), Philip (1991), Hogarth *et al. (1991)*. A major aim of some of these papers is concerned with modelling the rapid changes in surface water content during infiltration and involve time to ponding. Further details of these solutions to the flow equation are considered in section 4.4.

From the definitions of infiltration and redistribution it is clear that infiltration is the process whereby water enters the soil surface and redistribution is the process whereby the infiltrated water makes its way through the soil profile. From a modelling perspective the distinction is not so clear. Whilst many researchers use the flow equation for redistribution (as detailed in the next chapter), not all share a common approach to infiltration. The model of Feddes et al., (1974) typifies one group of researchers that use the infiltration rate (as a function of time) as a boundary condition for the flow equation. In the contrasting treatment, the soil is considered as a stack of layers with the infiltrating volume of water "filling" the first layer before it cascades to the lower layer and so on. The model of Rowse and Stone (1978) makes use of this method, because they state that modelling infiltration using the solution to the flow equation does not handle hysteresis.

It is also stated that the solution to the flow equation would result in large amounts of computer time which would not appear to be the concern now as it was then. In their model, it is considered that each soil layer has a soil water deficit equal to the difference between its actual water content and that of nominal field capacity. Water infiltrates the layer from the surface until half the deficit is replaced before progressively moving downward. This continues whilst water is infiltrating the surface and then gives way to redistribution as described by the flow equation after infiltration ceases.

A similar treatment of the infiltration process is given by Saxton et al., (1974) whereby excess water drains to succeeding lower layers once the upper layer has reached 90% of saturation. That same condition held for each of the lower layers. Baier and Robertson (1966), whilst not concerned with the mechanism of redistribution, used a totally empirical formula to determine the volume of infiltrating water and then assumed that this water would bring the moisture content of the top zone to field capacity and the remainder draining to the next zone and so forth until no more water infiltrates or all layers were at field capacity with the surplus draining away (deep percolation).

2.2.3 Water Uptake by Roots

Water uptake by roots is a difficult area because the process is not fully understood. Hillel (1977) points out the some of the problems in giving an exact physical description of soil-water uptake by plant roots. Uncertain areas such as the variation of root growth in terms of differing directions, spacings and rates together with the variations in root uptake as determined by age underscore the problem. As Hillel puts it, "How the root system of a plant senses the root zone as a whole and integrates its response so as to utilise soil moisture to best advantage has long been a subject of great interest" (Hillel, 1977,p. 155).

Whilst many processes are uncertain, it is a fact that water flows according to potential

gradients. The following discussion considers the origin of these gradients.

As the water molecules leave the leaf through the stomata due to the evaporative powers of the sun, the air spaces in the leaf interior adjacent to the stomata becomes momentarily devoid of the equivalent water pressures that exist in the xylem vessels which supply water to the leaves. This water pressure incongruence is dynamically corrected with water molecules supplied by the xylem. Thus the evaporative forces of the sun are responsible for creating the water pressure gradient that results from the domino-type effect as the water pressure reaches equilibrium xylem vessel by xylem vessel, down the stem, to the roots. The actual structure of the xylem vessel assists in the maintenance of this transpiration stream and is a topic of Plant Physiology texts. It is clear then that a pressure difference will develop at the soil-root interface and the flow of water into the root will then depend on the permeability of the root membrane, the magnitude of this pressure difference and the water supplying ability of the soil. This water supplying ability is dependent on the resistances to flow in the soil as related to the hydraulic conductivity of the particular soil.

Two main approaches have been taken in the mathematical modelling of this process. The *microscopic* approach considers the radial flow of soil water to a single root, whereas the *macroscopic* approach considers the root system as a whole and disregards the flow of soil water to individual roots.

Microscopic Approach.

In this situation an individual root may be seen as a cylindrical sink of infinite length. The flow equation is written in cylindrical coordinates by using Darcy's law in radial form i.e. $q = -K\, dH/dr$, (q is the volume of water per unit area per second or volume flux, H is hydraulic head and r is the radial distance from the root) and solved for the distribution of potentials, water contents and fluxes from the root outward. Here it is assumed that the

water content is spatially dependent only on the radial coordinate. Along the length of this sink the properties are considered to be constant, with a collection of such equally spaced cylindrical sinks comprising the entire root system. Herein lies a shortcoming of this approach - this approximation denies the complexity of the structure and geometry of plant roots. However, once the flow to a single "typical" root is determined the results are then multiplied by an average root density to project the entire plant-soil system.

The microscopic approach to modelling has been employed by Gardner (1960), Hillel *et al.* (1975), Taylor and Klepper (1975), and Herkelrath *et al.* (1977). These are considered in more detail below.

Gardner (1960) assumed:

- a stationary cylindrical root,
- a constant initial water content,
- constant diffusivity and conductivity and
- a constant flux at the root.

Gardner considered the one dimensional (vertical) transient state or unsaturated flow equation to treat the radial flow to a line sink such as an individual root, that is,

$$\frac{\partial \theta}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(rD\frac{\partial \theta}{\partial r}\right),$$

where θ = water content on a volume basis,

D = diffusivity,

t = time and

r = radial distance from the axis of the root.

By using the appropriate initial conditions and boundary conditions, Gardner solved this equation for constant D. For t sufficiently large,

$$\psi_s - \psi_r = \frac{q}{4\pi K}\left(\ln\frac{4Dt}{r^2} - \gamma\right), \qquad (2.5)$$

where ψ_s and ψ_r are the matric potentials in the bulk soil and at the root surface respectively,

q is the uptake volume of water per unit length of root, per unit time,

K is the hydraulic conductivity and

$\gamma = 0.57722$ (Euler's constant).

Calculations performed by Gardner on the suction distributions as a function of distance from the root based on the above solution indicate that the equation is realistic for only short periods of time or for low values of conductivity.

As a result, the solution of this equation for transient flow was further facilitated by Gardner, in approximating this flow as a series of steady states. This approximation permitted an analytical solution. The steady-state solution to the radial flow equation is:

$$\psi_s - \psi_r = \frac{q}{4\pi K}\ln\left(\frac{r_1^2}{r_2^2}\right),$$

where r_1 and r_2 are radii of the root and half the average distance between neighbouring roots respectively.

Hillel *et al.* (1975) avoided these possibly restrictive assumptions by using a numerical solution to the flow equation cast in the radial coordinates. This model further attempted to take into account the possible effects of solute convergence toward the root and their subsequent osmotic effects. This was done by introducing a water extraction flux analogous to Ohm's law:

$$q_{ex} = \frac{(\Phi_m + \Phi_o - \Phi_o)}{(R_s + R_r)},$$

where q_{ex} is the volume of water extracted per unit time,

Φ_m is the matric potential of some finite ring of soil immediately surrounding any particular root,

Φ_o is the osmotic potential of the soil solution in that same ring which has hydraulic resistance R_s, and

R_r is the hydraulic resistance of the root.

Hillel *et al. (1975),* introduce the parameter Φ_c termed "crown potential". This is the singular potential at the base of the stem where all roots converge and where the plant emerges from the ground. It was stated that the main intention of this model was not to simulate field conditions directly but rather to investigate the localised microscale effects of both matric and osmotic components and thus avoid the various problems of underestimation of water stress evident in the macroscale approach that neglects these effects. The model was not tested experimentally.

Taylor and Klepper (1975) indicate that it is difficult if not impossible to measure the water potentials at the soil-root interface and therefore it is difficult to test these microscopic models experimentally. Since the potentials may be measured with more certainty at the outer edge of the root xylem, then Taylor and Klepper suggest restating the solution to the model of Gardner (1960) in the analogous form but with different boundaries:

$$q_r = \frac{-2\pi K_{sys}(\psi_{root\ xylem} - \psi_s)}{\ln \frac{r_{cyl}}{r_{stele}}},$$

where q_r is the rate of water uptake per centimeter of root,

K_{sys} is the hydraulic conductivity of the combined soil-root radial pathway,

$\psi_{root\ xylem}$ is the value obtained from root xylem measurements,

ψ_s is the pressure potential of the water at r_{cyl} (with r_{cyl} being the same as

Gardner's r_1), and

r_{stele} is the radius of the root stele (the root xylem).

The results of the subsequent experiment indicated that plant resistance is much greater than soil resistance to radial water flow throughout a wide range of soil-water contents, and that water uptake is proportional to rooting density and to the water potential difference between bulk soil and plant xylem.

Herkelrath *et al.* (1977) found that the standard theory of root water uptake as presented by Gardner (1960) did not compare favourably with experiment, specifically in an experiment conducted by Herkelrath *et al.* (1977), the extraction rates predicted by standard theory were as much as eight times larger than the measured values. It was found that a reasonable fit between experiment and theory could only be made by assuming a rooting density 100 times smaller than that measured in experiment. This suggests that not all of the surface of the root contributed to the uptake of water and this gave rise to the Root Contact model whereby as the soil dries, the surface area of the roots in contact with the soil decreases. This assumption would attribute the water uptake to a lesser proportion of the surface area of the root system and subsequently this would manifestly be equivalent to the average root resistance increasing. This is consistent with the results of Taylor and Klepper (1975) who also found the major resistance to radial water flow was in the roots and not the soil. Herkelrath *et al.* (1977) introduce a root permeability parameter per unit length (ρ), presumably inversely proportional to the combined resistances of both soil and root membrane, that is,

$$q = \rho(\psi_1 - \psi_r) \ ,$$

where ψ_1 is the soil water potential at the root surface and ψ_r is the water potential inside

the root membrane. This equation was then modified to allow for root contact by assuming that the effective conductivity of a root segment is proportional to the wetted fraction of the surface area of that segment. The wetting fraction factor (f) was introduced with

$$q = f\rho(\psi_1 - \psi_r) \ .$$

Herkelrath *et al.* found that by using this root contact theory as a modification to the microscopic approach, a possible solution to the dilemma of why the total resistance to flow in the soil-plant system increases with soil dryness when theory implies that soil resistance should be negligible may have been provided.

The preceding survey of microscale approaches to water uptake was certainly not exhaustive. It was intended to provide a cross-section of such approaches to contrast with the forthcoming discussion on macroscopic approaches.

Macroscopic Approach.

If the flow of soil-water to individual roots were not so important as the amount of water taken in and the distribution of this intake in relation to the root system, then it would be reasonable to model the root system as a diffuse sink (as opposed to a series of line sinks) that permeates the entire soil profile to the depth of the root system. This macroscale approach avoids the geometrical complexity of the microscale model and is represented mathematically by adding a volumetric sink term (S) to the conservation equation so that the rate of change of water content of a volume of soil balances with the flux through the volume and with the water that is withdrawn by the roots:

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial z} - S(z,t) \ .$$

The driving force of the water passing into the root is the pressure head difference between the soil and the root interior.

The sink term is generally expressed as an extraction rate per volume of soil and, as such, the sum of all these extraction rates over the entire root system equals the transpiration rate, that is,

$$\int_0^v S(z)\,dz = T ,$$

where $S(z)$ = the moisture extraction rate per unit volume of soil,

z = the vertical distance positive downwards,

v = the vertical length of the root system, and

T = the transpiration rate per unit area of soil surface.

Many researchers have employed various macroscopic models i.e. Gardner (1964), Molz and Remson (1970), Feddes and Rijtema (1972), Nimah and Hanks (1973a), Feddes *et al.* (1974), Hayhoe (1981), Hayhoe and Dejong (1988) and many more. The following discussion considers the major schools of thought in this field.

The microscopic approach was concerned with the flow of water to the individual roots, i.e. the volume of water entering unit length of the root per unit time (this flux was previously denoted by q), whereas the macro approach is more concerned with the volume of water taken up by roots in a volume of soil per unit time. The latter approach does not consider individual roots but rather treats the root system as if it were a diffuse sink distributed evenly throughout the volume of soil. Therefore the microscopic model may be extended to the macroscopic model by introducing a parameter representing the effective root length per unit volume of soil. The term 'effective' meaning the portion of

roots effective in absorbing moisture. Gardner (1960) did this to account for flow into a nonuniform root system and derived the equation:

$$\frac{\partial\theta}{\partial t} = \frac{mL(\psi_L - \psi_s)}{R(\theta,Z)}, \qquad (2.6)$$

where ψ_L is the suction at the plant leaves,

ψ_s is the average soil suction,

L is the effective root length per unit volume of soil,

m is a constant which lumps together constant factors from his earlier microscopic equation (2.5) and

R is the sum of the resistance to the water movement in the soil and resistance to entry into the plant.

This equation neglects the soil-water flow. Gardner (1964) continued this work with the following equation resulting from (2.6):

$$S = \frac{(\psi_r - \psi_s)}{I_p + I_s}, \qquad (2.7)$$

where ψ_r and ψ_s represent suction of roots and average matric suction of soil respectively and I_p and I_s are impedance to water movement in plant roots and soil respectively. Arguing further that root impedance may be small compared with soil impedance and that $I_s = 1/BKL$ where B is a constant, K is unsaturated conductivity and L is the length of root in the unit volume of soil, Gardner arrived at a finite difference form for water uptake with the aim that the effect of root distribution on water uptake and availability could be analysed. The finite difference form is as follows:

$$S_i = B(\psi_r - \psi_s - z_i) K_i L_i,$$

where S_i is the rate of water uptake per unit cross section of the *ith* layer of soil, z_i is the distance from the soil surface to the centre of the *ith* layer and K_i and L_i are conductivity and length of root per volume respectively, evaluated in the *i*th layer.

The idea that plant resistance is not negligible compared to soil resistance, (Taylor and Klepper (1974)), casts some concern over the assumptions used in the derivation of the equations of Gardner. As stated previously the root contact model of Herkelrath *et al.* tends to support the notion of the importance of plant resistance in relation to soil resistance.

Molz and Remson (1970) recognised that a serious problem with the microscopic approach is the difficulty of specifying the boundary conditions at the root surface and that the macroscopic approach has significant advantages. Among these, Molz and Remson list that the boundary conditions (usually at the soil surface) are easier to apply and are quite realistic in that they allow for phenomena such as rainfall and evaporation (and no doubt, irrigation) to be included. Unlike Gardner (1964), Molz and Remson (1970) did not extend the micro model into a macro model but rather they began at the macro level with the flow equation (diffusivity form) including a volumetric sink term and then considered what form this term should take to model reality. The first of the two extraction terms presented depends only on depth and transpiration rate. This is an empirical term fitted to the commonly used extraction pattern of 40%, 30%, 20% and 10% of total transpiration coming from each successive deeper quarter of the root zone:

$$S(z) = -\frac{1.6T}{v^2}z + \frac{1.8T}{v} \qquad 0 \leq z \leq v \tag{2.8}$$

where variables are as described above and v is the length of the root system.

It can be shown that when (2.8) is summed over the entire root zone that the total transpiration results. A derivation of this model equation is given in section 5.1. The growing root can be easily incorporated here by substituting $v(t)$ for v. It is pointed out in this paper that the shortcoming in these simple models occur when the upper layers dry and cannot supply sufficient water to maintain the percentage extraction ratio. Molz and Remson (1970) then introduced an extraction term that depends on moisture content, depth, and transpiration rate:

$$S(z,\theta) = T\left[\frac{R(z)D(\theta)}{\int_0^v R(z)D(\theta)dz}\right].$$

This more mechanistic approach leads to the proposal of the term "effective rooting density", which refers to that portion of roots effective in absorbing moisture. Whilst this extraction term was derived in a "somewhat arbitrary manner", the "fraction" of transpiration rate allotted to the various depths is realistically greater if the amount of absorbing roots is great in a given volume as well as the ease of transport of water through the soil matrix is also great. It was found that this model fitted reasonably with experiment. This paper goes further to describe the numerical solutions to the flow equation incorporating extraction terms of the types outlined and these will be considered in detail in Chapter IV.

From the earlier discussion of the microscopic approach by Gardner (1960) it was evident that the flow of water into a single root under steady state conditions depended on the conductivity (or inversely, the resistance) and the head (or suction) drop. Gardner pointed out that this result may be extended to the entire root zone. An analogous equation to (2.7), extended to the entire root zone, assumes that the rate of uptake is proportional to

the soil hydraulic conductivity K and to the head drop. Thus the sink term can be represented as:

$$S = \frac{-K(h_r - h)}{b}, \tag{2.9}$$

where S = volumetric rate of water uptake per unit volume of soil,

h_r = pressure head at the root-soil interface,

h = pressure head in the soil, and

$1/b$ is a coefficient of proportionality.

In a review by Feddes *et al.* (1974) it is pointed out that most authors had used expressions similar to (2.9) for the volumetric uptake term and that the $1/b$ term has been assigned various meanings. The reason given for the variations on the meaning of the $1/b$ term is that there is a lack of understanding of the physics involved in this process and this empirical entity lumps the finer physical detail into a solitary, workable term. This $1/b$ term is basically equivalent to Gardner's (1964), BL which, in Gardner's equations accounted for root activity, root density and root geometry. Feddes *et al.* speculate that the $1/b$ term is proportional to the specific area of the soil-root interface and inversely proportional to the impedance of the soil-root interface. Contending that advantages of the simple simulation model that includes $1/b$ outweigh the disadvantage of gross oversimplification, Feddes *et al.* adopted this form of the uptake term and substituted it into the conductivity form of the flow equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\frac{\partial(h+z)}{\partial z}\right] + \frac{K(\theta)[h_r - h(z)]}{b(z)},$$

where h = matrix pressure head,

h_r = (assumed uniform) pressure head at the root-soil interface.

Osmotic pressures are neglected. It was found that *1/b* was proportional to root mass and that both varied nearly exponentially with depth, and since the root distribution varies with both depth and time, *1/b* would need to be carefully calibrated for each application. This model is considered in greater detail in Chapter III.

The preceding water uptake model was modified from the model of Nimah and Hanks (1973a) whose objective was to propose and test the model under field conditions. The root extraction term in this case was defined as:

$$A(z,t) = \frac{[H_{root} + (RRES \cdot z) - h(z,t) - s(z,t)] \cdot RDF(z) \cdot K(\theta)}{\Delta x \cdot \Delta z},$$

where H_{root} is an effective water potential in the root at the soil surface ($z = 0$),

RRES is a root resistance term equal to *1+Rc*,

(Rc is a flow coefficient in the plant root system assumed to be 0.05),

h(z,t) is the soil pressure head,

s(z,t) is the osmotic potential,

RDF(z) is the proportion of total active roots in depth increment Δz, and

Δx is the distance between the plant roots at the point in the soil where potentials are measured and is assumed to be arbitrarily one.

Hydraulic conductivity and pressure head-water content relation are considered constant with time. Comparing this with that of Feddes *et al.* (1974) it can be seen that they are effectively the same with *1/b(z)* corresponding to $RDF(z)/\Delta x \Delta z$.

Whilst Gardner (1964) was not concerned with the flow of soil-water other than that

which flowed to the roots, Hillel *et al.* (1976) found it of interest to establish how the pattern of soil water extraction by roots related to the flow of water within, through, and below the root zone. Considerations such as insufficient drainage causing accumulation of salts and excess drainage leading to unnecessary loss of water and nutrients led to such interest. The model of Hillel *et al. (1976)* sought to embrace the basic physical mechanisms of transport of soil and solutes through soil and into roots. With this model came a direction to achieve some practical goal - in this case the hope that such a model will contribute to an improvement in the optimisation of "agronomic, hydrologic, and environmental aspects of soil-water management". The extraction term was similar to that of Gardner (1964), that is,

$$S = \frac{\phi_{soil} - \phi_{plant}}{R_{soil} - R_{roots}},$$

where ϕ_{soil} is the total potential of soil water including matric, gravitational and osmotic potentials,

ϕ_{plant} is the "crown potential" as described earlier,

R_{soil} was as defined in Gardner (1964),and

R_{roots} is the sum of resistance to absorption and conduction of roots (the resistance to conduction is considered to be a function of the depth of any particular group of roots).

Rowse, Stone and Gerwitz (1978) use a similar uptake term to this except the plant potential is considered to be a constant value throughout the root xylem and not just at the "crown" of the plant root. This group of models differ to those of Molz and Remson (1970) in two ways:

- they are more mechanistically based and

- they incorporates several parameters that vary as functions of time and depth.

The macroscopic model of Feddes *et al.* (1976) moves away from the earlier sink term which included the product of the difference in pressure head between soil and root-soil interface, the hydraulic conductivity of the soil and some empirical root function, in an attempt to define a more simple expression. The sink term that was defined was a function of soil-water content which varied according to whether water was plentiful (but not excessive) or not easily available or somewhere in between. Water uptake was considered to be at a premium when soil-water pressure head was between -400cm and -50 cm. The lower limit corresponded to a point where water begins to limit plant growth (as determined in the Thesis of Feddes (1971)), whereas the upper limit of -50 cm corresponded to anaerobis point where oxygen is denied to the roots because the water occupies the air spaces in the soil matrix. The water uptake maximum falls to zero above anaerobis point. Water uptake was also considered to be zero below "wilting point" (-15 000 cm). Of course, these figures vary according to the soil type. The water uptake for the plant, S, is assumed to decrease linearly with time with θ between h = -400 cm and h = -15 000 cm. Certainly the mechanistic modeller would argue that these static soil indicators are not intrinsic soil properties. With further approximations the sink term was defined to be

$$S(\theta) = \alpha(\theta)\frac{2T}{Z},$$

where $\alpha(\theta)$ is the dimensionless variable $S(\theta)/S_{max}$,

T is the actual transpiration rate, and

Z is the rooting depth.

The conclusions drawn by Feddes *et al.* to results of the experiment used to verify this model were that it did not predict the distribution of soil-water content with depth very

accurately but it did simulate the cumulative effect of uptake over the entire root zone properly.

The model of Hoogland *et al.* (1981) was an extension of Feddes *et al.* (1976) whereby the maximum root extraction is taken to be a decreasing function with depth rather than constant with depth as in the earlier paper. The modification was based on observations of an experiment carried out by Feddes, (1971) where it was found that the magnitude of root extraction was generally small at the top of the profile, increasing to a maximum zone then decreasing to zero at the bottom of the zone. In the modified model it was assumed that S_{max} varies linearly with depth from some surface value found from the literature data:

$$S_{max} = a - bz, \qquad z \leq z_r,$$

where a and b are constants; and z_r is the rooting depth. The modified sink term then became:

$$S = \alpha(h).S_{max}(z).$$

Hoogland *et al.* (1981) could not determine from their experimentation whether the modified sink term had any advantage over the original one.

Some of the models outlined to this point have either included a root surface area parameter or a root length density parameter. As pointed out by Klepper and Taylor (1979), these characteristics of roots are more useful for inclusion with uptake terms rather than root dry weight, which, although can be determined more easily, are overly influenced by larger, older, woodier and less absorptive commonly found near the surface. It could be concluded that root effectiveness distribution, is not directly proportional to root dry weight distribution. Nevertheless, Hayhoe (1981), Dejong and Hayhoe (1984) and Hayhoe and Dejong (1988) all use a root sink term incorporating a root weight

function, that is,

$$S(\theta,z,t) = C(z)K(\theta)(\psi_r - \psi(\theta))W(z)$$

where $W(z)$ is the root weight function in grams per cubic centimetre,

$C(z)$ is a root activity function,

ψ_r is the suction head at the root-soil interface, and

$\psi(\theta)$ is the soil-water suction head function.

This model is similar to that of Feddes *et al.*(1974) in that the *1/b* of Feddes now manifests itself as $C(z)W(z)$ (recalling that Feddes *et al.* (1974) found *1/b* to be exponentially related to root mass). This model, as do many others, uses empirical relations of Clapp and Hornberger (1978) to specify $K(\theta)$ and $\psi(\theta)$ for various values of water content. The model as described by Hayhoe (1981) differed slightly from the other two in that the root activity parameter was considered a constant and not a function of depth as in the later two. One suggestion made for improvement of the root activity constant in Hayhoe (1981) was that to make it a function of root age and therefore account for the decreasing effectiveness of roots with age. The model of Hayhoe (1981) was tested by Dejong and Hayhoe (1984) on native grassland conditions where it was found that a better fit with measured data could be obtained by decreasing the lower limit of water availability to plant roots during dry periods.

Hayhoe and Dejong (1988) compare the model just described with another macroscopic sink term based only on a knowledge of rooting depth. The second sink term was limited by a maximum uptake rate which is a function of potential transpiration which was assumed to decrease linearly with depth. This maximum rate was defined by:

$$M(z) = \frac{2T(Z_r - z)}{Z_r^2},$$

where $M(z)$ is the maximum uptake, Z_r is the rooting depth and T is the potential evaporation. This results in the new sink term:

$$S(\theta,z) = C(z)K(\theta)(\psi_r - \psi(\theta)), \qquad S(\theta,z) < M(z),$$

$$\text{and} \quad S(\theta,z) = M(z), \qquad \textit{otherwise.}$$

The measured data indicated that the second uptake term estimates the actual evapotranspiration better than the one based on root weight distribution. A second advantage was that whilst the uptake term based on the weight function may estimate cumulative uptake quite well, it may not estimate the uptake distribution over time with any accuracy, whereas the uptake term specified with the linearly decreasing function is regulated such that at any depth the entire demand cannot be met, which is not realistic anyway.

The preceding discussion was designed to provide an overview of the types of models both microscopic and macroscopic, that have been developed. It has been evident that the models vary in degrees of empiricism and are largely a result of the balance between oversimplification in an effort to be reasonably practical and overmechanisation whereby parameters would be not readily available. In any case the mechanisms are not well known as acknowledged by Hillel *et al.* (1976), Hayhoe (1981) and Feddes and Zaradny (1978), thus there is a necessity for some degree of empiricism as borne out in the models of Feddes *et al.* (1974) and all the models based upon it (Hayhoe (1981), Dejong and Hayhoe (1984) and Hayhoe and Dejong (1988). Indeed Feddes and Zaradny (1978) stated that "A complete and physically - mathematically sound description of water uptake and transport by living root systems seems to be hardly possible". A more optimistic Klepper

and Taylor (1979) contend that "The day will surely come when, with appropriate identification of soil, climate and plant characteristics, we can predict the time courses for transpiration and for water content changes within a profile."

2.2.4 Evaporation, Transpiration and Drying

For a bare uncropped soil, water losses by evaporation could amount to 50% or more of total precipitation, Hillel (1980). In a cropped soil, water can also evaporate from the leaf surface, this process being called *transpiration.* The two processes, *evaporation* and *transpiration*, are closely related, this being emphasised by the fact they are usually grouped together in the process *evapotranspiration.* Just how the total evaporative losses are apportioned between the two component processes depends on the stage of development of the crop. If the crop is just emerging, clearly there is not much difference between that situation and bare soil. If the crop is in advanced stages and with much canopy cover shading the ground then evaporation from the soil surface is decreased and the transpiration, by virtue of the large leaf surface area, is increased. In modelling the soil-plant-atmosphere water movement, the processes therefore will have changing prominence as the crop grows. Consider now the two processes individually.

Evaporation From The Soil Surface.

This section will consider only the case of evaporation from bare soil where there is no high water-table that will permit rewetting of the soil profile in the case of loss of water due to evaporation and redistribution. This soil drying process consists of three identifiable stages:

- The initial *constant rate stage* where the soil is wet and evaporation is restricted only by the amount of energy supplied to the surface. For this reason this stage may also be called the *energy-limiting stage.* Thus the soil properties have little

to do with the rate of evaporation, but rather meteorological conditions dictate the rate. Hillel (1977) states that the end of this stage is considered to have occurred when the surface of the soil has desiccated to the point of "air-dryness".

- When moisture becomes limiting, the evaporation is controlled by the conductivity of the soil in restricting the rate of upward flow of water to the surface. This *falling-rate* or *soil-limiting* stage is where the rate of evaporation falls below its potential rate.
- The *slow-rate* or vapour diffusion stage is the third stage and it may persist for long periods of time. In this stage the upper layers are dry and will not permit the upward flow of liquid water and so water traverses these layers by the process of vapour diffusion.

So far as the relationship between evaporation and redistribution, experimentation of Gardner *et al.* (1970b) indicates that evaporation has little effect on redistribution. This gives some credence to the simplifying assumption of Saxton *et al.* (1974) who considers that the soil evaporation portion of total evapotranspiration comes only from the top 15 cm of soil. In the experiments of Gardner *et al.* (1970b), it was found that redistribution greatly detracted from evaporation. Cumulative evaporation was reduced by about three-fourths of what it would have been had redistribution not taken place.

Evaporation From The Plant Surface -Transpiration.

An outline of the process of transpiration was given in section 2.2.3 when dealing with water uptake by plant roots. The root uptake of water is driven by the energy supplied to leaf by the sun and not as a process of active transport of water by the roots. As such, the process of transpiration does not require an expenditure of energy by the plant itself.

Some water may indeed enter the plant root due to osmotic gradients but this is small in comparison with the sun-induced movement. The plant does have some regulatory powers over water loss in that the stomata will close as the plant loses water thus severing the connection between internal leaf air spaces and the external atmosphere hence halting the need to correct potential gradients between the two and stopping the loss of water.

Modelling Evapotranspiration.

The various approaches to modelling the consumptive use of crops or evapotranspiration has been introduced in Chapter I to demonstrate methods used in determining the soil-water availability to plants and how it is monitored. Two empirical models were outlined, that is, the models of Thornthwaite and of Blaney-Criddle. They will be considered no further in preference to the classic mechanistic model of Penman (1948).

Just as the discussion on redistribution and subsequently the development of the flow equation formed a useful perspective for further discussion of current work in that area, similarly, the following development of *Penman's equation* also provides useful background.

The Penman equation was designed to calculate the evaporative power of the atmosphere. This would permit the determination of the evaporation from the soil surface and since transpiration (the water uptake and loss of water by plants) is also driven by atmospheric demand, it too could be calculated as the collective term - evapotranspiration. Since the equation was designed to calculate the maximum possible rate at which the atmosphere is capable of extracting from a field, it yields **potential evapotranspiration.**

Penman defined potential evapotranspiration as "the amount of water transpired in unit time by a short green crop, completely shading the ground, of uniform height and never

short of water." This definition requires some elucidation.

For a surface to give up its water at its **potential rate**, two conditions need to be met. Firstly, energy must be supplied (by the sun, say) to the water surface to separate the molecules from liquid phase, and in doing so, work is done against internal cohesive forces. As the molecules leave the water surface, further work is done against surrounding molecules as the now water vapour expands outwards. It is to be noted that the energy absorbed by these water molecules now in vapour state is stored as Latent Heat (or Potential energy) leading to no rise in temperature.

Secondly, the equilibrium of the water vapour immediately above the water surface must constantly be disturbed by sweeping the particles away else the molecules returning to the surface and those breaking away will be in equal numbers with no resultant evapotranspiration. With the sweeping away of the particles as they break away from the liquid phase, partly dry air remains and as the new equilibrium is established, evapotranspiration is at a premium. It is to be pointed out that these two processes are not wholly independent since the incoming air may be warm thus suppling further energy with the transformation of this sensible heat into latent heat of vaporisation as before.

So it is clear that external energy is required as well as convection of air over the surface (advection if we consider the simultaneous transport of heat with the air movement). These two components are external and for potential evapotranspiration to be maintained the surface must keep up the supply of water for the subsequent conversion to water vapour and this is therefore a condition of the surface. Hence, the 'never short of water' clause ensures the definition of potential evapotranspiration is independent of the state of wetness of the surface and, as such, a point of reference has been established.

The clauses 'short green crop' and 'completely shading the ground', standardise the affects of external components already mentioned. Hot winds have been shown to cause evapotranspiration in stalky rough open vegetation to far exceed that for smooth, close vegetation by virtue of the greater transpiring surface area that the hot winds come in contact with. The 'short green crop' seeks to standardise this 'clothesline effect' as it has been termed by Tanner, 1957. One would reason however if the definition of potential evapotranspiration might not be improved by extending the clause to 'an **extensive uniform** green crop' since if the cropped area is small, the advective heat inflow from the surrounding area may be large (or at least quite different) leading to greater evapotranspiration than if the advection was indeed from a similarly cropped area also freely transpiring. The example given in Hillel, 1980, is that of arid lands where small irrigated fields are often surrounded by an expanse of dry land and it is a common sight for poor growth of the plants near the windward edge of the field where penetration of warm dry winds contributes energy for evapotranspiration. Finally, 'completely shading the ground' indicates that the crop cover must be uniform thus completing the definition of potential evapotranspiration to form a reference by which to gauge the level of evapotranspiration.

As previously stated, two external conditions need to be met if a surface is to give up its water at its potential rate. The **Dalton equation** largely represents one of these conditions -that of convection of air over the surface.

The Dalton equation for evaporation from a saturated surface is

$$LE = (e_s - e)f(u), \tag{2.10}$$

where e_s is vapour pressure related to the state of the surface,

e is the vapour pressure of the air at two metres above the surface,

LE is the energy absorbed as latent heat, and

$f(u)$ is a function of wind speed.

If this is to be solved then the humidities of the surface and above the surface need to be known. Since surface saturated vapour pressure (e_s) requires knowledge of the surface temperature (T_s), which is a quantity rarely available from routine measurements and subject to errors from complex instrumentation, this equation is not practical in assessing evaporation. This equation on its own may be not sufficient but as will be shown further analysis incorporates this 'convection' mechanism to finally lead to the Penman equation.

Solar radiation provides the energy necessary to drive evaporation from a wet surface, herein lies the second condition. The atmosphere scatters a large proportion of incoming radiation with the remainder absorbed by the earth's surface or involved in other heat processes. These processes may be the absorption of energy as latent heat, the increment of sensible heat (that is, heat detected by our senses) of the atmosphere and a major process is the re-emission as long wave radiation. These processes may be summarised in the following equation:

$$J_n = LE + A + S + M, \tag{2.11}$$

where J_n is the net radiation,

LE is the energy absorbed as latent heat,

A is the sensible heat flux (heating the air),

S is the stored heat, and

M is the miscellaneous component encompassing photosynthesis, respiration etc.

It must be elaborated here that *LE* is comprised of two terms as follows, *L*, which is the latent heat of vaporisation (Joules/kg) and *E*, which is the rate of water evaporation (kg/m^2.s). The term *LE* incorporates these two with a resultant meaning of the rate of energy utilisation in evapotranspiration, that is to say, the heat used to evaporate water per unit area and per unit time. (Joules/m^2.s).

Due to the previously expounded problems associated with an equation for evaporation containing surface temperature (T_s) as a parameter, Penman eliminated this quantity in the derivation of the Penman equation. A derivation of the Penman equation to illustrate this point is given in Appendix B. The resulting Penman equation is:

$$L.E = \frac{\left[\frac{\Delta}{\gamma}\right] J_n - L.E_a}{\left[\frac{\Delta}{\gamma}\right] + 1},$$

where $L.E_a = 0.35(e_a - e)(0.5 + 5U_2/800)$,

U_2 = mean wind speed in kms/day at 2m above the surface,

e_a is the saturated vapour pressure of air,

γ is the **psychrometric constant** and

Δ is the slope of the saturated vapour pressure - temperature curve.

The equation above is one form of the Penman equation and it is to be noted that whilst T_s does not appear explicitly it is implicit within Δ. In practice Δ is evaluated at T_a, the temperature of the air some distance above the surface. The error due to this approximation is small since Δ appears in both the numerator and denominator and errors would divide out to be negligible. It is a fact that Penmans equation is physically based and this is borne out in that the inputs are net radiation, air temperature, vapour pressure and wind velocity at one level above the field. Since this equation was derived from a

combination of the energy balance and water vapour transport equations it is often referred to as the Penman *combination* equation.

Penman's equation defines a mechanistic model for evapotranspiration and can be evaluated from readily available data in any locality. It was seen that since surface temperature was not easily obtainable, the surface was effectively raised an arbitrary distance to eliminate that unknown, by introducing the Dalton equation on two occasions and that end was achieved.

The Penman equation, either in the form to determine potential evaporation from a open water surface (Penman 1948), potential evapotranspiration from a short green crop with abundant water supply (Penman 1948), or evaporation from a drying soil and transpiration from a crop with restricted water supply (Penman 1949), has been used by many workers. Stern (1965) uses the potential open water evaporation form to calculate potential evaporation as a standard by which to compare evapotranspiration on safflower as deduced from the water balance equation.

Ritchie (1972) introduces semiempirical relations to Penmans equation in order to calculate daily evaporation rates from soil surfaces and plant surfaces from a soil with row cropped canopies. These equations of Ritchie (1972) have been subsequently used by Feddes *et al.* (1974), Feddes *et al.* (1976), and Saxton *et al.* (1974) to enable these workers to apportion potential evaporation to soil and plant fractions and, in the latter case to calculate evaporation from the soil in both constant rate and falling rate stages. Ritchie (1972) incorporates a factor called Leaf Area Index (*LAI*) defined as leaf area per unit ground area that would indicate to what extent the ground would be shaded and soil evaporation reduced.

A modified Penmans equation was employed by Wright and Jensen (1978) to compute a reference potential evapotranspiration that was used to incorporate empirical factors which enabled improved evapotranspiration estimates to be made as a basis for an irrigation schedule. Nimah and Hanks (1973a) calculated potential evaporation from a free water surface using Penmans equation to which they multiplied a crop factor thus obtaining potential evapotranspiration. The resulting evapotranspiration was apportioned between potential transpiration and potential evaporation from the soil surface in a ratio of 9:1. This crude division is to be contrasted with the method of Feddes *et al.* (1974) as described earlier and of Hayhoe (1981) who used the same method of Feddes *et al.* (1974) in partitioning the evaporation between the plant and soil surface as determined by crop cover.

As may be deduced from the foregoing short survey of the modelling approaches to evapotranspiration, the Penman equation forms the basis for many and is testimony to the appeal of such a mechanistic approach.

The diversity of the mathematical modelling approaches to the individual water movement processes in the foregoing sections is evident. The phrase 'Soil-Plant-Atmosphere Continuum' is indeed an apt one to expose the interrelatedness of this complex system. The modelling of such a system is inherently difficult particularly when mechanisms are incorporated. The next chapter considers mathematical models of the entire system.

CHAPTER III

WATER IN SOILS - MATHEMATICAL MODELS

In the previous chapter, the individual processes together with modelling approaches were considered. In this chapter the entire system in terms of water relations with soil and plants will be considered. The models presented here are not exhaustive but rather are tendered as representing the major schools of thought in the area. It will be seen that the models vary greatly in complexity and practicality. Some are primarily research models with others more useful for management purposes.

Rather than present these models in an isolated sense, they will be described within the framework of which category they belong. Classifying the models provides insight into the reason for a models development, provides a historical perspective, and tenders a niche for the development of further models. The classification system is described below.

3.1 GENERAL TYPES OF MATHEMATICAL MODELS

A mathematical model is an equation or set of equations which is used to represent a system with the aim of emulating its behaviour with a degree of accuracy, often with the intent of predicting future behaviour of the system. Models may be classified as :

- DYNAMIC or STATIC
- DETERMINISTIC or STOCHASTIC
- MECHANISTIC or EMPIRICAL

As pointed out by Hillel (1977), these groups are not mutually exclusive and a complex model may encompass features of several of these.

Consider the distinction between dynamic and static models. Static models do not contain the time variable explicitly but may capture the nature of a system at an instant. In contrast, dynamic models are specifically concerned with changes over a period of time or of instantaneous changes. Clearly, dynamic models usually include differential equations.

Stochastic models acknowledge the random element of a system so that an outcome of such a model will produce some probability distribution and associated variances. Deterministic models, on the other hand, produce a definite outcome for a given set of inputs. It would seem that a system would need to be fully understood in order to be modelled deterministically and that any departure from a full understanding would necessitate a stochastic element. Without certain simplifications, any modelling would soon become over-burdening if a stochastic element were introduced each time. For what is the reason one models if it is not to simplify a complex system in order to provide insights into such a system.

