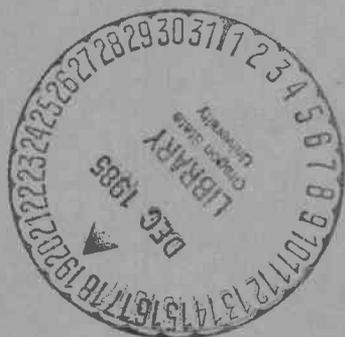


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# OR-NATURE: THE NUMERICAL ANALYSIS OF TRANSPORT OF WATER AND SOLUTES THROUGH SOIL AND PLANTS

## VOLUME I. THEORETICAL BASIS



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OR-NATURE: THE NUMERICAL ANALYSIS OF  
TRANSPORT OF WATER AND SOLUTES THROUGH SOIL AND PLANTS

VOLUME 1. THEORETICAL BASIS

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This is one of five volumes about numerical analysis  
of water and solute transport through soil.

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## FOREWORD

This report presents numerical solutions for the problems of transient, one-dimensional transfer of water and solutes in the layer of soil important for plant growth. It presents solutions to problems of infiltration of rainfall or irrigation water, evaporation, redistribution of water in the soil, and uptake of water and nutrients by plant roots. The numerical analysis presented in this report was prepared in response to the recognition that computer programs which deal with these problems are usually only applicable to very specific problems and are not easily generalized. This report was written on the premise that a manual should be available for the numerical analysis of these problems, one which can be used by persons not highly skilled in using computers. The program can be used by research workers who have a limited understanding of computer programming.

The report is presented in five volumes. The first volume gives the theoretical background of the program and should be of most interest to research workers familiar with the mathematical analysis of the problem and computer programming. The second volume presents the manual for the use of the program. The user does not have to be familiar with, or understand, the content of the first volume to use the manual. A discussion of potential numerical problems and a listing of computer generated error messages are given in Volume three. The fourth volume presents examples of the use of the program, and the fifth volume is a listing of the program.

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This publication reports work initiated under a Research Grant from the Pacific Northwest Forest and Range Experiment Station, Portland, Oregon, entitled "Physical and Chemical Factors Affecting the Transport and Distribution of Nutrient Ions in Soils Developed on Volcanic Materials" (FSPNW-GRANT Number 20). Dr. L. Boersma was project leader. Michael Unga and Suntaree Akrotanakul were graduate students at Oregon State University during the conduct of the studies reported here.

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OR-NATURE: THE NUMERICAL ANALYSIS OF  
TRANSPORT OF WATER AND SOLUTES THROUGH SOIL AND PLANTS  
VOLUME I. THEORETICAL BASIS

1. THEORETICAL BASIS OF THE MODEL

1.1 Introduction

The interest of soil scientists in the development of the capability to describe transfer processes in soils was prompted by the desire to be able to predict accurately the behavior and movement of water, solutes, and energy in the soil as it affects plant growth.

This interest received renewed emphasis from recent concerns about the impact of agricultural and forestry practices on water quality. The basic goal of forestry and agriculture is to manage the land for maximum rate of production of fiber and food. Although this effort has been successful, it has not been without cost or sacrifice. Management practices have resulted in increased erosion and have added to the natural burden of nutrient elements in streams.

There are many misunderstandings about the consequences of specific management practices on degradation of soils, groundwater, and surface waters. These can only be resolved by a clear understanding of the transfer processes in soils and the effect of management practices on these transfer processes. Further interest in the prediction of transfer processes in soil was prompted by the growing use of land for the disposal of a wide variety of waste products. There is an urgent need to predict the long-term consequences of these practices with respect to the quality of soil and groundwater.

This report considers the transient, one-dimensional problem of water and solute movement in the layer of soil important for plant growth. It considers problems of infiltration of rainfall or irrigation water, evaporation, redistribution of water in the soil, and uptake of water by plant roots.

The distribution of ions in soils is determined by sources and sinks, the form of the exchange isotherm, the exchange equilibria, diffusion and dispersion, convection, and storage and release by plant material. The part played by each of these factors is shown in Figure 1.1. Soil pores are assumed to be filled with water with a high concentration of ions near the surface. An equilibrium exists between ions in water (free phase) and ions retained on exchange sites of soil particles (sorbed phase). As a result of concentration gradients in the pore water, diffusion occurs. Some of the ions at the moving diffusion front are removed from the free phase by adsorption onto soil particles, thus maintaining a concentration gradient. Movement of ions as a result of mass flow of water also occurs. It is accompanied by sorption at the moving front and desorption at the tail. When mass flow occurs, diffusion is usually less important. Ions which are not removed from the root zone with water passing through it are available as plant food. This sink is no longer present when vegetation is removed and the potential then exists for nutrient loss from the soil to the ground water.

#### 1.1.1 The Sources of Ions

The ions in the soil solution are obtained from many sources. The natural soil system releases ions to the soil solution as a result of the dissolving action of soil water. The rate at which ions go into solution depends on, among other variables, the pH, the temperature of the water and the rate of removal of the ions by the leaching process. In a dynamic system with plants present, ions also become available from the decaying material at the soil surface and roots below the soil surface.

The natural system can be disturbed by activities of man. Among the disturbances are application of fertilizers to vegetation, removal of trees, and burning. When crops are removed, much organic material is left at the soil surface. The disturbance with respect to the ion balance involves, first of all, the removal of the sink. Ions removed by plant growth are available for leaching. An ion source at the soil surface also is added from decaying organic material.

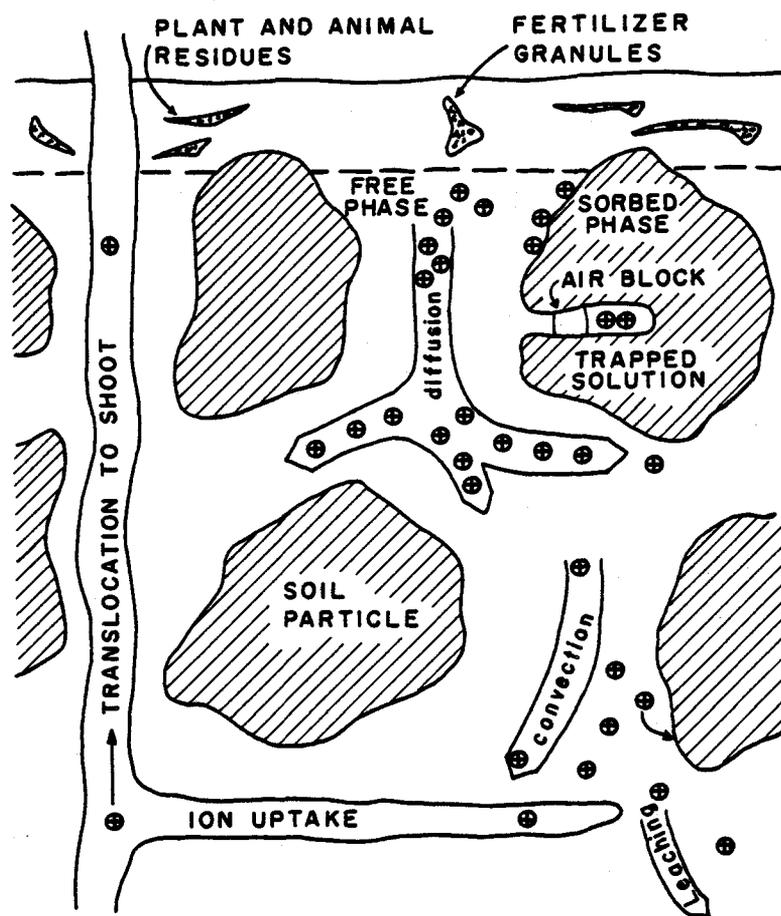


Figure 1.1 Schematic diagram of the mechanisms involved in the distribution of chemicals in soils.

A different situation arises when soil is used for disposal of waste materials. These can be in the form of solid waste or liquid waste. In this case, the loading of the soil with chemicals is greatly increased and the ability of the soil to absorb the materials is not clearly understood. This report presents numerical methods which may be used in the analysis of transfer problems through soils.

### 1.1.2 The Translocation Processes

The principles of diffusion and dispersion as well as exchange mechanisms between the free and sorbed phases are well understood and have been described in detail (Graham-Bryce, 1963; Frissel and Poelstra, 1967; Frissel, Poelstra, and Reiniger, 1970; Lindstrom and Boersma, 1970; Lindstrom and Boersma, 1971; Nye and Tinker, 1977). On a field

scale, the problem of ion translocation, however, is, very complex and has not been treated in a quantitative manner. The greatest complications are brought about by continuous changes in soil water content. A simple series of events may be recognized. In many areas, soils are at or near freezing temperatures while a layer of snow accumulates on the surface. In early spring, snow melts and water enters the soil to gradually increase the water content. During this time, adsorbed ions go into solution, diffusion to lower soil layers occurs, and ions may become evenly distributed throughout the soil profile.

What happens as the seasons progress depends on the amount of water available. In some geographic regions, there is just enough water to saturate the profile without deep seepage occurring. The nutrients remain in solution where they are available for plant growth. If more water is available, it passes through the profile and carries ions with it. The sequence of events described on a seasonal scale also occurs on a shorter time base within a season as during a series of drying and wetting periods resulting from intermittent rainfall.

Predicting ion movement in soils is clearly a complex problem. There is extensive literature about the movement of chemicals through soils (Nye and Tinker, 1977; Frissel, 1978). Little use has been made of this information for quantitative predictions. This lack of practical application of existing theory must be attributed to the problem of applying solutions developed for idealized steady-state systems to situations where nonisotropism is important, the boundary conditions are ill-defined, and the processes are transient in nature.

Given these circumstances, it is not surprising that the advances which have been made in the development of predictive capabilities have been based on sampling techniques. In this approach, a high volume of data is collected with the hope that upon analysis, results will show sequences which can be correlated with certain physical and chemical properties of the systems (Gessel and Cole, 1965; Johnson et al., 1968; Keller, 1970).

For example, a seasonal cycle in the concentration of a certain ion in streams may be observed which is correlated with changes in physical properties of a watershed. The properties of the watershed can be

changed--through vegetation removal, for example--and how the previously observed stream concentrations change can be determined.

Such a procedure has many drawbacks. It is costly and very slow. Several years of data collection are required to calibrate the system. Upon imposing the desired perturbations on the system many additional years of data collection are required and, in the end, even upon establishment of certain correlations, it is still difficult to assign fundamental explanations to causal relationships.

The problem also may be approached through numerical analysis. In this case, a mathematical model is developed which is based on a physical description of the process to be studied. Analytical models differ from statistical models. They are based on a statement of physical laws which govern the process to be studied, and may be for steady-state or transient conditions. This report describes a procedure for the numerical analysis of the problem of water and chemical transport in soils.

## 1.2 Flow of Water

The general partial differential equation of flow of water in soil in a vertical direction is given by Philip (1969) as

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K(\theta) \frac{\partial \psi}{\partial z} \right] - \frac{\partial K(\theta)}{\partial z} \quad \left[ \frac{L_w^3}{L^3/T} \right], \quad (1.1)$$

where  $\theta$  is the volumetric water content  $[\frac{L_w^3}{L^3}]$ ;  $\psi$  is the matric potential of the soil water  $[L_p]$ , which is a negative quantity when the soil is unsaturated;  $z$  is the vertical coordinate  $[L]$ , positive downwards;  $t$  is time  $[T]$ ; and  $K(\theta)$  is the hydraulic conductivity  $[\frac{L_w^3}{L^2/T}]$ . Equation (1.1) is usually solved as a function of water content rather than matric potential, to reduce the effect of hysteresis in the hydraulic conductivity function (Hillel, 1971) and to reduce the large change in the hydraulic conductivity during infiltration of dry soils.

Equation (1.1) holds for homogeneous soils as long as the effects of hysteresis on the function  $K(\theta)$  are ignored. It cannot be used to describe conditions where deep surface ponding occurs or where a fluctuating water table occurs. However, it can be used with saturated boundaries such as those which occur with shallow ponding or a fixed water

table. The equation will be solved using either the volumetric water content,  $\theta$ , or the water potential  $\psi$  as the dependent variable. Both solutions are computed and are printed out by the computer program OR-NATURE. A solution using the diffusivity potential obtained by the Kirchhoff transformation will also be presented.

### 1.2.1 Solution Based on $\theta$

In a homogeneous soil where  $K$  and  $\psi$  are single-valued functions of  $\theta$ , i.e., no hysteresis, a function  $D$  may be defined such that

$$D = K \frac{\partial \psi}{\partial \theta} \cdot \text{CNVRSN} \quad [L^2/T], \quad (1.2)$$

where CNVRSN converts the units of potential to the units of pressure head. The function  $D$  is called the diffusivity function. This nomenclature is based on its analogy to thermal diffusivity.

The transient, isothermal, one-dimensional equation based on water content for the vertical movement of water with a root sink term can then be written as

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} [-q_z] + A(z, \theta, \psi_{ps}) \quad [L_w^3/L^3/T], \quad (1.3a)$$

$$q_z = -D(\theta) \frac{\partial \theta}{\partial z} + K(\theta) \quad [L_w^3/L^2/T] \quad (1.3b)$$

where  $\psi_{ps}$  is the water potential  $[L_p]$  in the plant at the point where the plant stem intersects the soil surface,  $A(z, \theta, \psi_{ps})$  is the rate of water uptake  $[L_w^3/L^3/T]$  by roots at a depth  $z$ , and  $q_z$  is the volumetric or Darcian flux  $[L_w^3/L^2/T]$ . The root uptake function  $A$  is a negative quantity. It is further described in Section 1.4.