The distinction between mechanistic modelling and empirical will be considered in greater detail in section 3.2.1. as it is central to later discussion on water-movement models. Thornley and Johnson (1986) use this system of classification but since they are fundamentally concerned with the mechanism/empiricism contrast, they do not use the respective methods of solution of models as a further means of categorisation. Hillel (1977) and Addiscott and Wagenet (1985) attach the distinction between analytic and numerical solution to more finely characterise models, in particular, models involving water movement. Analytical models, of course, are those that can be solved by the

classical methods of analytical mathematics whereas numerical models make use of numerical analysis to home in on a solution and usually require the use of a computer to be effective.

3.2 CLASSIFYING WATER MOVEMENT MODELS

The general classification system described above will be used as the basis of classifying the water movement models. The broadest division is that between *deterministic* models and those that are *stochastic*. The deterministic models lead to unique outcomes for any given set of input parameters whereas water distribution models such as Feinerman et. al., 1989, contain random variables that attempt to account for the uncertainty of an outcome.

Within the deterministic models the division is due to how physically based the model may be. Models that incorporate the actual mechanism by which water moves within the plant or soil are called mechanistic. Those that are less physically based tend towards being empirical whereby simplifications are made that effectively reduce the input requirements. Another characteristic distinction between mechanistic and empirical models is that mechanistic models usually contains a rate of change of water content term. The empirical models do not include this but rather involve the change of water content from field capacity. As such, mechanistic models involving a rate of change term are driven by time whereas an empirical model including a volumetric water content term are more driven by events that change that volume such as inputs of water such as rainfall and irrigation. As will be expounded later, not all models fit neatly into these two seemingly polarised groups, but rather are spread by degrees from one extreme to the other. Figure 3.1 emphasises this by diagrammatically depicting the models considered later in this chapter along the 'empiricism-mechanism continuum'.

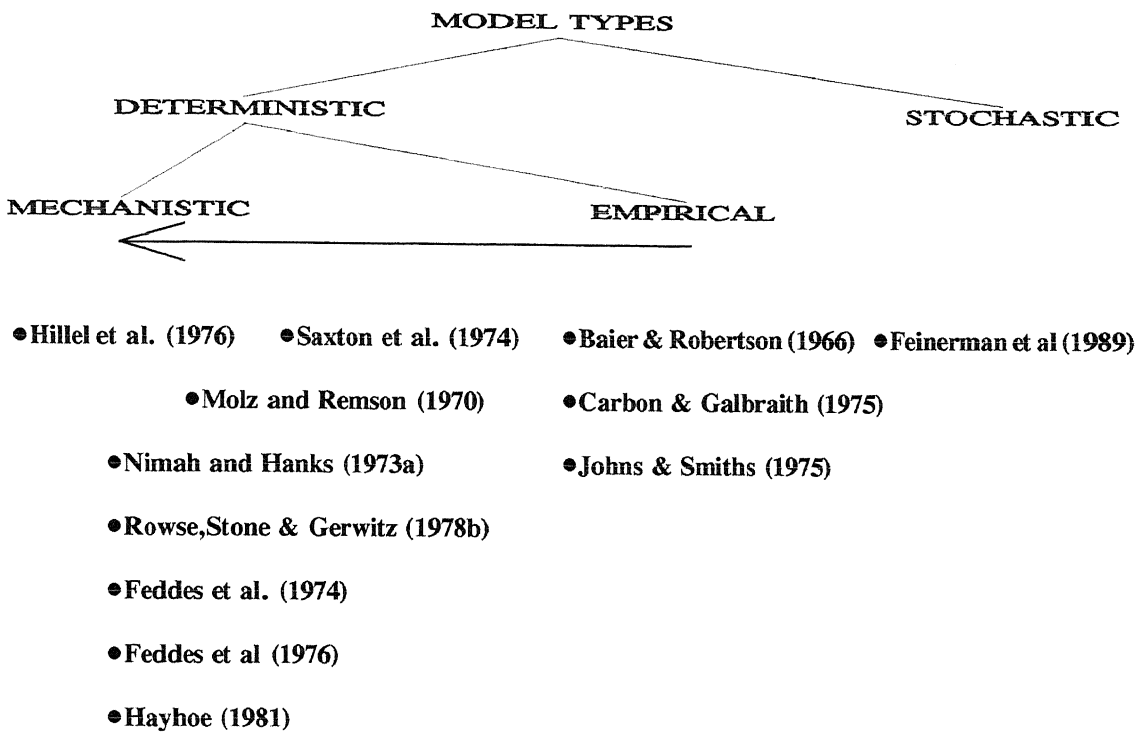


Figure 3.1. Models of water movement in soils on an arbitrary scale from empirical models to mechanistic models.

3.2.1 Mechanism vs Empiricism

As stated above, a mechanistic approach is where the modeller attempts to embody the actual physical processes that drive the system within the model. Another way to stress this distinction is by considering mechanistic models as *explanatory* models and empirical models as *descriptive* models whereby no attempt is made to explain a system, only to describe it with some accuracy.

In the case of water movement, the mechanism may be described in terms of energy gradients. The empirical approach, on the other hand, incorporates none of this mechanism but simply describes the system based on curve-fitting procedures derived from previously gathered statistical data. For example consider potential evaporation from a

surface. Various methods (Thornthwaite 1948, Oliver 1963) sought to find empirical relationships between potential evaporation and temperature of the air, humidity and wind using data collected over long periods. The problem with such empirical methods is that they are specific to the conditions from which the data was collected. Problems are certainly not confined to empirical modelling, however. Mechanistic approaches have problems of their own particularly when the mechanism that is to be modelled is not well understood. Hillel *et al., (1976)* states that this is the case with water uptake by a root system. Whilst the uptake surely is in response to potential gradients, just how the root system detects the spatial variability of the water over its entire root zone and alters uptake patterns and coordinates the 'efforts' of individual roots in response to this is quite a mystery.

Whilst it is possible for a model to be entirely empirical, no model involving the movement of water through soils and uptake into roots can be fully mechanistic. Mechanistic approaches must therefore include statistical or empirical components that arise due to the various simplifying assumptions that must be used to overcome those processes that are not well understood. As stated earlier, there would be no need to model any system that was fully understood. Herein lies the dilemma: a modeller who seeks to develop a fully mechanistic model cannot do so since any system worthy of modelling can not be comprehensively described and subsequently its mechanisms are not adequately known. So does the modeller concede that the system is to complex to model with any fidelity? The answer to this question specifies the final level of organisation of the water-movement models. If a modellers intention was to fully mechanistically model the water regime with the aspiration that the model will be simple enough to be accepted and used by the agricultural community to practically schedule irrigations, the modeller would most certainly concede that the two objectives conflict. On the other hand if the modeller

set out with the intention that the model would be primarily a research tool and that by its development some advance would be made toward a greater understanding of the mechanisms involved then this modeller would continue unabated. Thus, the final level of classification could be based on the reasons for the development of the model. These may be for research or for water management purposes. It is to be noted that Addiscott and Wagenet (1985) found that the distinction between research and management models broadly corresponded to mechanistic and empirical-type models.

3.3 THE MODELS IN DETAIL

A useful way to classify the various models involved in the movement of water through soils is to consider the various component processes of water movement and determine the degree of mechanism used to model each of these. The processes as described in an earlier chapter are : *infiltration, redistribution, evaporation, transpiration* and *water uptake by roots.*

The models of primary concern here are those deterministic models that range from largely empirical to largely mechanistic. Stochastic models will not be included.

In modelling water redistribution through soils, a large number of models are based on Darcy's Law for water flow together with the Law of Conservation of Matter. Darcy's Law stated in words is that 'if the change in potential is increased per unit distance then the discharge rate of water through an area (perpendicular to the direction of the increased gradient) will be increased'. These laws form the basis of some of the fundamental mechanisms of water movement in soils. For this reason any model based on the Flow equation will be considered basically mechanistic. This will be despite the fact that the solution of the Flow equation in unsaturated soil requires relationships between **K**, θ and ψ and these are found empirically.

The summary for each of the selected models follows. The variables will only be defined if they have not been encountered before. The variables are not necessarily the same as used in the papers where they were published because an attempt has been made here to standardise the notation to allow easier comparison. The notation is largely consistent with that used in Chapter II. In each summary the classification of the model will be given according to how each of the processes are modelled. A general description will also be given detailing the purpose of the development of each model, outlining various assumptions made and the method of solution will be briefly described. Verification of the model in field tests will also be considered.

MODEL SUMMARY Molz and Remson (1970)

MODEL TYPE: Mechanistic with regards to redistribution with an empirical, macroscopic sink term. Infiltration and soil evaporation are forced to be zero. Steady state assumed. Numerical solution.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D\frac{\partial \theta}{\partial z}\right) - \frac{\partial K}{\partial z} - \left(-\frac{1.6T}{l^2} + \frac{1.8T}{l}\right)$$

GENERAL DESCRIPTION: It was the purpose of these authors to develop a reasonable model for macroscopic moisture extraction. The model incorporated an early macroscopic sink term and was based on the diffusivity form of the flow equation, where it is assumed that conductivity and diffusivity are single valued functions of water content. As described in Chapter II, the sink term was developed by fitting a function to the well-known empirical approximate extraction pattern for roots i.e. 40%, 30%, 20% and 10%

extraction for successively deeper quarters of the root zone. It is empirical because there is no physical significance attached to the proportions. It was pointed out that the water uptake model fails where the surface layers dry and therefore cannot sustain their contribution to the total uptake. This problem was avoided by making the further assumption that the system was in a steady state i.e. $\partial\theta/\partial t = 0$ (this means that water content does not significantly change with time). Since one of the independent variables has now effectively been eliminated, the partial differential equation has been reduced to an ordinary differential equation that was solved using an Adams predictor-corrector method started by a Runge-Kutta procedure. This procedure could only be applied to an initial value situation so to solve the equation with the boundary conditions (as assumed here) of zero surface flux (no infiltration, no soil surface evaporation) and constant water content at the lower boundary, a shooting method was used.

MODEL SUMMARY Nimah and Hanks (1973a)

MODEL TYPE: Mechanistic, in terms of redistribution and evapotranspiration. Macroscopic sink term. Transient water regime. Numerical solution (finite difference method).

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left(K(\theta)\frac{\partial H}{\partial z}\right) + S(z,t)$$

where $$S(z,t) = \frac{[H_{root} + (RRES \cdot z) - H(z,t) - s(z,t)] \cdot RDF(z) \cdot K(\theta)}{\Delta x \cdot \Delta z}$$

and *RRES* is a root resistance term, H is the soil pressure head, s is the osmotic potential and *RDF(z)* is the proportion of total active roots in a depth increment.

GENERAL DESCRIPTION: The model was based on the conductivity form of the flow equation and was solved numerically using finite differences (Crank-Nicholson method as discussed in Chapter IV). The model was developed to predict water content profiles, evapotranspiration, water flow from or to the water table, root extraction and root water potential at the surface under transient conditions. The sink term is mechanistic to the extent that it includes pressure and osmotic potentials as the driving force of the water extraction as well as a root resistance factor. H_{root} could be compared with the 'crown' potential of Hillel et. al. 1976, which may well be related to leaf stomatal resistance as described be van Bavel and Hanks, 1983. Potential evapotranspiration was calculated using the Penman equation. A degree of empiricism is evident here as the potential evapotranspiration was partitioned between soil evaporation and transpiration in the ratio 1:9. The surface flux condition permitted evaporation at potential rate from the soil until the surface was air-dry and also permitted infiltration to occur at maximum rate until saturated surface conditions prevailed.

The model assumes that Hydraulic conductivity and pressure head-water content relations do not change with time and that the root density function is invariant with time.

This model was field tested (Nimah and Hanks (1973b)), with findings being that water content-depth profiles were in poor agreement directly after irrigation but good agreement 48 hours after irrigation.

This model was further modified by Feddes *et al.* (1974), to exclude osmotic pressures but to include a more physically based method for partitioning evapotranspiration into transpiration and soil surface evaporation to include certain properties that effect transpiration as described in Chapter II.

MODEL SUMMARY Hillel, Talpaz and van Keulen (1976)

MODEL TYPE: Mechanistic with regards to redistribution and the macroscopic sink term analogous to Ohm's law. No infiltration considered and the regime is transient. Numerical solution.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\frac{\partial(H_m - z)}{\partial z}\right] - \frac{H_{soil} - H_{crown}}{R_{soil} + R_{roots}}$$

where H_m, H_{soil} and H_{crown} are the matric, total soil and "crown" potentials respectively. The "crown" potential is the xylem water potential at ground level. R_{soil} and R_{roots} are resistances due to water flow in soil towards the root (as given by Gardner (1964)), and the hydraulic resistance of the roots, including resistances to absorption and conduction in the root respectively.

GENERAL DESCRIPTION: This model attempts to formulate a water uptake term in terms of the basic physical mechanisms and in doing so claims to be more mechanistic than those macroscopic terms of Molz and Remson (1970) and Nimah and Hanks (1973). Confirming the lack of understanding of the root uptake mechanism, a degree of empiricism is still evident in the root resistance term where an empirical constant representing root-length activity is introduced i.e. $R_{soil} = 1/BKL$. (K is hydraulic conductivity, L is total length of active roots in a unit volume of soil). The B term was introduced by Gardner (1964) and discussed critically by Taylor and Klepper (1975). This model was designed to produce as output, the patterns of soil moisture depletion as well as the leaching of salts below the root zone. The model was not field tested and was

used as a research tool to investigate how changes in root density and depth, root resistance, initial soil wetness and differing evaporative regimes effect water uptake patterns. Transpirational demand was considered to fluctuate diurnally according to a sinusoidal function and evaporation rate was considered to be 2% of transpiration rate (an empirical judgement). Infiltration is not considered to be a surface flux possibility but rather the simulation is commenced by using an initial soil moisture profile, constant throughout the root zone (the constant being roughly field capacity for their given soil). In the root extraction term, (which needs to be determined at each depth layer) the only unknown is "crown" potential. Since the root extraction term may be summed over the root zone to give transpiration rate, the value of H_{crown} can be obtained at successive times. This model does not allow for a growing root system.

MODEL SUMMARY Rowse, Stone and Gerwitz (1978b)

MODEL TYPE: Mechanistic in terms of redistribution, water uptake and the apportioning of evapotranspiration into transpiration and soil evaporation components. Infiltration is modelled empirically. Numerical solution by finite difference method.

$$\frac{\partial \theta}{\partial z} = \frac{\partial}{\partial z}\left[D(\theta)\frac{\partial \theta}{\partial z} - K(\theta)\right] - \frac{\Delta z L(H_{soil} - H_{plant})}{R_{soil} + R_{plant}}$$

where L is the root length per unit volume of soil, and all other variables as defined in this chapter.

GENERAL DESCRIPTION: The model was developed to enable the flow of water, the water content and the matric potential to be calculated at any depth for a cropped soil. It

is based on the numerical solution to the flow equation in diffusivity form. Unlike those models of Nimah and Hanks (1973) and Feddes *et al.* (1974), in this model transpiration and evaporation are considered independent processes and are apportioned in a different manner. Transpiration is calculated to be the sum of all uptake rates and is considered to be equal to $f.E$ at the energy limiting rate, where f is the fraction of plant ground cover and E is the Penman potential transpiration or equal to a rate at which water can be extracted from soil at a critical plant water potential, whichever is lesser. This critical potential is where stomatal closure is assumed to occur. The rate of evaporation from the surface is calculated to be that of an open water surface in energy-limiting phase (F_{EL}) or as in soil-limiting phase (F_{SL}) as described in Chapter II (such evaporation being considered to follow a half sine wave during daylight hours and zero at night). This potential evaporation is then adjusted by multiplying by $(1-f)$ where f is the fraction of plant ground cover. Infiltration rate is considered to be the smaller of F_{EL} (rainfall/irrigation rate) or F_{SL}. During an infiltration event this water is assumed to be distributed in the empirical manner or saturating the top layer before moving down to the next layer as described more fully in Chapter II. The root water extraction term is analogous to Ohm's law but differs from the uptake rate of Hillel *et al.* (1976) in that H_{plant} is considered to be constant throughout the root xylem and not thought of as a "crown" potential.

The model was field tested with the outcome of good agreement with field measurements and the conclusion that such models will be useful to help understand the effect of factors such as weather,soil type and root distribution on water and nutrient uptake.

MODEL SUMMARY Saxton, Johnson and Shaw (1974)

MODEL TYPE: Hybrid type in terms of basing redistribution on the flow equation and using reasonably strong empirical approaches to all other processes. Numerical solution.

GENERAL DESCRIPTION: This model was designed to strike a balance between the complexities of the largely mechanistic models and the lack of generality of the wholly empirical approaches and to estimate daily actual evapotranspiration and soil moisture profiles. The energy for evapotranspiration is considered the principal driving force for the water movement with soil water potentials playing a secondary role. This tends to lean towards the conventional approach to irrigation scheduling as described in Chapter I. In this so-called Soil-Water-Plant-Water (SPAW) model, the soil water balance is considered by modelling the processes as occurring sequentially. The evapotranspiration is firstly calculated (from a modified Penman equation), infiltration is then added and finally water is redistributed among the soil layers.

Potential evapotranspiration is apportioned between transpiration and soil evaporation according to canopy cover (using a canopy % graph from previously collected data). Potential transpiration is sequentially reduced by :

- the crop's phenological stage (empirical data),
- distribution to each soil layer depending on the root distribution and
- effect on potential evapotranspiration due to the plant suffering moisture stress and closing its stomata.

The actual evapotranspiration is then calculated by adding soil evaporation and reduced crop evapotranspiration. Soil evaporation was considered to come from the top 15cm of

soil and is calculated using the two-stage method of Ritchie (1972). Daily infiltration is as described previously in Chapter II and is similar to that of Rowse and Stone (1978). After infiltrated water was added, redistribution is initiated by using the flow equation and using empirical moisture-tension and moisture conductivity relationships.

The model is best described using the flow chart of actual evapotranspiration calculations and soil moisture movement as presented in Saxton, Johnson and Shaw (1974) or Hayhoe and De Jong (1988). The model was tested and calculated and observed soil moisture profiles were in good agreement.

MODEL SUMMARY Baier and Robertson (1966)

MODEL TYPE: Simple water budget approach using empirical algorithms.

$$AE_i = \sum_{j=1}^{n} \left[k_j \frac{S^*_{j(i-1)}}{S_j} Z_j PE_i e^{-w(PE_j - PE^*)} \right]$$

where AE_i = actual evaporation for day i ending at the morning observation of day $i+1$,

$\sum$ = summation from zone $j=1$ to zone $j=n$,

k_j = coefficient accounting for soil and plant characteristics in the jth zone,

$S^*_{j(i-1)}$ = available soil moisture in the jth zone at the end of day $i-1$,

S_j = capacity for available water in the jth zone,

Z_j = adjustment factor for different types of soil dryness curves,

PE_i = potential evapotranspiration for day i,

w = adjustment factor accounting for effects of varying PE rates on AE/PE ratio,

PE^* = average PE for month of season.

GENERAL DESCRIPTION: This model estimates daily soil moisture using standard meteorological data and is designed to monitor soil moisture without having to resort to soil sampling. The model has been termed the Versatile Budget (VB). The VB claims to be superior over direct measurement of soil moisture since such measurements provide readings for a specific area at a particular point in time. The model makes use of the potential evapotranspiration concept as the major driving force of soil-water depletion. The empirical assumption that all moisture from an upper zone is "evapotranspired" at the potential rate until all available moisture is withdrawn before any extraction occurs in the layer immediately below was a feature of earlier budget approaches and was abandoned in the VB. Also abandoned was the idea that if daily potential evapotranspiration rate is such that all cannot be accommodated by the topmost layer then the water in the next layer down is drawn upon and so on until the rate has been attained. In its place the VB considered water to be withdrawn simultaneously from different depth zones (in the root zone), in proportion with the available soil moisture in each zone until the transpirational demand is met. As such this model aimed to reflect a more accurate distribution of soil moisture.

A standout feature of the equation for estimating daily AE , above, is the number adjustment type factors: k_j , Z_i and w, - a feature of empirical models. These must be determined for a particular location and crop. The method by which infiltrating water enters the system is as described in section 2.2.2, with the infiltration equation being empirically based. The model achieved good agreement with measured values during field testing.

CHAPTER IV

METHODS OF SOLUTION OF ROOT-SOIL-WATER MODELS

4.1 THE GENERAL MODEL

The previous two chapters have presented a wide range of modelling approaches to both individual soil-water-root processes and the overall process of water movement throughout the so-called Soil-Plant-Atmosphere-Continuum. It is one thing to develop a ideal mathematical model and it is quite another to have the resources to solve it. This chapter outlines methods of solution both analytical (where possible) and numerical. It will also consider any assumptions that were used to simplify or otherwise change the model to aid in solution. The discussion will focus directly on models based on the flow equation as such a mechanistic approach will be targeted here.

Consider firstly, the most general situation to be encountered in the field, that of vertical, unsaturated subsurface flow of (liquid) water with cropped, homogeneous soil under isothermal conditions, where osmotic effects are negligible and with periods of infiltration and evaporation. The presence of a high water table and hysteresis will be neglected in this situation. With hysteresis neglected, a unique, single valued relation between matric potential and soil wetness can be assumed. Furthermore, the arguments of Van Bavel and Hanks (1983) support that liquid flow under anisothermal conditions and vapour flow of water under any conditions are of little practical significance.

The general model as detailed in Chapter II is

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\psi)\frac{\partial \psi}{\partial z} - K(\psi)\right] - S$$

$$= \frac{\partial}{\partial z}\left[K(\psi)\frac{\partial \psi}{\partial z}\right] - \frac{\partial K(\psi)}{\partial z} - S \ .$$

(4.1)

where all variables are defined as in Chapter II. It is to be noted that the hydraulic conductivity may be expressed as a function of suction (as it is here) or of water content. The above conductivity form can be cast in a basically equivalent diffusivity form as detailed in Chapter II. In making this change, there is a gain in mathematical simplification but a loss of generality since the diffusivity equations fail if the hysteresis effect if appreciable or when soil is layered, or in the presence of thermal gradients (Hillel (1971)). As these conditions were precluded in the base assumptions of this section, the diffusivity form will be pursued.

The diffusivity form is

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta)\frac{\partial \theta}{\partial z}\right] - \left[\frac{dK(\theta)}{d\theta}\right]\frac{\partial \theta}{\partial z} - S \ .$$

(4.2)

The computational advantages of the diffusivity form of the flow equation are at least threefold. Whereas the conductivity form contained both θ and ψ, the diffusivity form takes advantage of a single-valued relationship between the two (under current assumptions) to eliminate one of these dependent variables. Secondly, Hillel (1971), indicates that the range of variation of diffusivity is smaller (by a factor of one thousand) than that of conductivity (although this is only an advantage in the absence of gravity).

The third advantage is dependent on the method of solution. Rowse and Stone (1978) who used a numerical method of solution, found that the diffusivity form enabled the same degree of accuracy to be achieved by dividing the soil into a smaller number of layers. The limitations of the diffusivity form will be considered in the last chapter.

Despite which equation is used, both are nonlinear because of the dependencies of K, ψ, and D on θ. Furthermore the sink term is, in general, nonlinear. To solve these equations the functional dependencies need to be determined, often by empirical means. Many papers use the data of Clapp and Hornberger (1978) to ascertain these dependencies. Clapp and Hornberger (1978), acknowledge that not all workers wish to undertake direct experimental determination of θ-K-ψ relationships and therefore have developed power curves relating the parameters.

Further complicating the solution of the Richards' equation is the fact that the initial and boundary conditions may be derivatives. These considerations dictate that analytical solution would be difficult and that the solution would be specific for the boundary condition used. Indeed, Van Der Ploeg and Benecke (1974), when referring to the flow equation without the sink term, state that no general analytical solution is known. This was indeed the case until Knight and Philip (1974) produced an analytical solution for the flow equation for redistribution in the absence of gravity. An analytical solution for the model would have the advantage that the solution would be exact and the approximations made in any numerical solution could be avoided. The next section outlines a brief history of the solutions, both analytic and numerical, and which would be most appropriate for the solution of the model in this case.

4.2 METHODS OF SOLUTION FOR THE RICHARDS' EQUATION

As already outlined earlier this chapter, this equation is complex and nonlinear thus making solution difficult. In 1967, Remson *et al.* indicated that analytical solutions had been successfully achieved for only a limited number of cases. Van Der Ploeg and Benecke (1974) stated that for simple initial and boundary conditions and one-dimensional flow, some analytical or quasianalytical solutions existed. Numerical techniques such as finite difference solutions, as indicated by De Smedt and Wierenga (1978), were not limited by restrictive initial and boundary conditions and may be applied in a variety of situations. On the same token, in 1977 Wierenga, claimed that numerical solutions need more input information such as K-ψ-θ relationships which are seldom available for field situations.

Philip (1969), as reported by Parlange (1971), "emphasised rightly the value of analytical over numerical results to grasp the fundamental structure of solutions", thus indicating a preference for analytical solutions to the Richards' equation by that author. Despite the fact that these are earlier references relative to the amount of work recently done in this area, the two sides of the story with respect to solution methods is apparent.

One side involves the numerical solution and the other, analytical solution. Both sides have their positive and negative points. Analytical methods "advance understanding of the mathematical shape and the physical structure of the infiltration process", Philip (1988). Also, "analytical-type methods enable an understanding of the physics of the problem to be well developed", Hogarth and Watson (1991). These methods did, and still to the present, suffer from the problem that for realistic initial and boundary conditions the solutions became increasingly complex.

Haverkamp *et al.* (1977), state that quasianalytical solutions by Philip (1957) and Parlange (1971) were subject to fairly restrictive and simple initial and boundary conditions. Further indicating that these initial and boundary conditions did not represent usual conditions Haverkamp *et al.*, justified their interest in presenting a review of the numerical approaches up till that time.

Perroux *et al.* (1981), indicate that numerical methods met with greater success in the early search for solutions to the flow equation with constant boundary flux with the pioneering works of Rubin and Steinhardt (1963). Perroux *et al.* went on to report that White *et al,* (1979) developed a gravity-free analysis of the flow equation and that they extended the White *et al.*, analysis to include the effect of gravity and constant-flux infiltration based on the flux-concentration relation where similarity methods reduce the number of independent variables to one.

Analytic solutions continued to become more generalised to include other initial and boundary conditions after this time. Parlange *et al.* (1985) present a solution that allows water content at the surface to be a function of time rather than constant. The analytic solution in this case had the advantage over numerical methods of that time since it was the most reliable method in predicting time till ponding even under high intensity rainfall. Broadbridge *et al.* (1988), developed a new exact solution during constant rate rainfall in a finite soil profile. These authors explain that the Richard's equation can be reduced to a linear convection-diffusion equation using nonlinear transformations which in turn increases the difficulty of solving the linear equation. Hogarth *et al.* (1989) found middle ground by reducing the flow equation to an ordinary differential equation by using first

integral techniques. The reduced equation, which allowed for realistic soil properties, was then able to be solved numerically with a shooting technique. The authors explain that the solution has an advantage over the full numerical solutions of Richard's equations (which has precision problems in the initial stages of infiltration) and may be used to validate numerical methods for arbitrary soil properties and boundary conditions.

Sander *et al.* (1991) derived the first exact analytical solution for nonlinear, nonhysteretic redistribution of water in a bounded soil column under gravity. The solution allows for a description of both infiltration and redistribution for arbitrary soil properties.

It appears that the ongoing co-evolution of both analytical and numerical methods is mutually beneficial since new exact methods can be used as validation tools for existing numerical techniques and that the less restrictive requirements of initial and boundary conditions on numerical methods allows a more generalised solution which provides a perpetual challenge to the analysts. Furthermore, Hogarth *et al.* (1991) report that validation of the various numerical techniques by analytical solutions generates a confidence to enable the numerical solutions to be used as the intermediary means of checking approximate theoretical approaches against exact approaches.

Chapter I outlined the rationale for this study was to apply a mathematical model for the movement of water in an agricultural system to the problem of irrigation scheduling. As such all processes in a typical irrigation cycle need to be modelled for a variety of soils. This would include infiltration, evaporation, transpiration and redistribution. Furthermore, the condition at the boundary may change from evaporative flux to infiltrative flux to zero flux to constant water content. At this point in time no analytical solution of the Richard's Equation can provide determination of the changing water content profile under all such

processes at the boundary and for universally realistic $K/D/\theta/\psi$ relations. To maintain the flexibility required in this application a numerical solution is pursued. The search for a suitable method begins with consideration given to the general class of equation and subsequent techniques for its solution.

4.3 PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

The broader class of problem is the partial differential equation since there are two independent variables in the flow equation namely, depth *(z)* and time *(t)*. Furthermore, since the order of the equation is greater than one, two or more values must be known to evaluate the constants of integration. Since, in the case of the flow equation, these values of the function (or its derivative) are usually given at the boundaries of the domain (surface or rooting depth), the problem may be classed as a boundary-value problem. Added to this, these boundary-values are usually in the form of a derivative of the function. In the solution of the flow equation, initial values may also be required (the initial wetness profile). The class of problem may further be refined by considering the characteristics of the partial differential equation. Consider the general second-order, partial differential equation in two independent variables:

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\left[x,y,u,\frac{\partial u}{\partial x},\frac{\partial u}{\partial y}\right] = 0$$

Depending on the value of $B^2 - 4AC$, the equation can be classified as:

Elliptic, if $B^2 - 4AC < 0$;

Parabolic, if $B^2 - 4AC = 0$;

Hyperbolic, if $B^2 - 4AC > 0$.

If the variables of the flow equation (4.2) are equated to those in the general equation above by letting z = x and t = y also letting θ = u, and by comparing the flow equation

to the form above, it can be seen that both the coefficient of the cross term (B) and the second order term in time (C) are zero, hence the equation is a parabolic partial differential equation. It should be noted that the sink term and the term due to gravity in the flow equation are lumped together in the general equation stated above with the coefficient of D, which is of no consequence in the classification of the partial differential equation in the context of parabolic, elliptic or hyperbolic.

Concluding the classification of the flow equation, it may be said that it is a nonlinear, parabolic partial differential equation in two variables (first order in time, second order in depth), with derivative boundary conditions.

4.4 THE NUMERICAL SOLUTION OF PARABOLIC PDE'S

Without further restrictive assumptions, only numerical solutions exist to the transient flow equation including water uptake by roots. Stroosnijder (1982) states that this equation can be solved by using the finite difference method. The finite difference method is where the variables of depth and time are divided into small intervals and the partial derivatives are expressed in the finite difference approximation form and is described below.

4.4.1 Finite Difference Method

The finite difference method requires that adjacent points of the independent variable domain are a finite difference apart. The system for denoting finite difference equations in this section requires this difference to be Δx and that $x_i = i(\Delta x)$. The subscript i takes on integral values from 0 to N where N is the total number of increments required. Where a second variable is involved (time, say) a second subscript (or superscript) of j's will be used where j ranges integrally between 0 and M. As an example the point $x_{i,j}$ is shorthand for the point $(i(\Delta x), j(\Delta t))$.

A derivative of a function that is everywhere differentiable, f(x), say, may be

approximated by first expanding f(x+Δx) into a Taylor's series about x=0,

$$f(x+\Delta x) = f(x) + \Delta x\frac{df}{dx} + \frac{(\Delta x)^2}{2!}\frac{d^2f}{dx^2} + \cdots$$

Rearranging,

$$\frac{df}{dx} = \frac{f(x+\Delta x) - f(x)}{\Delta x} + O(\Delta x) ,$$

$$\frac{df}{dx} \approx \frac{f(x+\Delta x) - f(x)}{\Delta x} ,$$

where $O(\Delta x)$ is the remainder of the series and in this case is said to be of order Δx.

This is called the "forward difference" approximation to the derivative of f, with truncation error of order Δx. If f(x) is expanded about x using Taylors Theorem, in the negative direction, the following "backward difference" approximation would result:

$$\frac{df}{dx} \approx \frac{f(x) - f(x-\Delta x)}{\Delta x} .$$

This form of approximation has the same truncation error as the forward difference approximation, but by combining the expansions in both positive and negative directions and forming the "central difference" approximation, the truncation error is reduced to $O((\Delta x)^2)$. The central difference form is

$$\frac{df}{dx} \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x} .$$

Second derivatives may be approximated in a similar way. Since the Taylors expansion in positive and negative directions cause similar terms to be of opposite sign, combining the two can eliminate the first derivative and result in a expression for the second order derivative. That is,

$$\frac{d^2f}{dx^2} \approx \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2}$$

4.4.2 Explicit Methods

When terms of a Partial Differential Equation (PDE) are replaced by the forward difference approximation to the derivative in time and the initial conditions (at t=0) are known, then the finite difference equation may be used to *explicitly* express the values of the dependent variable at the first time step in terms of those known initial values of the dependent variable. As an example consider the classical one-dimensional diffusion equation:

$$\frac{\partial u}{\partial t} = K\frac{\partial^2 u}{\partial x^2} .$$

Approximating this equation using the explicit method results in

$$\frac{u_i^{j+1} - u_i^j}{\Delta t} = K\frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\Delta x)^2} .$$

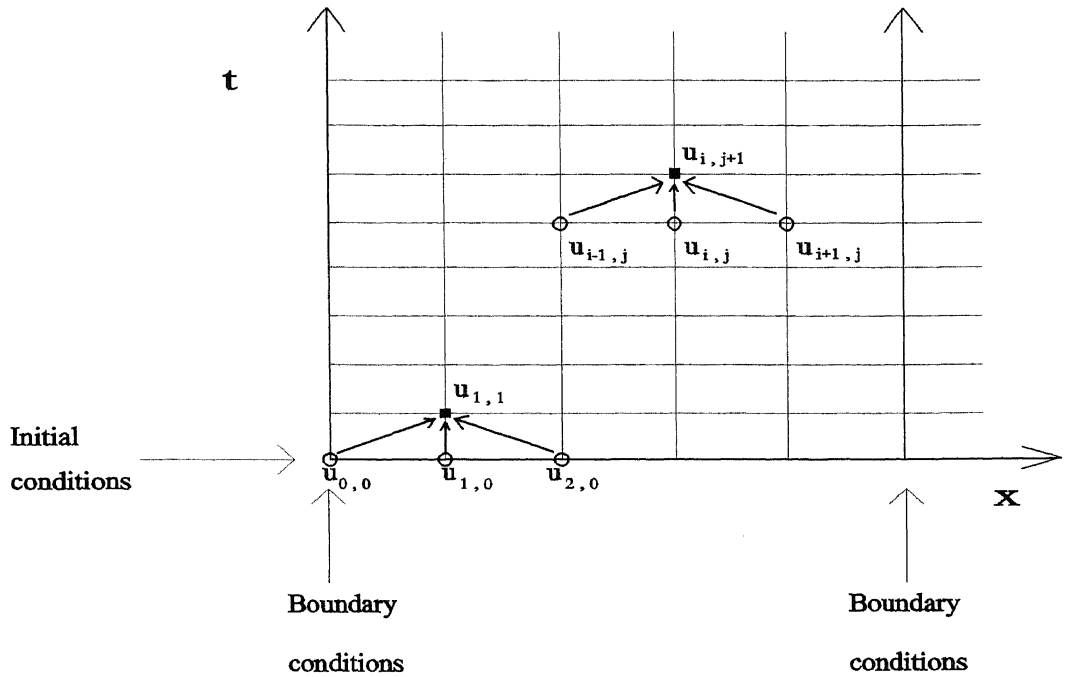
Thus obtaining,

$$u_i^{j+1} = u_i^j + \frac{K\Delta t}{(\Delta x)^2}(u_{i+1}^j - 2u_i^j + u_{i-1}^j) . \qquad (4.3)$$

A diagrammatic representation of this may be given using a grid as shown in Figure 4.1. Each horizontal division is of width Δx, multiples of which are denoted by *i's* and each vertical division represents Δt, the number of Δt's being denoted by *j's*. It is clear how boundary and initial values are used to provide the values of u at the $(t + \Delta t)$*'th* level. The problem with the use of the forward difference approximation and subsequent 'Explicit Method' is that as Δx and Δt approach zero, the approximation does not *unconditionally* converge to the actual values of the function and as t approaches infinity, the errors of the approximation are amplified unless certain conditions are met (Remson *et al.* (1971) pp 71-77).

This explicit method was the technique employed by Stroosnijder (1982) using a time step of $\Delta t < (\Delta z)^2/D(\theta)$, which avoided oscillation. The problem with this approach, as

described by Stroosnijder (1982) was that with soils that had high diffusivity, small time steps were required and subsequently, calculations were at a premium.



■ are values to be determined,

○ are known values required to calculate the unknown ■ values.

Figure 4.1. Grid illustrating the Explicit Method of solution of finite difference equations. It is evident that all values on a time step may be calculated from values on the previous time step only with the initial conditions providing the springboard for the process.

4.4.3 Implicit Methods

A way of improving convergence and stability of a finite difference approximation is to reformulate the PDE using a backward difference approximation for the time derivative thus achieving the so-called implicit approximation. Once again, consider the PDE

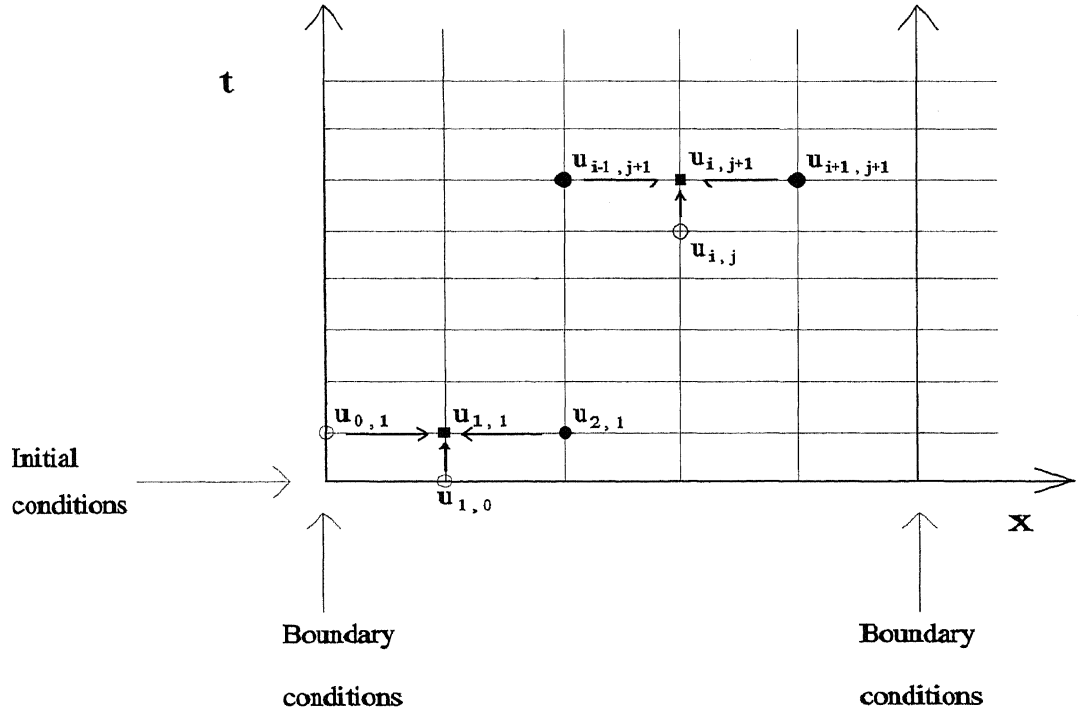
$$K\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

and replacing derivatives as described above and rearranging,

$$u_i^{j+1} = \frac{u_i^j + \frac{K\Delta t}{(\Delta x)^2}\left(u_{i+1}^{j+1} + u_{i-1}^{j+1}\right)}{1 + 2K\Delta t/(\Delta x)^2} . \qquad (4.4)$$

In contrast with the explicit derivation (4.3), the terms on the right hand side are not all known i.e. $u_{i+1,j+1}$ and $u_{i-1,j+1}$ as they are on the same time step. The following grid, Figure 4.2, accentuates this difference between implicit and explicit methods.