There is no general analytical solution for Equation (1.3) because the functional relationships between  $D$  and  $\theta$  and  $K$  and  $\theta$  are non-linear. Typically,  $D$  and  $K$  vary through five to six orders of magnitude when the soil water content ranges from wet to dry (Figure 1.2). Philip (1955, 1957) developed quasi-analytical solutions to Equation (1.3) for several sets of special boundary conditions (Vol. III, Section 6.5). Most of the quasi-analytical solutions use the Boltzmann similarity transform.

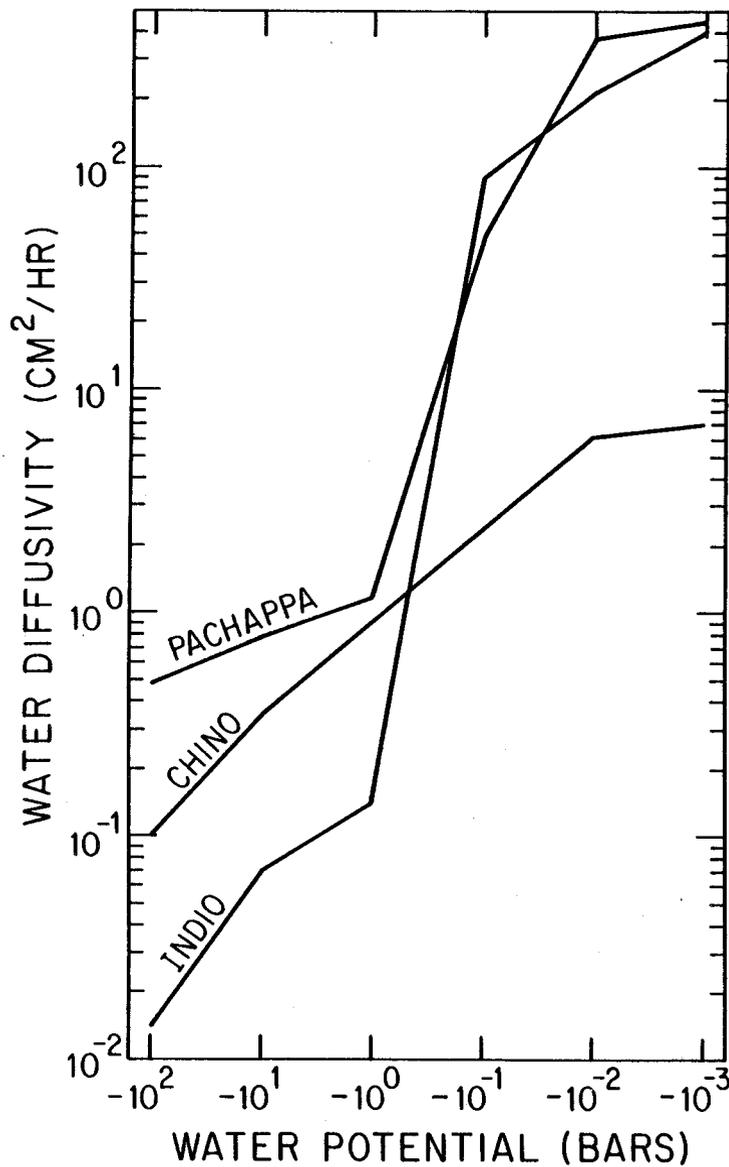
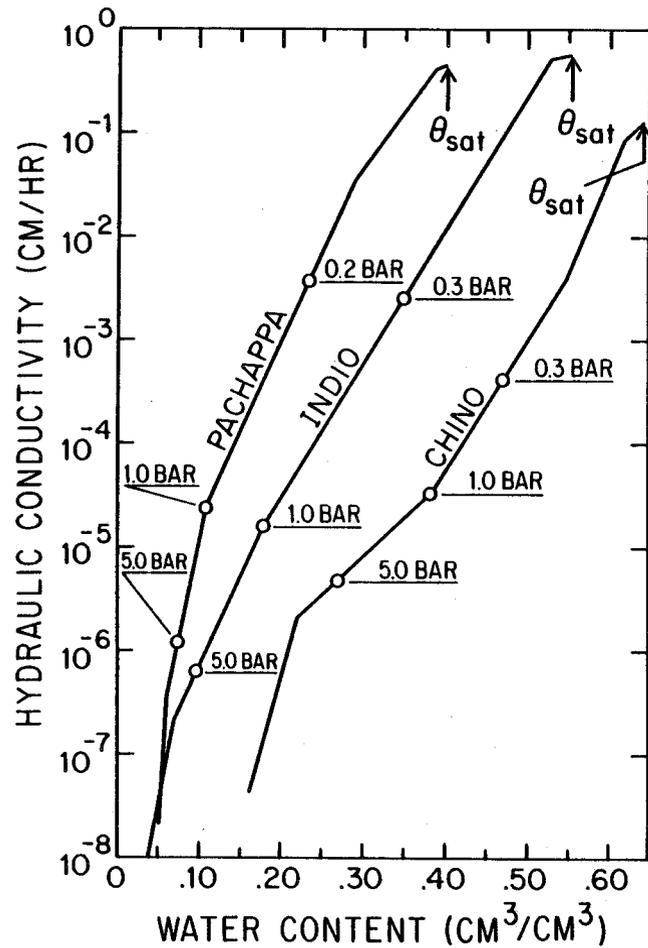


Figure 1.2. a. Soil water diffusivity as a function of soil water content. Functions shown were drawn after Gardner (1960).



b. Hydraulic conductivity as a function of soil water content. Functions shown were drawn after Gardner (1960).

This technique can not be used when flux type boundary conditions are specified. The Kirchhoff transform of the flow equation, however, can be used and is described in Section 1.2.3. The case where A is zero has been solved numerically by many investigators, including Hanks and Bowers (1969), Rubin and Steinhardt (1963), and Bresler (1973).

The water content is subject to the physical constraints that

$$\theta_d \leq \theta(z,t) \leq \theta_s \quad [L_w^3/L^3], \quad (1.4)$$

where the subscripts d and s denote air-dry and saturated conditions. For computational purposes, Feddes et al. (1974) determined that in the absence of field data one may define  $\theta_d$  as the water content which is at equilibrium with an environment at very low relative humidity,

$$\theta_d = \theta(\psi_d) \quad [L_w^3/L^3], \quad (1.5)$$

such that the potential

$$\psi_d = \left[ \frac{RT_o}{M_w g} \ln(RH) \right] / CNVRSN \quad [L_p], \quad (1.6)$$

where R is the universal gas constant ( $ML^2/T^2/^\circ K/mole$ ),  $T_o$  is the absolute temperature [ $^\circ K$ ],  $M_w$  is the molecular weight of water [ $M/mole$ ], g is the acceleration due to gravity [ $L/T^2$ ], and RH is the relative humidity of the air above the soil surface, given as a ratio.

The matric potential can be obtained by using the soil-water characteristic curve to convert from water content to water potential. Ignoring hysteresis and assuming the soil to be homogeneous, the soil-water characteristic curve gives a unique, one-to-one relationship between matric potential and water content (Figure 1.3). Such a curve,  $\psi(\theta)$ , must be experimentally determined and is unique for each specific soil.

To obtain a unique solution to Equation (1.3), the initial condition and the upper and lower boundary conditions in the soil column must be specified.

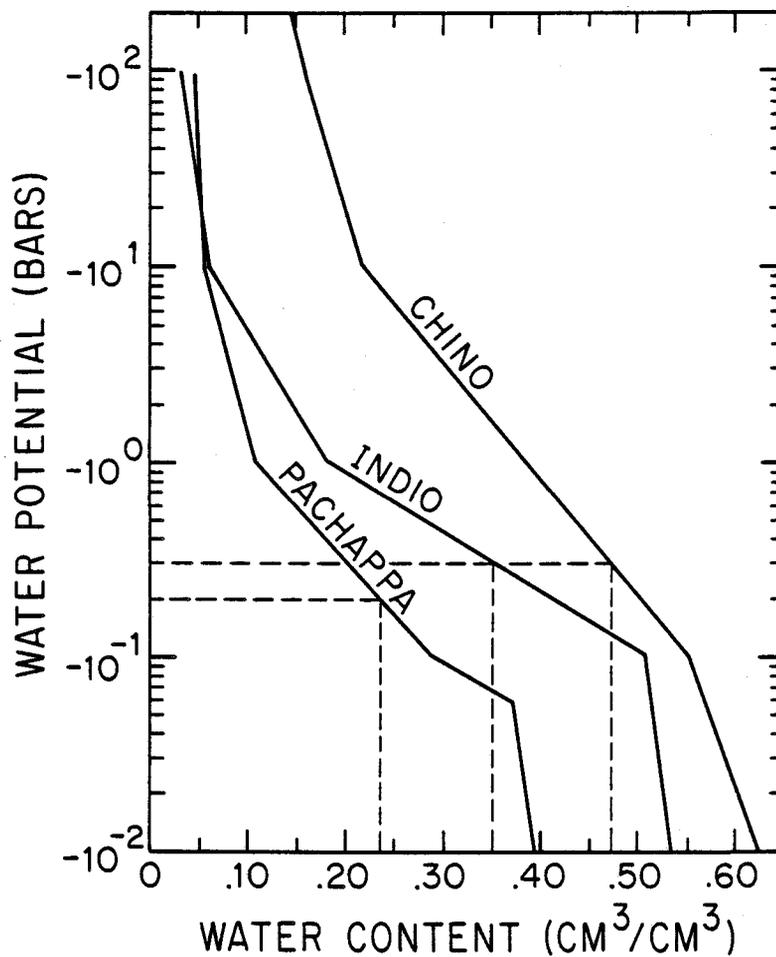


Figure 1.3. Soil water potential as a function of soil water content. Functions shown were drawn after Gardner (1960).

The initial condition is expressed as

$$\theta(z,0) = \theta_0(z), \quad t = 0, \quad 0 \leq z \leq z_{\max} \quad [L^3/L^3], \quad (1.7)$$

where  $z_{\max}$  is the depth [L] of the lower boundary and the subscript 0 denotes the initial condition. Hence, the initial water content of the soil is a function of depth only and is obtained from field data. The initial soil water content  $\theta_0(z)$  does not have to be constant with depth.

The three most common boundary conditions that may be specified are the Dirichlet, the Neumann, and the flux boundary conditions, also referred to as 1st, 2nd, and 4th type boundary conditions.

1st type: Dirichlet, specifies the water content,  $\theta$ .

2nd type: Neumann, specifies the water content gradient,  $\frac{\partial \theta}{\partial z}$ .

4th type: specifies the surface flux,  $R = -D \frac{\partial \theta}{\partial z} + K$ .

Calling the flux condition a 4th type boundary condition is arbitrary but strictly speaking, there is no 3rd type boundary condition. A truly 3rd type boundary condition would be of the form  $[a\theta + b(\partial\theta/\partial z)]$ , where  $a$  and  $b$  are coefficients independent of  $\theta$ . The 3rd type boundary condition as defined here does not occur in soil systems.

Boundary conditions must be independently specified for the upper and lower surfaces. The upper surface is located at  $z = 0$  and the lower surface at  $z = z_{\max}$  for either vertical or horizontal coordinate orientations. Table 1.1 lists the typical types of boundary conditions that may be encountered.

Table 1.1. Types of boundary conditions for the flow equation based on water content

Physical process	Type of boundary condition
Evaporation (surface flux)	4
Infiltration (surface flux)	4
Redistribution (zero flux)	4
Shallow surface ponding (surface irrigation)	1
Stationary water table at lower surface*	1
Semi-infinite soil column	2
Impervious barrier to water (reflective boundary)	2

\*The model presented here cannot be used with a fluctuating water table.

Typical boundary conditions that may be encountered are illustrated by the following example. Consider a soil column sufficiently long so that there is no change in the water content gradient at the lower boundary. A flux condition is specified on the upper boundary.

- i) At the lower boundary of soil column,  $z = z_{\max}$ , a second or Neumann type boundary condition specifies that there is no change in the water content gradient

$$\frac{\partial \theta}{\partial z} (z_{\max}, t) = 0, \quad t \geq 0 \quad \left[ \frac{L^3}{w L^4} \right]. \quad (1.8)$$

ii) At the upper boundary,  $z = 0$ , a general flux condition is specified by

$$- D \frac{\partial \theta}{\partial z} + K = R(0,t) \quad [L_w^3/L^2/T], \quad (1.9)$$

where  $R(0,t)$  equals the potential surface flux,  $[L_w^3/L^2/T]$ , after accounting for irrigation, rainfall, and evaporation rates. The three most common cases considered for  $R(0,t)$  are characterized by:

$$\begin{aligned} R(0,t) > 0 & \quad \text{infiltration} \\ R(0,t) = 0 & \quad \text{redistribution or drainage} \\ R(0,t) < 0 & \quad \text{evaporation} \quad [L_w^3/L^2/T]. \end{aligned} \quad (1.10)$$

Note that the flux has a positive value when the flux moves in the positive  $z$  direction (e.g., downwards) and a negative value when the flux moves in the negative  $z$  direction (e.g., upwards).

It should be pointed out that the "potential" flux rate,  $R(0,t)$ , for a given soil depends only on atmospheric conditions and is specified as a function of time. The actual flux across the surface,  $q(0,t)$ , is determined by the ability of the soil to transmit water through the soil surface. Thus, the exact flux at the soil surface cannot be predicted a priori but is subject to the condition that its magnitude be as large as possible, but not greater than the magnitude of the potential rate,

$$|q(0,t)| \leq |R(0,t)| \quad [L_w^3/L^2/T] \quad (1.11)$$

and that the resulting water content profile does not violate the air-dry and saturation limits of Equation (1.4). In general, the potential flux,  $R(0,t)$ , is specified and the computer program solves for the actual surface flux,  $q(0,t)$ , subject to Equations (1.4) and (1.11) by iteration. Additional details are given in Section 3.4.

### 1.2.2 Solution Based on $\psi$

The flow equation for transient, isothermal, one-dimensional conditions with flow in the vertical direction can be written in terms of matric potential as

$$\frac{\partial \psi}{\partial t} \left( \frac{\partial \theta}{\partial \psi} \right) = \frac{\partial}{\partial z} \left[ K \frac{\partial \psi}{\partial z} \cdot \text{CNVRSN} - K \right] + A(z, \psi, \psi_{ps}) \quad (1.12)$$

$$[L_w^3/L^3/T],$$

where  $(\partial\theta/\partial\psi)$  is the "specific water capacity," i.e., the slope of the soil-water characteristic curve. All other terms were defined earlier. Equations (1.3) and (1.12) are numerically identical, even though the notation is different. The soil-water characteristic function,  $\theta(\psi)$ , is needed to evaluate the specific water capacity term and to convert matric potential to volumetric water content. Thus, when Equation (1.12) is solved numerically, the computer program converts the potential to water content when evaluating  $K(\theta)$ .

The solution of Equation (1.12), the potential-based flow equation, is subject to the limits on water content at air-dry and saturated conditions, initial conditions, and boundary conditions. The range of matric potentials is bounded by the potentials for air-dry and saturated soils

$$\psi_d \leq \psi(z, t) \leq \psi_s \quad [L_p]. \quad (1.13)$$

In general, saturation is defined by

$$\psi_s = 0 \quad [L_p]. \quad (1.14)$$

Matric potential is defined as a negative quantity when the soil is unsaturated and a positive or zero quantity when the soil is saturated. The flow equation based on matric potential (Equation 1.12) is valid only for unconfined, unsaturated ( $\psi \leq 0$ ) soil conditions. However, Equation (1.12) can be used when the soil is saturated at the boundary ( $\psi \geq 0$ ). Thus, either surface ponding or a stationary water table can be specified at the boundaries.

The initial condition is:

$$\psi(z, 0) = \psi_0(z) \quad \text{at } t = 0, \quad 0 \leq z \leq z_{\max} \quad [L_p], \quad (1.15)$$

where subscript 0 denotes the initial condition.

The boundary conditions for the upper and lower boundaries are identical to those of the equations based on water content with appropriate changes in notation. The three types of boundary conditions are defined as

1st type: specified potential,  $\psi$ ,

2nd type: specified gradient,  $\frac{\partial \psi}{\partial z}$ ,

4th type: specified surface flux,  $R = -K \frac{\partial \psi}{\partial z} \text{ CNVRSN} + K$ .

### 1.2.3 Solution Based on Diffusivity Potential (Kirchhoff Transform)

Numerous investigators, including Remson et al. (1971), Bear (1972), and Braester (1972), introduce a new variable, called the diffusivity potential,  $F$ . A variable of this type is usually referred to as a Kirchhoff transform variable and is defined as either

$$F(\theta) = \int_{\theta'=\theta_d}^{\theta} D(\theta') d\theta' \quad [L_w^3/L/T], \quad (1.16)$$

or as

$$F(\psi) = \text{CNVRSN} \int_{\psi'=\psi_d}^{\psi} K(\psi') d\psi' \quad [L_w^3/L/T], \quad (1.17)$$

where  $D(\theta)$  is the soil water diffusivity and  $K(\theta)$  is the hydraulic conductivity. For a given soil-water characteristic curve,  $\theta$  and  $\psi$  are uniquely related, hence

$$F(\theta) = F(\psi) \quad [L_w^3/L/T]. \quad (1.18)$$

Braester (1972) gives several tables of  $F$  for different soils. The lower limit of  $F$  is defined as

$$F(\theta_d) = 0 \quad [L_w^3/L/T], \quad (1.19)$$

$$F(\psi_d) = 0 \quad [L_w^3/L/T]. \quad (1.20)$$

$F$  is always defined as a positive quantity which monotonically increases in value when going from air-dry to saturated conditions.

Using the Leibnitz rule for differentiating an integral obtains the following by differentiating Equations (1.16) and (1.17):

$$\frac{\partial F}{\partial t} = \frac{\partial \theta}{\partial t} D; \quad \frac{\partial F}{\partial t} = \text{CNVRSN} \cdot \frac{\partial \psi}{\partial t} K \quad [L_w^3/L/T^2], \quad (1.21)$$

$$\frac{\partial F}{\partial z} = \frac{\partial \theta}{\partial z} D; \quad \frac{\partial F}{\partial z} = \text{CNVRSN} \cdot \frac{\partial \psi}{\partial z} K \quad [L_w^3/L^2/T]. \quad (1.22)$$

Substitution of the Kirchhoff transform from Equations (1.21) and (1.22) into Equation (1.3) obtains the transformed flow equation

$$\frac{1}{D} \cdot \frac{\partial F}{\partial t} = \frac{\partial}{\partial z} \left( \frac{\partial F}{\partial z} - K \right) + A \quad [L_w^3/L^3/T]. \quad (1.23)$$

Similarly, the flow equation based on matric potential (Equation 1.12) reduces to

$$\frac{\partial \theta}{\partial F} \cdot \frac{\partial F}{\partial t} = \frac{\partial}{\partial z} \left( \frac{\partial F}{\partial z} - K \right) + A \quad [L_w^3/L^3/T], \quad (1.24)$$

where D and K are now expressed as functions of F.

The Kirchhoff transformed flow equation based on the water content according to Equation (1.23) is uniquely specified with the addition of the initial condition and boundary conditions. The initial condition is defined as

$$F(z,0) = \int_{\theta'=\theta_d}^{\theta(z,0)} D d\theta' \quad [L_w^3/L/T], \quad (1.25)$$

where  $\theta(z,0)$  is the initial water content of Equation (1.7). The 1st type boundary condition is computed as

$$F(z',t) = \int_{\theta'=\theta_d}^{\theta(z',t)} D d\theta' \quad [L_w^3/L/T], \quad (1.26)$$

where  $z'$  refers to the boundary  $z = 0$  or  $z_{\max}$  and where  $\theta(z',t)$  is the specified water content at the boundary. The 2nd type boundary condition is computed as

$$\frac{\partial F}{\partial z} (z',t) = \text{RHS}(t) \cdot D \quad [L_w^3/L^2/T], \quad (1.27)$$

where  $\text{RHS}(t) = \frac{\partial \theta}{\partial z}(z', t)$  is a specified function of time on the boundary (e.g., Equation (1.8)) and where  $D$  is the soil water diffusivity evaluated at the boundary. The 4th type boundary condition is computed as

$$-\frac{\partial F}{\partial z} + K = \text{RHS}(t) \quad [L_w^3/L^2/T], \quad (1.28)$$

where  $\text{RHS}(t) = (-D \frac{\partial \theta}{\partial z} + K)$  is a specified surface flux (e.g., Equation (1.9)).

The range of the transform variable is

$$F_d \leq F(z, t) \leq F_s \quad [L_w^3/L/T], \quad (1.29)$$

where  $F_s = F(\theta_s)$  and  $F_d = F(\theta_d)$ .

The Kirchhoff transformed flow equation can also be expressed in terms of matric potential, such as in Equation (1.24). Then the initial condition is

$$F(z, 0) = \int_{\psi'=\psi_d}^{\psi(z, 0)} K d\psi' \cdot \text{CNVRSN} \quad [L_w^3/L/T], \quad (1.30)$$

where  $\psi(z, 0)$  is the initial matric potential of Equation (1.15). The 1st type boundary condition, at  $z = 0$  or  $z = z_{\max}$  is

$$F(z', t) = \int_{\psi'=\psi_d}^{\psi(z', t)} K d\psi' \cdot \text{CNVRSN} \quad [L_w^3/L/T], \quad (1.31)$$

where  $\psi(z', t)$  is the specified matric potential at the boundary. The 2nd type boundary condition is

$$\frac{\partial F}{\partial z}(z', t) = \text{RHS}(t) \cdot K \cdot \text{CNVRSN} \quad [L_w^3/L^2/T], \quad (1.32)$$

where  $\text{RHS}(t) = \frac{\partial \psi}{\partial z}(z', t)$  is a specified function of time on the boundary and where  $K$  is the conductivity evaluated at the boundary. The 4th type boundary condition is

$$-\frac{\partial F}{\partial z} + K = \text{RHS}(t) \quad [L_w^3/L^2/T], \quad (1.33)$$

where  $\text{RHS}(t) = (-K \frac{\partial \psi}{\partial z} \cdot \text{CNVRSN} + K)$  is a specified surface flux. The range of the transform variable is the same as in Equation (1.29).

#### 1.2.4 Choice of Flow Equation to Use

Four forms of the flow equation have been described, i.e.,  $\theta$ ,  $\psi$ ,  $F(\theta)$ ,  $F(\psi)$ . The four expressions are numerically equivalent. They only differ in the dependent variable which is chosen for expressing changes in water content and in the manner in which the changes are calculated. It is difficult to decide beforehand which equation to use. Some comments can be made which may be helpful in making this choice.

- a) Conceptually, all solutions of the flow equation are the same. However, each solution is subject to a different type of numerical error.
- b) The flow equation based on water content  $\theta$  is usually the simplest to solve and has the least number of numerical steps.
- c) The Kirchhoff transform,  $F$ , is best used in conjunction with problems with infiltration into a soil which is initially very dry and has a high rate of infiltration.
- d) The Kirchhoff transform technique requires the greatest number of numerical steps and hence is subject to more numerical error and takes more time.
- e) It may be useful to try all four flow variables for a few time steps and then compare the results for speed of convergence and for accuracy. An estimate of accuracy is obtained by checking the mass balance that is printed out by the program.
- f) It is useful to use the Kirchhoff transform for the first few time steps when describing the rapid wetting of an initially dry soil, then switch back to the non-transform flow equation after the water profile has become stable. This is done by using the START procedure, which is explained later (Vol. II, Section 4.5.3).
- g) Solving in terms of matric potential avoids the need to evaluate the diffusivity coefficient,  $D(\theta)$ . However, it is then necessary to determine the soil-water characteristic function  $\theta(\psi)$ .
- h) In general, if one has a choice in using either  $\theta$  or  $\psi$ , use  $\theta$ .

### 1.3 Solute Displacement Equation

The displacement of solute by mass flow of water is described by Dutt et al. (1972) and Bresler (1973) as follows:

$$\frac{\partial\{\theta c\}}{\partial t} = \frac{\partial}{\partial z} \left\{ \theta D_{sz} (v) \frac{\partial c}{\partial z} \right\} - \frac{\partial\{q_z c\}}{\partial z} - \frac{\partial S}{\partial t} + G(z, t, \theta, c, S) \quad (1.34)$$

$[M/L^3/T],$

where  $c$  is the solute concentration in solution (liquid phase)  $[M/L_w^3]$ ,  $S$  is the local solute concentration in the sorbed or solid phase  $[M/L^3]$ ,  $D_{sz}$  is the apparent solute dispersion coefficient  $[L^2/T]$ ,  $G$  is the solute source/sink term  $[M/L^3/T]$ ,  $q_z$  is the volumetric or Darcian flux  $[L_w^3/L^2/T]$ ,  $v$  is the magnitude of the pore-water velocity,  $v = |q_z/\theta|$   $[L/T]$ , and  $t$  is the time  $[T]$ .

The first term on the right-hand side of Equation (1.34) describes the solute flux caused by diffusion and by hydrodynamic dispersion processes. The apparent solute dispersion coefficient,  $D_{sz}$ , includes the effect of hydrodynamic dispersion and molecular diffusion. The second term in Equation (1.34) represents the solute flux from mass transport processes.

The equation as stated allows diffusion to occur when the mass flow rate of water or the convection term is zero. It also includes an expression for the sorption or desorption of the solute onto soil particles and a solute source or sink term. The source/sink term can describe the addition of solute to the soil in the form of fertilizers, slow decay of organic matter, addition of hazardous chemicals, slow leaks from storage tanks for hazardous chemicals, and solute uptake by roots.

#### 1.3.1 Solute in the Liquid Phase

To obtain a unique solution to Equation (1.34), initial conditions and boundary conditions on the upper and lower soil surfaces must be specified. The initial concentration of the liquid phase is

$$c(z, 0) = c_0(z) \quad [M/L_w^3]. \quad (1.35)$$

There are three common types of boundary conditions that can be specified for the liquid phase solute. These are the Dirichlet, Neumann, and the Cauchy types.

1st type: Dirichlet, specifies surface concentration,  $c$ .

2nd type: Neumann, specifies the concentration gradient,  $\frac{\partial c}{\partial z}$ .

3rd type: Cauchy, specifies solute flux through the soil surface,  $f = q_z c - \theta D_{sz} (\partial c / \partial z)$ .