Suppose now, that for each time step there are n steps in space. Since the end-points are known, there are *(n-2)* unknowns each time step. Furthermore, since *(n-2)* finite difference equations may also be formed at each time step, then a solution is possible. In fact, the resulting system of equations form a tri-diagonal coefficient matrix for which methods of solution are well documented.



■ are values to be determined,

○ are known values required to calculate the unknown ■ values, and

● are unknown values required to calculate the unknown ■ values.

Figure 4.2. Grid illustrating the Implicit Method of solution to finite difference equations. In contrast with Figure 4.1, an unknown u requires adjacent (in space) unknown values on the same time step to be solved simultaneously. Fortunately a solvable system of equations results to overcome this.

4.4.4 Crank-Nicolson Method

It has been found that a finite difference scheme with small truncation error and increased accuracy from the previously described methods is the Crank-Nicolson approximation which is another implicit method. Consider the PDE used in the examples so far. In this method the forward difference approximation in time is now considered to be the central difference approximation (with associated reduced truncation error) about the midpoint of the time interval, that is, at $(j+½)$. The second derivative is approximated as a central difference about that same midpoint of the time interval by averaging the central difference approximations at the beginning and end of the time interval, that is,

$$\frac{u_i^{j+1} - u_i^j}{\Delta t} = \frac{K}{2}\left(\frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{(\Delta x)^2} + \frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{(\Delta x)^2}\right).$$

Once again, a set of simultaneous equations needs to be solved at each time step, but the tedium is reduced since the system is also tri-diagonal and solved using *LU* decomposition. The Crank-Nicolson method has proven popular in the solution of the flow equation with gravity taken into account. Hanks and Bowers (1962), Nimah and Hanks (1973) and Feddes *et al.*, (1974), used this method.

Molz and Remson (1970) considered the flow equation and sink term of the form

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D\frac{\partial \theta}{\partial z}\right) - \frac{\partial K}{\partial z} - S(z,t,\theta,\frac{\partial \theta}{\partial z}) .$$

The Douglas-Jones predictor-corrector method was used to solve this since it results in linear finite difference equations with tri-diagonal coefficient matrix (even though the above equation is highly non-linear). The Douglas-Jones approximation uses two equations. The *predictor* is a modified implicit approximation with the *corrector* being a modification of the Crank-Nicolson equation. The predictor marches the equation to

halfway through a time interval, the corrector takes it to the end of that time step. Whilst Molz and Remson restricted their flow equation to zero flow conditions at the boundaries, derivative boundary conditions may be handled as now described.

4.4.5 Derivative Boundary Conditions

Remson *et al.*(1971) state that the specification of the derivative of a function instead of the function itself at a boundary adds that function as another unknown to the system. Suppose a surface derivative condition is given. The space domain is extended one step before the surface boundary and this fictitious point is eliminated by forming two equations - one , expressing the boundary condition as a central difference about the surface and the other, obtained by writing the actual finite difference equations to include the nodes at the surface. That is, by writing the derivative boundary condition in finite difference form using the central difference approximation, this allows the fictitious value to be found in terms of other values at the same time step. Including this new-found value in the finite difference equations as before allows the surface value to be evaluated as part of the set of simultaneous equations on that time step. In effect, at the imaginary depth above the surface, the dependent variable is evaluated to form a finite difference approximation of the derivative boundary condition to form a new set of pre-boundary conditions, with that actual boundary values of the dependent variable becoming incorporated in the simultaneous equations. Demonstration of this technique will be given in Chapter VI.

4.4.6 The Tridiagonal Matrix

It has been stated that the elegance of the finite difference formulations above is in the fact that they reduce to a matrix system of the tridiagonal form. A typical Tridiagonal system is shown in equation 4.5 where *L, D, U* represent the lower diagonal, diagonal and upper diagonals of the tridiagonal matrix and form the coefficient matrix. The dependent

variable is represented by u_i's and the B's represent the solution vector of the system. One algorithm for solving this system is the Thomas Algorithm which is documented widely and may be found in von Rosenberg, 1969, Appendix A.

$$\begin{bmatrix} D_1 & U_1 & 0 & . & . & . & 0 \\ L_2 & D_2 & U_2 & 0 & . & . & 0 \\ 0 & L_3 & D_3 & U_3 & 0 & . & 0 \\ . & 0 & . & . & . & . & . \\ . & . & . & . & . & . & 0 \\ 0 & . & . & 0 & L_{N-1} & D_{N-1} & U_{N-1} \\ 0 & . & . & . & 0 & L_N & D_N \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ . \\ . \\ u_{N-1} \\ u_N \end{bmatrix} = \begin{bmatrix} B_1 \\ B_2 \\ B_3 \\ . \\ . \\ B_{N-1} \\ B_N \end{bmatrix} \tag{4.5}$$

The computational implementation of this algorithm will be used in the computer simulation of Chapter VII.

4.5 SOME SIMPLIFYING ASSUMPTIONS

The short and certainly not exhaustive section that follows provides a list of common assumptions required to necessitate fairly straight forward solution to the flow equation.

A first assumption may be made to introduce diffusivity. This assumption is that a single-valued relationship between ψ and θ exists. This implies no hysteresis. The resulting diffusivity form (4.2) may only be solved numerically. It is from this form that various assumptions may lead to one of three directions.

Consider the three assumptions:

(1) If diffusivity is assumed constant in relation to water content, equation (4.2) reduces to a linear PDE and may be solved analytically using the same methods as for the equations of Heat. Black *et al.* (1969) used this approach.

(2) If gravity is assumed negligible, the Boltzmann Transformation may be introduced (Gardner (1959)) and the resulting Ordinary Differential Equation (ODE) is amenable to analytical solution by separation of variables.

(3) If steady state is assumed, that is, $\partial\theta/\partial t=0$, a non-linear ODE results. Molz and Remson (1970) solved the resulting ODE numerically by using the Adams predictor corrector method.

The correspondence between the assumption and the situation in the field are now considered.

(1) Gravity negligible: Gardner *et al.* (1970a) states that "if the depth of infiltration is very shallow and matric suction dominates over gravitational effects, then the second term of the right hand side (of 4.2) is negligible. The resulting equation is similar to that of horizontal flow. For vertical flow in irrigation situations this would not be the case since, the surface would be saturated and with the wetting of the soil, the matric suction would reduce until the influence of gravity would be most significant.

(2) Diffusivity constant: Diffusivity would be relatively constant only if the range of water content was small, eg. the soil was constantly wet. In agricultural soils the range of wetness would not be small but rather become saturated at irrigation time becoming drier due to evapotranspiration until the next irrigation.

(3) Steady State Assumption: Darcy's Law adequately describes the steady state condition, but in general soil variability leads to source,sinks, water storage in the profile and subsequent variable potential gradient. The equation of

continuity was introduced in section 2.2.1 in the derivation of the flow equation to allow for this **transient** flow. In some situations the steady flow condition has certain relevance. Rawlins (1973) indicates that with high frequency irrigation the water pulses are damped out a few centimetres below the surface and flow becomes essentially steady for most soils.

Finally, a note on assumptions. It is apparent that some assumptions are made to avoid insignificant processes and conditions cluttering up the model, whereas other assumptions have been made only to facilitate the solution of the model. Both assumptions have their place. The latter reason for assumptions epitomises that all mathematical pursuits need not be reflected directly in reality, however such pursuit invariably sheds some light on the real processes under investigation. The former reason for assumptions highlights the direct applications side of mathematics where tangible results will issue forth if assumptions are well founded.

CHAPTER V

A NEW MODEL

5.1 NEW MODELS FROM OLD

Addiscott and Wagenet (1985) highlight a rarity for a model for solute leaching in soils to be independently validated. These workers found few examples of analytical solutions to the various mechanistic models for solute transport being used by other authors. Indeed Addiscott and Wagenet found even fewer authors using anothers numerical solution. A similar situation has been observed in the closely related field of water movement in soils where no entire model developed by one author was used by another independent author as the subject of a field test. On no occasion was the work of one author developed further along the same lines by another except in the instance that they were co-authors. Feddes, Bresler and Neuman (1974), Feddes *et al.* (1976) and Hoogland, Feddes and Belmans (1981) provided one example whereby a model was continually modified according to a common theme.

Addiscott and Wagenet (1985) provide some explanation of such a phenomenon where it is stated that:

- models tend to reflect the interests and environments of the modeller,
- models may contain built-in suppositions of the modeller that are not stated explicitly or remain in the sub-conscious, and
- there is usually more credit to be obtained from developing and testing a new model than from validating an existing one, which, they state, could be critical for a graduate student.

To this list it could be added that models tend to reflect the *ethos* of the institution at which the modellers are employed, probably because such an institution attracts workers with similar interests and inclinations and communication would be facilitated.

It is the purpose of this chapter to present a model for water movement through the 'soil-plant-atmosphere continuum' that is based on the flow equation and incorporating an original sink term based on the sink term of Molz and Remson (1970). The flow equation has been developed in Chapter II. Molz and Remson did not derive the sink term in their paper. A possible derivation of the term will be presented in the following section.

5.1.1 A Derivation of the Molz and Remson (1970) Uptake Term

A rule of thumb used when considering extraction patterns of soil water by a root system is that water is extracted from successively lower quarters of the root zone in the ratio of 40:30:20:10 of the total transpiration rate. Molz and Remson state that the following volumetric sink term satisfies this distribution:

$$S(z) = -\frac{1.6T}{v^2}z + \frac{1.8T}{v}, \qquad 0 \leq z \leq v,$$

where T = transpiration rate per unit area of soil surface,

v = vertical length of root system,

z = soil depth vertically down, and

S = uptake rate.

The derivation of this term is based on Figure 5.1.

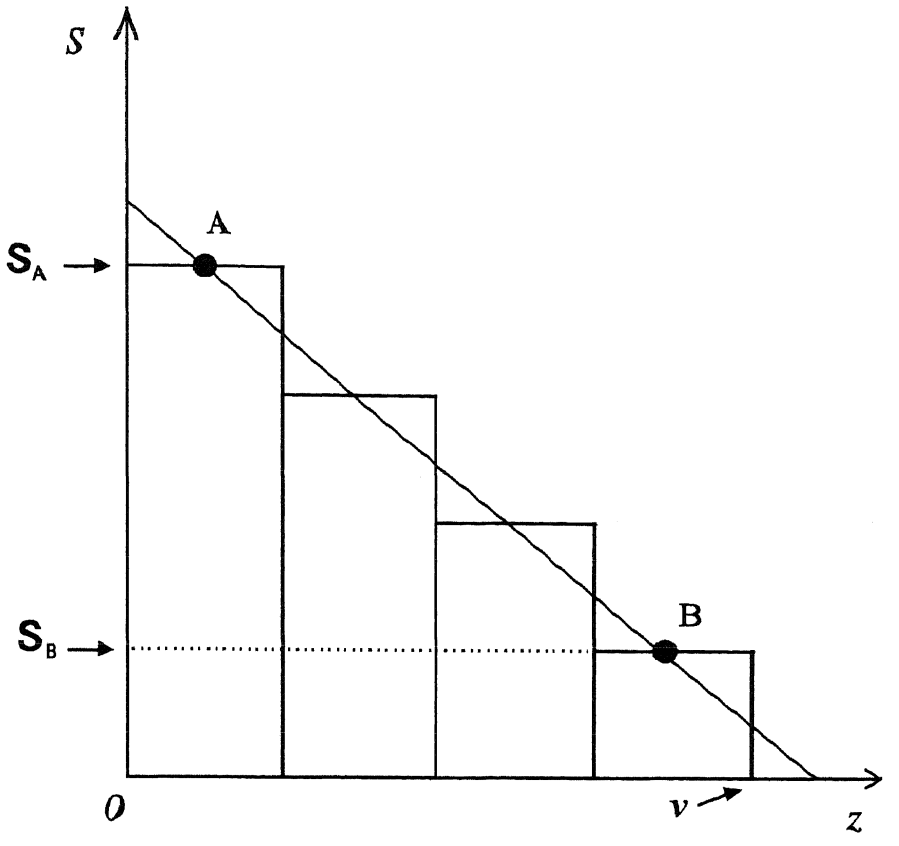


Figure 5.1. Graph depicting the relative proportions of uptake rates in successively deeper quarters of the root zone. The area of the bars represents transpiration fractions.

The sink term (S) can be represented by linear function of the depth z and is given by the line passing through points **A** and **B**. From Figure 5.1, the following relations are deduced from the areas of the largest and smallest rectangles:

$$0.4\ T = S_A.v/4 \qquad \text{giving,} \qquad S_A = (1.6\ T)/v \quad \text{and}$$

$$0.1\ T = S_B.v/4 \qquad \text{giving,} \qquad S_B = (0.4\ T)/v.$$

Thus, the points **A** and **B** have the coordinates:

$$\mathbf{A}(v/8\ ,\ (1.6\ T)/v) \quad \text{and} \quad \mathbf{B}(7v/8\ ,\ (0.4\ T)/v).$$

Denoting the gradient of the line through **A** and **B** by m_{AB},

$$m_{AB} = \frac{\dfrac{1.6T - 0.4T}{v}}{\dfrac{v}{8} - \dfrac{7v}{8}} = \frac{S - \dfrac{1.6T}{v}}{z - \dfrac{v}{8}},$$

gathering terms,

$$\frac{1.2T/v}{-3v/4} = \frac{S - (1.6T)/v}{z - v/8},$$

and simplifying yields:

$$S(z) = -\frac{1.6T}{v^2}z + \frac{1.8T}{v}, \qquad 0 \le z \le v, \tag{5.1}$$

as required.

5.1.2 Extending the Molz and Remson Sink Term

It was noted by Molz and Remson that this model failed when upper layers dried. Indeed, for the mechanistic modeller this model has a twofold shortcoming:

(1) It is not physically based to any extent and the 40:30:20:10 ratios have no mechanistic significance, and

(2) As the top layers dry, the empirical assumption of 40% of total transpiration rate being met by the top quarter of the root zone cannot be met, because of insufficient water in that zone.

The first consideration can be rationalised in the following way. The proportion of extraction met by the various zones is in direct proportion to the rooting density in those zones and if extraction capacity of roots were equal, then the ratios would be loosely justified. Furthermore, the purpose of the this model development is to predict the timing and extent of irrigations and as such, if a root system is provided with as

much water as is necessary for uninhibited growth and development, the anomalies leading to the breakdown of this model such as excessive surface drying will not occur. In section 1.3 it was indiciated that a movement towards the use of mechanistic models is desirable. Sections 2.2.3 and 3.2.1. support that in this case the mechanism is not well known. This, together with the fact that this empirical model will presently be extended to account for the second shortcoming above ratifies the use of the model in this case.

In summary, the processes whereby a root system may adjust its spatial uptake of water to satisfy demand under a range of conditions is quite mysterious, consideration to the relative merits of empirical versus semi-mechanistic water uptake terms are not at issue here, but rather how accurately the real situation may be modelled.

The second shortcoming may be overcome if the "*evaporation or drying front*" phenomenon is introduced. To elaborate, consider the three stages of drying as discussed in Chapter II. The first stage is characterised by potential evaporation - this is where evaporation from the soil surface is dictated fully by atmospheric demand and that the soil is sufficiently wet to maintain this evaporation rate. A point in time is reached whereby the soil cannot transmit the water to fulfil this potential rate. At this point the soil surface evaporation rate declines and the soil surface dries. Without further water infiltration, this zone of drying descends and water from deeper in the profile is transmitted in vapour form through this dry zone to the surface at a slow rate.

To illustrate the evaporation front concept more fully, consider Figures 5.2, 5.3 and 5.4. Figure 5.2 depicts the situation immediately following an irrigation event. In this situation all parts of the profile are above critical water content and the roots are absorbing water according to the 40:30:20:10 empirical ratio to meet the current

transpirational demand. After a period of drying, Figure 5.3 shows a small evaporation front having developed as the surface layers dry. The water content/depth profile indicates the depth at which the critical water content has been surpassed. It has been supposed in these diagrams that transpiration rate has remained at the same level, this being demonstrated by a proportionally longer "box" in Figure 5.3a than its counterpart in Figure 5.2a. It is to be noted that the level of transpiration rate used in this situation is *for illustrative purposes only* and need not be constant from timestep to timestep. In actuality the transpiration data will be calculated from some method such as Penmans method. It has been useful to use a constant transpiration requirement for the description of the evaporation front since the effect of the root activity with respect to water uptake increasing with depth as the evaporation front deepens is well represented.

It has also been assumed in this series of diagrams that the time frame that permits the evaporation front to advance to such a level is small in relation to time taken for the root front to move deeper. A straightforward modification can be made to allow for a growing root system as long as vertical length extension of the root is known as a function of time.

In Figure 5.4 the evaporation front has advanced to such a depth that a decision needs to be made about switching on of irrigation. To determine this the following questions need to be addressed: Are the top layers of soil too dry thus disabling a significant percentage of the roots transpiring to the detriment of the plant **or** are the young, advancing roots at the root front being deprived of water and is one situation more prevalent or important than the other? Which event occurs first and which is more significant is the subject of the ensuing computer simulation which incorporates the sink term presently derived.

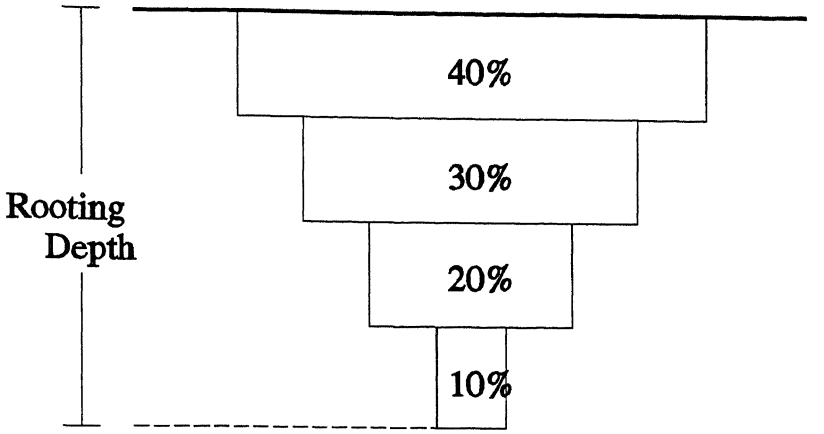


Figure 5.2a Extraction pattern immediately following an infiltration event

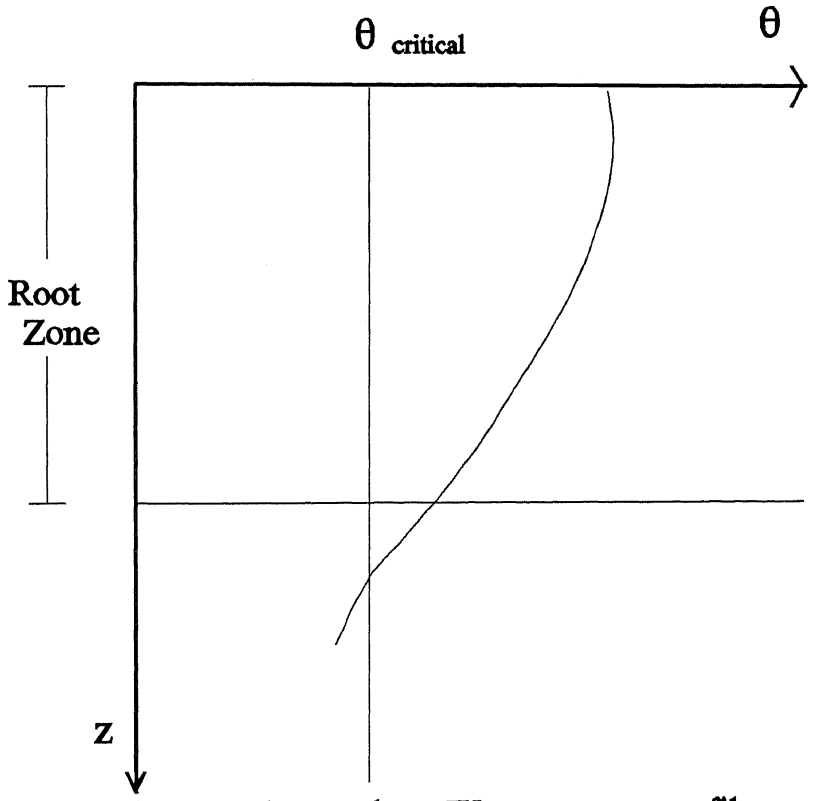


Figure 5.2b Depth vs Water content profile in the corresponding situation as 5.2a

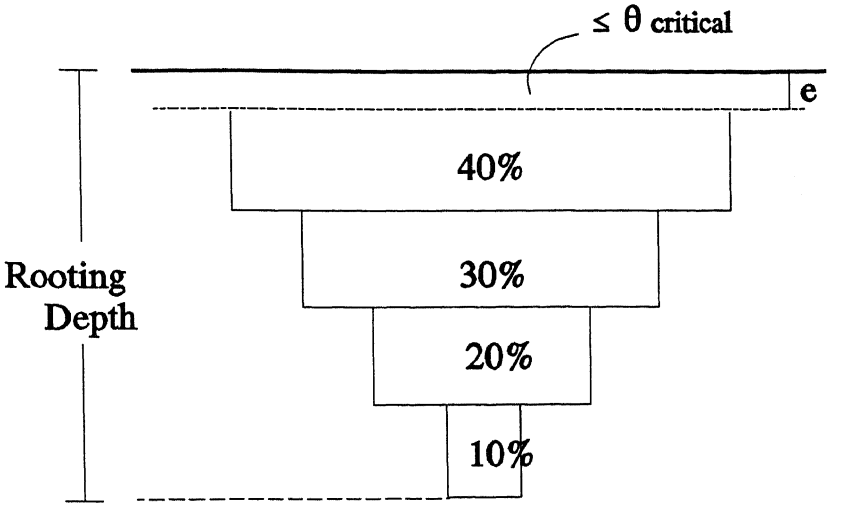


Figure 5.3a Extraction pattern for rooting system after some drying

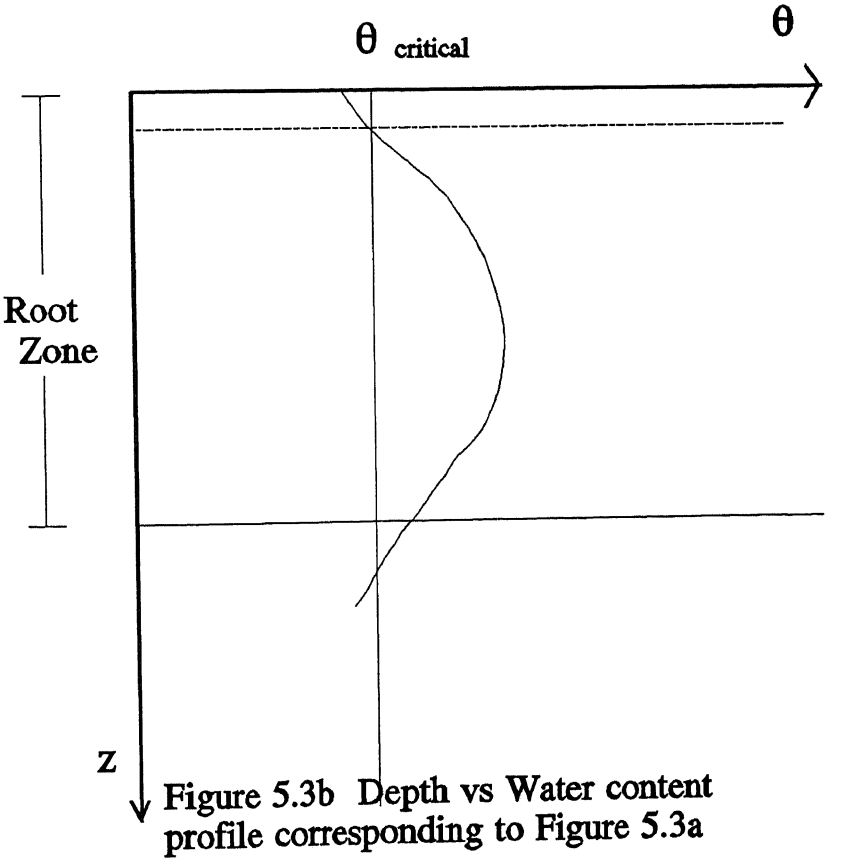


Figure 5.3b Depth vs Water content profile corresponding to Figure 5.3a

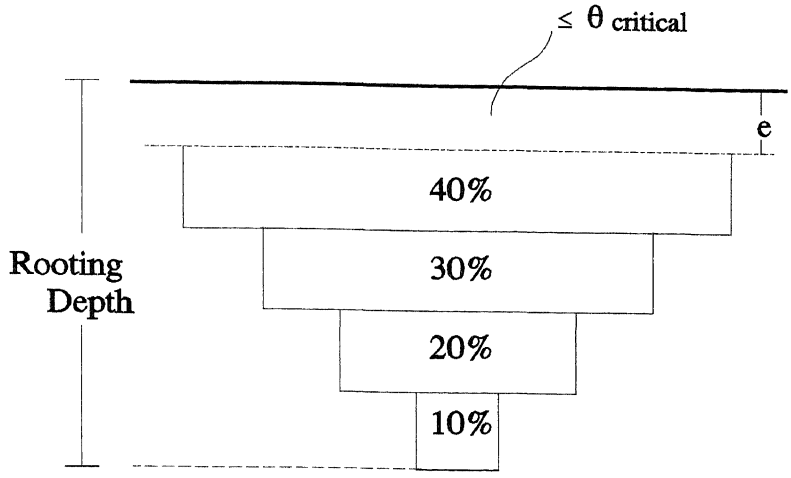


Figure 5.4a Extraction pattern of root system after substancial evapotranspiration

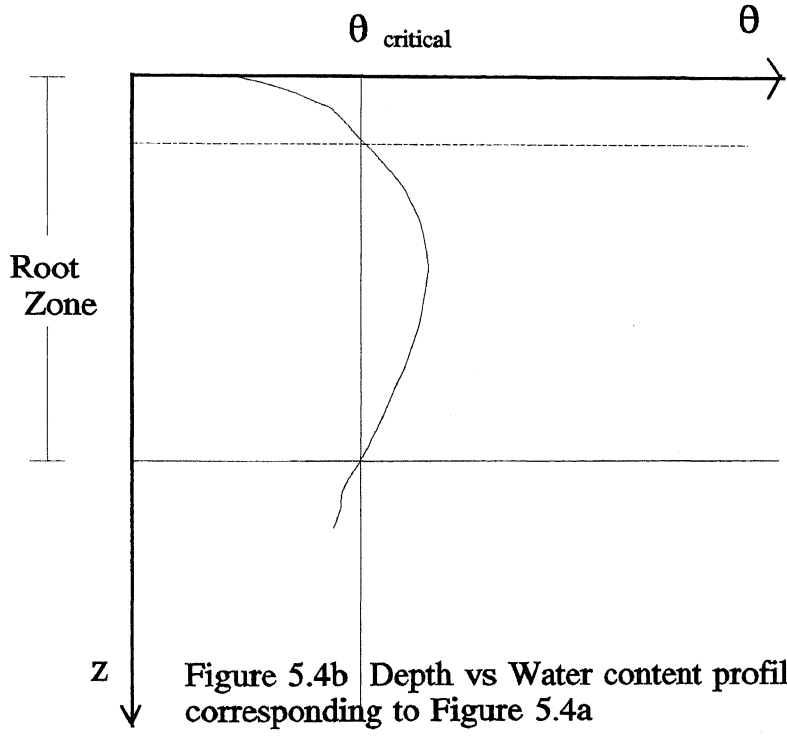


Figure 5.4b Depth vs Water content profile corresponding to Figure 5.4a

Consider a new derivation, similar to that in section 5.1.1, that includes this evaporation front from which no extraction demands can be met. Figure 5.5 shows the uptake pattern (shaded area) required from a profile in which an evaporation front has developed to a depth *e*. This uptake pattern is superimposed on the original pattern

where the surface has not yet dried and extraction is as for the Molz and Remson model. As the evaporation front deepens, the root zone is redefined as the zone from the evaporation front to the depth of the root system, a distance of *v-e*. The assumption here is that the four quarters of this **redefined** root zone can meet the total transpiration demand **for a given timestep** from successively lower quarters in the 40:30:20:10 ratio. In effect the lower zones of roots compensate for the loss of water drawing puissance of the topmost layers. This is not unlike the actual situation as the root zone required to compensate most is the next densest zone of roots.

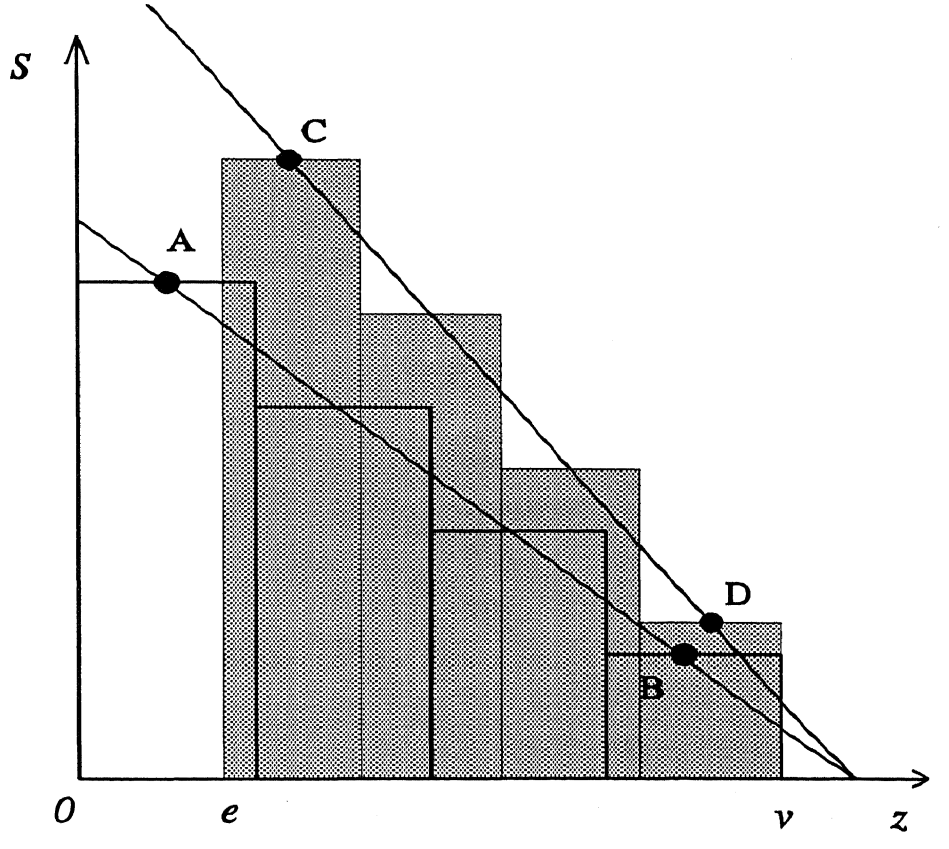


Figure 5.5. Graph showing the extraction pattern of roots in the presence of an *evaporation front* (shaded area). The unshaded bars indicate the extraction pattern with no evaporation front. Note that the sum of areas of both sets of bars are equal and sum to total transpiration rate only in the case where transpiration rate is constant in time.

As in section 5.1.1, the sink term may be represented by a linear function of S and z and is given by the line passing through the points **C** and **D**. In a similar manner to

before the coordinates of **C** and **D** may be determined by equating areas under the largest and smallest rectangles to 0.4 T and 0.1 T respectively. This gives:

C$(e + \frac{1}{8}(v - e)\ ,\ (1.6\ T)/(v - e))$ and **D**$(e + \frac{7}{8}(v-e)\ ,\ (0.4\ T)/(v - e))$.

Denoting the gradient of **CD** by m_{CD},

$$m_{CD} = \frac{\frac{1.6T}{v-e} - \frac{0.4T}{v-e}}{\left(e + \frac{(v-e)}{8}\right) - \left(e + \frac{7(v-e)}{8}\right)} = \frac{S - \frac{1.6T}{v-e}}{z - \left(e + \frac{(v-e)}{8}\right)} .$$

Rearranging to obtain an expression for S,

$$S = \frac{-1.6T}{(v-e)^2} z + \frac{(1.8v - 0.2e)T}{(v-e)^2} . \qquad (5.2)$$

This sink term (5.2) will be used in the computer simulation in the next chapter. It is to be noted that when $e=0$, the new sink term becomes identical to that of Molz and Remson.

5.1.3 A Description of the Whole Model

The objective for the development of this model is to determine the water distribution in relation to the root system throughout a succession of irrigation and evaporation events so that a criterion for switching irrigation on or off may be ascertained. For this reason all aspects of the SPAC must be modelled. Since monitoring water content is one method of determining the water distribution, a likely place to progress from would be the flow equation expressed in the diffusivity form with water content as the dependent variable as is equation 4.2. Solving the flow equation would provide water content at any depth and time as long as the initial water content distribution was known (by measurement) and that any sources or sinks were specified.

Other values required to solve the flow equation are those of diffusivity (**D**) and Hydraulic conductivity (**K**). Since the situation of interest includes unsaturated soils, both **D** and **K** are functions of water content (θ). As no physically based functional relationship has been determined between these entities, empirical methods are resorted to. Two such methods are feasible. One method is to use a table of relations measured in the field for a similar soil and within the θ range of interest (and interpolate unknown values). The other method is to adopt some empirical functions such as the exponential forms or the equations of Clapp and Hornberger (1978). They developed power functions that related the entities as long as certain parameters were known. Since the parameters were determined for a wide range of soil textures and types, this method is quite viable. The power functions of Clapp and Hornberger (1978) are

$$\psi(\theta) = \Psi_s(\theta/\theta_s)^{-b}, \qquad 0 \le \theta \le \theta_s,$$

and $$K(\theta) = K_s(\theta/\theta_s)^{2b+3},$$

where b, θ_s, Ψ_s, and K_s are the parameters to be specified for a particular soil type. The subscript s specifies that the values are at a saturated water content.

All that remains to be specified are the sources and sinks that effect the water content profile. One such sink (or source) occurs at the surface. During an infiltration event the source equates to the flux at the surface and during evaporation the flux at the surface is a sink. This condition manifests itself as a derivative boundary condition as will be described in the next chapter. A final sink is that due to root uptake or transpiration. The sink term was derived in section 5.1.2. What are the unknowns in such a term? For the rate of water uptake to be determined, transpiration rate, rooting depth and depth of evaporation front need be first evaluated. It is proposed that the

transpiration rate be deduced by taking the difference between evapotranspiration and surface evaporation adjusted to include the percentage ground shaded by the crop. The rooting depth will be estimated from previous work on the specific crop in question at a given time of development. A further improvement will be to incorporate a root growth function to allow for the dynamic situation in the field.

This leaves only the evaporation front depth to be assessed. If this imaginary delineation was defined as the boundary between soil at water contents above and below 'wilting point' water content, then this depth may be ascertained by solving the flow equation with e initially set to zero (or any value), determining the water content profiles, with e to then be updated before the next iteration of the solution process. This is feasible because if e were initially zero, say, and during an evaporation event, then water will be extracted from the entire root zone according to the uptake term. As the water is used and drains without replacement the water content will eventually fall below the critical θ value and the evaporation front will be redefined, and used for the next water content profile calculation. The next chapter compiles the computational forms of the equations described here with the final chapter implementing the simulation.

CHAPTER VI

THE COMPUTER SIMULATION

- THE FINITE DIFFERENCE EQUATIONS

6.1 METHOD OF FINITE DIFFERENCES

The preceding chapters have formed the foundation for a proposal of a working model to predict the movement of water through soils and its solution using the method of finite differences. It is intended that the model embody a degree of mechanism particularly where the mechanism is well known (evapotranspiration, redistribution). The model makes way for empiricism where the actual processes of water movement are not effectively described using relatively readily available input data (water uptake by roots).

Since the explicit, forward difference approximation of derivatives leads to restrictive relations between the size of the time and depth steps (von Rosenberg, 1969) and that both forward and backward differences are only correct to the first order in time, the Crank Nicolson method will be employed. In this method all finite differences will be written about the point z_i, $t_{j+½}$, that is, halfway between known and unknown time intervals. Several more advantages of Crank Nicolson as applied to non-linear parabolic differential equations of the type required to be solved in this water movement application are outlined in von Rosenberg (1969). Some of these reasons are: the approximations are second order correct in both time and in space; it is

relatively more efficient than forward or backward difference equations and it is stable for all sizes of depth step to time step ratios. Furthermore, the Crank Nicolson method is easily coupled with other methods to handle non-linear coefficients and the set of resulting equations are tridiagonal and may be solved using the Thomas algorithm (for example).

6.1.1 The Continuous Form of the Model

Consider the following Partial Differential Equation (PDE) form of the model for water movement in the soil,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}[D(\theta)\frac{\partial \theta}{\partial z} - K(\theta)] - S(z) , \qquad (6.1)$$

with boundary conditions at the surface resulting from evaporation from the soil surface (E_{soil}) or infiltration ($I(t)$). At the lower boundary, any one of several conditions could occur such as zero flux (possibly the water table or impermeable layer), but in this case a known distribution of water contents will be used. The initial conditions are $\theta(z,0)=\theta_0(z)$,that is a known distribution of water contents down the profile. As developed in Chapter V, the sink term $S(z)$ is defined (using the notation of the previous chapter) making provision for a growing root, that is, using $v(t)$ instead of v to represent the rooting depth:

$$S(z,t) = \frac{-1.6T}{(v(t) - e)^2} z + \frac{(1.8v(t) - 0.2e)T}{(v(t) - e)^2} . \qquad (6.2)$$

6.1.2 The Finite Difference Grid

In order to express these equations using finite differences, a grid is established similar to those in Chapter IV, using j's to represent the number of time steps each of length

Δt and i's to represent the number of depth steps each of length Δz. As will become evident, the grid needs an adjustment so that a value of $i=0$ does **not** correspond to the surface of the soil where $z=0$. This is because the following central difference approximation of the flow equation gives rise to a need to evaluate diffusivity and conductivity at water contents at a depth corresponding to one half a depth step above the actual surface of the soil. A similar adjustment was made by both Hanks and Bowers (1962) and Feddes, Kowalik and Zaradny (1978). As shown in Figure 6.1, a value of $i=0$ matches with a depth of $\Delta z/2$ from the surface, that is, $z_i = (i-½)\Delta z$ i=1,2,...,N. No adjustment is made to the time steps.

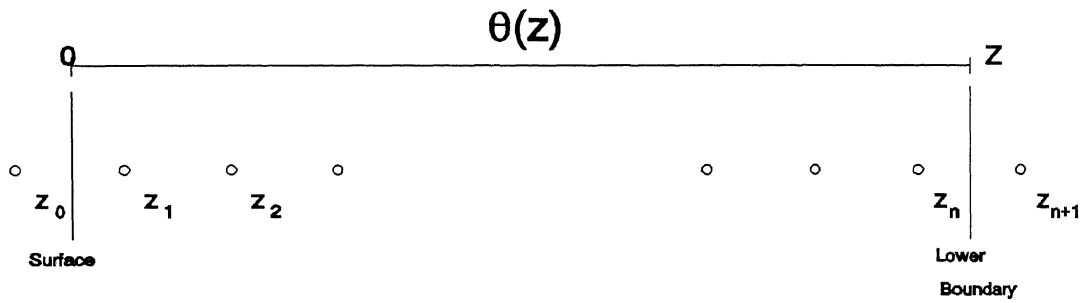


Figure 6.1 Adjusted Finite Difference Grid with depth points shifted one-half a step from the boundaries.

Apart from the advantage of this grid adjustment to the application at hand, there are two further advantages. The first benefit is not one of improvement of computational accuracy but rather an improvement to the applicability of the set of equations formed to a wider variety of situations. It is found that under the grid arrangement with the surface corresponding to i=0, the number of resulting finite difference equations varied with the type of boundary condition. For example, where all boundary values are

known explicitly, N-2, equations needed simultaneous solutions whereas if the top and bottom boundary conditions were given as derivatives, another equation was produced for each boundary, giving rise to N equations. If the grid is as arranged in Figure 6.1, N equations will always be produced despite the nature of the boundary conditions since the values at z_0 and z_{n+1} are always eliminated in finite difference equation formulation. This leads to a simplification of the testing of a variety of such conditions.