Table 1.2 lists the more common types of boundary conditions that may be encountered. Details about third type boundary conditions are given by Bresler (1973). If we define  $f(t)$  as the liquid phase solute flux through the soil surface with  $z = 0$  at the upper surface

$$f(t) \Big|_{z=0^-} = \{-\theta \cdot D_{sz} \frac{\partial c}{\partial z} + q_z c\} \Big|_{z=0^+} \quad [M/L^2/T], \quad (1.36)$$

then

for infiltration  $f(t) = q_z(0^-, t)c(0^-, t)$ ,

for redistribution  $f(t) = 0, q_z(0^-, t) = 0$ ,

for evaporation  $f(t) = 0, q_z(0^-, t) < 0, [M/L^2/T], \quad (1.37)$

where superscript (-) indicates above the boundary and superscript (+) indicates below the boundary. The solute flux,  $f(t)$ , that moves in the positive  $z$  direction (e.g., downward) is computed as a positive flux and a flux that moves in the negative  $z$  direction (e.g., upwards) is computed as a negative flux. Usually a zero gradient condition can be assumed for the lower surface

$$\frac{\partial c}{\partial z} (z_{\max}, t) = 0 \quad [M/L^3/L]. \quad (1.38)$$

However, Equation (1.38) cannot be used to describe movement in a short soil column where the solute reaches the end of the soil column.

### 1.3.2 Solute in the Solid Phase

To solve Equation (1.34), the sorption term,  $S$ , must be described mathematically. Many different models for sorption have been proposed. Boast (1973) and van Genuchten and Cleary (1979) give a detailed review of

these. In choosing any one of the models, the limitations imposed on their derivations should be recognized. All the models imply a homogeneous sorbing medium in the sense that the activation energy of the sorbing reaction is invariant within the medium, i.e., the soil is comprised of only one mineral.

Another serious limitation of most models is the fact that the analyses are based on a steady-state, saturated flow. The application of such models to a real soil and unsaturated conditions may be limited by this. Certain discrepancies between results obtained with these models and experiments are expected. The equilibrium or kinetic reaction constants may vary with local changes in water content. Reaction rates differ between wet and dry soils. Assuming a homogeneous soil and a steady-state condition, Lindstrom et al. (1970, 1971) and Lindstrom and Boersma (1970) put forth a kinetic model (Table 1.3) which appropriately accounts for forward and backward activation energies. The model can be applied to both adsorption and desorption. When van Genuchten et al. (1974) extended the model to a saturated soil column, they found that the model was inadequate to handle the non-homogeneity of the medium. In particular, the model does not incorporate the effect of residence time of chemical in the sorption process which results in greater deviation from the experimental values at higher pore-water velocities. Clearly, more study is needed to obtain a realistic sorption model which will satisfactorily circumvent the complexity of the soil (Yingjajaval, 1979).

Listed in Table 1.3 are some of the sorption models for equilibrium reactions which have been incorporated in the computer program. Non-equilibrium models are given in Table 1.4. The equilibrium models are special cases of the non-equilibrium models, with  $\partial S/\partial t$  having been set to zero.

The user must use his judgment in selecting one of these models. He should choose one which he thinks is most appropriate to his experimental conditions. The models shown in Tables 1.3 and 1.4 assume that sorption and desorption are defined by the same equation. Additional details of the use of these models are in Sections 2.2 and 3.6.

Table 1.2. Types of boundary conditions for the equation describing solute flow in the liquid phase

Physical process	Type of boundary condition
Solute flux during water evaporation	3
Solute flux during water redistribution	3
Solute flux during water infiltration	3
Specified solute concentration	1
Impervious barrier to solute (reflective boundary)	2
Semi-infinite soil column	2

Table 1.3. Equilibrium models for sorption of solute onto soil particles under isothermal conditions.  $k_1$ ,  $k_2$ ,  $k_3$  and  $k_4$  are specified constants for each model

Name	Sorption model	Reference
Linear	$S = k_1 c + k_2$	Lapidus and Amundson (1952)
Langmuir	$S = \frac{k_1 c}{(1+k_2 c)} + k_3$	Tanji (1970)
Freundlich	$S = k_1 c^{k_2} + k_3$	Lindstrom and Boersma (1970)
General non-linear	$S = F(S, c)$	
such as:	$S = \frac{k_1 c}{c + (k_2 - c) \exp[k_3 - k_4 c]}$	Lai and Jurinak (1971)

Table 1.4. Non-equilibrium models for sorption of solute onto soil particles under isothermal conditions.  $k_1$ ,  $k_2$ ,  $k_3$  and  $k_4$  are specified constants for each model

Name	Sorption model	Reference
Linear	$\frac{\partial S}{\partial t} = k_1 c + k_2 S + k_3$	Lapidus and Amundson (1952)
Bilinear	$\frac{\partial S}{\partial t} = k_1 c + k_2 S + k_3 c S + k_4$	Gupta and Greenkorn (1973)
Langmuir	$\frac{\partial S}{\partial t} = \frac{k_1 c}{(1+k_2 c)} + k_3 S + k_4$	
Freundlich	$\frac{\partial S}{\partial t} = k_1 c^{k_2} + k_3 S + k_4$	
General non-linear	$\frac{\partial S}{\partial t} = F(S, c)$	
such as:	$\frac{\partial S}{\partial t} = k_1 c^{k_2} S^{k_3}$	Enfield et al. (1976)
	$\frac{\partial S}{\partial t} = k_1 e^{k_2 S} \{k_3 c e^{-2k_2 S} - S\}$	Lindstrom et al. (1971)
	$\frac{\partial S}{\partial t} = k_1 (k_2 - S) \sinh(k_3 [1 - \frac{S}{k_4}])$	Leenheer and Ahlrichs (1971)

Experimentally, it may be more convenient to define the sorption term in units of mass of chemical per soil mass,  $s$ , rather than in units of mass of chemical per unit volume as indicated by  $S$ .  $S$  can be related to  $s$  by

$$S = s \cdot BD \quad [M/L^3] \quad (1.39)$$

where  $BD$  is the bulk density of the soil  $[M_{soil}/L^3]$  and  $s$  is the sorption on a mass basis  $[M/M_{soil}]$ .

The computer program does not use Equation (1.39) and the above is only given for general interest. The program assumes the sorption term,  $S$ , to have units of  $[M/L^3]$ .

#### 1.4 Water Uptake by the Roots

Leaves evaporate water in response to the evaporative demand of the atmosphere. The rate corresponding to the evaporative demand of the atmosphere is called the potential transpiration,  $q_{ps}$ . The water lost by the leaves is replaced by water adsorbed by the roots from the soil and transferred along the plant stem. When the rate of water supply from the roots to the leaves does not equal the evaporative demand, the potential of the water in the leaf cells decreases, which results in stomatal closure. The model used in this report is based on a "plant surface potential",  $\psi_{ps}$ , which is the potential of the water in the plant stem at the soil surface. Some authors call this the root-collar potential. Other authors (Gardner, 1964; Whisler et al., 1968; Molz and Remson, 1971; Nimah and Hanks, 1973; Neuman et al., 1975; Taylor and Klepper, 1975; Farnum, 1977; Molz, 1981) have used similar models. Several modifications have been used in the analysis presented here.

The root uptake model, developed by Ungs et al. (1977), is given as

$$A = \frac{\{[\psi_{ps} - \psi] \cdot CNVRSN + z + RPF\}}{\{\frac{1}{K} + \frac{1}{K_r}\}} \cdot RAF \quad [L_w^3/L^3/T]. \quad (1.40)$$

This model is based on the following concepts:

a) The actual rate of transpiration,  $T_r$ , is some fraction of the potential evaporative demand,  $q_{ps}$  of the atmosphere. This fraction is determined by the stomatal correction factor,  $c_{st}$ , which is a known function of the plant water potential at the soil surface. Then the actual transpiration rate is described by

$$T_r = q_{ps}(t) \cdot c_{st}(\psi_{ps}) \quad [L^3_w/L^2/T]. \quad (1.41)$$

The potential evaporative demand depends only on climatic conditions and is given as a function of time.

b) The plant surface potential,  $\psi_{ps}$ , is not a priori known and changes at each time step in response to the potential demand and soil supply conditions. A value of  $\psi_{ps}$  is "hunted" for until the total amount of water extracted by the plant roots over the soil column occupied by roots equals the actual transpiration rate,  $T_r$ . The plant surface potential  $\psi_{ps}$  is bounded by the condition that

$$\psi_{wilt} \leq \psi_{ps} \leq 0, \quad [L_p], \quad (1.42)$$

where  $\psi_{wilt}$  is the water potential at which the plant permanently wilts and dies.

c) The water potential of the root,  $\psi_r$ , is equal to the sum of the plant surface potential, the distance from the soil surface to the root (gravity potential), and RPF, which is a specified function describing the friction loss incurred by the water flowing through the root xylem to the soil surface

$$\psi_r(z, \theta, \psi_{ps}) = \psi_{ps} + \{z + RPF\}/CNVRSN \quad [L_p]. \quad (1.43)$$

d) The flow of water from the soil to the root is proportional to the difference between the soil matric potential,  $\psi$ , and the potential of the root

$$(\psi_r - \psi) \quad [L_p], \quad (1.44)$$

where  $\psi$ , corresponding to a given value of  $\theta$ , is computed from Equation (1.12) or from the soil-water characteristic function.

e) The hydraulic conductivity through the soil-root system,  $K_{sys}(\theta) [L^3_w/L^2/T]$ , is proportional to the conductivities of the soil

$K(\theta)$  and the root cortex  $K_r(\theta)$  as follows

$$1/K_{\text{sys}}(\theta) = 1/K(\theta) + 1/K_r(\theta), \quad [L^2T/L^3_w], \quad (1.45)$$

where  $K(\theta)$  and  $K_r(\theta)$  are known functions of  $\theta$ .

f) Water uptake by the root at a given depth is proportional to the root absorption function, RAF. The root absorption function is determined by root density,  $R_d$  and root uptake activity,  $R_a$  such that

$$\text{RAF}(z, \theta, t) = b \cdot R_d \cdot R_a \quad [1/L^2]. \quad (1.46)$$

RAF is a positive quantity;  $b$ , which is called the effective root length coefficient, is defined (Feddes and Rijtema, 1972; Taylor and Klepper, 1975) as

$$b = 2 \cdot \pi / \ln(R_{\text{cyl}}/R_{\text{stele}}) \quad [L/L_r], \quad (1.47)$$

where  $R_{\text{cyl}}$  is the radius of the cylinder of soil through which water is moving to the root. In our program it is assumed that this is the half-distance between randomly dispersed roots (Taylor and Klepper, 1975), thus

$$R_{\text{cyl}} = 1/\sqrt{4R_d} \quad [L_r]. \quad (1.48)$$

Some authors (Cowan, 1965; Farnum and Carey, 1981) define  $R_{\text{cyl}} = 1/\sqrt{4\pi R_d}$  but we will use the form given by Eq. (1.48).  $R_{\text{stele}}$  is defined (Taylor and Klepper, 1975) as the radius of the root stele, which is considered to be two-thirds of the actual root radius,  $R_r$  (Huck et al., 1970). Hence

$$R_{\text{stele}} = R_r \cdot 2/3 \quad [L_r]. \quad (1.49)$$

The root density,  $R_d [L_r/L^3]$ , is a function of depth and time and must be specified.

The root uptake activity expressed as a ratio

$$R_a = R_a(\theta) \cdot R_a(c) \quad [1], \quad (1.50)$$

is a function of a water activated term and a liquid phase solute activated term, both of which must be specified.

g) The flux of water withdrawn from each soil layer by the roots in that layer is defined by the root uptake term,  $A$ , where

$$A(z, \theta, \psi_{ps}) = K_{sys} \cdot \text{RAF} \cdot \{\psi_r - \psi\} \cdot \text{CNVRSN} \quad [L_w^3/L^3/T] \quad (1.51)$$

and upon substitution of Equation (1.43), the root uptake at the  $i$ -th soil layer is

$$A_i = K_{sys} \cdot \text{RAF} \cdot \{(\psi_{ps} - \psi) \cdot \text{CNVRSN} + z + \text{RPF}\} \quad [L_w^3/L^3/T]. \quad (1.52)$$

However, if  $A_i > 0$ , set  $A_i = 0$ .

h) The actual transpiration rate,  $T_r$ , from step a) must equal the sum of the amounts of water withdrawn from all soil layer sinks

$$T_r = \sum_{i=2}^{n-1} A_i \frac{(z_{i+1} - z_{i-1})}{2} \quad [L_w^3/L^2/T]. \quad (1.53)$$

The sum is from  $i = 2, \dots, n-1$  since it is assumed there is no uptake of water by roots at the top and bottom nodes.

To determine the actual transpiration rate,  $T_r$ , the computer program uses an iterative scheme:

- Step i) Specify the potential transpiration demand,  $q_{ps}$ , and guess the soil matric potential for each soil layer.
- Step ii) Guess the plant surface potential,  $\psi_{ps}$ , subject to the conditions of Equation (1.42).
- Step iii) Compute the actual transpiration rate,  $T_r$ , using the guessed value of  $\psi_{ps}$  and Equation (1.41).
- Step iv) Compute the root uptake term  $A_i$  for each soil layer from Equation (1.52).
- Step v) Compute the actual transpiration rate,  $T_r$ , using Equation (1.53).
- Step vi) If the transpiration rate of step iii) does not equal the transpiration rate of step v), then make a new guess of the plant surface potential  $\psi_{ps}$  and return to step ii).

The iterative process stops when step vi) converges. The results of this iterative process (Section 3.2) depend on the initially guessed values of soil matric potential,  $\psi$ . An additional iterative process is

required in which the correct soil matric potential, subject to Equations (1.12) and (1.13), is determined.

In actual practice, the iteration scheme for computing  $\psi_{ps}$  converges within three to five iterations. The matric potential iterator scheme, however, may take 5 to 10 iteration cycles to compute  $\psi$ . Additional details are given in later sections.

### 1.5 Solute Uptake

The source/sink term in Equation (1.34) describes release processes such as from fertilizer, organic matter, or from added hazardous chemicals and uptake of nutrients by plants, changes in composition during chemical reactions such as nitrification, precipitation or dissolution.

Unfortunately, little progress has been made in the understanding of the absorption of ions by plant roots. This is mainly because of the limited knowledge about the transfer of ions across root tissues.

Gardner (1965) proposed several models for the uptake of nutrients by plants:

1. Concentration independent uptake

i)  $G = k_1$ .

This equation describes a constant rate of uptake.

ii)  $G = G(x)$ .

This equation describes a rate of uptake which depends on biological activity,  $x$ .

2. Concentration dependent uptake, passive transport

iii)  $G = k_2 cA$ .

This equation describes passive uptake which is linearly dependent on concentration,  $c$ , and root water uptake,  $A$ .

iv)  $G = \frac{k_3 cA}{1 + k_4 c}$ .

This equation describes passive uptake based on the Michaelis-Menten model. Uptake is a non-linear function of concentration and a linear function of root water uptake.

### 3. Concentration dependent uptake, active transport

$$v) G = k_5 c.$$

For root systems, this equation describes root solute uptake as a function of solute concentration. Solute transport into the root is independent of root water uptake. This implies an active membrane transport mechanism.

For non-root systems, this equation implies a decay/addition of solute that is linearly proportional to the solute concentration in the soil (Vol. IV, Section 7.5, for example).

$$vi) G = \frac{k_6 c}{1+k_7 c}.$$

This equation describes root solute uptake as a Michaelis-Menten model. However, unlike iv), the uptake can be a non-linear function of both concentration and root water uptake. Hence,  $k_6 = k_6(A)$ , and  $k_7 = k_7(A)$ .

A more detailed discussion of the above models, including the effect of soil temperature on root solute uptake, is given by Ungs et al. (1982).

In subroutine SOLUTE, the solute source/sink term is evaluated at the  $i$ -th spatial node, at time level  $(k + 1/2)$  and is written as

$$\text{Passive: } G(i) = \text{GCOEF} \cdot A(i) \quad [M/L^3/T], \quad (1.54a)$$

$$\text{Active: } G(i) = \text{GCOEF} \quad [M/L^3/T], \quad (1.54b)$$

where  $A(i)$  is the rate of water uptake by the roots  $[L_w^3/L^3/T]$  at node  $i$  and time level  $(k + 1/2)$  and GCOEF is the source/sink coefficient of solute  $[M/L_w^3]$ ,  $[M/L^3/T]$  at node  $i$ . Table 1.5 lists the form of coefficient GCOEF for some of the models given above. Variable  $G(i)$  is a negative quantity for sink models (root uptake, solute decay, and positive for source models (solute release). Variable  $A(i)$  is always negative for root uptake.

Table 1.5. Source/Sink models of solute

Name	Source/Sink model
Constant	GCOEF = $k_1$
Linear	GCOEF = $k_2 \cdot c_i^{k+1/2}$
Michaelis-Menten	GCOEF = $\frac{k_3 \cdot c_i^{k+1/2}}{(1+k_4 \cdot c_i^{k+1/2})}$

where  $c_i^{k+1/2}$  is defined in Equation (3.31)

The total amount of solute taken up by the source/sink system at any instant is given by the sum of the amounts of solute added or withdrawn from all soil layers

$$T_{cr} = \sum_{i=2}^{n-1} G_i \frac{(z_{i+1} - z_{i-1})}{2} \quad [M/L^2/T]. \quad (1.55)$$

The sum is from  $i = 2, \dots, n-1$  since it is assumed that there is no source/sink at the top and bottom nodes. Also note that  $G_i$  is evaluated at  $(i, k + 1/2)$ , i.e., the half-time step level.

## 2. FORMULATING SOLUTIONS BY FINITE-DIFFERENCE METHODS

### 2.1 Flow of Water

#### 2.1.1 Solution Based on $\theta$

The water flow equation is solved by employing the time-centered finite-difference scheme of Crank-Nicolson (von Rosenberg, 1969). In finite-difference form, Equation (1.3) is evaluated about the interior  $i$ -th space node and the  $(k+1/2)$  time level, such that Equation (1.3) becomes

$$\begin{aligned} \frac{\theta_i^{k+1} - \theta_i^k}{\Delta t^{k+1}} = & \left[ \frac{D(\theta_{i+1/2}^{*k+1/2}) \{ \theta_{i+1}^{k+1} + \theta_{i+1}^k - \theta_i^{k+1} - \theta_i^k \}}{2\Delta z_2} \right. \\ & \left. - \frac{D(\theta_{i-1/2}^{*k+1/2}) \{ \theta_i^{k+1} + \theta_i^k - \theta_{i-1}^{k+1} - \theta_{i-1}^k \}}{2\Delta z_1} \right] \frac{1}{\Delta z_3} \\ & - \text{GRAV} \cdot \left[ \frac{K(\theta_{i+1/2}^{*k+1/2}) - K(\theta_{i-1/2}^{*k+1/2})}{\Delta z_3} \right] \\ & + A(z_i, \theta_i^{*k+1/2}, \psi_{ps}^{k+1/2}) \quad i = 2, \dots, n-1, \quad (2.1) \end{aligned}$$

where  $n$  is the total number of space nodes and the root uptake term,  $A(z, \theta, \psi_{ps})$ , is defined by Equation (1.52), evaluated at time  $(k+1/2)$ . The subscript " $i$ " refers to the  $i$ -th vertical or horizontal distance node, i.e.,  $i = 1$  refers to the surface,  $z = 0$ , the superscript " $k$ " refers to the current time level  $t^k$ , and  $(k+1/2)$  is half-time step into the future. GRAV is the gravity coefficient which is set equal to one for vertical flow and equal to zero for horizontal flow. The superscript "\*" indicates that this variable has an estimated value.

The finite-difference solution of Equation (2.1) allows the use of variable time as well as variable space step-sizes. The space step-size is defined by

$$\begin{aligned} \Delta z_1 &= z_i - z_{i-1}, \\ \Delta z_2 &= z_{i+1} - z_i, \\ \Delta z_3 &= (z_{i+1} - z_{i-1})/2, \end{aligned} \quad (2.2)$$

and the time step-size is defined by

$$\begin{aligned}\Delta t^k &= t^k - t^{k-1}, \\ \Delta t^{k+1} &= t^{k+1} - t^k.\end{aligned}\tag{2.3}$$

The half-time step can be related to the full-time step by

$$*\theta_{i+1/2}^{k+1/2} = (*\theta_{i+1}^{k+1} + *\theta_i^{k+1} + \theta_{i+1}^k + \theta_i^k)/4,\tag{2.4a}$$

$$*\theta_i^{k+1/2} = (*\theta_i^{k+1} + \theta_i^k)/2,\tag{2.4b}$$

$$*\theta_{i-1/2}^{k+1/2} = (*\theta_i^{k+1} + *\theta_{i-1}^{k+1} + \theta_i^k + \theta_{i-1}^k)/4.\tag{2.4c}$$

There is a total of  $n$  space nodes but Equation (2.1) is evaluated only at the interior nodes of the soil column, from  $i=2, \dots, n-1$  at time level  $(k+1/2)$ . The boundary conditions are evaluated at the first and last node at time level  $(k+1)$  and are evaluated by a backward-difference scheme. Hence the  $n-2$  interior flow equations of Equation (2.1) and the upper and lower boundary expressions comprise a total of  $n$  equations and  $n$  unknowns for time level  $(k+1)$ .

The initial condition of Equation (1.7) is expressed as

$$\theta_i^{k=0} = \theta_0(z_i) \quad i = 1, \dots, n.\tag{2.5}$$

Three types of boundary conditions for the upper soil surface are allowed, namely the Dirichlet (1st type), the Neumann (2nd type), and the 4th type involving a surface flux. These are backward-differenced as

1st type:

$$\theta_1^{k+1} = \text{RHS}(t^{k+1}),\tag{2.6a}$$

2nd type:

$$\left\{ \frac{\theta_2^{k+1} - \theta_1^{k+1}}{z_2 - z_1} \right\} = \text{RHS}(t^{k+1}),\tag{2.6b}$$

4th type:

$$\frac{\theta_1^{k+1} - \theta_1^k}{\Delta t^{k+1}} = D(\theta_{1+1/2}^{*k+1}) \cdot \frac{\{\theta_2^{k+1} - \theta_1^{k+1}\}}{(z_2 - z_1)^2} - \frac{K(\theta_{1+1/2}^{*k+1})}{(z_2 - z_1)} \cdot \text{GRAV} + \frac{q_0^{k+1}}{(z_2 - z_1)} \quad (2.6c)$$

In the above equations  $\text{RHS}(t^{k+1})$  corresponds to the specified value of the boundary condition at time  $t^{k+1}$ . The term  $q_0^{k+1}$  is the actual surface flux as defined by Equation (1.11), evaluated at node 1/2 (which lies above the soil surface,  $z=0$ ) and time level  $(k+1)$ . In addition,  $\theta_{1+1/2}^{*k+1}$  is defined as

$$\theta_{1+1/2}^{*k+1} = (\theta_1^{*k+1} + \theta_2^{*k+1})/2. \quad (2.7)$$

There are also three types of boundary conditions for the lower soil surface. These are backward-differenced as

1st type:

$$\theta_n^{k+1} = \text{RHS}(t^{k+1}), \quad (2.8a)$$

2nd type:

$$\left\{ \frac{\theta_n^{k+1} - \theta_{n-1}^{k+1}}{z_n - z_{n-1}} \right\} = \text{RHS}(t^{k+1}), \quad (2.8b)$$

4th type:

$$\frac{\theta_n^{k+1} - \theta_n^k}{\Delta t^{k+1}} = -D(\theta_{n-1/2}^{*k+1}) \cdot \frac{\{\theta_n^{k+1} - \theta_{n-1}^{k+1}\}}{(z_n - z_{n-1})^2} + \frac{K(\theta_{n-1/2}^{*k+1})}{(z_n - z_{n-1})} \cdot \text{GRAV} - \frac{q_n^{k+1}}{(z_n - z_{n-1})}, \quad (2.8c)$$

where  $q_n^{k+1}$  is the actual surface flux, evaluated at node  $n+1/2$  (which lies below the lower soil surface,  $z=z_{\text{max}}^+$ ) and time level  $(k+1)$ . In addition,  $\theta_{n-1/2}^{*k+1}$  is defined as

$${}^* \theta_{n-1/2}^{k+1} = ({}^* \theta_n^{k+1} + {}^* \theta_{n-1}^{k+1})/2 . \quad (2.9)$$

To evaluate the non-linear coefficients A, D, and K of Equation (2.1), the water content must be estimated by iteration. The problem is non-linear because the coefficients A, D, and K are non-linear functions of the water content or of the variable being calculated.

At the beginning of each new time level, a first estimate of  ${}^* \theta_i^{k+1}$  is made by linear extrapolation from the previous time level (Rubin and Steinhardt, 1963; Neuman et al., 1975) as follows:

$${}^* \theta_{i+1}^{k+1} = \theta_{i+1}^k + \text{ACL RAT} \cdot \left( \frac{\Delta t^{k+1}}{\Delta t^k} \right) (\theta_{i+1}^k - \theta_{i+1}^{k-1}), \quad (2.10a)$$

$${}^* \theta_i^{k+1} = \theta_i^k + \text{ACL RAT} \cdot \left( \frac{\Delta t^{k+1}}{\Delta t^k} \right) (\theta_i^k - \theta_i^{k-1}), \quad (2.10b)$$

$${}^* \theta_{i-1}^{k+1} = \theta_{i-1}^k + \text{ACL RAT} \cdot \left( \frac{\Delta t^{k+1}}{\Delta t^k} \right) (\theta_{i-1}^k - \theta_{i-1}^{k-1}), \quad (2.10c)$$

where ACLRAT = 1 for linear extrapolation and ACLRAT = 1.4 for accelerated linear extrapolation (Hanks and Bowers, 1969).

The linear extrapolation technique described above has been found to give an excellent first guess for the water content iterator at each new time level. However, the extrapolator cannot be used until the third time step because  $\theta^k$  and  $\theta^{k-1}$  are not defined. The values given in Table 2.1 are used during the first two time steps as initial guesses. Table 2.1 is arbitrary, but it has been found to give good starting results.

Using the initial estimates of  ${}^* \theta_i^{k+1}$  from Equation (2.10), the coefficients in Equations (2.1), (2.6), and (2.8) can be evaluated and then the resulting tri-diagonal matrix can be solved by the Thomas algorithm (von Rosenberg, 1969) to obtain computed values of  $\theta_i^{k+1}$  (Table 2.2). Because of the non-linear nature of the coefficients, the computed values of  $\theta$  will not be the same as the estimated values. The solution can be improved by an iterative process. At each additional iteration about time level  $t^{k+1}$ , the most recent computed values of  $\theta_i^{k+1}$  are used to obtain an improved estimate of  ${}^* \theta_i^{k+1}$  either by setting



$$*\theta_i^{k+1}(\text{new estimate}) = \{*\theta_i^{k+1}(\text{old estimate}) + \theta_i^{k+1}(\text{computed})\}/2. \quad (2.11)$$

according to Neuman et al. (1975) or by using a Newton-Raphson scheme (Section 3.3) in the fourth and/or subsequent iteration. The iterative procedure continues until a satisfactory degree of convergence is obtained, usually within 10 cycles, depending on the accuracy required. The criterion for convergence is

$$\max \left| \frac{*\theta_i^{k+1} - \theta_i^{k+1}}{*\theta_i^{k+1}} \right| \leq \text{WRATIO} \quad i = 1, \dots, n, \quad (2.12)$$

where WRATIO is the maximum allowed difference, expressed as a ratio.