A second benefit of the adjusted grid was determined by Douglas (1961) as reported by von Rosenberg (1969). Douglas found that for certain derivative boundary conditions, the dependent variable at the boundary oscillates for the original grid configuration but does not occur with the adjusted grid.

Perhaps one shortcoming of the adjusted grid is that the dependent variable is not found explicitly at either boundary but may be found by averaging the exterior point (deduced by boundary conditions) and the first interior point. This arithmetic averaging is clearly a problem with nonlinear boundary conditions.

6.1.3 The Finite Difference Form

As indicated above, an implicit method of expressing the PDE 6.1 in finite difference form will be used by employing a central difference approximation of the derivatives about the point $z_i, t_{j+½}$. To handle the non-linearity arising from the product of $\partial\theta/\partial t$ and $D(\theta)$, von Rosenberg (1969) formulates the first derivative of the space derivative at the points $z_{i-½}$, $t_{j+½}$ and $z_{i+½}$, $t_{j+½}$. A consequence of this is that the coefficients $D(\theta)$ and $K(\theta)$ need to be evaluated at these points also. The method of achieving these approximations is detailed later. The finite difference equation formed in this manner is:

$$\frac{\theta_i^{j+1} - \theta_i^j}{\Delta t} = \frac{\left[D\left(\theta_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right)\left(\frac{\partial\theta}{\partial z}\right)_{i+\frac{1}{2}}^{j+\frac{1}{2}} - K\left(\theta_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right)\right] - \left[D\left(\theta_{i-\frac{1}{2}}^{j+\frac{1}{2}}\right)\left(\frac{\partial\theta}{\partial z}\right)_{i-\frac{1}{2}}^{j+\frac{1}{2}} - K\left(\theta_{i-\frac{1}{2}}^{j+\frac{1}{2}}\right)\right]}{\Delta z} - S(z,t)_i^j \tag{6.3}$$

The partial derivatives in depth are estimated at the *(j+½)*th time step by averaging at the *j* and *j+1* time levels, then by using central difference approximations with respect to depth. This approximation eliminates the need to evaluate the derivatives at the half time and half depth steps. Mathematically,

$$\left(\frac{\partial\theta}{\partial z}\right)_{i+\frac{1}{2}}^{j+\frac{1}{2}} = \frac{\left(\frac{\partial\theta}{\partial z}\right)_{i+\frac{1}{2}}^{j+1} + \left(\frac{\partial\theta}{\partial z}\right)_{i+\frac{1}{2}}^{j}}{2}$$

and substituting for

$$\left(\frac{\partial\theta}{\partial z}\right)_{i+\frac{1}{2}}^{j+1} = \frac{\theta_{i+1}^{j+1} - \theta_i^{j+1}}{\Delta z},$$

and

$$\left(\frac{\partial\theta}{\partial z}\right)_{i+\frac{1}{2}}^{j} = \frac{\theta_{i+1}^{j} - \theta_i^{j}}{\Delta z},$$

gives

$$\left(\frac{\partial\theta}{\partial z}\right)_{i+\frac{1}{2}}^{j+\frac{1}{2}} = \frac{\left(\theta_{i+1}^{j+1} + \theta_{i+1}^{j}\right) - \left(\theta_i^{j+1} + \theta_i^{j}\right)}{2\,\Delta z}. \tag{6.4}$$

Similarly,

$$\left(\frac{\partial\theta}{\partial z}\right)_{i-\frac{1}{2}}^{j+\frac{1}{2}} = \frac{\left(\theta_i^{j+1} + \theta_i^{j}\right) - \left(\theta_{i-1}^{j+1} + \theta_{i-1}^{j}\right)}{2\,\Delta z}. \tag{6.5}$$

Since the diffusivity, *D*, and the conductivity, *K*, are always corresponding to water contents at the *(j+½)th* time step, the following notation will be used as it is less

cumbersome: $D_{i+1/2}^{j+1/2}$, $D_{i-1/2}^{j+1/2}$, $K_{i+1/2}^{j+1/2}$ and $K_{i-1/2}^{j+1/2}$ denoting diffusivity or conductivity calculated at water contents at a half a depth step above or below that of the *ith* step.

Substituting for the partial derivative approximations (6.4) and (6.5), into (6.3), simplifying and writing the unknowns on the left hand side gives,

$$\begin{aligned} & D_{i-1/2}^{j+1/2}\theta_{i-1}^{j+1} - \left(D_{i-1/2}^{j+1/2} + D_{i+1/2}^{j+1/2} + A\right)\theta_i^{j+1} + D_{i+1/2}^{j+1/2}\theta_{i+1}^{j+1} \\ & = -D_{i-1/2}^{j+1/2}\theta_{i-1}^{j} + \left(D_{i-1/2}^{j+1/2} + D_{i+1/2}^{j+1/2} - A\right)\theta_i^{j} - D_{i+1/2}^{j+1/2}\theta_{i+1}^{j} \\ & \quad + 2\,\Delta z\left(K_{i+1/2}^{j+1/2} - K_{i-1/2}^{j+1/2}\right) + 2\,\Delta z^2 S_i^j , \end{aligned} \tag{6.6}$$

where $A = 2\Delta z^2/\Delta t$ and the finite discrete form of the sink term is given by:

$$S_i^j = \frac{-1.6\,T_j}{\left(v(\Delta t.j) - e_j\right)^2}\,\Delta z.(i-1/2) + \frac{\left(1.8\,v(\Delta t.j) - 0.2\,e_j\right)T_j}{\left(v(\Delta t.j) - e_j\right)^2} . \tag{6.7}$$

with the j subscripts denoting that both transpiration (T) and evaporation front (e) depend on time. It is to be noted that to be precise the sink term needs to be evaluated at the same time as the derivatives and parameters are evaluated, that is, $j+½$. It will be assumed that the change in water uptake from one time to the next half time step is negligible and that the sink evaluated at the jth timestep will be used. One justification of this would be that to determine the sink at time $j+½$ the previous sink would need to be averaged with the future sink at time $j+1$ and that the prediction forward in time of transpiration rate may be inaccurate thus forcing the half time step sink to be inaccurate. It is difficult to assess at this time which method would be least inaccurate hence the simpler of the two is chosen. An evaluation of the two sink terms is presented in Appendix E.

Equation 6.6 will be referred to hereafter as the Primary Finite Difference Equation

(Primary FDE).

6.1.4 Boundary Conditions

Equation 6.6 holds for i=2 to i=n-1 since the boundary conditions will lead to change in 6.6 for i=1 and i=n. As indicated in section 6.1.1 the surface condition will depend on the soil evaporation or infiltration at any time these surface flux conditions give rise to a derivative boundary condition. The surface derivative boundary condition needs to be given as the rate of change of water content with respect to depth. It is to be recalled that Darcy's Law for water flux under gravity is given by:

$$q(t) = -K(\psi)\left(\frac{\partial \psi}{\partial z} - 1\right), \tag{6.8}$$

where the variables are as defined in Chapter II and that at the surface the flux (q) may be the evaporation or infiltration rates. The origin of z is taken at the surface with the downward direction considered positive. Expressing equation 6.8 in terms of water content (θ) (by introducing diffusivity) gives:

$$q(t) = -D(\theta)\frac{d\theta}{dz} + K(\theta).$$

and rearranging,

$$\frac{d\theta}{dz} = \frac{K(\theta) - q(t)}{D(\theta)}. \tag{6.9}$$

At the surface, that is $i=½$, the derivative in equation 6.9 may be approximated by the second order correct, central difference analog

$$\left(\frac{d\theta}{dz}\right)_{1/2}^{j+1} \approx \frac{\theta_1^{j+1} - \theta_0^{j+1}}{\Delta z}. \tag{6.10}$$

Substituting 6.10 into 6.9 and evaluating the other parameters at the same point gives

an expression for the dependent variable at the external point one-half a depth step above the surface, that is,

$$\theta_0^{j+1} = \theta_1^{j+1} + \frac{\Delta z}{D(\theta_{1/2}^{j+1})}\left(q_{1/2}^{j+1} - K(\theta_{1/2}^{j+1})\right). \qquad (6.11)$$

It can be seen here that the implementation of this surface flux condition requires a knowledge of the water contents and flux at the immediate future timestep. This is a major source of error and the subject of making reasonable estimates where possibly a linear estimate is not sufficiently accurate. These projections are the subject of the next section 6.1.5: "Forward Projections of Water Content in Time and Space". The flux at the surface as indicated earlier may be due to evaporation or infiltration. These are now considered in turn.

Evaporation at the Surface.

For an evaporation event, equation 6.11 is substituted into the primary finite difference equation to produce the FDE that holds for $i=1$. In fact the expression for θ_0 at both the jth and $(j+1)$st timesteps are substituted for both their occurrences in the primary finite difference equation.

Consider firstly the primary FDE expressed for $i=1$ as in equation 6.12. The two fictitious above-ground points are evident here and the boundary condition equation is combined with 6.12 to eliminate them.

$$\begin{aligned} D_{1/2}^{j+1/2}\theta_0^{j+1} - \left(D_{1/2}^{j+1/2} + D_{3/2}^{j+1/2} + A\right)\theta_1^{j+1} + D_{3/2}^{j+1/2}\theta_2^{j+1} \\ = -D_{1/2}^{j+1/2}\theta_0^{j} + \left(D_{1/2}^{j+1/2} + D_{3/2}^{j+1/2} - A\right)\theta_1^{j} - D_{3/2}^{j+1/2}\theta_2^{j} \\ + 2\,\Delta z\left(K_{3/2}^{j+1/2} - K_{1/2}^{j+1/2}\right) + 2\,\Delta z^2 S_1^j \,. \end{aligned} \qquad (6.12)$$

Using equation 6.11 to substitute for θ_0^{j+1} , 6.12 becomes:

$$
\begin{aligned}
&- \left(D_{3/2}^{j+1/2} + A\right)\theta_1^{j+1} + D_{3/2}^{j+1/2}\theta_2^{j+1} \\
&= -D_{1/2}^{j+1/2}\theta_0^{j} + \left(D_{1/2}^{j+1/2} + D_{3/2}^{j+1/2} - A\right)\theta_1^{j} - D_{3/2}^{j+1/2}\theta_2^{j} \\
&\quad -D_{1/2}^{j+1/2}\Delta z\left(q_{1/2}^{j+1} - K_{1/2}^{j+1}\right)/D_{1/2}^{j+1} + 2\,\Delta z\left(K_{3/2}^{j+1/2} - K_{1/2}^{j+1/2}\right) \\
&\quad + 2\,\Delta z^2 S_1^{j} ,
\end{aligned}
\tag{6.13}
$$

where θ_0 at the jth timestep is as follows:

$$
\theta_0^{j} = \theta_1^{j} + \frac{\Delta z}{D(\theta_{1/2}^{j})}\left(q_{1/2}^{j} - K(\theta_{1/2}^{j})\right) . \tag{6.14}
$$

At the $(j+1)$st timestep, it is to be noted that the first term of the right hand side of equation 6.11 becomes part of the left hand side of the primary FDE and as such will "solved" as part of the tridiagonal system. The second term of equation 6.11 requires evaluation/estimation and is incorporated into the right hand side of the primary FDE and subsequently forms part of the solution vector in the tridiagonal system.

Infiltration at the Surface.

In theory, equation (6.13) can be used for positive (infiltration) and negative (evaporation) fluxes however in practice, it is feasible only for evaporation due to the complex nature of infiltration. Infiltration rates could be expressed as functions of time as in equations of Philip, 1957 or Green and Ampt, 1911. In both cases several more empirically fitted parameters would need to be introduced thus complicating the entire process and adding more room for lack of generality and increased error. Despite both equations having their roots in physically based derivation, certain criteria need be met for their applicability. Both equations demonstrate the phenomenon of reduction in

infiltration rate with increase in water content. One way to avoid this estimation of the infiltration rate over time to be used in equation 6.13 is to redefine the surface boundary condition under infiltration to be at saturated water content for the duration of infiltration. Clearly this will overestimate the real situation since the ground is not instantaneously saturated on the surface when irrigation begins. Furthermore the surface is not guaranteed an even and thorough coverage of water. This surface condition may correspond more closely for the process of flood irrigation. Some advantages of this method are that it is computationally simple, the infiltration rate is intrinsically contained within the solution and needs not be estimated and that the mechanism whereby infiltration rate reduces with irrigation time is also a built in feature of the solution of the flow equation. The finite difference equation that embodies this saturated surface condition is developed as follows. It becomes still a matter of eliminating the two above ground water contents at j and at $j+1$ times in equation 6.12. By virtue of the grid formation as described in section 6.1.2 the surface condition of saturated water content can be expressed as an average of the above-ground point and the point at $i=1$, that is $\theta_{1/2} = (\theta_0 + \theta_1)/2$. Since $\theta_{1/2} = \theta_{saturated}$ during infiltration,

$$\theta_0^{j+1} = 2\theta_s - \theta_1^{j+1} ,$$

where θ_s is saturated water content for the given soil.

Substituting the values for θ_0 at both j and $j+1$ timesteps into 6.12 gives,

$$\begin{aligned} -\left(2D_{1/2}^{j+1/2} + D_{3/2}^{j+1/2} + A\right)\theta_1^{j+1} + D_{3/2}^{j+1/2}\theta_2^{j+1} \\ = \left(2D_{1/2}^{j+1/2} + D_{3/2}^{j+1/2} - A\right)\theta_1^{j} - D_{3/2}^{j+1/2}\theta_2^{j} \\ + 2\,\Delta z\left(K_{3/2}^{j+1/2} - K_{1/2}^{j+1/2}\right) - 4D_{1/2}^{j+1/2}\theta_s \\ + 2\,\Delta z^2 S_1^j . \end{aligned} \qquad (6.15)$$

The Lower Boundary.

The lower boundary condition of known water contents is treated in a similar manner to the surface saturated water content situation. In this case however, it is the instances of θ_{N+1} that need elimination. Consider the primary FDE at $i=N$:

$$\begin{aligned} & D^{j+1/2}_{N-1/2}\theta^{j+1}_{N-1} - \left(D^{j+1/2}_{N-1/2} + D^{j+1/2}_{N+1/2} + A\right)\theta^{j+1}_{N} + D^{j+1/2}_{N+1/2}\theta^{j+1}_{N+1} \\ & = -D^{j+1/2}_{N-1/2}\theta^{j}_{N-1} + \left(D^{j+1/2}_{N-1/2} + D^{j+1/2}_{N+1/2} - A\right)\theta^{j}_{N} - D^{j+1/2}_{N+1/2}\theta^{j}_{N+1} \\ & \quad + 2\,\Delta z\left(K^{j+1/2}_{N+1/2} - K^{j+1/2}_{N-1/2}\right) + 2\,\Delta z^2 S^{j}_{N} . \end{aligned} \tag{6.16}$$

Now let the value of the water contents at the bottom boundary, that is, at $i=N+½$ be denoted by θ_L's. Also,

$$\theta^{j}_{N+1} = 2\theta^{j}_{L} - \theta^{j}_{N} . \tag{6.17}$$

Hence equation 6.16 becomes:

$$\begin{aligned} & D^{j+1/2}_{N-1/2}\theta^{j+1}_{N-1} - \left(D^{j+1/2}_{N-1/2} + 2D^{j+1/2}_{N+1/2} + A\right)\theta^{j+1}_{N} \\ & = -D^{j+1/2}_{N-1/2}\theta^{j}_{N-1} + \left(D^{j+1/2}_{N-1/2} + D^{j+1/2}_{N+1/2} - A\right)\theta^{j}_{N} - D^{j+1/2}_{N+1/2}\theta^{j}_{N+1} \\ & \quad - 2D^{j+1/2}_{N+1/2}\theta^{j+1}_{L} + 2\,\Delta z\left(K^{j+1/2}_{N+1/2} - K^{j+1/2}_{N-1/2}\right) + 2\,\Delta z^2 S^{j}_{N} . \end{aligned} \tag{6.18}$$

where θ_{N+1} at the jth timestep is given by 6.17.

6.1.5 Forward Projections of Water Content in Time and Space

Some Necessary Estimates.

There are several instances of where water content (and its dependent values of Conductivity and Diffusivity) are required to be projected forward in either time or space or both. One such instance is involved with the surface flux where the elimination of the above-ground water content requires a knowledge of the water content one step in the future as in the $j+1$ version of equation 6.14. For long periods

of evaporation where the profile is not changing greatly between time steps, a simple linear projection from the previous one or two water contents at the same depth is quite accurate, however at the surface where an evaporation event may be succeeded by an infiltration event, water contents are subject to wide variation. Given that a change of water content from 0.2 cm^3/cm^3 to 0.29 cm^3/cm^3 in Silt Loam soil results in a 300-fold increase in Conductivity, any inaccuracies are magnified greatly. One method used by the writer to reduce this error was to monitor 'switching' times from infiltration to evaporation and at these times no linear forward projection was used, particularly at the surface where the fluctuations were more critical. These methods are elaborated upon in Chapter VII in conjunction with detailing the computer program.

Another instance of forward projection, this time in space, occurs after the tridiagonal system is solved at each timestep. Since the grid used does not explicitly give the surface water content it needs to be found by averaging the above-ground water content ($i=0$) and the water content at the top grid point ($i=1$). The problem here is due to the non-linearity of the surface boundary condition and therefore to find the above-ground value by using equation 6.14, the surface water content needs to already be known. The method employed here was to make an initial linear estimate of the water content at the boundary then to use this in equation 6.14 then to average this new-found above-ground value and top grid point value as described above. The linear estimate made use of the values of water content at $i=1$ and $i=2$ at a given time and projected upwards so: $\theta_0 = (3\theta_1 - \theta_2)/2$. Error here was reduced by decreasing the depth step so that the projections occurred over a small distance. An iterative procedure was considered but as there was no assurance of convergence it was abandoned.

Crank-Nicolson Requirements- Projecting a Half Step Forward in Time and Space.

As a consequence of achieving second order correctness for all analogs of derivatives in time and depth, the time derivative was evaluated about a point one-half a time step ahead of known values, that is, at $(z_i, t_{j+½})$ and the derivatives in depth were evaluated at this same point but by averaging values at $z_{i-½}$ and $z_{i+½}$. Because of this the diffusivity and conductivity need to be evaluated at these points also. Since this model will use the equations of Clapp and Hornberger (1978), to provide empirical functional relationships between K, ψ and θ, it becomes a matter of approximating θ at the points $(z_{i\pm½}, t_{j+½})$ and then using:

$$\psi(\theta) = \Psi_s(\theta/\theta_s)^{-b}, \qquad 0 \le \theta \le \theta_s, \tag{6.19}$$

and

$$K(\theta) = K_s(\theta/\theta_s)^{2b+3}, \tag{6.20}$$

where b, θ_s, Ψ_s, and K_s are the parameters to be specified for a particular soil type. The subscript s specifies that the values are at a saturated water content. These equations may be used in determining $D(\theta)$, which, as described in Chapter II, is defined so:

$$D(\theta) = -d\psi/d\theta\, K(\theta). \tag{6.21}$$

Differentiating equation 6.19 with respect to θ and substituting into 6.21 gives

$$D(\theta) = -b\Psi_s K_s(\theta_s)^{-(b+3)}\theta^{b+2}.$$

Two methods may be used to project the value of water content forward in space and in time. Feddes, Kowalik and Zaradny, (1978) and Hayhoe (1978) use a simple geometric method whereas von Rosenberg (1969) uses a Taylors series expansion. These methods are considered in the following section.

(a) The Geometric Method of Projection.

This method uses the grid in figure 6.2.

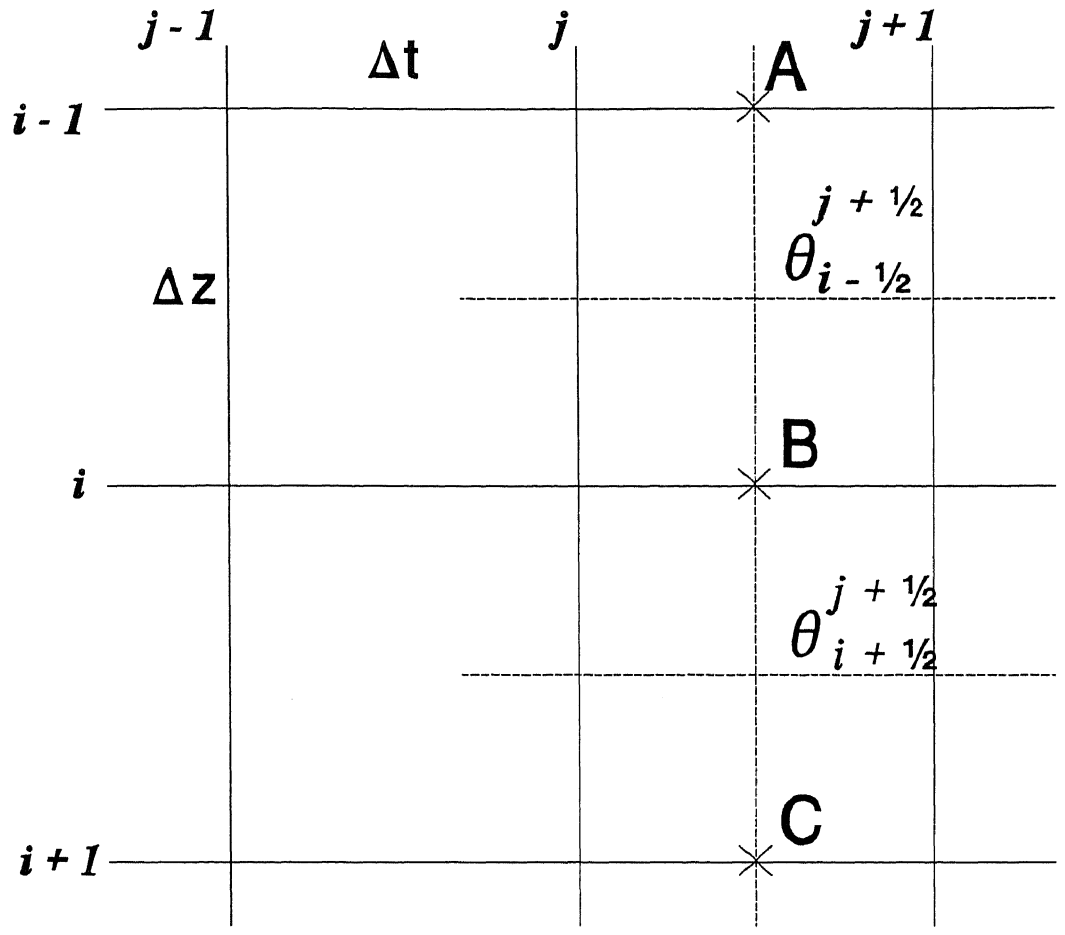


Figure 6.2 Grid showing the location of water content to be evaluated.

Water contents are projected forward in time at the depths z_i and z_{i+1} using the values of water content at the *(j-1)st* and *jth* time steps. This external division projects to the $j+½$ water contents. For example, to find the water content at *C*:

$$\theta^{j}_{i+1} - \theta^{j-1}_{i+1} = \frac{2}{3}\left(\theta^{j+1/2}_{i+1} - \theta^{j-1}_{i+1}\right).$$

This gives $\theta^{j+1/2}_{i+1} = \frac{3}{2}\theta^{j}_{i+1} - \frac{1}{2}\theta^{j-1}_{i+1}$ and similarly at *B*, $\theta^{j+1/2}_{i} = \frac{3}{2}\theta^{j}_{i} - \frac{1}{2}\theta^{j-1}_{i}$.

Averaging gives the required values,

$$\theta_{i+1/2}^{j+1/2} = \tfrac{3}{4}\left(\theta_{i+1}^{j} + \theta_{i}^{j}\right) - \tfrac{1}{4}\left(\theta_{i+1}^{j-1} + \theta_{i}^{j-1}\right) ,$$

$$\text{and} \quad \theta_{i-1/2}^{j+1/2} = \tfrac{3}{4}\left(\theta_{i-1}^{j} + \theta_{i}^{j}\right) - \tfrac{1}{4}\left(\theta_{i-1}^{j-1} + \theta_{i}^{j-1}\right) . \qquad (6.22)$$

(b) The Taylors Series Expansion Method.

The first step in this method towards approximating water content projected half a time step forward at the $(i+½)$th depth step is to use an average in depth of water contents at the two adjacent known depth steps as in equation 6.23,

$$\theta_{i+1/2}^{j+1/2} = \frac{\left(\theta_{i+1}^{j+1/2} + \theta_{i}^{j+1/2}\right)}{2} . \qquad (6.23)$$

The water contents at the known depth steps, on the right hand side of the equation, are then projected forward in time from the known *jth* time step using a Taylors series expansion truncated after the second term. This truncation maintains the second order correctness. Consider such an expansion:

$$\theta_{i}^{j+1/2} = \theta_{i}^{j} + \left(\frac{\partial\theta}{\partial t}\right)_{i}^{j}\left(\frac{\Delta t}{2}\right) \qquad (6.24)$$

The problem now amounts to finding a reasonable approximation of $\partial\theta/\partial t$ at the (z_i, t_j) point. This is obtained from equation 6.1, that is,

$$\left(\frac{\partial\theta}{\partial t}\right)_{i}^{j} = \left[\frac{\partial}{\partial z}\left[D(\theta)\,\frac{\partial\theta}{\partial z} - K(\theta)\right] - S(z)\right]_{i}^{j} . \qquad (6.25)$$

From this point various expansions could be implemented. To maintain second order correctness, equation 6.25 could first be expressed in terms of a forward difference for the first depth derivative, followed by a backward difference for the second depth

derivative. This analog together with other analogs for equation 6.25 are given below. The **forward difference** for the first depth derivative yields:

$$\left(\frac{\partial\theta}{\partial t}\right)_i^j = \frac{\left[D\left(\theta_{i+1}^j\right)\left(\frac{\partial\theta}{\partial z}\right)_{i+1}^j - K\left(\theta_{i+1}^j\right)\right] - \left[D\left(\theta_i^j\right)\left(\frac{\partial\theta}{\partial z}\right)_i^j - K\left(\theta_i^j\right)\right]}{\Delta z} - S(z_i,t_j).$$

(6.26)

Similarly, the backward difference for this derivative gives:

$$\left(\frac{\partial\theta}{\partial t}\right)_i^j = \frac{\left[D\left(\theta_i^j\right)\left(\frac{\partial\theta}{\partial z}\right)_i^j - K\left(\theta_i^j\right)\right] - \left[D\left(\theta_{i-1}^j\right)\left(\frac{\partial\theta}{\partial z}\right)_{i-1}^j - K\left(\theta_{i-1}^j\right)\right]}{\Delta z} - S(z_i,t_j).$$

(6.27)

The depth derivatives in equation 6.26 may then be expressed as a forward difference again to form what could be termed the **forward/forward** approximation:

$$\left(\frac{\partial\theta}{\partial t}\right)_i^j = \frac{\left[D\left(\theta_{i+1}^j\right)\left(\frac{\theta_{i+2}^j - \theta_{i+1}^j}{\Delta z}\right) - K\left(\theta_{i+1}^j\right)\right] - \left[D\left(\theta_i^j\right)\left(\frac{\theta_{i+1}^j - \theta_i^j}{\Delta z}\right) - K\left(\theta_i^j\right)\right]}{\Delta z} - S(z_i,t_j).$$

(6.28)

The **forward/backward** approximation is similarly,

$$\left(\frac{\partial\theta}{\partial t}\right)_i^j = \frac{\left[D\left(\theta_{i+1}^j\right)\left(\frac{\theta_{i+1}^j - \theta_i^j}{\Delta z}\right) - K\left(\theta_{i+1}^j\right)\right] - \left[D\left(\theta_i^j\right)\left(\frac{\theta_i^j - \theta_{i-1}^j}{\Delta z}\right) - K\left(\theta_i^j\right)\right]}{\Delta z} - S(z_i,t_j).$$

(6.29)

In a similar manner the depth derivative in (6.27) can be written as a backward difference to form the **backward/backward** approximation:

$$\left(\frac{\partial\theta}{\partial t}\right)_i^j = \frac{\left[D\left(\theta_i^j\right)\left(\frac{\theta_i^j - \theta_{i-1}^j}{\Delta z}\right) - K\left(\theta_i^j\right)\right] - \left[D\left(\theta_{i-1}^j\right)\left(\frac{\theta_{i-1}^j - \theta_{i-2}^j}{\Delta z}\right) - K\left(\theta_{i-1}^j\right)\right]}{\Delta z} - S(z_i,t_j)\,. \tag{6.30}$$

The requirements of these various analogs determine where they may be used in the computer simulation. For example, the forward/forward analog used to find the water contents in (6.23) would require the range of water contents at the *j*th timestep from the *i*th depth to the *(i+3)*th depth - quite a problem if the approximation was required near the lower boundary as the water contents beyond the boundary are unknown. A similar problem occurs with both the forward/backward and backward/backward analogs if they are used at the surface. A solution to this is to use the forward/forward analog for projecting forward from the values near the surface ($i \leq 2$), backward/backward near the lower boundary ($i \geq N\text{-}2$) and use the forward/backward elsewhere.

Evaluation of θ at $z_{i+½}, t_{j+½}$ When i=1 or When j=1.

The methods outlined in the previous sections for finding water content at $z_{i\pm½}, t_{j+½}$ needs special consideration when $i=1$ or when $j=1$. If the method of Feddes et al (1978) is used, knowledge of the water contents at all depths for the previous time steps (*jth* and *(j-1)st*) needs to be recalled for use in equation 6.16. A problem arises when $j=1$ since there is no prior knowledge of the water contents before this time. A possible solution is to begin each simulation with the soil profile having drained to field capacity which, by virtue of its definition, will allow an assumption of initial unchanging water content (unchanged from field capacity).

If the method involving Taylors expansion is used, the evaluation of $\theta_{i-½,j+½}$ at $i=1$ requires a knowledge of $\theta_{0,j}$ in order to find the time derivative at $(z_{½}, t_j)$ using equation

6.21. One possible avenue is to take this surface water content to be in equilibrium with the atmosphere in an evaporation event or saturated during an infiltration event. However, these two assumptions would be extreme approximations and may unduly influence the solution. A more representative value of the topmost layer may be found by averaging the surface flux obtained by the method described in section 6.1.2 (by using the fictitious external point) and the above-mentioned extreme values. At the very first time iteration however, some estimate needs to be made of this surface water content as part of the initial conditions. Enforcing the initial field capacity initial condition mentioned above will provide a starting point. In reality, field measurement of the initial water profile by neutron probe would be necessary.

Special consideration needs to be given to the evaluation of this half-step water content at the last iteration, that is, when $i=N$. In both the methods of evaluating this water content, knowledge of the external (to the adjusted grid) point is required. When $j=1$, that is the first time level, the initial conditions need to include this external point and it needs updating with each time iteration. This should not be a problem at these lower depths as the water content would not change greatly with depth as it does in the uppermost layers. This leads to water contents numbering N+2 initially and a requirement that all N+2 be updated at the end of each time step.

6.1.6 The Finite Difference Equations - a Summary

The preceding discussion served to develop the finite difference equations and to emphasise any points of consequence to this application. The set of finite difference equations (6.31)-(6.36), are collated below in their entirety.

The depth steps are defined as $z_i = (i-\frac{1}{2})\Delta z$ and N depth steps are used.

For $2 \leq i \leq (N-1)$:

$$\begin{aligned} & D_{i-1/2}^{j+1/2}\theta_{i-1}^{j+1} - \left(D_{i-1/2}^{j+1/2} + D_{i+1/2}^{j+1/2} + A\right)\theta_i^{j+1} + D_{i+1/2}^{j+1/2}\theta_{i+1}^{j+1} \\ & = -D_{i-1/2}^{j+1/2}\theta_{i-1}^{j} + \left(D_{i-1/2}^{j+1/2} + D_{i+1/2}^{j+1/2} - A\right)\theta_i^{j} - D_{i+1/2}^{j+1/2}\theta_{i+1}^{j} \\ & \quad + 2\,\Delta z\left(K_{i+1/2}^{j+1/2} - K_{i-1/2}^{j+1/2}\right) + 2\,\Delta z^2 S_i^j \,, \end{aligned} \tag{6.31}$$

where $A = 2\Delta z^2/\Delta t$ and the finite discrete form of the sink term is given by:

$$S_i^j = \frac{-1.6\,T_j}{\left(v(\Delta t.j) - e_j\right)^2}\Delta z.(i-\tfrac{1}{2}) + \frac{\left(1.8\,v(\Delta t.j) - 0.2\,e_j\right)T_j}{\left(v(\Delta t.j) - e_j\right)^2} \,. \tag{6.32}$$

For $i = 1$ with an Evaporation event:

$$\begin{aligned} & -\left(D_{3/2}^{j+1/2} + A\right)\theta_1^{j+1} + D_{3/2}^{j+1/2}\theta_2^{j+1} \\ & = -D_{1/2}^{j+1/2}\theta_0^{j} + \left(D_{1/2}^{j+1/2} + D_{3/2}^{j+1/2} - A\right)\theta_1^{j} - D_{3/2}^{j+1/2}\theta_2^{j} \\ & \quad -D_{1/2}^{j+1/2}\Delta z\left(q_{1/2}^{j+1} - K_{1/2}^{j+1}\right)/D_{1/2}^{j+1} + 2\,\Delta z\left(K_{3/2}^{j+1/2} - K_{1/2}^{j+1/2}\right) \\ & \quad + 2\,\Delta z^2 S_1^j \,, \end{aligned} \tag{6.33}$$

where θ_0 at the jth timestep is as follows:

$$\theta_0^j = \theta_1^j + \frac{\Delta z}{D(\theta_{1/2}^j)}\left(q_{1/2}^j - K(\theta_{1/2}^j)\right). \tag{6.34}$$

For $i = 1$ with an Infiltration event:

$$\begin{aligned} & -\left(2D_{1/2}^{j+1/2} + D_{3/2}^{j+1/2} + A\right)\theta_1^{j+1} + D_{3/2}^{j+1/2}\theta_2^{j+1} \\ & = \left(2D_{1/2}^{j+1/2} + D_{3/2}^{j+1/2} - A\right)\theta_1^{j} - D_{3/2}^{j+1/2}\theta_2^{j} \\ & \quad + 2\,\Delta z\left(K_{3/2}^{j+1/2} - K_{1/2}^{j+1/2}\right) - 4D_{1/2}^{j+1/2}\theta_s \\ & \quad + 2\,\Delta z^2 S_1^j \,. \end{aligned} \tag{6.35}$$

For $i = N$:

$$
\begin{aligned}
& D_{N-1/2}^{j+1/2}\theta_{N-1}^{j+1} - \left(D_{N-1/2}^{j+1/2} + 2D_{N+1/2}^{j+1/2} + A\right)\theta_N^{j+1} \\
& \quad = -D_{N-1/2}^{j+1/2}\theta_{N-1}^{j} + \left(D_{N-1/2}^{j+1/2} + D_{N+1/2}^{j+1/2} - A\right)\theta_N^{j} - D_{N+1/2}^{j+1/2}\theta_{N+1}^{j} \\
& \qquad - 2D_{N+1/2}^{j+1/2}\theta_L^{j+1} + 2\,\Delta z\left(K_{N+1/2}^{j+1/2} - K_{N-1/2}^{j+1/2}\right) + 2\,\Delta z^2 S_N^{j} ,
\end{aligned}
\tag{6.36}
$$

where $\theta_{N+1}^{j} = 2\theta_L^{j} - \theta_N^{j}$.

This chapter presented and collated the main mathematical ideas behind the computer simulation. It has not explicitly outlined the algorithm for simulating the water movement. The next chapter considers this in detail and further describes details of the simulation as well as presenting results.

CHAPTER VII

THE COMPUTER SIMULATION

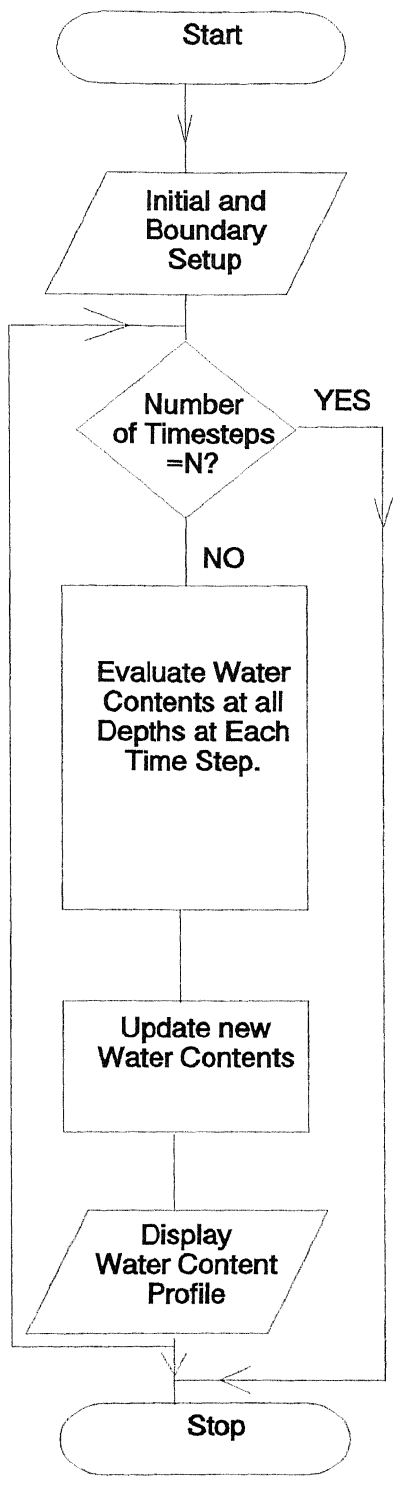
- PROGRAM DEVELOPMENT AND RESULTS

7.1 FROM ALGORITHM TO CODING

The method employed in the development of the full simulation was to simulate a series of evaporation events only, then simulate a series of infiltration events only and then merge the two together so that a choice would be given to the user to irrigate at the end of each "day" or not. In this way the program could simulate drying in the field and determine an appropriate time to irrigate. The simulation could then also be used to determine the effect of the new sink term.

The simulation was set up for a Silty Clay soil with the parameters from Clapp and Hornberger, 1978. The initial wetness profile was arbitrarily chosen and is given in the results section. To give the full effect of the sink term the root length was taken to be that of a mature plant (120 cms). The evapotranspiration profile for the simulation was taken to be values commensurate with the soil type and how readily it would give up water at the soil surface.

The algorithm within which the equations developed in Chapter VI were incorporated is shown in Diagram 7.1.



Load initial water content profiles, evapotrans. data and lower boundary profile. Set depth, depth stepsize, time of simulation, time stepsize and set evaporation front value to zero.

This procedure uses the finite difference equations in Chapter VI, i.e. (6.31), (6.33) and (6.36), to set up the coefficient and solution matrices to be solved. The water contents are first estimated half-way between known and unknown timesteps by a Taylors approximation.

A Triadiagonal matrix is set up at each timestep and the system is then solved using the Thomas Algorithm.

The solutions of the Thomas Algorithm form the new "days" water content profile. Also as the water contents are updated, the evaporation front is monitored and updated if necessary.

Diagram 7.1 Flow chart illustrating the algorithm for the solution of the flow equation incorporating the evaporative flux boundary condition.

In this case it is evident that the algorithm is straight forward and similarly the coding. As with the evaporation boundary condition program, the extended infiltration simulation posed no further problems other than the inherent mathematical difficulties of projecting forward in time and space in a highly non-linear system and the previously described question of overestimating irrigation with the top surface assumed at saturated water content.