Some authors (Rubin and Steinhardt, 1963) have assumed that the guess obtained by linear extrapolation of Equation (2.10) is sufficiently accurate so that no iteration is attempted. Others solve the non-linear coefficients at the old time level,  $t^k$ , thereby reducing the finite-difference equation of the water flow equation to a linear one. In general, small time steps are necessary when a non-iterative technique is used. How small these time steps should be is a difficult question to answer. Convergence criteria and failure to converge problems for the iterative schemes presented in this report are further discussed in Volume III.

### 2.1.2 Size of Time Step

Usually the choice of size of the time step is one of convenience. Both the centered Crank-Nicolson and the backward-difference schemes are unconditionally stable for all ratios of  $\Delta z$  and  $\Delta t$  (von Rosenberg, 1969). However, mass balance and numerical oscillation problems can occur if the size of the time step chosen is too large. Furthermore, the water content iterator becomes very inefficient when large time steps are used since the rate of convergence decreases dramatically and, in fact, failure to converge may occur.

Program OR-NATURE provides four methods to determine the size of the time step in subroutine STEP.

i) use the method of Hanks and Bowers, by setting the parameter  
 $KIDELT = 0$ .

ii) use a general formula, by setting  $KIDELT = 1$ , with

$$\Delta t^{k+1} = a + b\Delta t^k + c t^k. \quad (2.13a)$$

iii) use a user specified empirical formula, by setting  $KIDELT = 2$ .

iv) fix the minimum and maximum step size such that

$$\Delta t = \Delta t_{\min} = \Delta t_{\max}.$$

The method of Hanks and Bowers defines the step size as the length of time required for the water to move in the soil from one node to the next at the maximum flux rate. Hanks and Bowers (1969) and Dutt et al. (1972) define

$$\Delta t^{k+1} \leq \min \left| \frac{\theta_{i+1/2}^{k-1/2} (z_{i+1} - z_i)}{q_{i+1/2}^{k-1/2}} \right| \quad i = 1, \dots, n-1, \quad (2.13b)$$

where the Darcian flux  $q_{i+1/2}^{k-1/2}$  is defined at the previous time level as

$$q_{i+1/2}^{k-1/2} = -D(\theta_{i+1/2}^{k-1/2}) \cdot \frac{(\theta_{i+1}^{k-1/2} - \theta_i^{k-1/2})}{(z_{i+1} - z_i)} + GRAV \cdot K(\theta_{i+1/2}^{k-1/2}). \quad (2.13c)$$

The size of the time step according to Equation (2.13b) is constrained to lie between the specified minimum and maximum step size limits

$$\Delta t_{\min} \leq \Delta t^{k+1} \leq \Delta t_{\max}. \quad (2.14)$$

If the computed time step-size violates Equation (2.14), it is set to the limiting value of either  $\Delta t_{\min}$  or  $\Delta t_{\max}$ .

The minimum and maximum time step-sizes are specified by the user as  $DTMIN$  and  $DTMAX$ . It is not possible to know in advance the best way of defining these limits. The main purpose of the limits on the size of the step size is to prevent subroutine  $STEP$  from generating an excessively small or large time step. From experience, the user will be able to determine  $\Delta t_{\min}$  and  $\Delta t_{\max}$ .

The general form of Equation (2.13a) can be used to specify three types of formulae for calculating the time step-size by adjusting the values of the  $a$ ,  $b$ ,  $c$  coefficients.

- 1) constant step size:  $\Delta t^{k+1} = a$  ( $b=0$ ;  $c=0$ );
- 2) step size is logarithmic in  $\Delta t$ :  $\Delta t^{k+1} = b\Delta t^k$  ( $a=0$ ;  $c=0$ );
- 3) step size is logarithmic with time:  $\Delta t^{k+1} = c t^k$  ( $a=0$ ;  $b=0$ ).

Note that  $\Delta t^{k+1}$  is always subject to the constraint of Equation (2.14). In the computer program,  $a = \text{ATCOEF}$ ,  $b = \text{BTCOEF}$ , and  $c = \text{CTCOEF}$ , which are specified on program card #7 and by setting  $\text{KIDELT}=1$  on program card #1 (Vol. II, Section 4.5.7).

If the user wishes to provide his own empirical formula for the time step-size, he can do so by setting  $\text{KIDELT}=2$  on program card #1 and by writing the appropriate FORTRAN statements in subroutine STEP between statements "80" and "100". The step size remains subject to the limits of Equation (2.14).

It is sometimes simpler to fix  $\Delta t$  by setting  $\text{KIDELT}=1$  and  $\text{DTMIN} = \text{DTMAX} = \Delta t$  on program card #5. Hence, the constraints of Equation (2.14) are always satisfied. The above procedure gives the same result as would be obtained by use of the general formula and setting  $\Delta t$  equal to a constant,  $\Delta t^{k+1} = a$ . But the procedure described here is faster.

### 2.1.3 Solution Based on $\psi$

The centered Crank-Nicolson representation of the flow equation based on matrix potential is obtained from Equation (1.12) and expressed as

$$\begin{aligned}
 \left(\frac{\partial \theta}{\partial \psi}\right)_i^{k+1/2} \left(\frac{\psi_i^{k+1} - \psi_i^k}{\Delta t^{k+1}}\right) &= K(\psi_{i+1/2}^{k+1/2}) \left[ \frac{\{\psi_{i+1}^{k+1} + \psi_{i+1}^k - \psi_i^{k+1} - \psi_i^k\}}{2\Delta z_2} \right. \\
 &\quad \left. - K(\psi_{i-1/2}^{k+1/2}) \frac{\{\psi_i^{k+1} + \psi_i^k - \psi_{i-1}^{k+1} - \psi_{i-1}^k\}}{2\Delta z_1} \right] \cdot \frac{\text{CNVRSN}}{\Delta z_3} \\
 &\quad - \text{GRAV} \cdot \left[ \frac{K(\psi_{i+1/2}^{k+1/2}) - K(\psi_{i-1/2}^{k+1/2})}{\Delta z_3} \right] \quad (2.15) \\
 &\quad + A(z_i, \psi_i^{k+1/2}, \psi_{ps}^{k+1/2}) \quad i = 2, \dots, n-1,
 \end{aligned}$$

where  $\Delta z$  and  $\Delta t$  are defined by Equations (2.2) and (2.3) and where  $(\partial\theta/\partial\psi)$  is the specific water capacity, evaluated at  $\psi_i^{*k+1/2}$ . The hydraulic conductivity function,  $K$ , is always specified by the user as a function of water content and not matric potential. So, for the program to evaluate  $K(\psi)$ , the following steps are taken by the computer:

- i) determine the desired value of matric potential,  $\psi$ ,
- ii) using the soil-water characteristic function  $\theta(\psi)$ , compute the value of water content,  $\theta$ , corresponding to the value of matric potential obtained with step i),
- iii) determine the hydraulic conductivity for the water content found in step i) above, then set  $K(\psi) = K(\theta)$ .

The superscript "\*" indicates that the variable is an estimate. The "starred" quantities are defined analogous to the definition of  $\theta$  in Equation (2.4). The  $n-2$  flow equations of Equation (2.15) for the interior nodes and the upper and lower boundary conditions make a total of  $n$  equations with  $n$  unknowns for time level  $(k+1)$ . The initial condition is given by

$$\psi_i^{k=0} = \psi_0(z_i) \quad i = 1, \dots, n. \quad (2.16)$$

The three upper boundary conditions, stated earlier, are backward-differenced.

1st type:

$$\psi_1^{k+1} = \text{RHS}(t^{k+1}). \quad (2.17a)$$

2nd type:

$$\left\{ \frac{\psi_2^{k+1} - \psi_1^{k+1}}{z_2 - z_1} \right\} = \text{RHS}(t^{k+1}). \quad (2.17b)$$

4th type:

$$\left( \frac{\partial\theta}{\partial\psi} \right)_{k+1/2} \left( \frac{\psi_1^{k+1} - \psi_1^k}{\Delta t^{k+1}} \right) = K(\psi_{1+1/2}^{*k+1}) \frac{\{\psi_2^{k+1} - \psi_1^{k+1}\}}{(z_2 - z_1)^2} \cdot \text{CNVRSN}$$

$$- \frac{K(\psi_{i+1/2}^{*k+1})}{(z_2 - z_1)} \cdot \text{GRAV} + \frac{q_0^{k+1}}{(z_2 - z_1)}. \quad (2.17c)$$

The lower boundary conditions are finite-differenced in the same manner as those of the water-based flow equation (Equation (2.8)).

The guessing and iterating scheme used for solving the water-based flow equation is also used for solving the flow equation based on matrix potential. At a given time level, the flow equation is assumed to have converged when

$$\max \left| \frac{\psi_i^{*k+1} - \psi_i^{k+1}}{\psi_i^{*k+1}} \right| \leq \text{WRATIO} \quad i = 1, \dots, n, \quad (2.18)$$

where WRATIO is the maximum allowed difference expressed as a ratio.

#### 2.1.4 Solution Based on the Kirchhoff Transform

The Kirchhoff transform variable,  $F$ , is defined by Equations (1.16) and (1.17) and is computed numerically by means of a numerical integration scheme in subroutines INTGRT and TRNSFM.

Several steps are taken by subroutine TRNSFM to solve Equation (1.16) and to create a table of 20 values of  $F$  versus  $\theta$ .

- i) Compute the transform variable  $F$  at 20 values of  $\theta$ , such that

$$F(\theta_j) = \int_{\theta'_d}^{\theta_j} D(\theta') d\theta' \quad j = 2, \dots, 20, \quad (2.19)$$

where  $F(\theta_1) = F(\theta_d)$  is defined by Equation (1.19) and where

$$\theta_j = \theta_d + (\theta_s - \theta_d) \cdot \text{PICK}(j) \quad j = 2, \dots, 20. \quad (2.20)$$

The values of  $\text{PICK}(j)$  are given in Table 2.3.

- ii) Numerically evaluate the integral of Equation (2.19) by subdividing the interval  $(\theta_d, \theta_j)$  into 40 intermediate points, such that

$$\theta_\ell = \theta_{\ell-1} + (\theta_j - \theta_d) / 39 \quad \ell = 2, \dots, 40, \quad (2.21)$$

where at  $\ell = 1$ ,  $\theta_1 = \theta_d$ .

- iii) Numerically integrate the 40 subpoint values of  $D(\theta_\ell)$  vs  $\theta_\ell$  by means of a second-order Taylor series expansion integration scheme which allows for unevenly spaced pivotal points (Section 3.7.2). Subroutine INTGRT returns with the integrated values of  $F(\theta_j)$ .
- iv) Repeat steps i) through iii) for all 20 values of  $\theta_j$ . The result is a table of  $F(\theta_j)$  vs  $\theta_j$  which is stored in data set FW.

Table 2.3. The values of PICK(j)

j	PICK(j)
1	0.0000
2	0.0050
3	0.0100
4	0.0175
5	0.0250
6	0.0500
7	0.0750
8	0.1000
9	0.2000
10	0.3000
11	0.4000
12	0.5000
13	0.6000
14	0.7000
15	0.8000
16	0.9000
17	0.9500
18	0.9700
19	0.9900
20	1.0000

The steps taken by subroutine TRNSFM to solve Equation (1.17) and to create a table of  $F$  vs  $\psi$  are listed below. The steps taken differ from those for the solution based on  $\theta$  because the integration variable  $\psi$  can vary over several orders of magnitude. It was found by trial and error that the procedure given below is fairly accurate and consistent.

- i) Compute the transform variable  $F$  at 40 different values of  $\psi$ , such that

$$F(\psi_j) = \text{CNVRSN} \int_{\psi'=\psi_d}^{\psi_j} K(\psi') d\psi' \quad j = 2, \dots, 40, \quad (2.22)$$

where  $F(\psi_1) = F(\psi_d)$  is defined by Equation (1.20) and where  $\psi_j = \psi(\theta_j)$ , such that

$$\begin{aligned} \theta_j &= \theta_{j-1} + (\theta_s - \theta_d)/39 \quad j = 2, \dots, 40, \\ \theta_{j=1} &= \theta_d. \end{aligned} \quad (2.23)$$

ii) Numerically evaluate the integral of Equation (2.22) by subdividing the interval  $(\psi_d, \psi_j)$  into 40 intermediate points, such that

$$\begin{aligned} \ln|\psi_\ell| &= \ln|\psi_{\ell-1}| + (\ln|\psi_j| - \ln|\psi_d|)/39 \quad \ell = 2, \dots, 40, \\ \psi_{\ell=1} &= \psi_d. \end{aligned} \quad (2.24)$$

- iii) Numerically integrate the 40 subpoint values of  $K(\psi_\ell)$  vs  $\psi_\ell$  from step ii) using an integration scheme based on a second-order Taylor series expansion which allows for unevenly spaced pivotal points (Section 3.7.2). Subroutine INTGRT returns with the integrated values of  $F(\psi_j)$ .
- iv) Repeat steps i) through iii) for all 40 values of  $\psi_j$ . The result is a table of  $F(\psi_j)$  vs  $\psi_j$  which is stored in data set FP.