7.2 THE FULL SIMULATION

It initially seems that to implement the full simulation of any combination of evaporation and infiltration events, that one would simply combine the two cases above with an opportunity after each "day" to switch irrigation on or off. If irrigation was switched on, for example, the set of FDE's for infiltration could be called instead of the evaporation set. A boolean variable could be used to **switch** between the two. This switching is equivalent to commencing either process with any possible profile and herein lies the problem.

It has already been established that, to develop FDE's using Crank-Nicolson, water contents projected a half time step forward and at half depth steps are required. This two step process then uses these θ's to form the sets of equations in finite difference form. Two methods for such projections were detailed in section 6.1.5 : the Geometric method and the Taylor's expansion method.

The geometric method requires a knowledge of the previous two days water contents to project forward in time. At least two problems arise with this method.

(1) During an extended evaporation event the fictitious above-ground water content becomes a very large negative as it is linearly projected upward in space and

this overly influences the projected θ at the surface. This does not occur with infiltration since the water content cannot exceed saturation in the soil profile hence any linear projection is at most vertical and would give an above ground value of saturation at most. Also,

(2) If an extended event is **switched** to the opposing event (several days of infiltration followed by evaporation, say), it is obvious that any projections from these previous values are in total contrast to the actual value, particularly at the surface. The projections would indicate wetting at the surface whereas in fact they would be drying in the case above.

Since the Taylor's Expansion method uses values on the previous time step only to project forward the extended history of the profile is not a problem but indeed the same shortcoming as in the geometric method is suffered to a similarly unworkable extent. For example if the initial profile was entirely saturated, and an evaporation event occurs, projecting forward from these values would be totally unreliable at the surface layers. Projecting from evaporation induced, drier values under an irrigation event is not a problem since it is assumed that the surface wets instantaneously to saturated water content and it is the surface projection the has room for greatest error. Taylor's method has another advantage over the Geometric method in that the forward/forward approximation (as detailed in Chapter VI), which draws its data from the firmer foothold of the less variable lower layers, is used at the surface.

So, if a trend can be ascertained from the previous day or two's data and that pattern is consistent with the current event then projecting forward using either method is quite feasible (except for extended evaporation using the Geometric method as described above). For example, if the previous two days indicate drying is taking place and the

current event is evaporation, then projecting forward geometrically or using Taylor's expansion will be operating in the "right" direction. However if the previous two days indicate a wetting of the profile and an evaporation event takes place then the half time step projection is invalid.

Clearly the switching times need to be monitored and no forward projection done from previous values at such times. However, with no projections at these times, the second order correctness fails since the premise for Crank-Nicolson centred difference is not adhered to, that is, to evaluate the dependent variable and all functions of it at the centre of the time interval, which is between j and $j+1$.

What is required in the practical sense is a reasonable approximation of water contents at some intermediate step into the future. How this is to be done becomes clear when considering the mathematics within its practical context.

The fundamental shortcoming in both methods is that in no place in projecting forward one half a time step is any allowance made for the surface condition. It is not until the actual Crank-Nicolson FDE's are used that the process would embody the boundary condition. Consider the two possible switching cases:

(a) evaporation→infiltration and

(b) infiltration→evaporation.

The first case, (a), is not a great problem since the critical area is the top surface and for infiltration this is assumed saturated and not projected. As a result the layers immediately below the surface are of greater concern as they are close enough to the surface to be effected by a surface event during the chosen time step. However if the soil is of a clay variety then these layers will be less effected. Sandy soils would pose

quite a different problem. Despite the soil, the top layers below the surface will soon be adjusted to be realistic after solving the Tridiagonal system the first time. Any forward projection after this would be best served by Taylor's method as it does not require the two previous days profiles. The lower layers of the profile are of much less concern as the surface condition has little immediate effect down the profile and projection can be done as usual.

The second case, (b), is where the major problem lies. How can realistic intermediate values be approximated if the effect of the boundary condition is not incorporated until the Tridiagonal set are formed? One possible solution is to monitor the switch, and do not project forward one half a step after the switch, but rather form and solve the Tridiagonal set using the present values of θ as a first approximation of the half time step projections (averaged in depth to provide half depth step values). In this manner the effects of the surface conditions are imposed and the new profile formed, which incorporates the effects of evaporation as well as gravity *and* sink effects. A second approximation of the half-step forward projected profile is accomplished by averaging the present water contents with the water contents projected forward as described above, that is, averaging the known values at j with the provisional $j+1$ set. The Tridiagonal set is formed again and solved and it is this solution profile that now forms the basis of further approximation using the standard methods. After the switch has occurred however, the usual projection forward is continued until the next switch. Taylor's method is preferred here also due to the problem mentioned above in approximating the extended evaporation events using the geometric method.

The algorithm for the full simulation resulting from this discussion is shown below in Diagram 7.2.

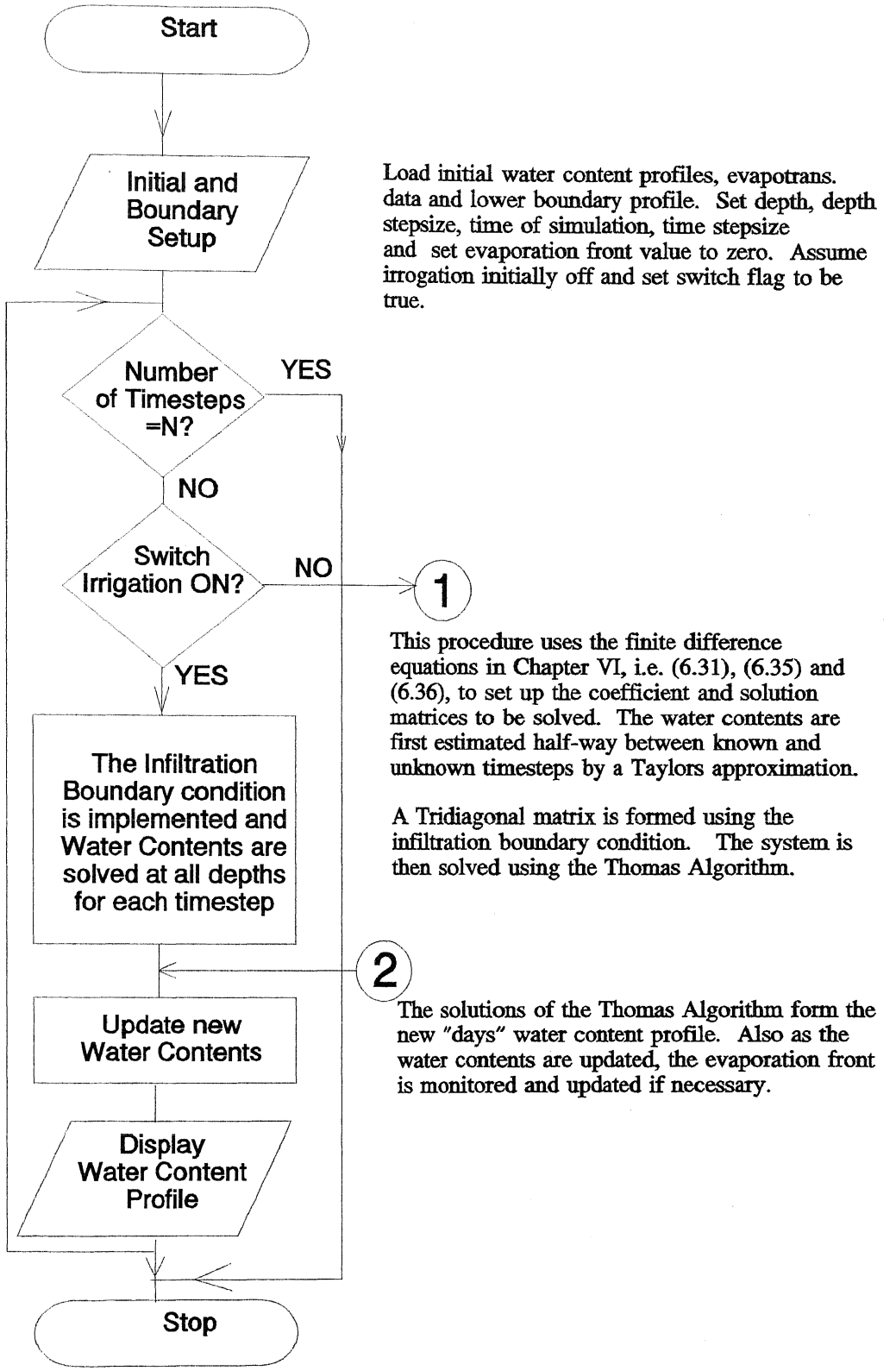


Diagram 7.2 Flow diagram indicating the algorithm for the full simulation including switching on or off irrigation.

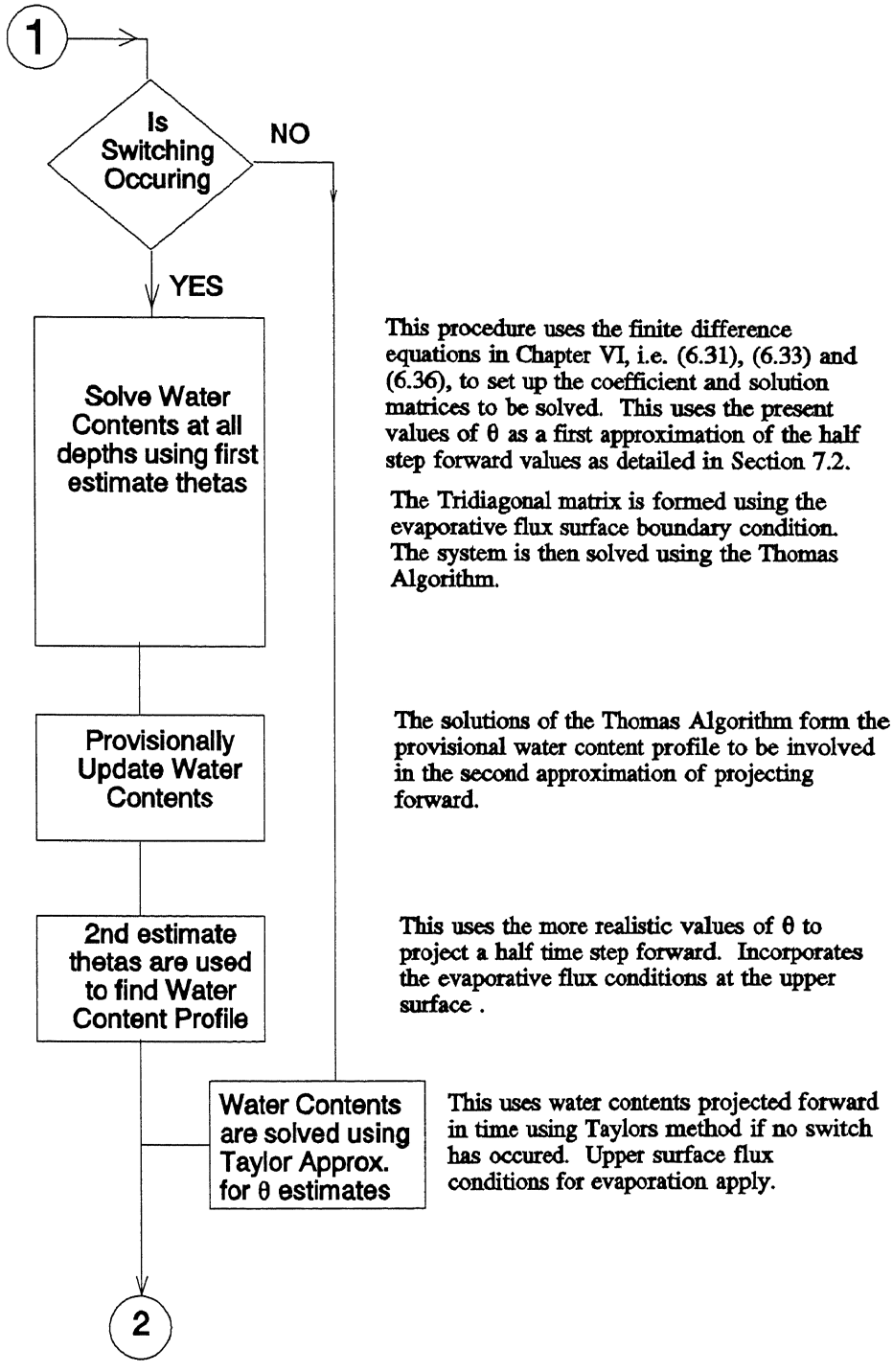


Diagram 7.2 *Continued* Flow diagram indicating the algorithm for the full simulation including switching on or off irrigation.

The entire program listing is in Appendix C.

7.3 RUNNING THE SIMULATION - RESULTS

The full simulation program allows for the simulation of a wide range of events. Events that are of interest here involve examining the sequence of soil water profiles over time of

- Uncropped soil with
  - (a) No surface evaporation - Redistribution only and,
  - (b) Simultaneous surface evaporation and redistribution.
- Cropped Soil with
  - (a) No surface evaporation or infiltration - Redistribution and Transpiration only,
  - (b) Extended surface evaporation, redistribution and transpiration with no infiltration,
  - (c) Comparison of the sink term developed in Chapter V with the sink term of Molz and Remson also detailed in Chapter V,
  - (d) Extended infiltration including all other processes, and
  - (e) Switching between infiltration and evaporation events.
- Interrelatedness of processes;
  - (a) The effect of Evaporation on Redistribution and
  - (b) The effect of the sink term.

In each of the simulations below the lower boundary condition will be considered to be known water contents for the duration of the run of 18 days. The lower profile will be fairly dry in keeping with no water table near the surface. Unless stated otherwise, all simulations use the parameters and input data now listed.

Clapp and Hornberger soil parameters:

$$\Psi_s = 17.40 \text{ cm}, \qquad \theta_s = 0.492 \text{ cm}^3/\text{cm}^3,$$

$\theta_{critical}$ = 0.210 cm³/cm³, K_s = 8.928 cm/day,

and b = 10.400.

The Initial Profile was:

Depth (cms)	0	4	12	20	28	36	44	52	60	68	76	84
θ (cm³/cm³)	0.345	0.340	0.328	0.320	0.325	0.340	0.338	0.310	0.284	0.277	0.280	0.284
Depth (cms)	92	100	108	116	124	132	140	148	156	164	172	180
θ (cm³/cm³)	0.295	0.304	0.297	0.265	0.258	0.249	0.240	0.232	0.224	0.216	0.208	0.201

The Evapotranspiration Data are as follows:

Day	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Total Evapotrans. (mm d^{-1})	7.2	7.2	7.2	7.2	7.7	7.7	6.8	6.8	5.9	5.9	5.9	5.0	5.0	5.0	5.0	3.8	3.8	3.8	3.8
E_{soil} (mm d^{-1})	1.6	1.6	1.6	1.6	1.6	1.6	1.1	1.1	0.9	0.9	0.9	0.7	0.7	0.7	0.7	0.5	0.5	0.5	0.5
Transpiration (mm d^{-1})	5.7	5.7	5.7	5.7	6.1	6.1	5.7	5.7	5.0	5.0	5.0	4.2	4.2	4.2	4.2	3.3	3.3	3.3	3.3

The water content distribution of the 18 day period at the lower bound, that is, at 184 cm, was held at 0.197 cm³/cm³.

It is to be noted that in all profile diagrams that follow, the numeric data has been omitted for clarity as the trends will be more evident. All corresponding numeric data is tabulated in Appendix D. Furthermore, on the point of readability of the profiles,

all data points were connected else the profiles are lost in the clutteredness of points and symbols. This was further made necessary by the fact that successive profiles needed to be overlayed to permit changes to be observed. This interpolation is clearly an approximation only but the advantages of clarity outweigh this problem.

A series of numerical accuracy trials were conducted to determine appropriate time and depth steps. The implementation of the Crank-Nicolson method as applied to this situation was run with an arbitrary initial timestep which was subsequently halved in each successive run until a suitable degree of accuracy was obtained. The depth step was held constant throughout this process. It was found that a Δt of 1 'day' provided accuracy to two decimal places. Further, it was found that a timestep of 1/8 day would be required for accuracy of three decimal places. A similar process was carried out on the depthstep. The procedure deviated from the halving process since the modified grid necessitated the use of depthsteps that provided solutions to water content at the same depths. This led to the use of depthsteps of $10/(2n+1)$, $n= 0,1,2,\ldots$. A depth step of 10 cm provided two decimal place accuracy. It was established that a depthstep of 2 centimetres gave four decimal place accuracy. Two decimal place accuracy was considered sufficient for this instance as it provided a balance between excessive computer time and sufficient accuracy to reveal trends and consider the effect of the sink term. Furthermore, fine depth and timesteps would require large amounts of input data such as a refined initial water content profiles and greatly detailed evapotranspiration data.

As a result of these trials the Time increment was chosen as 1 day and the depth increment, 8 centimetres.

7.3.1 Uncropped Soils

In the case of uncropped soils the processes effecting the movement of soil water are those of gravity, other soil potentials and evaporation at the soil surface. With no roots permeating the soil profile the sink term is equated to zero. Consider the following two simulation cases for uncropped soils.

(a) No Surface Evaporation

This may occur when the upper surface is mulched or as in the experiments of Gardner, Hillel and Benyamini, (1970a), covered with sheets of polyethylene. The only process occurring here is redistribution. Changes to the simulation program are minimal with each call to the Sink function equated to zero and the soil evaporation data, which is read from a text file, overwritten with zeroes. The results of the 18 day run are illustrated in Figure 7.1a. On the scale used by Figure 7.1a it is evident that very little redistribution has taken place as would be expected in a soil with parameters for that of clay as used in the simulation.

To provide a more detailed view of the profiles the axes were expanded and adjusted so that the range of the water content scale was 0.265 cm^3/cm^3 to 0.345 cm^3/cm^3 as shown in Figure 7.1b. It can be seen here that the initial profile on day 0 is soon "straightened" out under the influence of soil-water potentials. Qualitatively, it is clear that no great amount of water is removed from the soil in the zone under consideration as the initially wetter zone at about 40cm depth progressively becomes drier and the initially drier zone at about 70cm progressively wets.

The profiles qualitatively resemble those of Gardner, Hillel and Benyamini, (1970a), (page 856). Indeed, very little redistribution occurs between profiles on the third and

18th days.

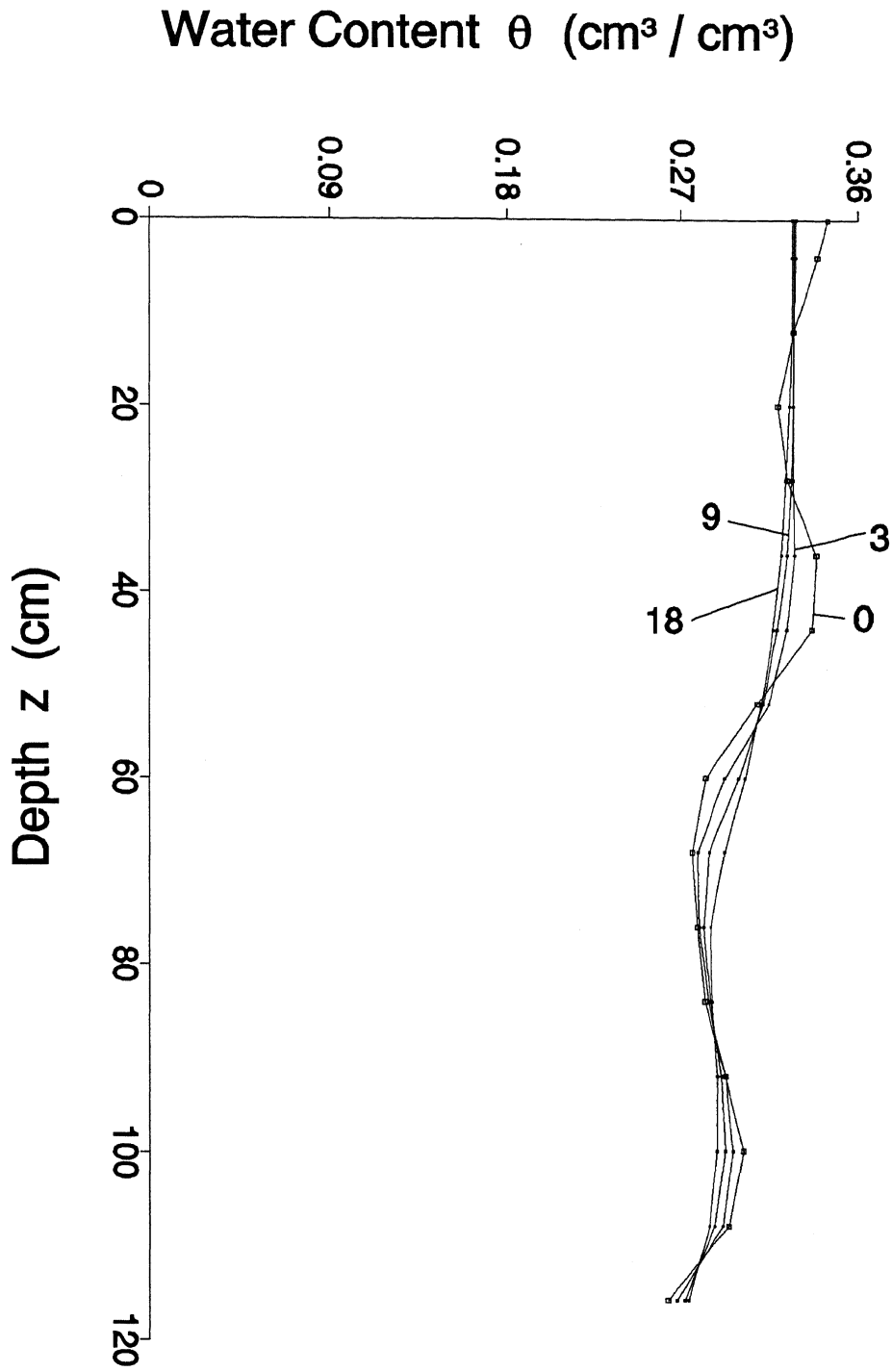


Figure 7.1a Soil water profiles after 3,9 and 18 days from the initial profile (day 0) for an uncropped soil with no surface flux.

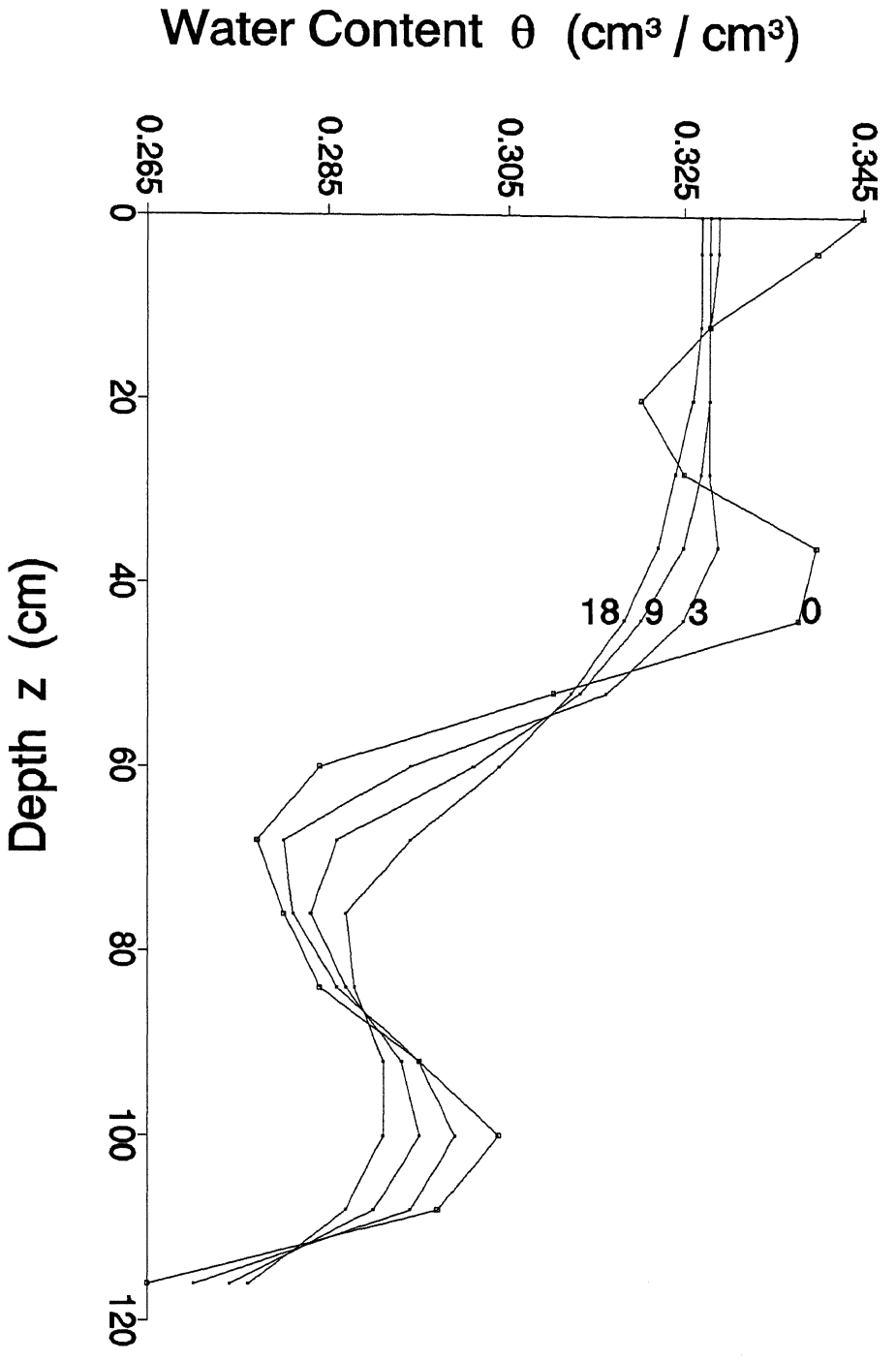


Figure 7.1b Soil water profiles after 3, 9 and 18 days from the initial profile (day 0) for an uncropped soil with no surface flux. The water content scale has been enlarged to show greater detail than Figure 7.1a.

(b) Simultaneous Evaporation and Redistribution

Once again the sink term is equated to zero to simulate uncropped soil. This time evaporation from the soil surface is permitted. Figure 7.2 shows profiles after 3, 10 and 18 days from the initial profile. The surface flux has clearly led to the surface drying out progressively until the 18th day where the very top layers of soil are air dry. Below this depth (about 12 cms), the profiles do not change markedly from the initial profile as it would be expected with no extraction by roots.

Once again there is a qualitative resemblance between these profiles and those of Gardner, Hillel and Benyamini, (1970b), (page 1149).

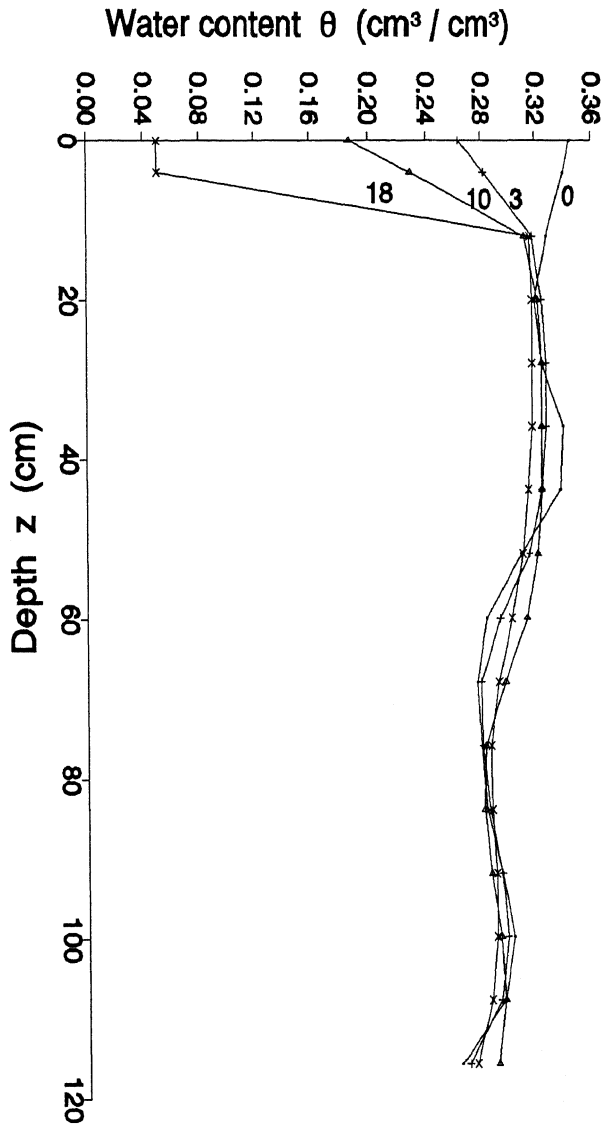


Figure 7.2 Soil water profiles after 3, 10 and 18 days of soil surface evaporation in an uncropped soil. The initial profile is labelled day 0.

7.3.2 Cropped Soil Simulations

In this case the sink term is reinstated to represent the withdrawal of water from the soil profile due to the roots. In the following simulations a mature root system with rooting depth 120 cms is considered to permeate the soil profile. Below this depth there will be no uptake of water due to roots. The evaporation front concept will be incorporated in the simulations.

(a) No Surface Flux

As in the corresponding simulation for uncropped soil, the surface may be mulched or in some other way covered so as to prevent soil surface evaporation. Furthermore this simulation requires no infiltration to occur either. This will permit the combined effects of redistribution and water uptake by roots to be examined. The successive profiles over the 18 day period are shown in Figure 7.3. It can be seen that drying occurs at proportionately lesser levels as deeper layers are reached. This is consistent with the 40:30:20:10 ratio of water extraction for successively lower quarters of the root zone as embodied in the sink term. With no surface flux the upper layers show no conspicuous increase or decrease in water content than that due to water uptake.

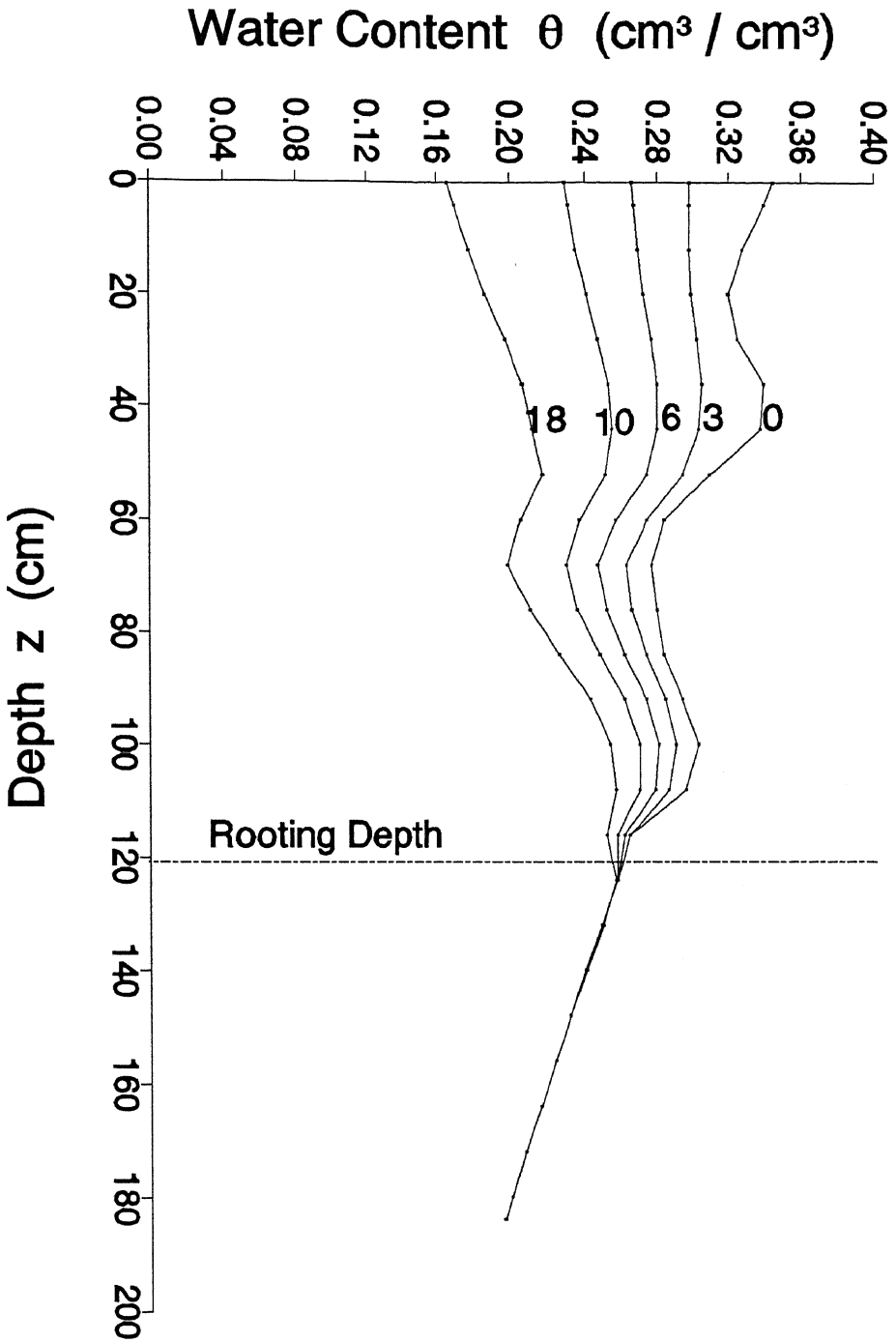


Figure 7.3 Soil water profiles after 3, 6, 10 and 18 days in a cropped soil with no evaporation or infiltration at the surface. The initial profile is labelled day 0.

(b) Extended Evaporation Event

No infiltration was allowed at the soil surface and so only the surface evaporation equations (6.31) to (6.34) were be used. It is to be recalled from section 1.2 that the conventional view to irrigation scheduling is basically to top up the water content of the root zone to a certain level after that zone has "lost" a volume of water determined by evapotranspiration to a level where the plant begins to 'struggle' in its process of absorbing water. The question arises, "is it possible that the amount of water supplied, whilst in terms of averages restores the entire root zone to field capacity, but does indeed leave parts of the profile very wet and other parts very dry"? In this simulation the drying cycle for a crop is considered with the aim of gaining insights as to where does the water distribute itself and when to irrigate.

The representative profiles from 18 days of drying are shown in Figure 7.4a. The combination of root uptake and surface evaporation at the surface leads to significant drying in the top layers. Figure 7.4b enlarges the top layers to show this more clearly. The linear interpolation approximations are evident in Figure 7.4b but even with a smooth curve drawn through the points the outcome would show the same trend in terms of the deepening *evaporation front.* In this case the evaporation front is delineated by the 0.210 cm^3/cm^3 water content which represents the lower limit at which the plant can absorb water from this type of soil without being subject to stress. From Figure 7.4b, after 18 days of drying, the top 21cm of the soil profile is below the critical water content for water uptake in that soil after 18 days of drying. This represents about 18% of the rooting depth which, under the 40:30:20:10 rule of thumb would usually supply about 30% of uptake demands. With this top section effectively dry, the rest of the root zone needs to compensate. If there is a depth of drying beyond which the rest of the root zone cannot effectively compensate, then the plant

and crop will suffer. As will be elaborated later this lowering of the *evaporation front* may form a criterion for irrigation scheduling.

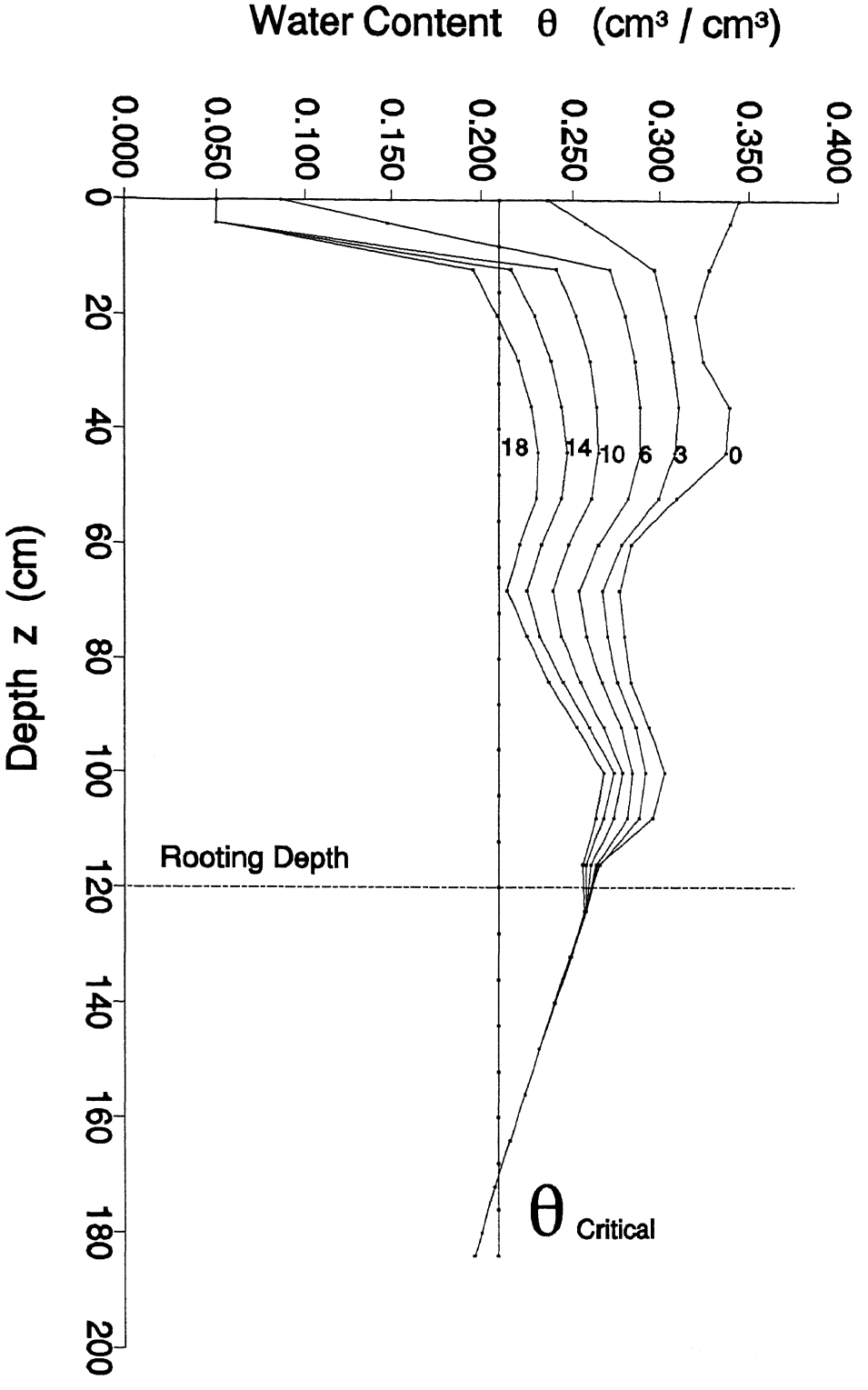


Figure 7.4a Soil water profiles from the initial profile (Day 0) to Day 18, under an extended evaporation event in cropped soil, as generated by the Full Simulation program of section 7.2.