## 2.2 Solute Equation

The centered in time Crank-Nicolson representation of Equation (1.34) at  $(i, k+1/2)$  is

$$\begin{aligned} \frac{\theta_i^{k+1} c_i^{k+1} - \theta_i^k c_i^k}{\Delta t^{k+1}} &= \left[ \theta_{i+1/2}^{k+1/2} \cdot D_{sz} (v_{i+1/2}^{k+1/2}) \cdot \left\{ \frac{c_{i+1}^{k+1} + c_{i+1}^k - c_i^{k+1} - c_i^k}{2\Delta z_2} \right\} \right. \\ &\quad \left. - \theta_{i-1/2}^{k+1/2} \cdot D_{sz} (v_{i-1/2}^{k+1/2}) \cdot \left\{ \frac{c_i^{k+1} + c_i^k - c_{i-1}^{k+1} - c_{i-1}^k}{2\Delta z_1} \right\} \right] \frac{1}{\Delta z_3} \\ &\quad - \left[ \frac{q_{i+1/2}^{k+1/2} \cdot c_{i+1/2}^{k+1/2} - q_{i-1/2}^{k+1/2} \cdot c_{i-1/2}^{k+1/2}}{\Delta z_3} \right] - \frac{\partial S}{\partial t} + G(i, k+1/2) \end{aligned} \quad (2.25)$$

$$i = 2, \dots, n-1,$$

where

$$\begin{aligned}
 c_{i+1/2}^{k+1/2} &= (c_{i+1}^{k+1} + c_i^{k+1} + c_{i+1}^k + c_i^k)/4, \\
 c_i^{k+1/2} &= (c_i^{k+1} + c_i^k)/2, \\
 c_{i-1/2}^{k+1/2} &= (c_i^{k+1} + c_{i-1}^{k+1} + c_i^k + c_{i-1}^k)/4,
 \end{aligned}
 \tag{2.26}$$

and where  $\Delta z_1$ ,  $\Delta z_2$ ,  $\Delta z_3$  are defined by Equation (2.2) and  $\Delta t^k$  and  $\Delta t^{k+1}$  are defined by Equation (2.3). The dispersion term,  $D_{sz}(v)$ , is assumed to be a function of the magnitude of the pore-water velocity, where

$$v_{i+1/2}^{k+1/2} = |q_{i+1/2}^{k+1/2} / \theta_{i+1/2}^{k+1/2}|,$$

and

$$v_{i-1/2}^{k+1/2} = |q_{i-1/2}^{k+1/2} / \theta_{i-1/2}^{k+1/2}|. \tag{2.27}$$

The dispersion term is evaluated in subroutine DSZ where it is defined by data set XDSZ and YDSZ, where XDSZ is the pore-water velocity and YDSZ is the corresponding value of dispersion. It is also possible to write an empirical formula in subroutine DSZ for the dispersion term,  $D_{sz}(v)$ , e.g.  $DSZI = .216*v + .192 \text{ (cm}^2/\text{hr)}$  and setting  $TBLDSZ = 0$ .

There is a total of  $n$  space nodes, but Equation (2.25) is evaluated only in the interior of the soil column, from  $i=2, \dots, n-1$  at time level  $(k+1/2)$ . The remaining two equations are provided by the boundary conditions.

The initial condition for the liquid phase solute equation is defined by Equation (1.35). Its finite-difference form is

$$c_i^{k=0} = c_0(z_i) \quad i = 1, \dots, n. \tag{2.28}$$

Three types of boundary conditions are allowed for the upper soil surface. The finite differences of these are

1st type:

$$c_1^{k+1} = \text{RHS}(t^{k+1}), \tag{2.29a}$$

2nd type:

$$\frac{c_2^{k+1} - c_1^{k+1}}{z_2 - z_1} = \text{RHS}(t^{k+1}), \tag{2.29b}$$

3rd type:

$$\frac{\theta_1^{k+1} c_1^{k+1} - \theta_1^k c_1^k}{\Delta t^{k+1}} = (\theta D_{sz})^{k+1/2} \cdot \left\{ \frac{c_2^{k+1} + c_2^k - c_1^{k+1} - c_1^k}{2(\Delta z_2)^2} \right\} \quad (2.29c)$$

$$- q_{1+1/2}^{k+1/2} \cdot \left\{ \frac{c_1^{k+1} + c_1^k + c_2^{k+1} + c_2^k}{4\Delta z_2} \right\} + \frac{f_0^{k+1/2}}{\Delta z_2},$$

where  $\Delta z_2 = z_2 - z_1$ ,  $q_{1+1/2}^{k+1/2}$  is the Darcian flux,  $\text{RHS}(t^{k+1})$  corresponds to the specified value of the boundary condition at time  $t^{k+1}$ , and  $f_0^{k+1/2}$  is the actual flux of solute through the upper surface as defined by Equation (1.37). Source/sink terms are not evaluated at the upper surface. The user must supply the value of RHS and f through subroutine BCCTOP.

There are also three types of boundary conditions for the lower soil surface. The finite differences of these are

1st type:

$$c_n^{k+1} = \text{RHS}(t^{k+1}), \quad (2.30a)$$

2nd type:

$$\frac{c_n^{k+1} - c_{n-1}^{k+1}}{z_n - z_{n-1}} = \text{RHS}(t^{k+1}), \quad (2.30b)$$

3rd type:

$$\frac{\theta_n^{k+1} c_n^{k+1} - \theta_n^k c_n^k}{\Delta t^{k+1}} = -(\theta D_{sz})^{k+1/2} \left\{ \frac{c_n^{k+1} + c_n^k - c_{n-1}^{k+1} - c_{n-1}^k}{2(\Delta z_1)^2} \right\} \quad (2.30c)$$

$$+ q_{n-1/2}^{k+1/2} \left\{ \frac{c_{n-1}^{k+1} + c_{n-1}^k + c_n^{k+1} + c_n^k}{4\Delta z_1} \right\} - \frac{f_n^{k+1/2}}{\Delta z_1},$$

where  $\Delta z_1 = z_n - z_{n-1}$ , and where  $f_n^{k+1/2}$  is the actual flux of solute through the lower surface as defined by Equation (1.37). The user supplies the values of RHS and f through subroutine BCCBTM.

The sorption terms are finite-differenced by means of the centered Crank-Nicolson method. These are listed in Tables 2.4 and 2.5, where

$$\frac{\partial S}{\partial t} = \frac{S_i^{*k+1} - S_i^k}{\Delta t^{k+1}}, \quad (2.31a)$$

$$c_i^{k+1/2} = (c_i^{k+1} + c_i^k)/2, \quad (2.31b)$$

$$S_i^{k+1/2} = (S_i^{k+1} + S_i^k)/2. \quad (2.31c)$$

Without sorption and the source/sink terms, Equation (2.25) is linear with respect to concentration,  $c$ . The non-linearity induced by the sorption term requires that Equation (2.25) be solved by iteration (Sections 3.5 and 3.6).

Table 2.4. The finite-difference forms of the equilibrium sorption terms according to the Crank-Nicolson scheme

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JSORB = 1 : Linear	$S_i^{k+1} = k_1 c_i^{k+1} + k_2$
JSORB = 2 : Langmuir	$S_i^{k+1} = \frac{k_1 c_i^{k+1}}{(1 + k_2 c_i^{k+1})} + k_3$
JSORB = 3 : Freundlich	$S_i^{k+1} = k_1 (c_i^{k+1})^{k_2} + k_3$

---

Table 2.5 The finite-difference forms of the non-equilibrium sorption terms according to the Crank-Nicolson scheme

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JSORB = 5 : Linear	$\left(\frac{S_i^{k+1} - S_i^k}{\Delta t^{k+1}}\right) = k_1 c_i^{k+1/2} + k_2 S_i^{k+1/2} + k_3$
JSORB = 6 : Bilinear	$\left(\frac{S_i^{k+1} - S_i^k}{\Delta t^{k+1}}\right) = k_1 c_i^{k+1/2} + k_2 S_i^{k+1/2} + k_3 (cS)_i^{k+1/2} + k_4$
JSORB = 7 : Langmuir	$\left(\frac{S_i^{k+1} - S_i^k}{\Delta t^{k+1}}\right) = \frac{k_1 c_i^{k+1/2}}{(1+k_2 c_i^{k+1/2})} + k_3 S_i^{k+1/2} + k_4$
JSORB = 8 : Freundlich	$\left(\frac{S_i^{k+1} - S_i^k}{\Delta t^{k+1}}\right) = k_1 (c_i^{k+1/2})^{k_2} + k_3 S_i^{k+1/2} + k_4$

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### 3. ITERATION ALGORITHMS

#### 3.1 Methods of Iteration

The computer program uses three basic methods of iteration in solving the water and solute flow equations, namely:

- a) successive averaging,
- b) Newton-Raphson iteration,
- c) Golden Section Search.

Iteration is required when the equation to be solved is a non-linear function of the dependent variable. The flow equation based on water content contains the non-linear functions of diffusivity, conductivity, and surface flux. The mass transport equation may have non-linear sorption and/or desorption terms. The iteration process may be thought of as a method of finding the roots of a transcendental equation.

##### 3.1.1 Successive Averaging

With the successive averaging approach, successive estimates are made of the dependent variable (e.g., water content) by averaging the most recent computed value with the previous estimate so that

$$\text{new guess} = (\text{old guess} + \text{computed value})/2. \quad (3.1)$$

The rate of convergence of this technique is usually very rapid, but depends a great deal on the first estimate. The linear extrapolation technique

$$x^{k+1} = x^k + \text{ACLRAT} \cdot \frac{\Delta t^{k+1}}{\Delta t^k} \cdot (x^k - x^{k-1}), \quad (3.2)$$

usually gives an excellent first guess for time level (k+1).

The method of successive averaging is usually reliable but it can fail to converge. This occurs when the iterator enters a repeating guess-compute cycle. Table 3.1 shows an example where the estimated and computed values of water content repeat every second iteration.

Table 3.1. Example of a guess-compute failure in the successive averaging method

Iteration	$\theta$ (guess)	$\theta$ (compute)
64	.3805E-01	.3563E-01
65	.3684E-01	.3950E-01
66	.3817E-01	.3537E-01
67	.3677E-01	.3932E-01
68	.3805E-01	.3563E-01
69	.3684E-01	.3950E-01
70	.3817E-01	.3537E-01

The conditions that lead to a repeating guess-compute cycle are not known beforehand. This type of failure occurs only on rare occasions. To eliminate this uncertainty, however, the successive averaging method has been replaced in the computer program described in this report by the Newton-Raphson technique. When the successive averaging method is used, it is restricted to only the first several iterations. The computer then switches to the Newton-Raphson scheme.

### 3.1.2 Newton-Raphson Iteration

The Newton-Raphson technique of iteration is based on a first-order Taylor series approximation of a function whose value is approaching zero.

$$H(x+dx) = H(x) + \frac{\partial H}{\partial x} dx \approx 0. \quad (3.3)$$

A new guess is defined by solving Equation (3.3) for  $dx$ , such that

$$x^{m+1}(\text{new guess}) = x^m(\text{old guess}) + dx, \quad (3.4)$$

where

$$dx = -H(x)/(\partial H/\partial x) \quad (3.5)$$

The Newton-Raphson method of iteration is very fast. It has a second-order rate of convergence in the neighborhood of the final solution. However, the method can diverge if the initial guess is too far from the final solution. It is, therefore, best to start out by using the linear extrapolation technique (Equation 3.2).

At the start of a new time step, program OR-NATURE uses the linear extrapolation technique to make the initial guess. On the next few

iterations OR-NATURE uses the successive averaging technique. During the final iterations, OR-NATURE uses the Newton-Raphson method until convergence is reached.

### 3.1.3 Golden Section Search

The most sophisticated technique for iteration used in the computer program described in this report is the so-called "Golden Section Search" method. It is a special case of a Fibonacci Section Search. A detailed description is presented in reviews by Aoki (1971) and by Jacoby et al. (1972). It can be shown that given the total number of times that a function is to be evaluated, a Fibonacci Section Search of a unimodal function is optimal. It minimizes the maximum possible interval of uncertainty in which the minimum of the function lies.

The Golden Section Search method to determine the location of the minimum of function H consists of several steps (Figure 3.1).

Step a) Choose two values  $a_0$  and  $b_0$  of the independent variable which bracket the minimum of function H. The initial interval of uncertainty in locating the minimum of function H is now defined as  $[a_0, b_0]$ .

Step b) Compute the values of the interior points

$$\begin{aligned}x_1 &= a_0 + .328(b_0 - a_0), \\x'_1 &= a_0 + .618(b_0 - a_0),\end{aligned}\tag{3.6}$$

and evaluate function H at the points  $x_1, x'_1$ . Set the iteration index  $m = 1$  and  $a_m = a_0, b_m = b_0$  and proceed with the next step.

Step c) There are two possible results of step b)

i) If  $H(x_m)$  is less than or equal to  $H(x'_m)$  the next interval of uncertainty is chosen as  $[a_{m+1}, b_{m+1}]$  such that

$$\begin{aligned}a_{m+1} &= a_m, \\b_{m+1} &= x'_m, \\x'_{m+1} &= x_m, \text{ and} \\x_{m+1} &= a_{m+1} + .328(b_{m+1} - a_{m+1}).\end{aligned}\tag{3.7}$$

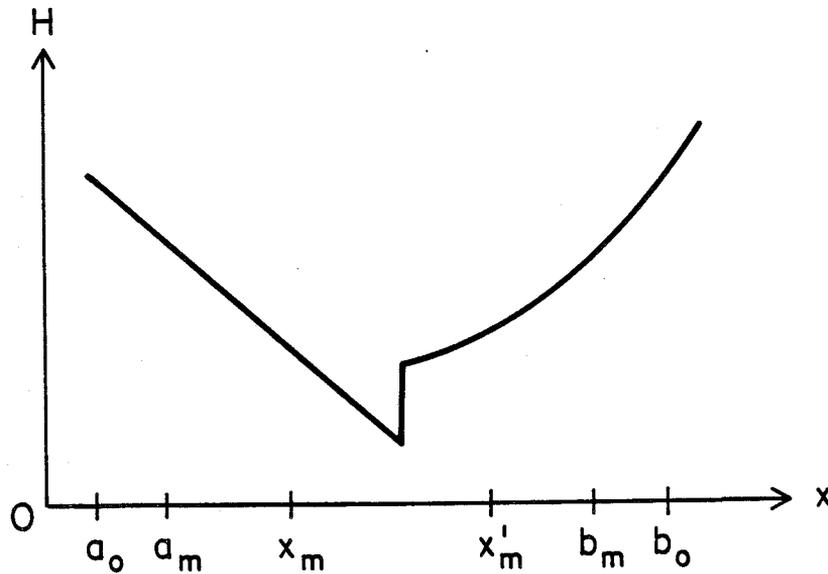


Figure 3.1. Schematic diagram showing details of method of the "Golden Section Search" for locating the minimum of a function H.