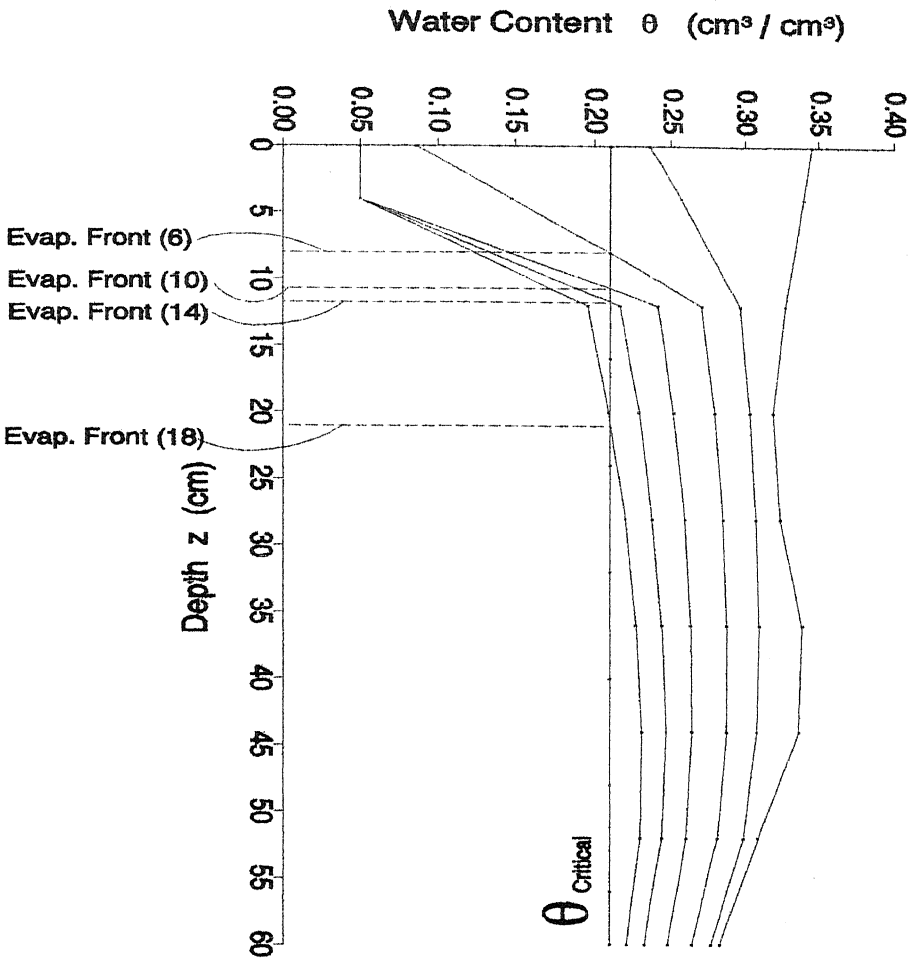


Figure 7.4b Macroscopic view of the top 60cms of the drying profiles in Figure 7.4. The evaporation front moves down as the profile dries.

(c) Comparison of Sink Terms

It was stated in section 5.1.2 that the sink term described in Molz and Remson, (1970) failed when the upper layers dried. This was the premise on which the development of the new sink term incorporating the 'evaporation front' was based. During the extended evaporation event of the previous simulation, the surface layers indeed did dry below the critical water content for extraction by roots. Since a fair proportion of the roots are located in these dry areas, the original sink must fail as the top quarter of the

root system could not then supply the requirement dictated by the original sink term (40%). Indeed, if the simulation in (b) reflects the real situation, the top 21cm of the soil profile is below the critical water content for water uptake in that soil. This represents about 18% of the rooting depth which, under the Molz and Remson model would need to supply 30% of extraction requirements. This clearly indicates the model deficiency. It is to be noted that in the earlier simulation the evapotranspiration data was not great and reduced with time. The drying situation would be increased if the evapotranspiration demands were increased further. For the simulation comparing sink terms the following data was used: Total evapotranspiration was kept at 9.2 mm/day, evaporation from the soil was 3.7 mm/day and the transpiration rate was maintained at 5.5 mm/day for the time of the run. These represent increases from the original data given in earlier this section.

Figure 7.5 illustrates the difference between the two sink terms after extraction for 18 days. With the increased evapotranspiration the *evaporation front* has deepened considerably. The effect of this has not been represented realistically by the Molz and Remson sink but the term incorporating the evaporation front reveals that as the front deepens the water extraction proportions are met deeper down the root system and subsequently altering the entire profile. With more water required to be taken up by deeper roots the lower layers are drier than those using the Molz and Remson term. With the Molz and Remson term failing here, the question is "Does the new sink term more closely represent reality"? Clearly the simulation assumes evapotranspiration is occurring at its potential rate yet as the evaporation front deepens there is no mechanism to consequently reduce evapotranspiration. As the plant stresses this rate would reduce - and the new model would eventually fail completely as it tries to extract

the same volume of water from smaller and smaller zones. However under the assumption that the regime for irrigation is optimal, (in terms of supplying abundant water as not to cause plant stress) the extent of drying leading to model failure will not be reached as an irrigation event will be scheduled before such time. If the model does approximately correspond to the situation in the field then the evaporation front in this case will have deepened to about 50cm and the remaining 60% of the root zone would be required to absorb the full complement of water.

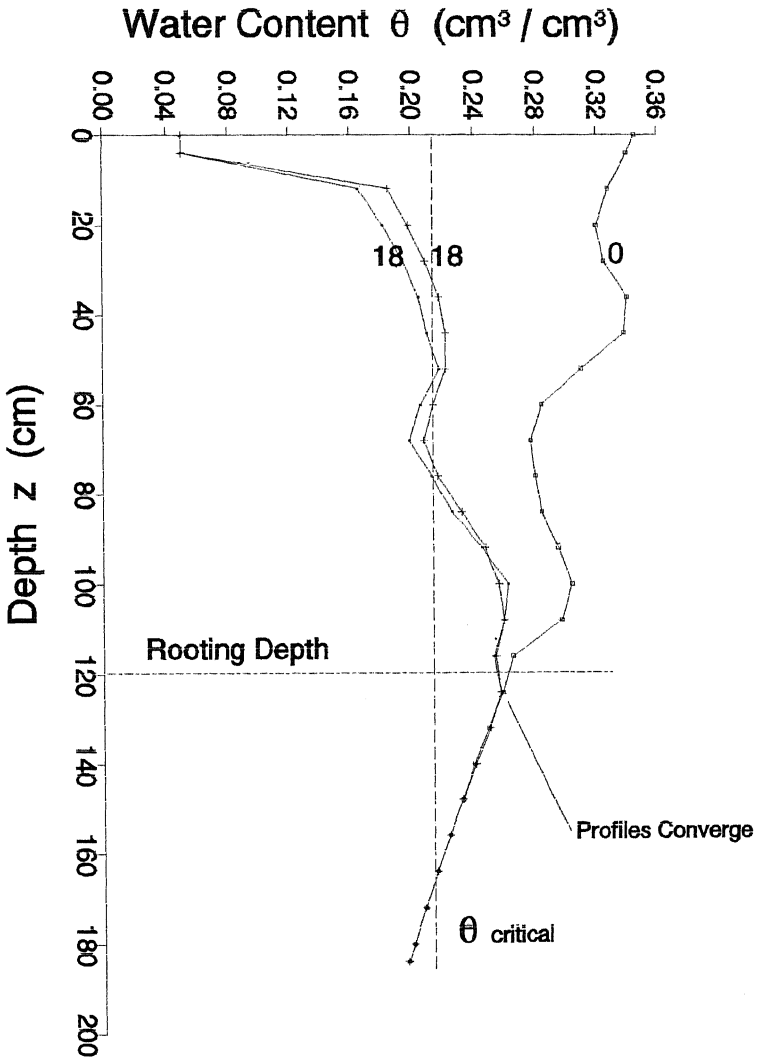


Figure 7.5 Soil water profiles comparing the sink term of Molz and Remson (1970) as indicated by the crosses (+), and the sink term incorporating the evaporation front after 18 days of evapotranspiration.

(d) Extended Infiltration

This simulation represents the case of irrigation or precipitation. The set of equations employed here are (6.31), (6.32), (6.35) and (6.36) where the surface is assumed to instantaneously reach saturation during infiltration. The profile after one day of such infiltration is given in Figure 7.6a. The next two days of continuous infiltration are shown in Figure 7.6b. As described in the literature the wetting front descends whilst the deeper layers are virtually unaffected.

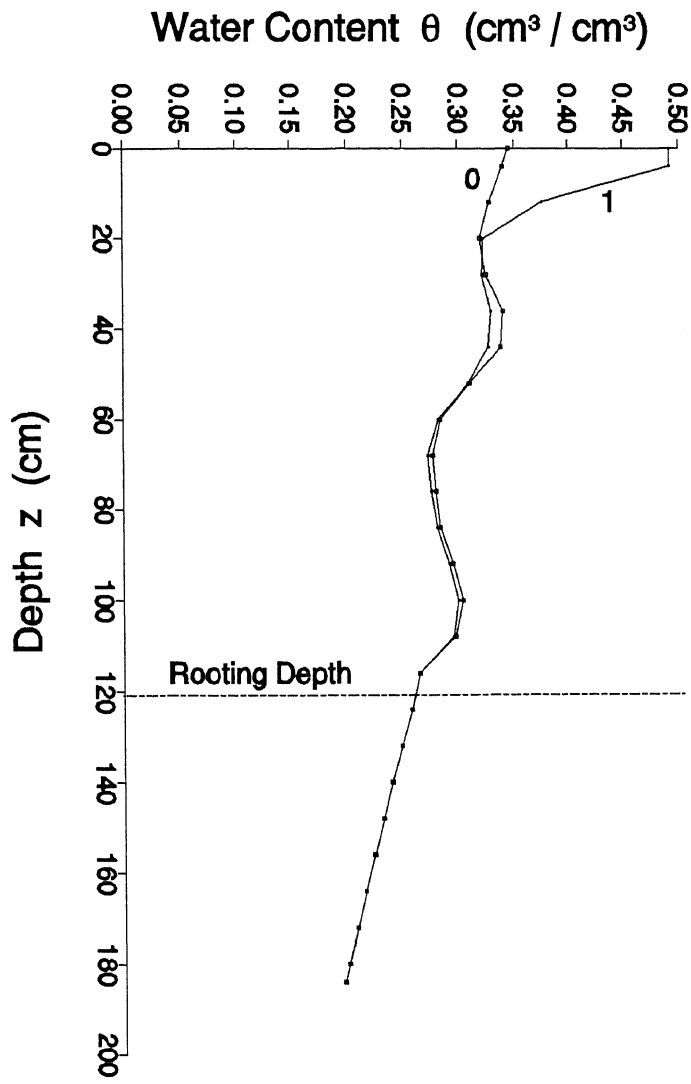


Figure 7.6a Water Content profile after one day of infiltration from the initial profile (day 0).

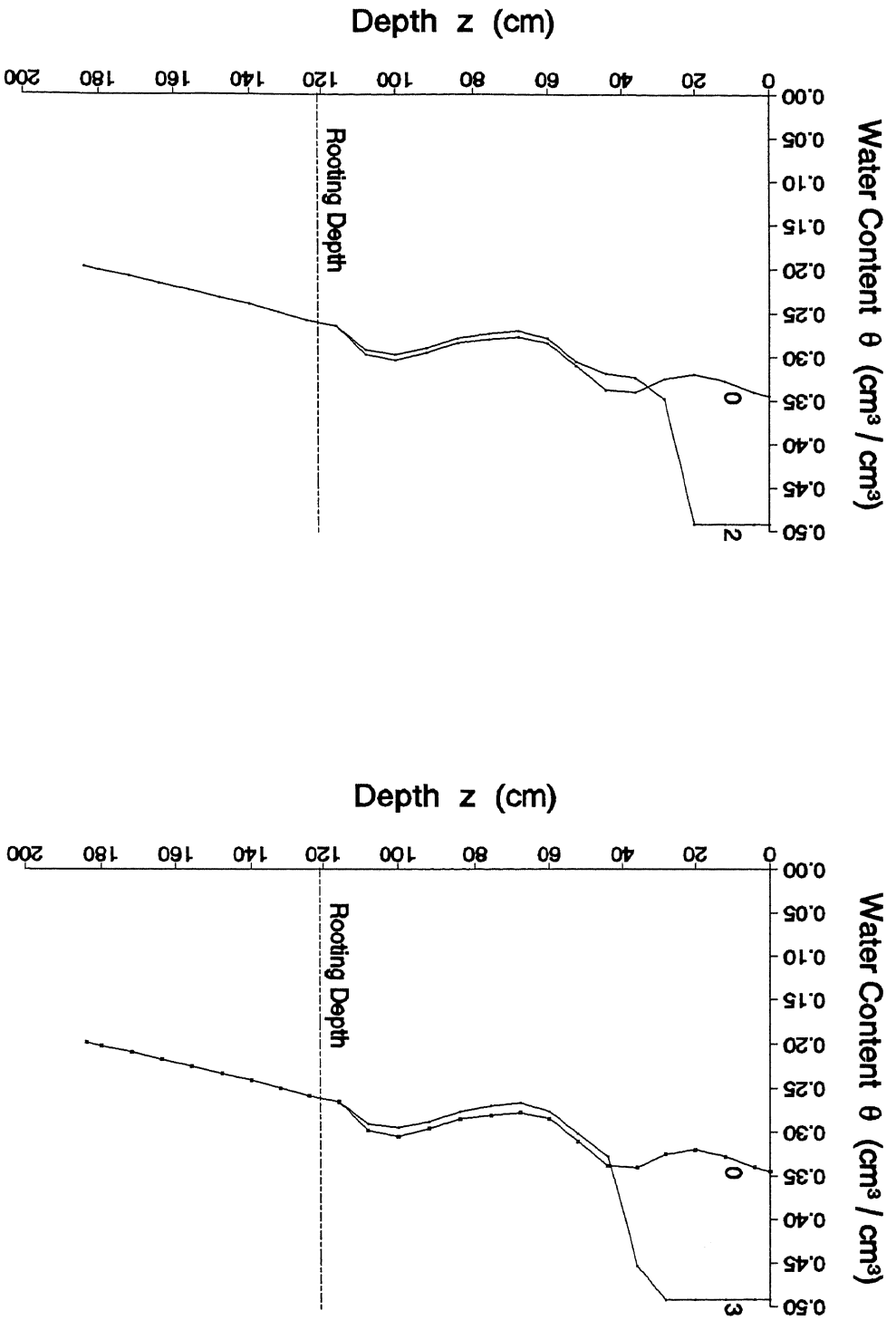


Figure 7.6b Profiles of the second and third successive days of continued maximum infiltration.

(e) Switching Between Evaporation and Infiltration Events

This is the full simulation of the field situation whereby a crop is permitted to dry for a period of time followed by an infiltration event for a certain time followed by another drying period and so on. The simulation that follows will simply illustrate the capability of the simulation program to switch between evaporation and infiltration and vice-versa. This is shown in Figures 7.7a, 7.7b,7.7c and 7.7d.

Consider Figure 7.7a, whereby four days of drying occur from the initial profile until irrigation is switched on. With infiltration occurring all day five, a wetting front forms and begins to deepen.

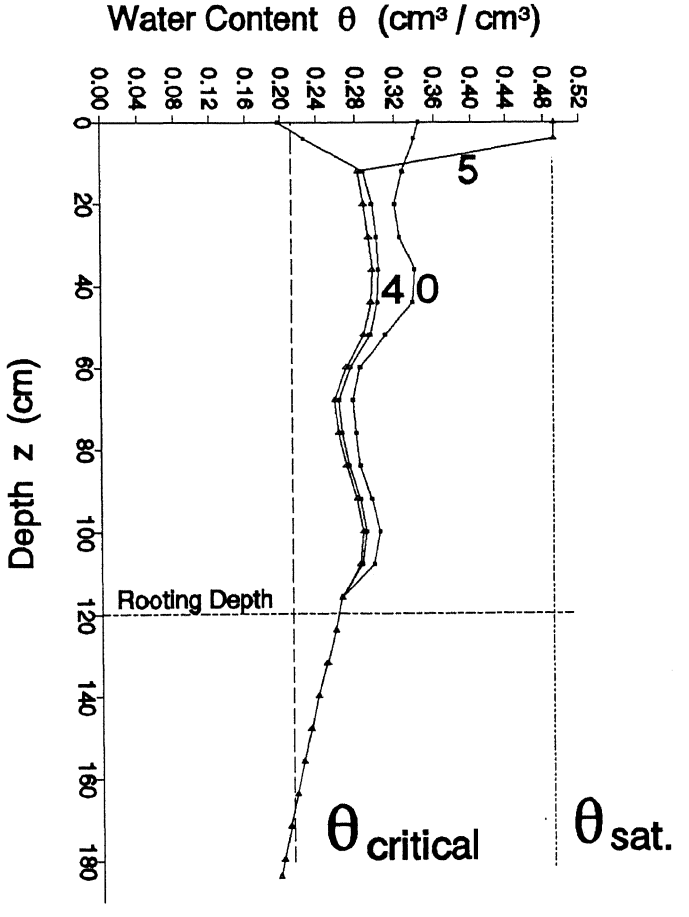


Figure 7.7a Water profiles of a soil subjected to four days drying from an initial distribution (day 0) to the drier day 4 profile. The day 5 profile is a result of constant maximum infiltration for one day.

Figure 7.7b shows the situation if infiltration was maintained at the maximal rate for days five, six and seven. The wetting front continues to deepen and the zone of saturation has reached a depth of over 20cm from the surface. Despite this it is seen that the effect of the root uptake is still evident lower in the profile as extraction continues to take place. In this simulation the infiltration event ceased after day seven and evaporation began.

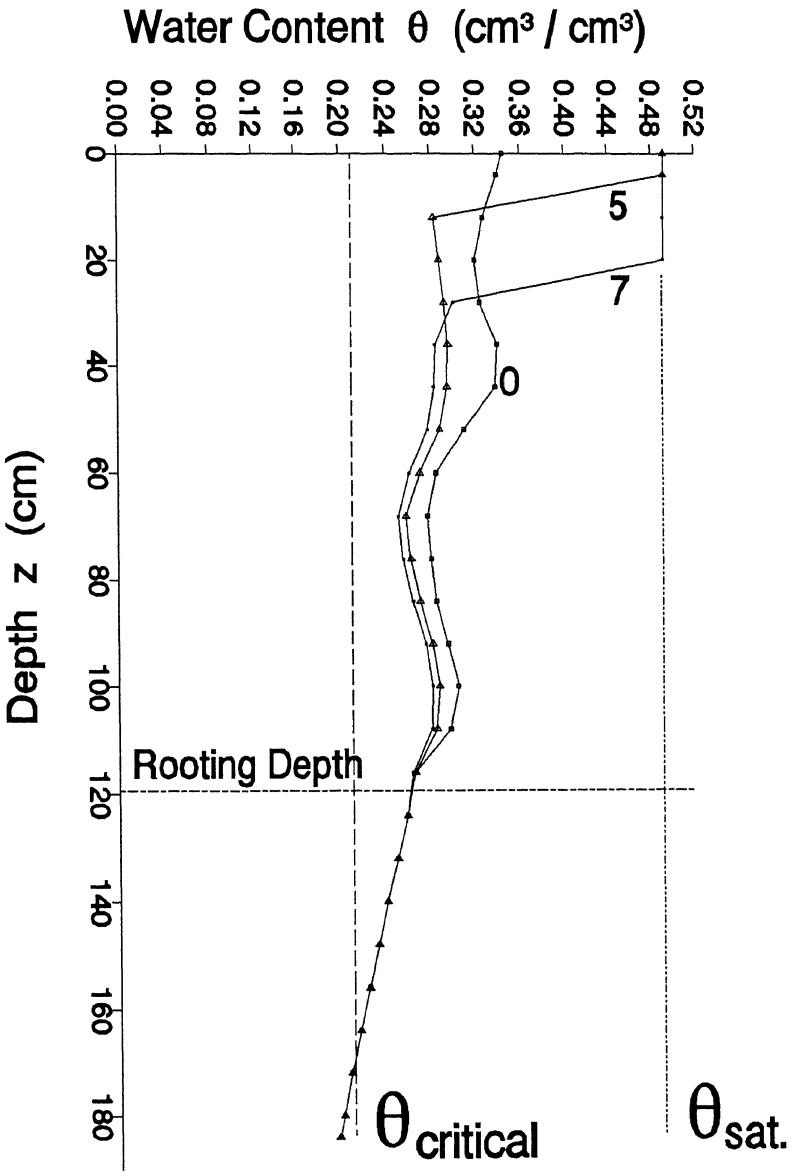


Figure 7.7b Soil water profiles of the same situation in Figure 7.7a but showing the profile on the seventh day, after three days of maximum infiltration.

Figure 7.7c shows the day eight profile where one full day of evapotranspiration has occurred. A wetting front continues down to about 40cm yet the effect of surface evaporation causes drying at the surface.

Evaporation continues for the next ten days with Figure 7.7d illustrating the drying sequence. The wetting front becomes less defined and the surface layers continue to dry. The profiles 'smooth' out as would be expected as redistribution takes place.

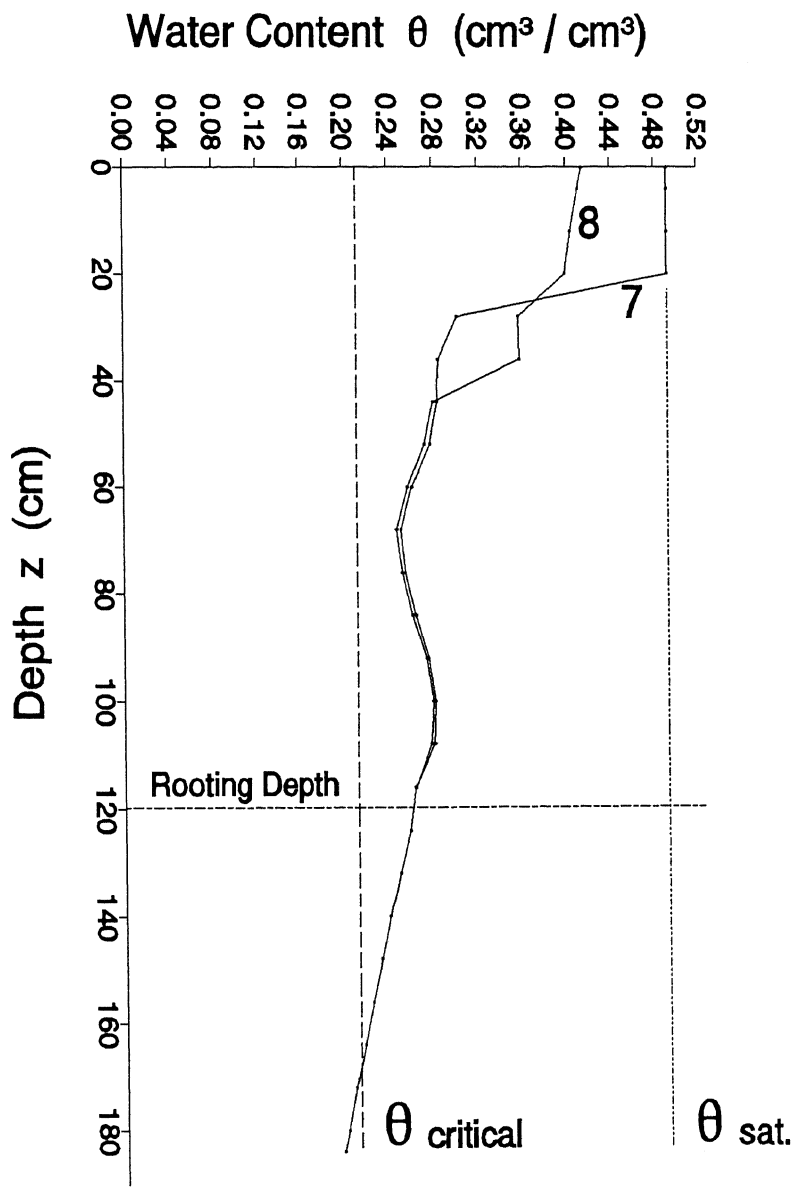


Figure 7.7c Soil water profiles of day 7 (the third and final day of irrigation) and day 8 which is after a complete day of drying.

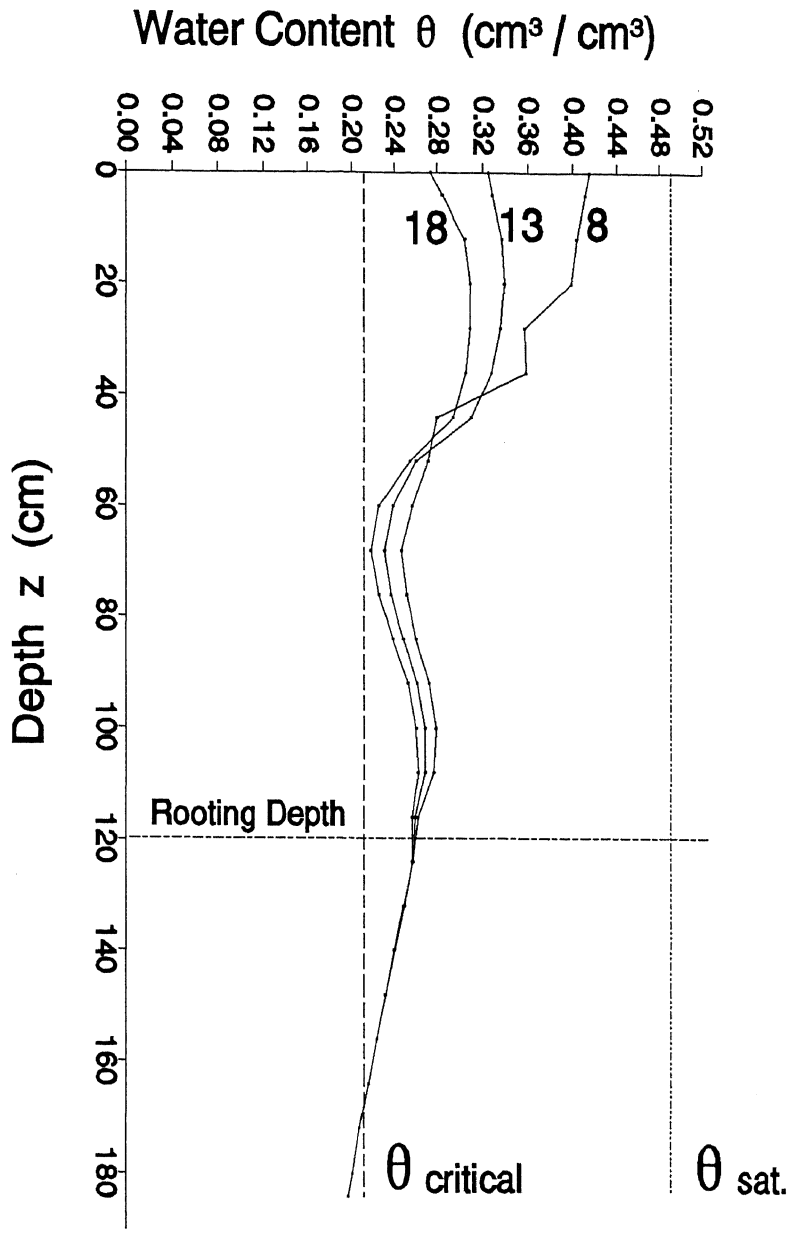


Figure 7.7d The drying sequence on days 8, 13 and 18 which represent one, six and eleven days of drying respectively after three days of maximum infiltration.

It still appears that the effect of this infiltration has not been evident below about 60cm as these layers continue to dry in response to transpiration. This is borne out if Figure 7.7d is compared to 7.4a where there was no infiltration. Both profiles are in close proximity to the critical water content line at about the 60cm depth. The effect of the infiltration has, however, strongly influenced the shape of the profile above this level.

7.3.3 Interrelatedness of Processes

The Effect of Evaporation on Redistribution.

The purpose of this simulation was to run an extended evaporation event (surface flux) in an uncropped soil and allow redistribution and then to run the same situation but with no surface flux thus controlling variables and allow a statement to be made about the effect of surface evaporation on redistribution. It may be thought that as soil evaporation reduces the water available for redistribution, then it may strongly effect that process.

Figure 7.8 shows the two profiles described after 18 days relative to the initial profile. Whilst the top layers have dried in the simulation with surface flux, there is little if no difference in the redistribution pattern between this and the profile with no surface flux. This conclusions of this simulation therefore agree with the findings of Gardner, Hillel and Benyamini, (1970b) who found experimentally that evaporation had little effect on drainage.

The Effect of the Sink Term

The effect of the sink term was isolated by comparing a simulation with surface flux and water uptake forced to zero with a simulation where only surface flux was zero and the sink term functioning. For comparison purposes the 18th day profile of redistribution only (zero sink) was superimposed on the graph in Figure 7.9. The simulation of the effect of the sink term and no surface flux was also run for 18 days.

It is clear that the sink term has a great influence on the profile and as expected, the top layers were proportionately drier than the lower layers where root density was less.

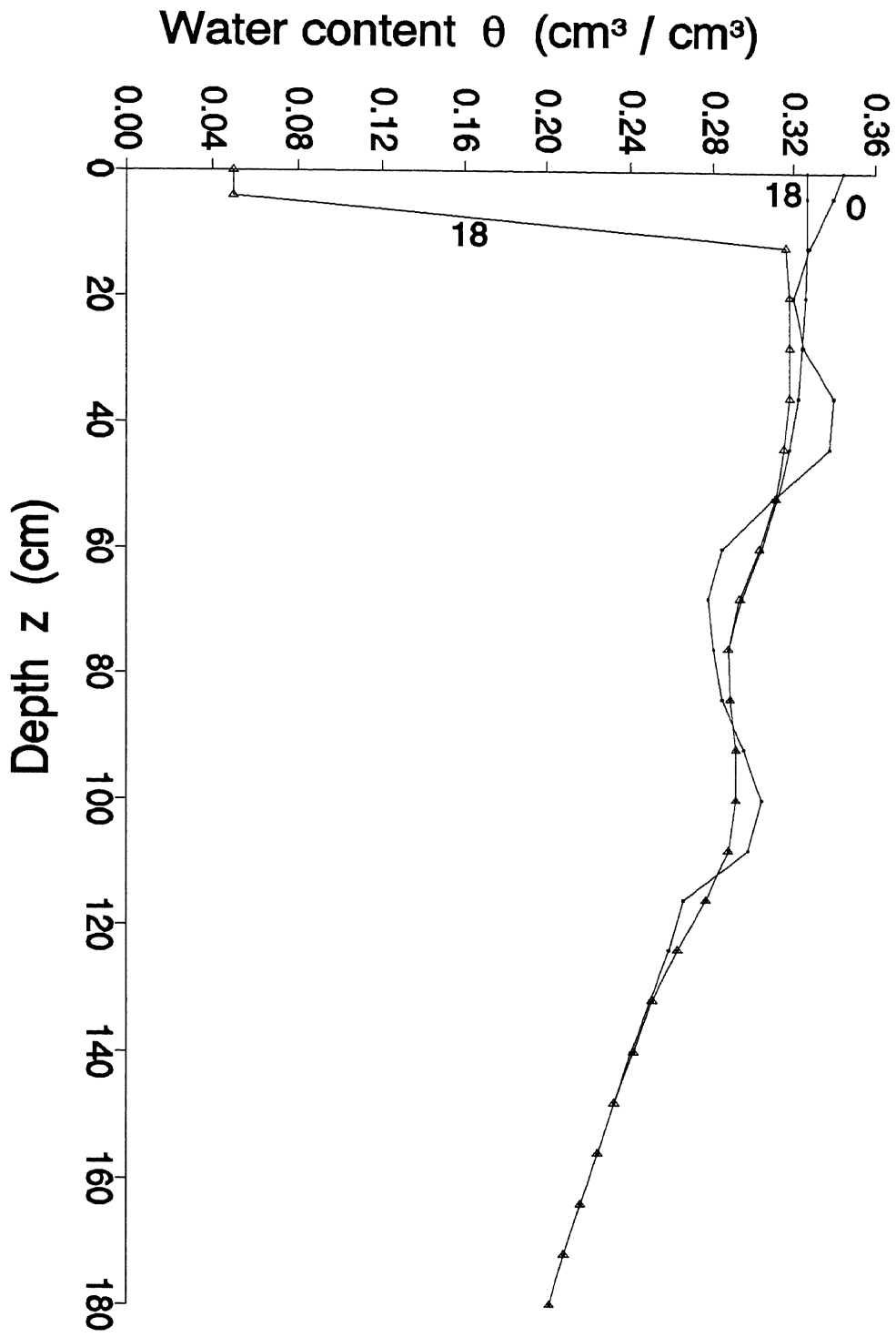


Figure 7.8 Soil water profiles comparing the effect of surface evaporation on redistribution. The initial profile (day 0) and the 18th day profiles for redistribution with and without surface evaporation are shown.

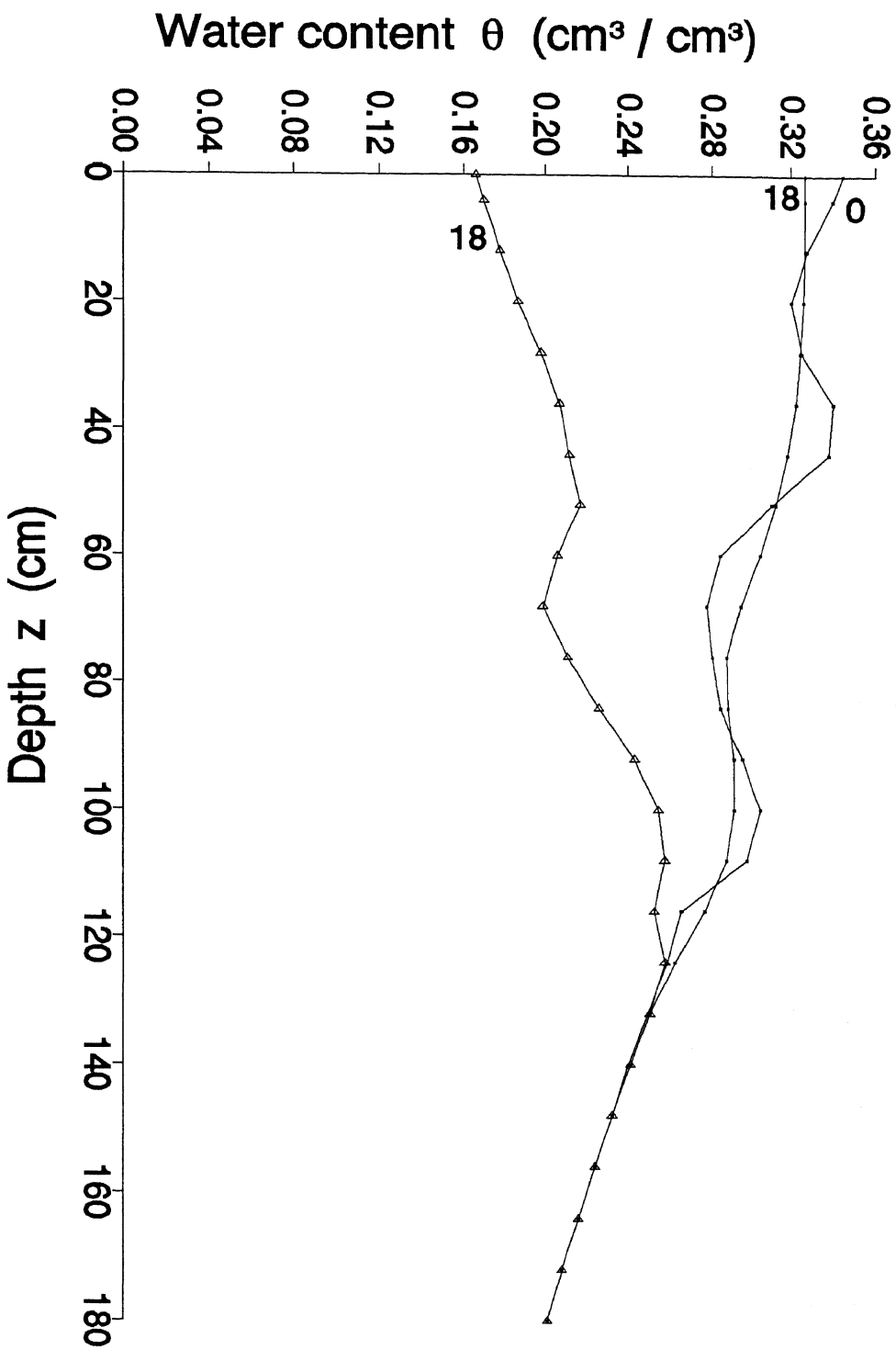


Figure 7.9 Water profiles illustrating the effect of the sink term. Both the profile resulting from the effect of the sink and the profile of redistribution only are calculated 18 days from the initial profile.

7.4 CONCLUSIONS

7.4.1 Scope for Simulations

The previous simulations demonstrate the wide variety of situations that may be investigated with such a mathematical model and computer solution. This simulation may be easily modified to encompass an even broader category of problem. Several enhancements would be:

- allowance for a growing root system,
- presence of a water table and
- provision for movement of Nitrates.

The growing root system is already built into the program in Appendix C. In the case of all the simulations in this chapter the stationary root system was used. This was because no satisfactory root growth model other than that of constant root growth could be found. For any root growth model it would simply be a matter of calling the Root Length function to return a rooting depth to the Sink term to utilise.

The presence of a high water table may be represented by a different set of lower bound water contents. In the simulations above, all lower bound values were relatively dry indicating a deep water table. If the lower bound water contents for the duration of the run was taken to be that of saturated water content for the soil under simulation and at an appropriate depth, this would represent a high water table.

The chromatographic theory of Dayananda et al., (1980), could be incorporated where the soluble ions could move with the pulsing saturated wetting front, thus building a model for the distribution of such soluble ions. This may form the basis for the control of leaching of such ions from the root system. Similarly it may provide some insight into the salinisation problem, in terms of the downward and upward movement of such

ions with the water movement.

It is acknowledged that the mathematical model has not been field tested and this may form the basis of further investigation to verify the model. The flow equation and the method employed for solution provide reasonable results in terms of trends that are comparable to the experimental findings of Gardner, Hillel and Benyamini, (1970a) and also the findings by the same authors in their second paper (Gardner, Hillel and Benyamini, (1970b).

Further support for the model comes from the fact that the initial profile, evapotranspiration data and soil parameters were loosely based on the experiment by Olsson and Rose (1988). The initial profile was taken from the graphical data of that paper, the evapotranspiration data was given and the soil type was of a layered variety. From the description given, Clapp and Hornberger soil parameters were chosen as to represent an 'average' of the layer types. Whereas the Olsson and Roses profile consisted of 16.5 cm of sandy loam over 43.5 cm of 54% clay soil which in turn overlayed a 40% clay soil until a depth of 150 cm, the soil parameters were chosen for a Silty clay with a 49% fraction of clay. It was found that after simulating that situation for the same 18 day duration with a depth step of four centimetres, the shape of the two final profiles was generally the same with the only difference being that the contours were not as accentuated. Figure 7.10 shows the comparison after 18 time steps. The evapotranspiration data employed as the surface flux condition was that which was calculated in the paper of Olsson and Rose and was noted to reduce in magnitude with the drying of the surface layers. The lower boundary condition was considered to be a known water content distribution taken from the graph on page 93 of Olsson and Rose. The departure of the simulated profile from the actual profile at

about 20 cms could be attributed to the nature of the heavier clay layer from 16.5 cm to 43.5 cm whereby redistribution is retarded due to attraction of water molecules to the clay particles. Furthermore, the 'humps' in the original Olsson and Rose profile resulted from the layers in the soil whereas the averaging of soil types in the simulation could not match this layering effect. Given the approximation in soil types, the similarity was extremely encouraging. The numerical data is tabulated in Appendix D.

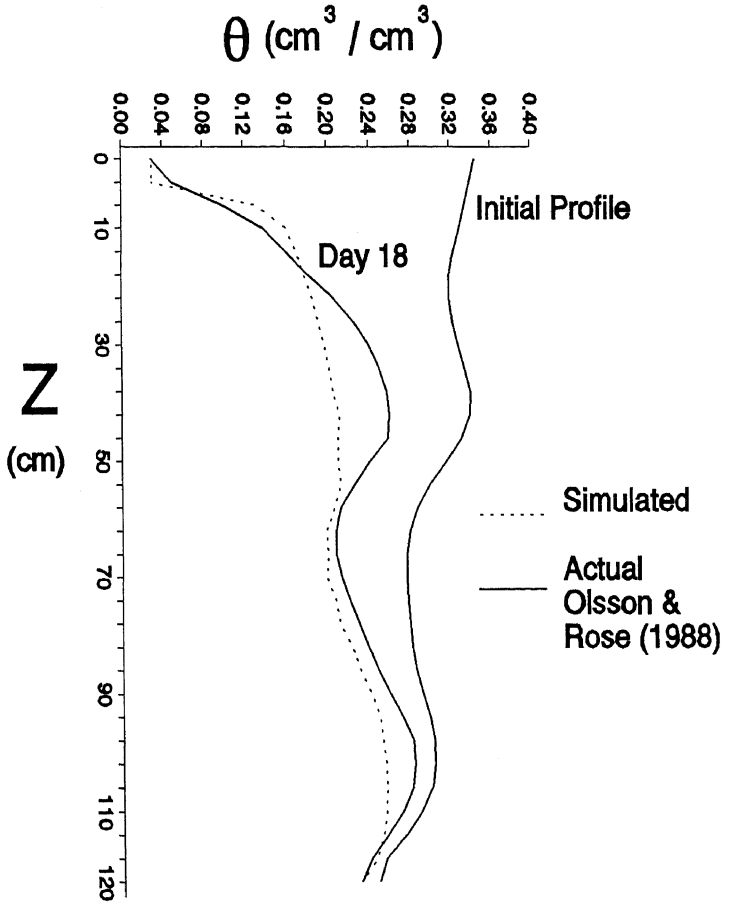


Figure 7.10 Comparison of the Olsson and Rose (1988) profile with the numerical simulation after 18 days of drying. The same initial and boundary conditions were used.

At least one shortfall cannot be rectified without field calibration and validation. It is acknowledged that the Clapp and Hornberger parameters have significant variance. For example, consider the parameters used in the above simulations. The parameter *b* had a value of 10.4 with a standard deviation of 4.45 and the saturated water content had

an average value of 0.492 with a standard deviation of 0.064. These deviations resulted from a sample size of 441 soils of this class.

7.4.2 A Direct Application

The significant application of this model is in irrigation scheduling. As indicated throughout, the development of a model that predicts the movement of water in soils can give insights into an optimal irrigation regime. The contribution of this model is the introduction of the evaporation front concept in the sink term and the employment of this as a criterion for irrigation scheduling. Clearly it will depend on the soil and the water table situation as to whether the surface will dry below the critical water content before the lower depths of the root system dry below the critical level or not. It has been stated that the conventional view to irrigation scheduling deals with the delivering of a volume of water to bring the root zone up to the an acceptable water content for plant root extraction. Consideration of movement of water in the soil profile leads to an idea that it is not so much the volume of water that is important but rather **where** the water is with respect to the roots. The simulation that follows was set up to provide an instance where the lowering evaporation front may be used as a criterion for irrigating.

The simulation allows the soil to dry to a fair extent before infiltration was switched on. Figure 7.11a shows that if the soil continues to dry under an evaporation event for seven consecutive days from the initial profile then an evaporation front forms to the depth of about 12cm or 10 per cent of the total rooting depth. This 10 per cent of the roots could account for 15-20 per cent of water uptake if the top layers were wet (according to the 40:30:20:10 ratio). If this was deemed to be sufficiently deep and further deepening of the evaporation front may cause plant stress and subsequent loss of crop quality, then irrigation may be switched on. It may be seen

in Figure 7.11a that one full day of irrigation brings the top layers up to saturation and the formation of a wetting front is evident. Figure 7.11b depicts the next two days of infiltration, with three days irrigation in all. The wetting front continues to deepen.

If the irrigation is switched off at the end of day 10 then the front is observed to continue to deepen and the surface to dry. Perhaps an insight that may be gleaned here is that whilst the depth of the evaporation front was used as a indicator for when irrigation was to be switched on, perhaps the state of the deeper layers would determine when to switch off as they have been virtually unaffected by the infiltration events. If the layers from about 60 cm and deeper continue to dry before the dissipating wetting front can effect them, then the roots deeper in the profile would be ineffective in water uptake thus the roots towards the surface would be required to satisfy the transpiration demand. The complication here is that the top layers dry fairly rapidly in response to the surface evaporative flux and it would not be long before the top layers were not sufficiently wet to maintain the evapotranspiration demand of the plant and atmosphere.

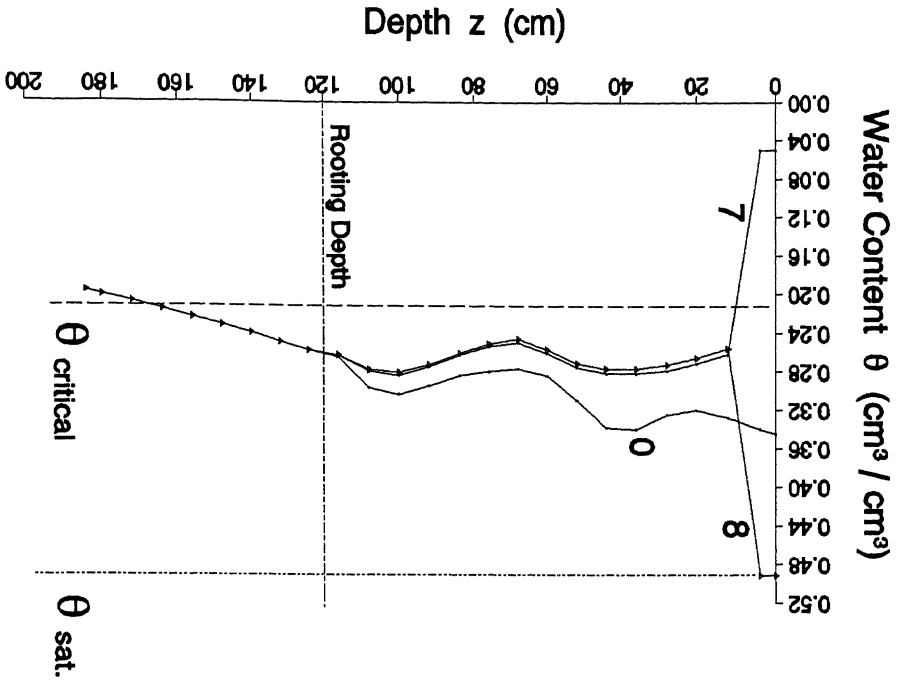


Figure 7.11a Water content profile day 7, represents the result of seven days drying from the initial profile on day 0. The profile of day 8 resulted from maximum infiltration for one full day from the day 7 situation.

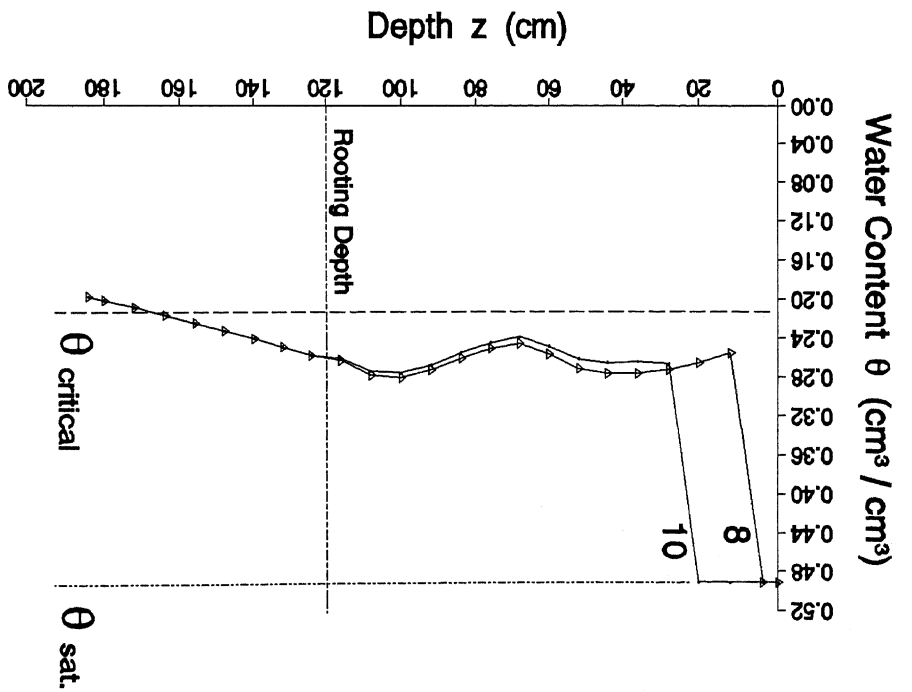


Figure 7.11b The day 10 profile follows three days of maximum infiltration from the first day of infiltration on day 8.

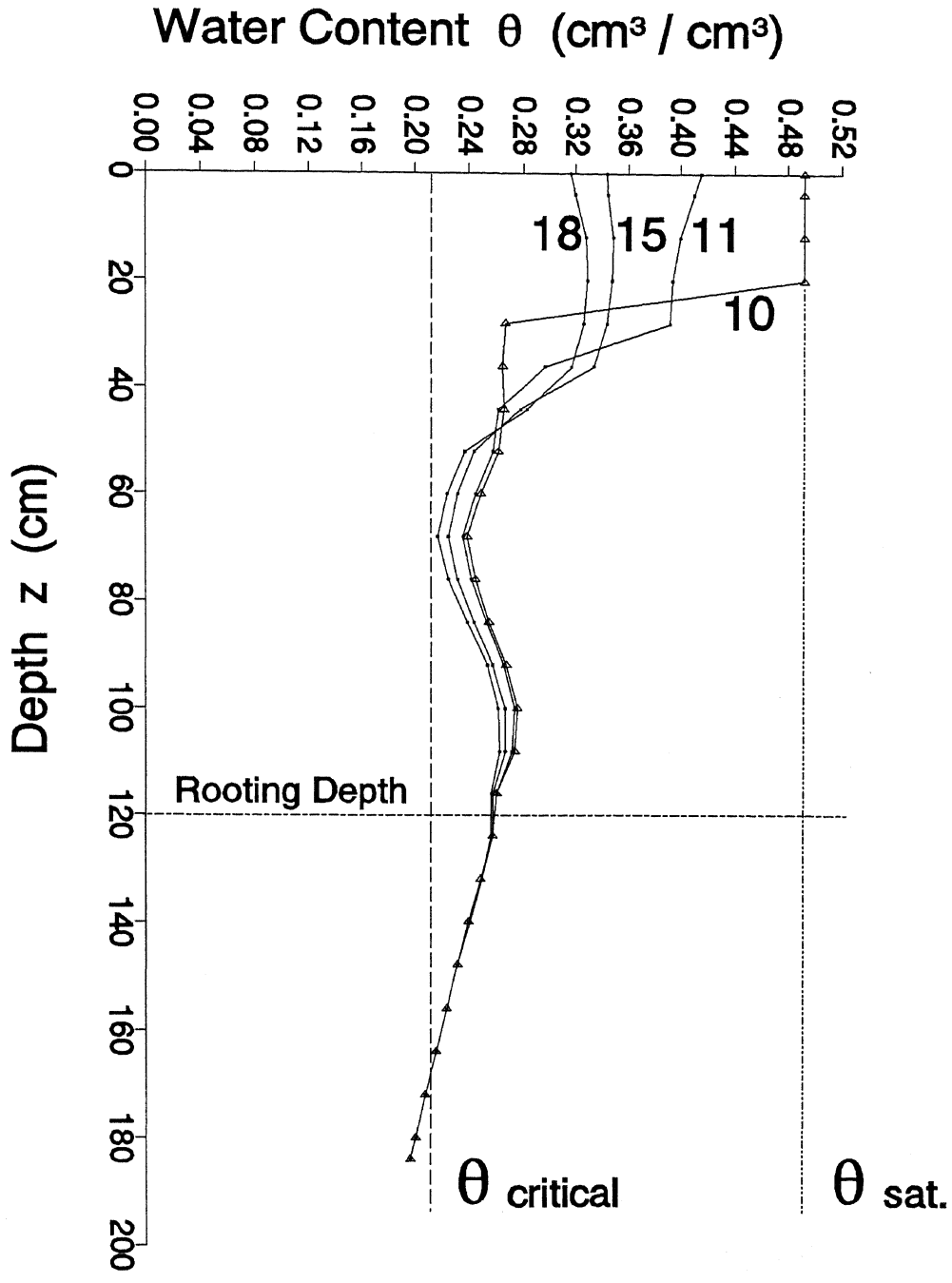


Figure 7.11c These series of profiles represent eight days of drying following the third and final day of maximum infiltration on day 10.

In conclusion, the only firm evaluation of the sink term and of the usefulness of the 'evaporation front' criteria for scheduling irrigations can come with field testing. However, as can be seen in the previous simulation, the rate of the lowering of the evaporation front and the fact that there is a high density of roots in the upper layers, presents a valid case for further investigation in the light of the following limitations.

7.4.3 Limitations of the Model

There are definite limitations to the model used in the simulations. Consider these in turn:

- The sink term which includes the evaporation front is a fully empirical model and incorporates none of the fundamental mechanism by which roots actually uptake water. A mechanistic model for water uptake would be preferable if such a model could be found that was both precise and applicable to a range of crops. The empiricism versus mechanism argument could come into play here as the shortcomings of the simple empirical model are weighed up against the mysteries surrounding the precise mechanisms of root uptake.
- The water content or diffusivity form of the flow equation as used as a basis of the foregoing model suffers from some disadvantages:

  (1) In many soils, the relationship between soil potentials and water content is not unique and single valued leading to the failure of the diffusivity equation since the functional relationship between $D(\theta)$ and $K(\theta)$ relies on the existence of $d\psi/d\theta$ as described in section 2.2.1. and,

  (2) Hogarth and Watson (1991) point out that in non-

homogeneous soils such as layered soils, water contents are discontinuous across the layer interface leading to a preference for the soil potential form of the flow equation for these soils since pressure head is continuous.

- There is no mechanism in the model to predict the time taken from when infiltration begins until the surface is saturated and ponding occurs, but rather the model assumes instantaneous saturation at the onset of infiltration which is clearly an overestimation in the general situation but reasonably models the case of flood irrigation. Several recent papers consider this issue in depth such as Haverkamp *et al.* (1977), Parlange *et al.* (1985), Hogarth *et al.* (1989) and Hogarth *et al.* (1991).
- The functional dependencies of D, K and θ are empirical and resulted from the development of power curves from measured data. The parameters of these functions have a high degree of variance.

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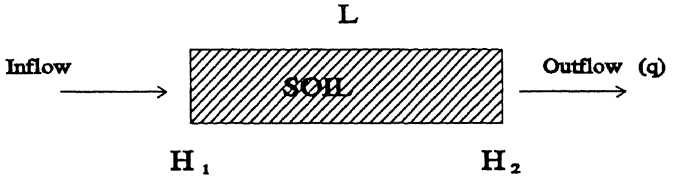
APPENDIX A

A DERIVATION OF THE FLOW EQUATION

Saturated Soils

Consider firstly, the situation where the soil is saturated, in which case hydraulic pressure is positive. The reference level for gravitational potential is arbitrary and is chosen to be in such a place so that gravitational potential is always positive or at least zero. Therefore, when soil water is saturated, the potentials are positive. The driving force of soil-water is the potential gradient. The potentials that are largely responsible for this movement are the hydraulic potentials which can be expressed in terms of hydraulic head. Therefore the driving force of soil water can be considered due to the hydraulic head gradient. If the head drop per unit distance is increased, the driving force is increased and consequently, the discharge rate through an area is increased. This discharge rate per area is called **flux** (q), and it is proportional to the hydraulic head gradient $\Delta H/L$.



and $\Delta H = H_2 - H_1$.

Mathematically, it can be written

$$q = K\,(\Delta H / L), \qquad \text{(A.1)}$$

where the proportionality constant K is called the **hydraulic conductivity**. It is related to the properties of the soil pertaining to its capacity to conduct liquid. The above equation is known as Darcy's Law.

For discussion of flow in three dimensions, Darcy's Law may be written in vector form

$$\boldsymbol{q} = -K\nabla \boldsymbol{H} \,, \tag{A.2}$$

where $\nabla \boldsymbol{H} = \frac{\partial H}{\partial x}\boldsymbol{i} + \frac{\partial H}{\partial y}\boldsymbol{j} + \frac{\partial H}{\partial z}\boldsymbol{k}$.

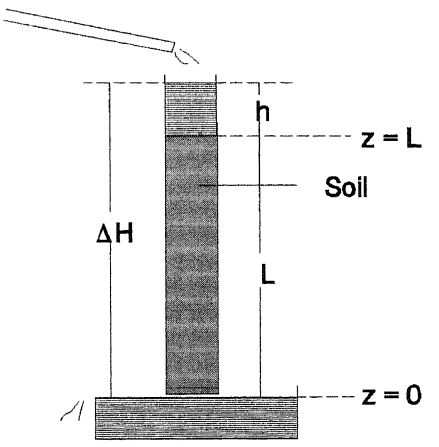
In one dimension (horizontally),

$$q = -K\frac{dH}{dx} \quad . \tag{A.3}$$

The negative sign indicates that the direction of the flux is in opposite sense to increasing potential gradient, since water moves from areas of high potential to low.

Consider Darcy's law now for the case of vertical flow, that is, where hydraulic head consists of both gravitational and pressure heads.

To determine the change in head, the head at the soil surface and the head at the base of the vertical column need be known. Let the height of the column be L cm, thus the gravitational head is L cm. If a head of water h cm high is maintained above the surface of the column, then the pressure head is h cm. The reference level is chosen at the bottom of the column and, as such, both the gravitational and pressure heads at the base are zero. Hence the change in head will be (h + L) cm.



$$\Delta H = H_{\text{surface}} - H_{\text{base}} = (h + L) - 0 \,.$$

Using Darcy's Equation with q being the flux at the bottom of the column,

$$q = K(\Delta H/L) = K(h + L)/L = K(h/L) + K .$$

If there is no ponded depth of water above the surface of the soil then the pressure head is zero $(h = 0)$. Darcy's equation now becomes simply $q = K$. In words, if the soil is saturated with no ponded depth of water then the flux is equivalent to the hydraulic conductivity.

Darcy's equation (A.1), relies on the constancy of flux (q) and head gradient. This is in fact the case for steady state flow but does not model that of transient flow, where water may flow into a volume of soil and some may be stored with the remainder forming the outflow. To overcome this difficulty in fully describing water movement, the equation of continuity, which embodies the conservation of matter principle, is introduced. In words this means that as the volume of stored water decreases over time, the rate of change in flux in a direction is increased. This can be expressed mathematically for one dimensional flow as,

$$\frac{\partial \theta}{\partial t} = -\frac{\partial q}{\partial x} , \qquad (A.4)$$

and for three dimensional flow as

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot q , \qquad (A.5)$$

where θ is the volumetric water content.

Combining Darcy's equation (A.2) with the continuity equation (A.5) the equation for three dimensional flow in saturated soils is obtained.

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot (-K \nabla H) , \qquad (A.6)$$

and in one dimension,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}\left(K \frac{\partial H}{\partial x} \right) .$$

In most agricultural situations, the soil is not saturated. In these cases the driving force for the flow of water in soil is no longer due to positive hydraulic pressures but rather is due to negative pressures or *matric suction* (ψ). Matric suction is defined as the negative of H_p. Furthermore hydraulic conductivity (K) is no longer constant in unsaturated soils. Indeed, K may vary by several orders of magnitude (Hillel, 1971) between saturated and unsaturated states.

Unsaturated Soils.

Consider now the unsaturated state. As has already been outlined, pressure and gravitational heads are positive in saturated soils, however the opposite is the case for pressure head in unsaturated soils. The term 'matric suction' emphasises this point. Matric suction (ψ), is the driving force for water flow in unsaturated soil. As suction changes so to does hydraulic conductivity, and this is expressed mathematically by writing $K(\psi)$.

Given a pressure head H_p, the matric suction ψ is expressed as $\psi = -H_p$. Given these comments it is noted that the development of Darcy's Equation (A.2) and the continuity equation (A.5) still hold for the study of flow in unsaturated soil and their combination gives,

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot q$$

$$= -\nabla \cdot [\, -K(\psi)\, \nabla H \,] .$$

Letting the hydraulic head (H) be separated into matric suction (ψ) and gravitational head (z), and substituting for H,

$$\frac{\partial \theta}{\partial t} = \nabla \cdot [\, K(\psi) \nabla (\psi - z) \,]$$

$$= \nabla \cdot \, (K(\psi) \, \nabla \psi) \, - \frac{\partial K}{\partial z}$$

The first term on the right hand side of the above equation is due to matric suction and the last term is a result of gravitational head.

For vertical flow,

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} K(\psi) \left(\frac{\partial \psi}{\partial z} \right) - \frac{\partial K}{\partial z} = \frac{\partial}{\partial z} \left(K(\psi) \frac{\partial \psi}{\partial z} - K(\psi) \right) \qquad \text{(A.7)}$$

This is one of the two major forms of the **flow equation.**

APPENDIX B

A DERIVATION OF PENMAN'S EQUATION

Since sensible heat flux (A), is proportional to the temperature gradient and the rate of latent transfer by water vapour from the field to the atmosphere (LE), is proportional to the vapour pressure gradient, then the ratio of sensible heat transport to latent heat transport becomes

$$\beta = \frac{A}{L.E} \approx \frac{\gamma(T_s - T_a)}{(e_s - e)} \qquad \text{(B.1)}$$

where β is the **Bowen Ratio** and γ is the **psychrometric constant.**

Since $LE = (e_s - e)f(u)$, equation (B.1) becomes:

$$\frac{A}{(e_s - e)f(u)} \approx \frac{\gamma(T_s - T_a)}{(e_s - e)} ,$$

from which it is obtained

$$A = \gamma f(u)(T_s - T_a). \qquad \text{(B.2)}$$

Equation (B.2) describes how the surface loses or gains heat by convection of sensible heat (advection).

Since there is no net rise in the temperature of the earth, stored heat is negligible in relation to LE and A. The miscellaneous energy term has been determined to be usually less than 5% of the total net energy and so too can it be considered negligible compared with LE and A. Therefore, the heat balance equation, (2.11) becomes

$$J_n = LE + A.$$

Dividing through by LE yields

$$\frac{J_n}{L.E} = 1+\frac{A}{L.E},$$

and substituting from equation (B.1) gives,

$$\frac{J_n}{L.E} = 1 + \frac{\gamma(T_s-T_a)}{(e_s-s)} . \qquad \text{(B.3)}$$

If e_a is the saturated vapour pressure of air, then

$$LE_a = (e_a - e)f(u).$$

Combining this equation and the Dalton Equation (2.10),

$$\frac{L.E_a}{L.E} = \frac{(e_a - e)f(u)}{(e_s - e)f(u)} .$$

Rearranging terms,

$$\frac{e_s - e_a}{e_s - e} = 1 - \frac{E_a}{E} .$$

Returning to (B.1),

$$\frac{J_n}{L.E} = 1 + \frac{\gamma(T_s - T_a)}{e_s - e}\times\frac{e_s - e_a}{e_s - e_a}$$

$$= 1 + \frac{\gamma(T_s - T_a)}{e_s - e_a}\times\frac{e_s - e_a}{e_s - e} .$$

Introducing,

$$\Delta = \frac{e_s - e_a}{T_s - T_a},$$

where Δ is the slope of the saturated vapour pressure - temperature curve, the equation becomes:

$$\frac{J_n}{L.E} = 1 + \frac{\gamma}{\Delta}(1 + \frac{E_a}{E}) .$$

Rearranging gives,

$$J_n\Delta = L.E(\Delta + \gamma) + \gamma L.E_a ,$$

$$L.E = \frac{J_n\Delta - L.E_a}{\Delta + \gamma} ,$$

with the common form being:

$$L.E = \frac{\left(\frac{\Delta}{\gamma}\right)J_n - L.E_a}{\left(\frac{\Delta}{\gamma}\right) + 1} ,$$

where $L.E_a = 0.35(e_a - e)(0.5 + 5U_2/800)$ and U_2 = mean wind speed in kms/day at 2m above the surface.

APPENDIX C

FULL SIMULATION PASCAL PROGRAM

```
Program SoilWaterSimulator;
uses dos,graph,CRT;
Const
  MaxVector = 60;
  bb = 10.4;    {Clapp & Hornberger's 'b bar' - all for Silty - Dimensionless}
  PSI = 17.4;   {Saturated Psi - cm   }
  ThetaS = 0.492;        {Saturated Water Content - cm³/cm³}
  Ks = 8.928;  {Saturated conductivity - cm/day}
  Ds = 3283.76;          {Saturated Diffusivity - cm²/day}
  ThetaCritical = 0.21;
  UpperSurface = 0;
  ThetaAirDry =0.05;

Type
  Counter = 0..MaxInt;
  SubIndex = 0..MaxVector;
  Float = Real;
  Vectors = Array[SubIndex] Of Float;
  Subtitle = string[40];
  Posint = 1..Maxint;
  METHOD = (Taylors,Geometric);

Var
  Ld, B, Ud, D,ThPresent,ThOld,K,ET,Esoil : Vectors;
  ThetaAbove,LowTheta:Vectors; { To hold fictitious points }
  Theta11,Theta12,D1,D2,T0,Transpiration : Float;
  A,deltaz,deltat, timelength, EvapFront,TotalUptake : Float;
  Infile : Text;
  I,J,LowerSurface: Counter;
  NumDepthSteps,m,n :Subindex;
  NumTimeSteps : Posint;
  depth,DaysInRow : integer;
  resp,ans  : Char;
  ThetaBoundary,ThetaAhead: Float;
  TranspirationUsed,IrrignOn,switch : Boolean;
  th1,th2,ThetaBelow : Float;
```

```
  METHOD1 : METHOD;
  gd,gm : integer;
  xstart,xrange,ystart,yrange :Real;
  Depthz,ThetaCrit :Vectors;
  clen :Subindex;

{*****************************************************************************}
{The code for graphing the results of the simulation was written by Dr. Russel Stonier, University of
Central Queensland, Rockhampton}
{*****************************************************************************}
  Function Checksize(xcord,ycord :Real) :Boolean;
  Begin
    If ((xcord < -1.0*maxint) or (xcord > 1.0*maxint)) then
      Checksize := false;
    If ((ycord < -1.0*maxint) or (ycord > 1.0*maxint)) then
      Checksize := false;
  End; {End of Checksize}

  Procedure writeongraph1(x, xs, xr, ys, yr, y : Real; color :Word);
  Var
    gmx, gmy : Integer;
    xcord,ycord : Integer;
    rxcord,rycord :Real;
  Begin
    gmx := Getmaxx;
    gmy := Getmaxy;
    rxcord := ((x - xs) * gmx / xr);
    rycord := gmy - 20 - ((y - ys) * (gmy - 40) / yr);
    If Checksize(rxcord,rycord) then
    Begin
      xcord := Round(rxcord);
      ycord := gmy - 20 - Round((y - ys) * (gmy - 40) / yr);
      setcolor(color);
      setfillstyle(1, color);
      pieslice(xcord, ycord, 0,round(9*gmy/10), 2);
    End;
  End;

  Procedure Drawaxes(xstart, x_range, ystart, y_range : Real;
                     PLottitle : Subtitle; colorset :Boolean);
  Var
    i, j, gmx, gmy, xvz, yhz : Integer;
```

```
  x0, xf, y0, yf : String[7];
  Empty : String[40];
  color : Word;
  Title : String;
Begin
  gmx := Getmaxx;
  gmy := Getmaxy;
  If (colorset = True) Then
     color := 15
  Else
     color := White;
  Setcolor(color);
  Title := 'Plot: ';
  Empty := '                                    ';
  If (PLottitle <> Empty) Then
  Begin
    Outtextxy(Round(gmx / 8) + 5, gmy - 10, 'Plot: ');
    Outtextxy(Round(gmx / 8) + 5 + TextWidth(Title), gmy - 10, PLottitle);
  End;
  If (colorset = True) Then
     color := 2;
  Setcolor(color);
  { Set position of the vertical axis}
  If (xstart >= 0.0) Then
    xvz := 0
  Else
    xvz := Round(- xstart * gmx / x_range);
  SetLineStyle(Solidln,0,Normwidth);
  Line(xvz, 20, xvz, gmy - 20);
  { Set position of the horizontal axis }
  If (ystart >= 0.0) Then
    yhz := gmy - 20
  Else
    yhz := gmy - 20 - Round(- ystart * (gmy - 40) / y_range);
  SetLineStyle(Solidln,0,Normwidth);
  line(0, yhz, gmx, yhz);
  { Set tags on the axes }
  For i := 0 To 10 Do
  Begin
    line(i * Round(gmx / 10), yhz + 2, i * Round(gmx / 10), yhz - 2);
    line(xvz - 2, 20 + i * Round((gmy - 40) / 10), xvz + 2,
        20 + i * Round((gmy - 40) / 10));
```

```
  End;
  For i := 0 To 10 Do
  Begin
    For j := 1 To 10 Do
      Putpixel( Round(i*gmx / 10), 20 + j * Round((gmy - 40) / 10),color);
  End;
  {Label the axes}
  Str(xstart:4:2, x0);
  Str((xstart + x_range):4:2, xf);
  Outtextxy(2, yhz + 10, x0);
  Outtextxy(gmx - 50, yhz + 10, xf);
  If (xvz = gmx) Then
  Begin
    Str(ystart:4:1, y0);
    Str((ystart + y_range):4:1, yf);
    Outtextxy(xvz - 50, gmy - 30, y0);
    Outtextxy(xvz - 50, 20, yf);
  End
  Else
  Begin
    Str(ystart:4:1, y0);
    Str((ystart + y_range):4:1, yf);
    Outtextxy(xvz + 4, gmy - 30, y0);
    Outtextxy(xvz + 4, 20, yf);
  End;
End; { End of Drawaxes }

Procedure Drawcurve(u, v : Vectors; no_of_terms : Subindex;
                    umin, u_range, vmin, v_range : Float);
Var
  gmx, gmy, i, k : Integer;
  ucord_i, vcord_i : Integer;
  ucord_k, vcord_k : Integer;
  rucordi, rvcordi :Float;
  rucordk, rvcordk :Float;
Begin
  gmx := Getmaxx;
  gmy := Getmaxy;
  i := 0;
  rucordi := ((u[i] - umin) * gmx / u_range);
  rvcordi := gmy - 20 - ((v[i] - vmin) * (gmy - 40) / v_range);
  While (checksize(rucordi,rvcordi) = false) do
```

```
    Begin
      i := i + 1;
      rucordi := (u[i] - umin) * gmx / u_range;
      rvcordi := gmy - 20 - ((v[i] - vmin) * (gmy - 40) / v_range);
    End;
    ucord_i := Round(rucordi);
    vcord_i := gmy - 20 - Round((v[i] - vmin) * (gmy - 40) / v_range);
    moveto(ucord_i, vcord_i);
    Setcolor(15);  {Color = white for Ega}
    For k := i To no_of_terms Do
    Begin
      rucordk := ((u[k] - umin) * gmx / u_range);
      rvcordk := gmy - 20 - ((v[k] - vmin) * (gmy - 40) / v_range);
      If Checksize(rucordk,rvcordk) then
      Begin
        ucord_k := Round(rucordk);
        vcord_k := gmy - 20 - Round((v[k] - vmin) * (gmy - 40) / v_range);
        SetLineStyle(Dashedln,0,NormWidth);
        Lineto(ucord_k, vcord_k);
      End;
      If keypressed Then Halt;
    End;
    Outtextxy(1, 1, 'Press <Return> to quit:');
    Reset(Input);
    ReadLn;
    {  write(ReadKey); }
    Closegraph;
  End; { End of Drawcurve }
{*************************************************************************}

  Procedure Tridiag(n : SubIndex;
                    Ld, D, Ud : Vectors;
                    Var B : Vectors);
{Uses the Thomas Algorithm}
  Var
    mult : Float;
    i, j : Integer;
  Begin
    For i := 2 To  n Do
    Begin
      mult := Ld[i] / D[i - 1];
      D[i] := D[i] - mult * Ud[i - 1];
```

```
      B[i] := B[i] - mult * B[i - 1];
    End;
    B[n] := B[n] / D[n];
    For j := 1 To n - 1 Do
      B[n - j] := (B[n - j] - Ud[n - j] * B[n - j + 1]) / D[n - j];
  End; { End of Tridiag }
{*************************************************************************}
Procedure SetConstants(var ND1:subindex;var NT1:Posint);
{Set size of timestep, number of timesteps, size of depthstep and number of steps}
Begin
  writeln('Enter the size of the time step in hours');
  readln (DeltaT);
  writeln('Enter the length of time to conduct the simulation in days');
  readln (timelength);
  NT1 := round(timelength/DeltaT);
  writeln('Enter the size of the depth step in centimetres');
  readln(DeltaZ);
  writeln('Enter the rooting depth in centimetres');
  readln(depth);
  ND1 := round(depth/DeltaZ);
  LowerSurface := ND1+1;
  A := (2*(DeltaZ*DeltaZ))/DeltaT;
End;
{*************************************************************************}
Procedure AcceptConstants(var ND2:subindex;var NT2:Posint);
Begin
  DeltaT := 1;
  timelength := 18;
  NT2 := round(timelength/DeltaT);
  DeltaZ := 8.0;
  depth := 184;
  ND2 := round(depth/DeltaZ);
  LowerSurface := ND2+1;
  A := (2*(DeltaZ*DeltaZ))/DeltaT;
End;
{*************************************************************************}
Procedure DrawHeader(ThPresent2:vectors;ND3:Posint);
Begin
   Writeln('  Time  ':7, ' Water Content Profile':50);
   Writeln('**********':7, '************************':50) ;
   T0 := 0.0;
   Write(t0:10:0);
```

```
  For I := 0 To ND3+1 Do          {The zero'th position represents the surface}
  Begin                           {From the 0'th to 1'st position is 1/2 depth step}
    Write( ThPresent2[I]:10:3);  {The n+1'th position is the lower boundary}
  End;
  Writeln;
End;
{*************************************************************************}
Procedure PrintResults(ThetaPresent3:vectors;ND3:Posint;J:counter);
Begin
  Write( j*DeltaT:10:6);
  For I := 0 To ND3 +1 Do
  Begin
    Write(ThetaPresent3[I]:10:3);
  End;
  Writeln;
  Writeln('ThetaAbove is: ',ThetaAbove[J]:10:3);
  writeln;
  writeln('ThetaBoundary is: ',ThetaBoundary:10:3);
End;
{*************************************************************************}
Function X_To_Y(x,y:Float) : Float;
Var r : Float;
Begin
  If x<0 Then writeln('One of Your powers is out of range')
  Else
  Begin
    r := y*Ln(x);
    X_To_Y := Exp(r);
  End;
End;
{*************************************************************************}
Function SINK(I1,J2 : Integer;
              EF2,T2 : Float):Float;
var S,v, EFdiff,RootDiff,TempTotal : Float;

 Function RootLength(J3: Integer) : Float;
  {Constant Root length function - may be changed}
 Begin
  {RootLength := 2 * J3*DeltaT;}
   RootLength := 120;
 End;
```

```
Begin
  v := RootLength(J2);
  EFdiff := v - EF2;
  RootDiff := v - (DeltaZ*(I1-0.5));
  If TotalUptake <> T2 Then
  Begin
    If (EFdiff <= 0) or (RootDiff <= 0) Then
    {If the evapfront is deeper than the roots or if no roots in the depth zone}
    begin
      if (RootDiff <= 0) and Not TranspirationUsed Then
      begin
        SINK := (T2 - TotalUptake)/DeltaZ;
        TranspirationUsed := True;
        TotalUptake := T2;
      end
      else SINK := 0;
    end
    Else
    begin
      S :=          -1.6*T2*(DeltaZ*(I1 - 0.5))/X_To_Y(EFdiff,2)
                    +T2*(1.8*v - 0.2*EF2)/X_To_Y(EFdiff,2);
      SINK := S;
      TempTotal := TotalUptake + S*DeltaZ;
      if (TempTotal > T2) and (NOT TranspirationUsed) then
      Begin
        SINK := (T2 - TotalUptake)/DeltaZ;
        TranspirationUsed := True;
      End
      else TotalUptake := TotalUptake + S*DeltaZ;
    end;
  End
  Else SINK := 0;
End;
{*************************************************************************}
Function KTheta(Th : Float) : Float;
Begin
    If Th <= ThetaAirDry Then Th := ThetaAirDry;
    KTheta := Ks*X_To_Y((Th/ThetaS),(2*bb+3));
End;
{*************************************************************************}
Function Diffusivity(Th : Float) : Float;
Begin
```

```
    If Th <= ThetaAirdry Then Th := ThetaAirdry;
    Diffusivity := ((bb*PSI*(X_TO_Y(ThetaS,bb)))/X_TO_Y(Th,bb+1))*KTheta(Th);
End;
{*************************************************************************}
Function Theta_half_time(ThPresent6:vectors;
                         J3,I2:integer;
                         EF3,T3:Float): Float;
var dTheta_dT,Th12 : Float;
Begin
 If I2 < 2 then
 begin
  dTheta_dT:=  ((Diffusivity(ThPresent6[I2+1])*(ThPresent6[I2+2]-ThPresent6[I2+1])/DeltaZ -
               KTheta(ThPresent6[I2+1])) -
               (Diffusivity(ThPresent6[I2])*(ThPresent6[I2+1]-ThPresent6[I2])/DeltaZ -
               KTheta(ThPresent6[I2])))/DeltaZ;
{This is using the forward/Forward difference analog for the space derivatives}
  end
  Else
    if I2 > (NumDepthSteps-1) then
    begin
    dTheta_dT:=          ((Diffusivity(ThPresent6[I2])*(ThPresent6[I2]-ThPresent6[I2-1])/DeltaZ -
                         KTheta(ThPresent6[I2])) -
                         (Diffusivity(ThPresent6[I2-1])*(ThPresent6[I2-1]-ThPresent6[I2-2])/DeltaZ -
                         KTheta(ThPresent6[I2-1])))/DeltaZ;
{This is using the backward/backward difference analog for the space derivatives}
    end
    else
    begin
      dTheta_dT:=((Diffusivity(ThPresent6[I2+1])*(ThPresent6[I2+1]-ThPresent6[I2])/DeltaZ -
                  KTheta(ThPresent6[I2+1]))-
                  (Diffusivity(ThPresent6[I2])*(ThPresent6[I2]-ThPresent6[I2-1])/DeltaZ -
KTheta(ThPresent6[I2])))/DeltaZ;
{ Forward/ Backward difference}
    end;
  If (I2-0.5) * DeltaZ > EF3 Then dTheta_dT := DTheta_dT - Sink(I2,J3,EF3,T3);
  {Do Not project forward using the sink if in the dry upper zone}
  Th12 := ThPresent6[I2] + dTheta_dT*DeltaT/2;
  if Th12 < ThetaAirDry Then Th12 := ThetaAirDry;
  Theta_half_time:= Th12;
End;
{*************************************************************************}
Function FindThetaLess(ThOld4,ThPresent4:vectors;
```

```
                        J2,I1:integer;
                        EF2,T2: Float;
                        IrrignOn2,switch2:Boolean) : Float;
var ThLess : Float;
Begin
 If METHOD1 = Taylors Then
 Begin
  If (I1 = 1) and IrrignOn2
  Then ThLess := ThetaS
  Else If (I1=1) and Not IrrignOn2
      Then ThLess := Theta_half_time(ThPresent4,J2,I1,EF2,T2)
      Else ThLess :=  (Theta_half_time(ThPresent4,J2 , I1,EF2,T2) +
                      Theta_half_time(ThPresent4,J2 , I1-1,EF2,T2))/2;
 End
 Else
 Begin {Geometric Method}
  if I1 = 1 then ThLess := (3*ThPresent4[I1-1] - ThOld4[I1-1])/2
  else  ThLess := 0.75*(ThPresent4[I1-1]+ThPresent4[I1]) - 0.25*(ThOld4[I1-1]+ThOld4[I1]);
 End;
 If ThLess < ThetaAirDry then ThLess := ThetaAirDry;
 If ThLess > ThetaS then ThLess := ThetaS;
 FindThetaLess := ThLess;
End;
{*************************************************************************}
Function FindThetaMore(ThOld5,ThPresent5:vectors;
                        J2,I1:integer;
                        EF2,T2 : Float;
                        IrrignOn2,switch2:Boolean) : Float;
var ThMore : Float;
Begin
 If METHOD1 = Taylors Then
 Begin
  If I1 = NumDepthSteps Then ThMore := (LowTheta[J2+1]+LowTheta[J2])/2
  Else ThMore := (Theta_half_time(ThPresent5,J2,I1+1,EF2,T2) +
                      Theta_half_time(ThPresent5,J2 , I1,EF2,T2))/2;
 End
 Else
 Begin {Geometric Method}
  If I1 = NumDepthSteps Then ThMore := (3*ThPresent5[I1+1] - ThOld5[I1+1])/2
  Else ThMore := 0.75*(ThPresent5[I1+1]+ThPresent5[I1]) - 0.25*(ThOld5[I1+1]+ThOld5[I1]);
 End;
 If ThMore > ThetaS Then ThMore := ThetaS;
```

```
  FindThetaMore:=ThMore;
End;
{*************************************************************************}
Procedure Init_and_Bound(var ThOld1,ThPresent1,ET1,Esoil1,LowTheta1:vectors;ND4,NT4:Posint);
{This procedure will read the initial conditions from a file}
var       I : integer;
    response : char;
begin
  Assign(Infile, 'c:\tp\flow\init8.DAT');
  Reset(Infile);
  For I := 0 to ND4+1  do
  {i=0 corresponds to the surface water content }
  begin
    Read(Infile, ThOld1[I]); {ThOldores the old thetas}
    readln(Infile, ThPresent1[I]); {ThPresent stores the current thetas}
    ThetaCrit[I] := ThetaCritical; {To later be graphed}
  end;
  Close(Infile);
  ThetaAbove[0] := 2*ThOld1[0] - ThOld1[1]; {Linear Projection above}
  ThetaAbove[1] := 2*ThPresent1[0] - ThPresent1[1];

  Assign(Infile, 'c:\tp\flow\ETrose.DAT');
  Reset(Infile);
  For I := 1 to NT4+1 do  {18 Days of Data}
  begin
    Read(Infile, ET1[I]);
    readln(Infile, Esoil1[I]);
  end;
  Close(Infile);

  Assign(Infile,'c:\tp\flow\LowBd8.dat');
  Reset(Infile);
  For I := 1 to NT4+1 do  {18 Days of Data}
  Readln(Infile, LowTheta1[I]);
  Close(Infile);
End;
{*************************************************************************}
Procedure FormTridiagE1(Theta1,Theta0:vectors;
                        T1,EF1 : Float;
                        J1 : Integer;
                        IrrignOn1,switch1:Boolean);
{Forms the tridiagonal system using the current Thetas as a first approximation
```

```
of the half time forward thetas in the case of switching off irrigation}
var  I : integer;
     z1,z2,z3 :float;
Begin
   For I := 1 To NumDepthSteps  Do  {Calculate the matrix elements in the tridiagonal system}
   Begin                            {at a given timestep - this time includes boudaries }
     if I=1 then Theta11:= Theta0[0]
     else Theta11 := (Theta0[I]+Theta0[I-1])/2;
     if i=NumDepthSteps Then Theta12 := LowTheta[J1]
     else Theta12 := (Theta0[I]+Theta0[I+1])/2;
     D1 := Diffusivity(Theta11);
     D2 := Diffusivity(Theta12);
     If  (I > 1) and (I < NumDepthSteps) then
     Begin
       Ld[I] := D1;
       D[I] :=  -(D1 + D2 + A);
       Ud[I] := D2;
       z1 :=     +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
       z2 :=     +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
       B[I] :=   -D1*Theta0[I-1]
                 +(D1+D2-A)*Theta0[I]
                 -d2*theta0[I+1] +z1 +z2;
     End
     Else
       If (I=1) Then
       Begin
         Ld[I] := 0;
         D[I]  := -(D2 + A);
         Ud[I] := D2;
         if J1=1 then
         begin
           ThetaBoundary := Theta0[0];
           ThetaAbove[1] := (2*ThetaBoundary-Theta0[1])/2;
           If ThetaBoundary <= ThetaAirDry Then ThetaAbove[J1] := ThetaAirDry;
         end
         else
         begin
           ThetaBoundary :=  Theta0[0]; {sqrt(Theta0[0]*Theta0[1])}
           If ThetaBoundary <= ThetaAirDry Then ThetaAbove[J1] := ThetaAirDry
           Else ThetaAbove[J1] := Theta0[I] +
                                  DeltaZ*(-Esoil[J1]/10-KTheta(ThetaBoundary))/
                                  Diffusivity(ThetaBoundary);
```

```
        end;
        ThetaAhead := 2*Theta11 - ThetaBoundary; {Needed for boundary flux term }
        If ThetaAhead <=ThetaAirDry Then ThetaAhead := ThetaAirdry;
        z1 :=   -DeltaZ*D1/Diffusivity(ThetaAhead)*(-Esoil[J1+1]/10-KTheta(ThetaAhead));
        z2 :=   +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
        z3 :=   +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);

        B[I]:=  -D1*ThetaAbove[J1]
                +(D1+D2-A)*Theta0[I]
                -D2*Theta0[I+1] +z1 +z2 +z3;
      End
      Else
        If (I=NumDepthSteps) Then
        Begin
          ThetaAhead := 2*Theta12-Theta0[NumDepthSteps+1];
          ThetaBelow :=2*LowTheta[J1]-Theta0[I];
          Ld[I] := D1;
          D[I]  := -(2*D2 + D1 + A);
          Ud[I] := 0;
          z1 :=   +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
          z2 :=   +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
          B[I]:=  -D1*Theta0[I-1]
                  +(D1 + D2 - A)*Theta0[I]
                  -D2*ThetaBelow
                  -2*D2*LowTheta[J1] + z1  +z2;
        End;
    End;
End;
{*************************************************************************************}
Procedure FormTridiagE2(Theta1,Theta0:vectors;
                        T1,EF1 : Float;
                        J1 : Integer;
                        IrrignOn1,switch1:Boolean);
{Forms a tridiagonal system from the water contents found in FormTriDiagE1}
var  I : integer;
     z1,z2,z3 :float;
Begin
    For I := 1 To NumDepthSteps  Do
    Begin
      if I=1 then Theta11:= (Theta0[0]+Theta1[0])/2
      else Theta11 := ((Theta0[I]+Theta0[I-1])/2+(Theta1[I]+Theta1[I-1])/2)/2;
      if I=NumDepthSteps Then Theta12 := LowTheta[J1]
```

```
else Theta12 := ((Theta0[I]+Theta0[I+1])/2+(Theta1[I]+Theta1[I+1])/2)/2;
D1 := Diffusivity(Theta11);
D2 := Diffusivity(Theta12);
If (I > 1) and (I < NumDepthSteps) then
Begin
 Ld[I] := D1;
 D[I] := -(D1 + D2 + A);
 Ud[I] := D2;
 z1 :=    +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
 z2 :=    +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
 B[I] :=  -D1*Theta0[I-1]
         +(D1+D2-A)*Theta0[I]
         -D2*theta0[I+1] +z1 +z2;
End
Else
 If (I=1) Then
 Begin
  Ld[I] := 0;
  D[I] := -(D2 + A);
  Ud[I] := D2;
  if J1= 1 then
  begin
   ThetaBoundary := Theta0[0];
   ThetaAbove[1] := 2*ThetaBoundary-Theta0[1];
   If ThetaBoundary <= ThetaAirDry Then ThetaAbove[J1] := ThetaAirDry;
  end
  else
  begin
   ThetaBoundary := Theta0[0]{(Theta0[0]*Theta0[1])};
   If ThetaBoundary <= ThetaAirDry Then ThetaAbove[J1] := ThetaAirDry
   Else ThetaAbove[J1] := 2*ThetaBoundary-Theta0[1];
  end;
  ThetaAhead := 2*Theta11 - ThetaBoundary; {Needed for boundary flux term }
  If ThetaAhead <=ThetaAirDry Then ThetaAhead := ThetaAirdry;
  z1 :=  -DeltaZ*D1/Diffusivity(ThetaAhead)*(-Esoil[J1+1]/10-KTheta(ThetaAhead));
  z2 :=  +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
  z3 :=  +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
  B[I] := -D1*ThetaAbove[J1]
          +(D1+D2-A)*Theta0[I]
          -D2*Theta0[I+1] +z1 +z2 +z3;
 End
 Else
```

```
        If (I=NumDepthSteps) Then
        Begin
          ThetaAhead := 2*Theta12-Theta0[NumDepthSteps+1];
          ThetaBelow := 2*LowTheta[J1]-Theta0[I];
          Ld[I] := D1;
          D[I]  := -(2*D2 + D1 + A);
          Ud[I] := 0;
          z1 := +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
          z2 := +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
          B[I]  := -D1*Theta0[I-1]
                   +(D1 + D2 - A)*Theta0[I]
                   -D2*ThetaBelow
                   -2*D2*LowTheta[J1] + z1  +z2;
        End;
    End;
End;
{*************************************************************************}
Procedure FormTridiagE3(Theta1,Theta0:vectors;
                        T1,EF1 : Float;
                        J1 : Integer;
                        IrrignOn1,switch1:Boolean);
{Forms a Tridiagonal system based on projecting one-half step forward from the current values of water
content}
var  I : integer;
     z1,z2,z3 :float;
Begin
    For I := 1 To NumDepthSteps  Do
    Begin
      Theta11 := FindThetaLess(Theta1,Theta0,J1,I,EF1,T1,IrrignOn1,switch1);
      Theta12 := FindThetaMore(Theta1,Theta0,J1,I,EF1,T1,IrrignOn1,switch1);
      D1 := Diffusivity(Theta11);
      D2 := Diffusivity(Theta12);
      If  (I > 1) and (I < NumDepthSteps) then
      Begin
        Ld[I] := D1;
        D[I] := -(D1 + D2 + A);
        Ud[I] := D2;
        z1 := +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
        z2 := +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
        B[I] :=  -D1*Theta0[I-1]
                 +(D1+D2-A)*Theta0[I]
                 -d2*theta0[I+1] +z1 +z2;
```

```
End
Else
  If (I=1) Then
  Begin
    Ld[I]  := 0;
    D[I]   := -(D2 + A);
    Ud[I]  := D2;
    if J1= 1 then
    begin
      ThetaBoundary := Theta0[0];
      ThetaAbove[1] := 2*ThetaBoundary-Theta0[1];
      If ThetaBoundary <= ThetaAirDry Then ThetaAbove[J1] := ThetaAirDry;
    end
    else
    begin
      ThetaBoundary := Theta0[0];{sqrt(Theta0[0]*Theta0[1]);}
      If ThetaBoundary <= ThetaAirDry Then ThetaAbove[J1] := ThetaAirDry
      Else ThetaAbove[J1] := Theta0[I] +
                             DeltaZ*(-Esoil[J1]/10-KTheta(ThetaBoundary))/
                             Diffusivity(ThetaBoundary);
    end;
    ThetaAhead := 2*Theta11 - ThetaBoundary; {Needed for boundary flux term }
    If ThetaAhead <=ThetaAirDry Then ThetaAhead := ThetaAirdry;
    z1 := -DeltaZ*D1/Diffusivity(ThetaAhead)*(-Esoil[J1+1]/10-KTheta(ThetaAhead));
    z2 := +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
    z3 := +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
    B[I] := -D1*ThetaAbove[J1]
            +(D1+D2-A)*Theta0[I]
            -D2*Theta0[I+1] +z1 +z2 +z3;
  End
  Else
    If (I=NumDepthSteps) Then
    Begin
      ThetaAhead := 2*Theta12-Theta0[NumDepthSteps+1];
      ThetaBelow :=2*LowTheta[J1]-Theta0[I];
      Ld[I] := D1;
      D[I]  := -(2*D2 + D1 + A);
      Ud[I] := 0;
      z1 := +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
      z2 := +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
      B[I] := -D1*Theta0[I-1]
              +(D1 + D2 - A)*Theta0[I]
```

```
                -D2*ThetaBelow
                -2*D2*LowTheta[J1] + z1  +z2;
        End;
    End;
End;
{*************************************************************************}
Procedure FormTridiagI(Theta1,Theta0:vectors;T1,EF1 : Float; J1 : Integer;IrrignOn1,switch1:Boolean);
var I : integer;
    z1,z2,z3 :float;
{Forms a Tridiagonal system using infiltration equations}
Begin
   For I := 1 To NumDepthSteps  Do
   Begin
     Theta11 := FindThetaLess(Theta1,Theta0,J1,I,EF1,T1,IrrignOn1,switch1);
       {Theta11 is at a 1/2 depthstep less and J+1/2}
     Theta12 := FindThetaMore(Theta1,Theta0,J1,I,EF1,T1,IrrignOn1,switch1);
       {Theta12 is at a 1/2 depthstep more and J+1/2}
     D1 := Diffusivity(Theta11);
     D2 := Diffusivity(Theta12);
     If  (I > 1) and (I < NumDepthSteps) then
     Begin
      Ld[I] := D1;
      D[I] := -(D1 + D2 + A);
      Ud[I] := D2;
      z1 :=  +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
      z2 :=  +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
      B[I] :=  -D1*Theta0[I-1]
             +(D1+D2-A)*Theta0[I]
             -d2*theta0[I+1] +z1 +z2;
     End
     Else
      If (I=1) Then
      Begin
       Ld[I]  := 0;
       D[I]   := -(2*D1+D2 + A);
       Ud[I]  := D2;

       z1 := -4*D1*ThetaS;
       z2 :=  +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
       z3 :=  +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
       B[I] := (2*D1+D2-A)*Theta0[I]
              -D2*Theta0[I+1] +z1 +z2 +z3;
```

```
        End
        Else
          If (I=NumDepthSteps) Then
          Begin
            ThetaAhead := 2*Theta12-Theta0[NumDepthSteps+1];
            ThetaBelow :=2*LowTheta[J1]-Theta0[I];
            Ld[I] := D1;
            D[I]  := -(2*D2 + D1 + A);
            Ud[I] := 0;
            z1 := +2*DeltaZ*(KTheta(Theta12)-KTheta(Theta11));
            z2 := +2*DeltaZ*DeltaZ*SINK(i,J1,EF1,T1);
            B[I] := -D1*Theta0[I-1]
                    +(D1 + D2 - A)*Theta0[I]
                    -D2*ThetaBelow
                    -2*D2*LowTheta[J1] + z1  +z2;
          End;
    End;
End;
{*************************************************************************}
Procedure UpdateThetas(var ThOld6,ThPresent6:vectors;
                       Day:Posint;
                       IrrigationOn:Boolean);
{Water contents for the day just gone are stored as ThOld6}
var FrontFound : Boolean;
    I,Maxi : integer;
    Max : Float;
Begin
{Copy  B into theta to update the thetas just calculated}
{so that they may be used as a base for the next set of calculations }
  FrontFound := False;
  Max := 0;
  Maxi := 1;
  For I := 1 to NumDepthSteps Do
  Begin
    ThOld6[I] := ThPresent6[I]; {Take a Copy of old thetas}
    ThPresent6[I] := B[I];   {Update newfound thetas}
    If ThPresent6[I] < ThetaAirDry Then ThPresent6[I] := ThetaAirDry;
    If ThPresent6[I] > ThetaS Then ThPresent6[I] := ThetaS;
  End;
  ThOld6[0] := ThPresent6[0];{N.B. ThPresent6[0] not yet updated}
  If  IrrigationOn then
      begin
```

```
      ThPresent6[0] := ThetaS;
      ThetaAbove[Day+1] := 2*ThetaS-ThPresent6[1];
    end
    else ThPresent6[0] := (3*ThPresent6[1] -ThPresent6[2])/2; {first Linear estimate to calc K&D }
ThPresent6[LowerSurface] := LowTheta[Day + 1];
If ThPresent6[UpperSurface] < ThetaAirDry Then ThPresent6[UpperSurface] := ThetaAirDry;
If ThPresent6[UpperSurface] > ThetaS Then ThPresent6[UpperSurface] := ThetaS;
For I := 1 to NumDepthSteps Do {Look For Evaporation Front}
begin
  if ThPresent6[I] > Max
  then
  begin
    Max := ThPresent6[I];
    Maxi := i
  end;
  IF IrrigationOn
  THEN
  Begin
    EvapFront :=0;
    FrontFound := True;
  End
  ELSE
  Begin
  {Check for a change in position of EvapFront}
    If (ThPresent6[I] < ThetaCritical) and (ThPresent6[I+1] > ThetaCritical) and Not FrontFound
    Then
    Begin
      EvapFront := (i-0.5) * DeltaZ;
      FrontFound := True;
    End;
   END;
 End;
 If Not FrontFound and (Max <= ThetaCritical)
 Then EvapFront :=(Maxi-0.5)*DeltaZ
 Else If (Max > ThetaCritical) and not FrontFound
     Then EvapFront := 0;
End;
{*************************************************************************}
Procedure UpdateThetasE(var ThOld6,ThPresent6:vectors;
                        Day:Posint;
                        IrrigationOn:Boolean);
{This updates the water contents provisionally after switching off irrigation}
```

```
var I : integer;
Begin
  For I := 1 to NumDepthSteps Do
  Begin
    ThOld6[I] := ThPresent6[I]; {Take a Copy of old thetas}
    ThPresent6[I] := B[I];   {Update newfound thetas}
    If ThPresent6[I] < ThetaAirDry Then ThPresent6[I] := ThetaAirDry;
  End;
  ThOld6[0] := ThPresent6[0];{N.B. ThPresent6[0] not yet updated}
  ThetaAbove[Day] := 2*ThetaAirDry-ThPresent6[1];
  ThPresent6[0] := (3*ThPresent6[1] -ThPresent6[2])/2;
  ThetaAbove[Day] := ThPresent6[1] +
                          DeltaZ*(-Esoil[Day]/10-KTheta(ThPresent6[0]))/
                          Diffusivity(ThPresent6[0]);
  ThPresent6[UpperSurface] := (ThetaAbove[Day] + ThPresent6[1])/2;
  If ThPresent6[UpperSurface] < ThetaAirDry Then ThPresent6[UpperSurface] := ThetaAirDry;
  If ThPresent6[UpperSurface] > ThetaS Then ThPresent6[UpperSurface] := ThetaS;
end;
{*************************************************************************}
{ End of procedures and functions }
{*************************************************************************}

Begin { Start of main program }
  clrscr;
  EvapFront := 0; {Reset evaporation front}

  writeln('Do you wish to alter the constants? Y/N');
  readln(resp);
  if upcase(resp) = 'Y' then SetConstants(NumDepthSteps,NumTimeSteps)
  else AcceptConstants(NumDepthSteps,NumTimeSteps);
  Init_and_Bound(ThOld,ThPresent,ET,Esoil,LowTheta,NumDepthSteps,NumTimeSteps);
     {Set Initial and Boundary Conditions}
  DrawHeader(ThPresent,NumDepthSteps);
  IrrignOn := False;
  Switch := True; {To signal the switch from On to Off and vice-versa}
  DaysInRow:=0; {To monitor how many days since a switch}
{********** Graphing Setup **********}
  xstart := 0;
  xrange := Depth+DeltaZ;
  ystart := 0;
  yrange := 0.5;
  Depthz[0] := 0.0;
```

```
Depthz[1] := 5.0;
For m := 0 to Numdepthsteps - 2 Do
  Depthz[2+m] := (DeltaZ+trunc(DeltaZ/2)) + m*deltaZ;
Depthz[LowerSurface] := Depth;
directvideo := False;
gd := detect;
Initgraph(gd, gm, 'c:\tp\bgi');
setgraphmode(1);
clen := LowerSurface;
Drawaxes(xstart, xrange, ystart, yrange,'Theta against z',False);
For m := 0 to Numdepthsteps+ 1 Do
  writeongraph1(depthz[m],xstart,xrange,ystart,yrange,ThetaCrit[m],white);
Drawcurve(depthz,ThPresent,clen, xstart, xrange, ystart, yrange);
{*********************************************************}

For J := 1 to NumTimeSteps Do
Begin
{ The J loop is for each timestep and within it calculations at all depths are done for a given timestep}
  Transpiration := (ET[J] - Esoil[J])/10;
  TotalUptake := 0;
  TranspirationUsed := False;
  writeln('Do you wish to irrigate at end of day ',J);
  readln(ans);
  if upcase(ans) = 'Y'
  Then
  Begin
    if not IrrignOn Then switch := True
    else Switch:= False;
    IrrignOn := True;
    EvapFront := 0;
    ThetaAbove[J] := ThetaS;{Fixes prob when switching from off to on}
    FormTridiagI(ThOld,ThPresent,Transpiration,EvapFront,J,IrrignOn,switch);
  end
  else
  begin
    If IrrignOn Then
    begin
      Switch := True;
      DaysInRow:=0;
    end;
    IrrignOn := False;
    If Switch or (DaysInRow <= 2) Then {Allows 2 timesteps for convergence}
```

```
      begin
        FormTridiagE1(ThOld,ThPresent,Transpiration,EvapFront,J,IrrignOn,switch);
        Tridiag(NumDepthSteps, Ld, D, Ud, B);
        UpdateThetasE(ThOld,ThPresent,J,IrrignOn);
        FormTridiagE2(ThOld,ThPresent,Transpiration,EvapFront,J,IrrignOn,switch);
        switch := false;
        DaysInRow := DaysInRow + 1;
      end
      Else FormTridiagE3(ThOld,ThPresent,Transpiration,EvapFront,J,IrrignOn,switch);
    end;
    Tridiag(NumDepthSteps, Ld, D, Ud, B); {Solve the tridiagonal system at this timestep}
    UpdateThetas(ThOld,ThPresent,J,IrrignOn);{This gives the thetas for the next timestep}
    PrintResults(ThPresent,NumDepthSteps,J);
{********************* Graph Results *********************}
    directvideo := False;
    gd := detect;
    Initgraph(gd, gm, 'c:\tp\bgi');
    setgraphmode(1);
    clen := LowerSurface;
    Drawaxes(xstart, xrange, ystart, yrange,'Theta against z',False);
    For m := 0 to Numdepthsteps+ 1 Do
      writeongraph1(depthz[m],xstart,xrange,ystart,yrange,ThetaCrit[m],white);
    {Draws Critical water content line}
    Drawcurve(depthz,ThPresent,clen, xstart, xrange, ystart, yrange);
    Closegraph;
{*********************************************************}
  End; { End Time iteration loop }
End. { End of the main program }
```

APPENDIX D

DATA TABLES FOR GRAPHS OF SIMULATIONS

Depth (cm)	Day of Simulation			
	0	3	9	18
0	0.345	0.329	0.328	0.327
4	0.340	0.329	0.328	0.327
12	0.328	0.328	0.328	0.327
20	0.320	0.328	0.327	0.326
28	0.325	0.328	0.326	0.324
36	0.340	0.329	0.324	0.322
44	0.338	0.325	0.320	0.318
52	0.310	0.316	0.313	0.312
60	0.284	0.294	0.301	0.304
68	0.277	0.280	0.287	0.294
76	0.280	0.281	0.283	0.287
84	0.284	0.286	0.287	0.288
92	0.295	0.295	0.293	0.291
100	0.304	0.299	0.295	0.291
108	0.297	0.294	0.290	0.287
116	0.265	0.270	0.274	0.286
124	0.258	0.258	0.259	0.262
132	0.249	0.249	0.250	0.250
140	0.240	0.240	0.240	0.251
148	0.232	0.232	0.232	0.232
156	0.224	0.224	0.224	0.224
164	0.216	0.216	0.216	0.216
172	0.208	0.208	0.208	0.208
180	0.201	0.201	0.201	0.201
184	0.197	0.197	0.197	0.197

Table A.1 Numeric data for Figures 7.1a and 7.1b - uncropped soil with no surface flux.

Depth (cm)	Day of Simulation			
	0	3	10	18
0	0.345	0.264	0.050	0.050
4	0.340	0.282	0.050	0.050
12	0.328	0.318	0.312	0.316
20	0.320	0.325	0.319	0.318
28	0.325	0.328	0.322	0.318
36	0.340	0.328	0.322	0.318
44	0.338	0.325	0.319	0.315
52	0.310	0.316	0.313	0.311
60	0.284	0.294	0.301	0.303
68	0.277	0.280	0.287	0.293
76	0.280	0.281	0.283	0.287
84	0.284	0.286	0.287	0.288
92	0.295	0.295	0.293	0.291
100	0.304	0.299	0.294	0.291
108	0.297	0.294	0.290	0.287
116	0.265	0.270	0.274	0.276
124	0.258	0.258	0.260	0.262
132	0.249	0.249	0.250	0.250
140	0.240	0.240	0.240	0.241
148	0.232	0.232	0.232	0.232
156	0.224	0.224	0.224	0.224
164	0.216	0.216	0.216	0.216
172	0.208	0.208	0.2018	0.208
180	0.201	0.201	0.201	0.201
184	0.197	0.197	0.197	0.197

Table A.2 Numeric data for Figure 7.2 - uncropped soil with surface evaporation.

Depth (cm)	Day of Simulation				
	0	3	6	10	18
0	0.345	0.299	0.266	0.229	0.166
4	0.340	0.299	0.267	0.231	0.170
12	0.328	0.299	0.269	0.235	0.178
20	0.320	0.300	0.272	0.241	0.187
28	0.325	0.303	0.277	0.247	0.198
36	0.340	0.306	0.280	0.253	0.207
44	0.338	0.304	0.280	0.255	0.212
52	0.310	0.295	0.274	0.251	0.217
60	0.284	0.274	0.257	0.237	0.206
68	0.277	0.263	0.247	0.230	0.199
76	0.280	0.266	0.252	0.236	0.211
84	0.284	0.274	0.262	0.248	0.226
92	0.295	0.285	0.294	0.262	0.243
100	0.304	0.291	0.281	0.270	0.256
108	0.297	0.287	0.279	0.270	0.257
116	0.265	0.265	0.262	0.258	0.252
124	0.258	0.258	0.258	0.258	0.257
132	0.249	0.249	0.249	0.249	0.250
140	0.240	0.240	0.240	0.240	0.241
148	0.232	0.232	0.232	0.232	0.232
156	0.224	0.224	0.224	0.224	0.224
164	0.216	0.216	0.216	0.216	0.216
172	0.208	0.208	0.208	0.208	0.208
180	0.201	0.201	0.201	0.201	0.201
184	0.197	0.197	0.197	0.197	0.197

Table A.3 Numeric data for Figure 7.3 - cropped soil with no surface flux. Evaporation front is indicated by shading.

Depth (cm)	Day of Simulation					
	0	3	6	10	14	18
0	0.345	0.236	0.086	0.050	0.050	0.050
4	0.340	0.257	0.148	0.050	0.050	0.050
12	0.328	0.297	0.271	0.241	0.216	0.196
20	0.320	0.304	0.280	0.252	0.229	0.209
28	0.325	0.308	0.286	0.260	0.238	0.220
36	0.340	0.311	0.289	0.264	0.244	0.227
44	0.338	0.309	0.289	0.265	0.247	0.231
52	0.310	0.300	0.282	0.261	0.244	0.230
60	0.284	0.278	0.265	0.248	0.233	0.221
68	0.277	0.267	0.254	0.239	0.225	0.214
76	0.280	0.270	0.258	0.244	0.232	0.225
84	0.284	0.276	0.267	0.255	0.245	0.237
92	0.295	0.287	0.278	0.268	0.260	0.253
100	0.304	0.293	0.285	0.279	0.274	0.268
108	0.297	0.289	0.282	0.274	0.268	0.264
116	0.265	0.266	0.264	0.261	0.258	0.256
124	0.258	0.258	0.258	0.258	0.258	0.257
132	0.249	0.249	0.249	0.249	0.250	0.250
140	0.240	0.240	0.240	0.240	0.241	0.241
148	0.232	0.232	0.232	0.232	0.232	0.232
156	0.224	0.224	0.224	0.224	0.224	0.224
164	0.216	0.216	0.216	0.216	0.216	0.216
172	0.208	0.208	0.208	0.208	0.208	0.208
180	0.201	0.201	0.201	0.201	0.201	0.201
184	0.197	0.197	0.197	0.197	0.197	0.197

Table A.4 Numeric data for Figures 7.4a and 7.4b - cropped soil with surface evaporation. The depth of the evaporation front is indicated by shading.

Depth (cm)	Day of Simulation		
	0	18 (Molz and Remson)	18 (Sink with Evap. Front)
0	0.345	0.050	0.050
4	0.340	0.050	0.050
12	0.328	0.183	0.166
20	0.320	0.198	0.182
28	0.325	0.209	0.195
36	0.340	0.218	0.205
44	0.338	0.222	0.210
52	0.310	0.222	0.218
60	0.284	0.214	0.206
68	0.277	0.208	0.199
76	0.280	0.217	0.213
84	0.284	0.232	0.226
92	0.295	0.247	0.245
100	0.304	0.256	0.262
108	0.297	0.259	0.259
116	0.265	0.254	0.253
124	0.258	0.257	0.257
132	0.249	0.250	0.250
140	0.240	0.241	0.241
148	0.232	0.232	0.232
156	0.224	0.224	0.224
164	0.216	0.216	0.216
172	0.208	0.208	0.208
180	0.201	0.201	0.201
184	0.197	0.197	0.197

Table A.5 Numeric data for Figure 7.5 - comparison of two sink terms, one with an evaporation front, the other without. The depth of the evaporation front is indicated by shading.

Depth (cm)	Day of Simulation			
	0	1	2	3
0	0.345	0.492	0.492	0.492
4	0.340	0.492	0.492	0.492
12	0.328	0.376	0.492	0.492
20	0.320	0.323	0.492	0.492
28	0.325	0.322	0.348	0.492
36	0.340	0.329	0.324	0.453
44	0.338	0.327	0.319	0.327
52	0.310	0.309	0.305	0.301
60	0.284	0.282	0.279	0.276
68	0.277	0.273	0.270	0.266
76	0.280	0.276	0.273	0.269
84	0.284	0.281	0.279	0.276
92	0.295	0.292	0.290	0.287
100	0.304	0.300	0.297	0.294
108	0.297	0.295	0.292	0.290
116	0.265	0.265	0.265	0.265
124	0.258	0.258	0.258	0.258
132	0.249	0.249	0.249	0.249
140	0.240	0.240	0.240	0.240
148	0.232	0.232	0.232	0.232
156	0.224	0.224	0.224	0.224
164	0.216	0.216	0.216	0.216
172	0.208	0.208	0.208	0.208
180	0.201	0.201	0.201	0.201
184	0.197	0.197	0.197	0.197

Table A.6 Numeric data for Figures 7.6a and 7.6b - cropped soil with three days of infiltration.

Depth (cm)	Day of Simulation						
	0	4	5	7	8	13	18
0	0.345	0.197	0.492	0.492	0.415	0.325	0.274
4	0.340	0.227	0.492	0.492	0.411	0.329	0.284
12	0.328	0.288	0.283	0.492	0.404	0.337	0.304
20	0.320	0.296	0.288	0.492	0.399	0.339	0.309
28	0.325	0.301	0.293	0.301	0.357	0.336	0.309
36	0.340	0.303	0.296	0.284	0.358	0.328	0.305
44	0.338	0.302	0.295	0.283	0.280	0.310	0.294
52	0.310	0.294	0.288	0.277	0.272	0.261	0.255
60	0.284	0.274	0.270	0.261	0.257	0.239	0.226
68	0.277	0.263	0.258	0.251	0.247	0.231	0.218
76	0.280	0.266	0.262	0.255	0.252	0.237	0.226
84	0.284	0.273	0.270	0.264	0.261	0.249	0.239
92	0.295	0.284	0.281	0.275	0.273	0.262	0.253
100	0.304	0.290	0.287	0.281	0.279	0.269	0.261
108	0.297	0.286	0.284	0.280	0.277	0.269	0.263
116	0.265	0.265	0.265	0.263	0.263	0.260	0.257
124	0.258	0.258	0.258	0.258	0.258	0.258	0.257
132	0.249	0.249	0.249	0.249	0.249	0.249	0.250
140	0.240	0.240	0.240	0.240	0.240	0.240	0.241
148	0.232	0.232	0.232	0.232	0.232	0.242	0.232
156	0.224	0.224	0.224	0.224	0.224	0.224	0.224
164	0.216	0.216	0.216	0.216	0.216	0.216	0.216
172	0.208	0.208	0.208	0.208	0.208	0.208	0.208
180	0.201	0.201	0.201	0.201	0.201	0.201	0.201
184	0.197	0.197	0.197	0.197	0.197	0.197	0.197

Table A.7 Numeric data for figures 7.7a, 7.7b, 7.7c and 7.7d - evaporation for four days, followed by infiltration for a further three days followed by 11 days of drying. The evaporation front depth is indicated by shading.

Depth (cm)	Day of Simulation						
	0	7	8	10	11	15	18
0	0.345	0.050	0.492	0.492	0.415	0.344	0.316
4	0.340	0.050	0.492	0.492	0.410	0.345	0.320
12	0.328	0.262	0.256	0.492	0.400	0.349	0.328
20	0.320	0.272	0.266	0.492	0.394	0.348	0.329
28	0.325	0.279	0.274	0.267	0.392	0.344	0.326
36	0.340	0.282	0.277	0.265	0.297	0.334	0.317
44	0.338	0.282	0.277	0.266	0.262	0.278	0.283
52	0.310	0.276	0.272	0.262	0.258	0.244	0.237
60	0.284	0.261	0.257	0.249	0.245	0.232	0.224
68	0.277	0.250	0.246	0.239	0.236	0.225	0.217
76	0.280	0.254	0.251	0.245	0.242	0.232	0.225
84	0.284	0.263	0.261	0.255	0.253	0.244	0.239
92	0.295	0.275	0.273	0.268	0.266	0.258	0.254
100	0.304	0.284	0.281	0.276	0.274	0.267	0.262
108	0.297	0.280	0.278	0.274	0.272	0.267	0.263
116	0.265	0.263	0.263	0.261	0.261	0.258	0.257
124	0.258	0.258	0.258	0.258	0.258	0.258	0.257
132	0.249	0.249	0.249	0.249	0.250	0.250	0.250
140	0.240	0.240	0.240	0.240	0.240	0.241	0.241
148	0.232	0.232	0.232	0.232	0.232	0.232	0.232
156	0.224	0.224	0.224	0.224	0.224	0.224	0.224
164	0.216	0.216	0.216	0.216	0.216	0.216	0.216
172	0.208	0.208	0.208	0.208	0.208	0.208	0.208
180	0.201	0.201	0.201	0.201	0.201	0.201	0.201
184	0.197	0.197	0.197	0.197	0.197	0.197	0.197

Table A.8 Numeric data for the full simulation illustrated in Figures 7.11a, 7.11b and 7.11c - seven days of drying followed by three days of infiltration followed by eight days of drying. The depth of the evaporation front is indicated by shading.

Depth (cm)	Day of Simulation		
	0	18 (Actual Data)	18 (Simulated Data)
0	0.345	0.030	0.030
2	0.340	0.050	0.030
6	0.335	0.100	0.132
10	0.330	0.139	0.161
14	0.324	0.161	0.171
18	0.320	0.183	0.179
22	0.320	0.207	0.186
26	0.323	0.226	0.192
30	0.329	0.240	0.198
34	0.335	0.250	0.202
38	0.341	0.258	0.206
42	0.340	0.260	0.212
46	0.332	0.259	0.211
50	0.317	0.241	0.211
54	0.300	0.226	0.213
58	0.288	0.213	0.207
62	0.280	0.209	0.199
66	0.277	0.209	0.200
70	0.277	0.214	0.199
74	0.278	0.222	0.208
78	0.280	0.230	0.212
82	0.282	0.239	0.223
86	0.286	0.248	0.231
90	0.292	0.260	0.241
94	0.299	0.272	0.249
98	0.303	0.281	0.252
102	0.304	0.281	0.255
106	0.302	0.281	0.256
110	0.290	0.272	0.255
114	0.275	0.257	0.252
118	0.255	0.240	0.245
120	0.248	0.231	0.231

Table A.9 Numeric data for Figure 7.10 - Comparison of the actual data of Olsson and Rose (1988) and of the simulation with $\Delta z = 4$ cm and $\Delta t = 1$ day.

APPENDIX E

FINITE DIFFERENCE SINK TERMS

In section 6.1.3 the continuous form of the model was couched in finite difference terms. As was pointed out the sink term needs to be evaluated at the same point in time and space as the other terms. Since the Crank-Nicolson method was used this point was $(z_{i+1/2}, t_{j+1/2})$. This section compares the effect of the sink term evaluated at this point and the sink term used in the model which was evaluated at $(z_{i+1/2}, t_j)$. The input data and parameters were the same as that used in section 7.3 with the following differences:

- $\Delta t = 1$ day and $\Delta z = 10$ cms,
- Depth of profile = 120 cms,
- evapotranspiration data was extended by one time step with the 19th 'day' the same as the 18th 'day',
- Upper surface evaporative flux condition maintained for the length of the run (18 timesteps),
- The initial profile is given in Table A.10.

The sink term evaluated at the half timestep ahead was determined by arithmetically averaging sinks on the *j*th and *(j+1)*th days. After running the comparative simulation for 18 timesteps it could be seen that the two profiles did differ as indicated in Table A.10. Given that the accuracy of the time and depth steps used was two-decimal places the difference is significant.

The results were as expected since the transpiration data used in this instance reduced over time. As the daily transpiration rate formed the upper bound for the sum of the

Depth (cm)	Day of Simulation Water Contents		
	0 Initial Profile	18 (using S^j)	18 (using $S^{j+1/2}$)
0	0.345	0.050	0.050
5	0.336	0.050	0.050
15	0.325	0.173	0.178
25	0.322	0.193	0.199
35	0.338	0.206	0.229
45	0.336	0.213	0.216
55	0.296	0.214	0.210
65	0.277	0.198	0.199
75	0.278	0.217	0.208
85	0.285	0.229	0.229
95	0.300	0.255	0.249
105	0.303	0.258	0.257
115	0.272	0.252	0.252
120	0.248	0.231	0.231

Table A.10 Comparison of two sink terms, one evaluated at the *j*th timestep, the other evaluated at the *(j+1/2)*th timestep. Two decimal place accuracy discrepancies are shaded.

sink terms over the rooting depth for any one day, then the effect of the averaging led to reduced uptake as demonstrated in the wetter layers for the sink term calculated at one half day ahead as shown in Table A.10. The reason for the upper layers being wetter and the lower layers much the same is that the distribution of uptake of the sink term employed in this case was greater in the upper layers and depends on the depth of the evaporation front. With greater evapotranspiration in the S^j term the evaporation front lowered quicker and resulted in greater withdrawal from the top layers as opposed to that due to the S^{j+1}.

The level of this significance of the difference between the two terms could well depend on the context within which the simulation was conducted. That is to say, whether the simulation was used as a predictor of the field situation given only current measured data or whether the model was being used to determine how well it represented reality in retrospect. To elaborate, it would be dictated by the circumstances that the simulation was designed for as to which term could be used. If the simulation was designed to test the accuracy of the numerical solution of the model as compared to measured field data then the forward evapotranspiration data in time would be known and the only term to use would be the proper Crank-Nicolson term, that is, $S^{j+1/2}$. If however the simulation was to be used to predict the relative distribution of water down the profile given the current days evapotranspiration data only as a decision making tool for irrigation scheduling, then the approximate S^j term could be used. As the simulations in this case were in a context where the $(j+1)$th days evapotranspiration data is not known *a priori*, the S^j term was used with the subsequent loss in fidelity.