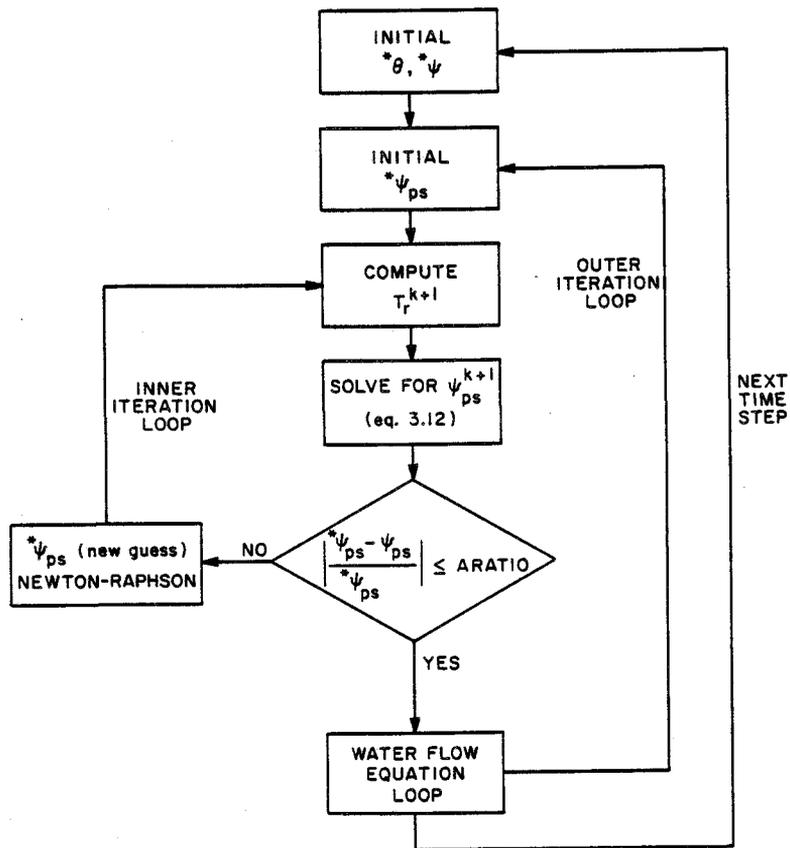


Figure 3.2. Flow chart of the method of iteration used to calculate the plant surface potential  $\psi_{ps}$ .

Evaluate the value of  $H(x_{m+1})$ , then set  $m = m+1$  and return to the beginning of step c).

- ii) If  $H(x_m)$  is greater than  $H(x'_m)$ , the next interval of uncertainty is chosen as  $[a_{m+1}, b_{m+1}]$  such that

$$\begin{aligned} a_{m+1} &= x_m, \\ b_{m+1} &= b_m, \\ x_{m+1} &= x'_m, \text{ and} \\ x'_{m+1} &= a_{m+1} + .618(b_{m+1} - a_{m+1}). \end{aligned} \quad (3.8)$$

Evaluate the value of  $H(x'_{m+1})$ , set  $m = m+1$  and return to the beginning of step c).

- Step d) The iteration procedure of step c) ends when the interval of uncertainty is reduced to some specified ratio of the original interval by the statement

$$\text{stop if } \left( \frac{b_{m+1} - a_{m+1}}{b_0 - a_0} \right) \leq \text{QRATIO}. \quad (3.9)$$

Test points  $x_m$  and  $x'_m$  are always within the interval  $[a_m, b_m]$  (Figure 3.1). However, during any given iteration, the program evaluates function  $H$  at only one of these points, the other points having been evaluated on the previous iteration. Thus, only one evaluation of function  $H$  is required per iteration.

The Fibonacci Section Search is the most efficient no-derivative line search procedure that guarantees a prescribed accuracy. The only condition required is that the function  $H$  be unimodal in the interval of the search. Except for this unimodal property, which is normally satisfied in some neighborhood of a minimum, the function may be irregular and discontinuous.

The interval of uncertainty, i.e., the location of the minimum of function  $H$ , is reduced very rapidly. The interval of uncertainty is reduced to one percent of the original interval in 11 iterations. In general, the interval of uncertainty on the  $m$ -th iteration is approximated by the formula

$$(b_m - a_m) = \frac{(b_0 - a_0)}{FB_{m+1}}, \quad (3.10a)$$

where the Fibonacci numbers  $FB_m$  are defined by

$$FB_m = FB_{m-1} + FB_{m-2} \quad m = 2, \dots, \infty, \quad (3.10b)$$

and where

$$FB_0 = FB_1 = 1. \quad (3.10c)$$

Thus, on the eleventh iteration,  $FB_{11}=144$  and  $(b_{10}-a_{10})/(b_0-a_0) = .007$ .

The number of iterations required to compute the minimizing value of a function to accuracy QRATIO is the greatest integer less than or equal to

$$1 + \left[ \frac{\ln(QRATIO)}{\ln(1-c)} \right] \quad (3.10d)$$

where  $c = (3-\sqrt{5})/2 = .381966$ .

### 3.2 Algorithm to Compute the Plant Surface Potential

To evaluate the root sink model as stated by Equation (1.52) at time level  $(k+1/2)$ , the plant surface potential,  $\psi_{ps}^{k+1/2}$  must be determined. However, the plant surface potential depends on the potential transpiration demand, the potential surface flux, the soil matric potential, and the root distribution. The correct value of  $\psi_{ps}$  for a given time step is found with an iterative algorithm.

- 1) Make an estimate of water content  $\theta_i^{k+1/2}$ , from Equations (2.4b) and (2.10b) and an estimate of water potential,  $\psi_i^{k+1/2}$ , where

$$*\psi_i^{k+1} = \psi_i^k + ACLRAT \left( \frac{\Delta t^{k+1}}{\Delta t^k} \right) (\psi_i^k - \psi_i^{k-1}), \quad (3.11a)$$

and

$$*\psi_i^{k+1/2} = (\psi_i^k + *\psi_i^{k+1})/2, \quad (3.11b)$$

for  $i = 1, \dots, n$  at time level  $(k+1/2)$ .

- 2) Make an initial estimate of the plant surface potential by linear extrapolation from the previous time step,

$$\psi_{ps}^{*k+1/2} = \psi_{ps}^{k-1/2} + \text{ACLRAT} \left( \frac{\Delta t^{k+1}}{\Delta t^k} \right) (\psi_{ps}^{k-1/2} - \psi_{ps}^{k-3/2}). \quad (3.12a)$$

- 3) Compute the actual rate of transpiration,  $T_r^{k+1/2}$ , based on the estimated plant surface potential and the potential rate of transpiration as described by Equation (1.41).
- 4) Set the actual transpiration demand of step 3) equal to the sum of the root sinks according to Equation (1.53) and solve for the plant surface potential. This is the computed value of  $\psi_{ps}^{k+1/2}$ ,

$$\psi_{ps}^{k+1/2} = \frac{T_r(\psi_{ps}^{*k+1/2}) - \sum_{i=2}^{n-1} [K_{\text{sys},i} \cdot \text{RAF}_i \cdot (z_i + \text{RPF}_i - \psi_i^{*k+1/2} \cdot \text{CNVRSN}) \cdot \left( \frac{z_{i+1} - z_{i-1}}{2} \right)]}{\sum_{i=2}^{n-1} [K_{\text{sys},i} \cdot \text{RAF}_i \cdot \left( \frac{z_{i+1} - z_{i-1}}{2} \right) \cdot \text{CNVRSN}]}, \quad (3.12b)$$

where  $K_{\text{sys},i}$ ,  $\text{RAF}_i$ , and  $\text{RPF}_i$  are evaluated with values of  $\theta_i^{*k+1/2}$ .

- 5) Compare the estimated and computed values of the plant surface potential. Convergence is reached when the ratio

$$\left| \frac{\psi_{ps}^{*k+1/2} - \psi_{ps}^{k+1/2}}{\psi_{ps}^{*k+1/2}} \right| \leq \text{ARATIO}, \quad (3.13)$$

where ARATIO is the specified convergence ratio. The iterator stops when Equation (3.13) is satisfied. At that time, the program proceeds to solve the water flow equation.

- 6) If a satisfactory degree of convergence is not obtained in Step 5), make an improved estimate of  $\psi_{ps}^{*k+1/2}$  by means of a Newton-Raphson iteration scheme. For this scheme, define the optimization function H as the difference between the computed and guessed values of plant surface potential

$$H = \psi_{ps}^{*k+1/2} - \psi_{ps}^{k+1/2}. \quad (3.14)$$

The objective is to iterate on  $\psi_{ps}^{*k+1/2}$  until H goes to zero. The derivative of H must be evaluated as a function of the guessed

value, specified by Equation (3.3). The superscript  $k+1/2$  of Equation (3.14) is dropped for convenience in further discussions.

$$\frac{\partial H}{\partial(\psi_{ps}^*)} = 1 - \frac{\partial(\psi_{ps})}{\partial(\psi_{ps}^*)}. \quad (3.15)$$

The second part of the right side of Equation (3.15) is obtained by differentiating Equation (3.12b), thus,

$$\frac{\partial(\psi_{ps})}{\partial(\psi_{ps}^*)} = \frac{\partial(T_r)}{\partial(\psi_{ps}^*)} \left[ \frac{1}{\sum_{i=2}^{n-1} K_{sys,i} \cdot \text{RAF}_i \cdot \left(\frac{z_{i+1} - z_{i-1}}{2}\right) \cdot \text{CNVRSN}} \right]. \quad (3.16)$$

Using Equations (3.4) and 3.5), an improved estimate of the plant surface potential is made by

$$\psi_{ps}^{*k+1/2}(\text{new guess}) = \psi_{ps}^{*k+1/2}(\text{old guess}) - \frac{H}{\partial H / \partial \psi_{ps}^*} \Big|_{(\text{old guess})} \quad (3.17)$$

where H is evaluated by using Equation (3.14) and the derivative by using Equations (3.15) and (3.16), all evaluated with the old guessed value of  $\psi_{ps}^{*k+1/2}$ .

- 7) Return to Step 3). The iteration algorithm of steps 3) to 6) continues for fixed values of  $\theta_i^{*k+1/2}$  until Equation (3.13) is satisfied. If the new estimate of  $\psi_{ps}^{*k+1/2}$  from Equation (3.17) violates the feasibility condition of Equation (1.42), then set  $\psi_{ps}^{*k+1/2}$  to the limiting value.

$$\text{If } \psi_{ps}^{*k+1/2} > 0, \quad \text{set } \psi_{ps}^{*k+1/2} = 0. \quad (3.18)$$

- 8) If the final converged value of  $\psi_{ps}^{*k+1/2} \leq \psi_{wilt}$ , the plant is assumed to be permanently wilted and dead. When wilted, transpiration and root uptake stops and the program no longer computes  $\psi_{ps}$ , A(i) or G(i).

The algorithm of steps 1) through 7) above requires the solution of two sequential iteration schemes called the "inner iteration" and "outer iteration" (Figure 3.2). Each time a new estimate is made of the water content,  $\theta_i^{*k+1/2}$ , during a given time step, the program must first solve

program must first solve the inner iterator routine which consists of steps 3) to 6). In the inner iterator, the program hunts for a value of  $\psi_{ps}^{k+1/2}$  for fixed values of  $\theta_i^{k+1/2}$ . Once a feasible value of  $\psi_{ps}^{k+1/2}$  is found, the program enters the outer iteration routine. The outer iterator finds an improved estimate of  $\theta_i^{k+1/2}$  for a fixed value of  $\psi_{ps}^{k+1/2}$ . This sequential process continues back and forth until both  $\psi_{ps}^{k+1/2}$  and  $\theta_i^{k+1/2}$  coverage.

### 3.3 Algorithm to Compute the Water Content

The water content must be estimated by iteration to evaluate the non-linear coefficients A, D, and K in Equation (2.1). Subroutine WATER uses the successive averaging technique on the first three iterations and then switches to a Newton-Raphson iteration scheme. In the Newton-Raphson scheme, the optimization function H is defined as the difference between the computed  $\theta_i^{k+1}$  and the guessed  $\theta_i^{k+1}$  at node i,

$$H_i = \theta_i^{k+1} - \theta_i^{k+1} \quad i = 1, \dots, n. \quad (3.19)$$

The objective is to iterate on  $\theta_i^{k+1}$  until  $H_i$  goes to zero for each node. In the following discussion, the subscript i will be dropped, but it is to be understood that the iterator scheme is simultaneously applied to each node. The superscript k+1 is also omitted, since all values of  $\theta$  are being evaluated at the future time level (k+1).

Function H is expanded by a Taylor series to the first-order about the previous guess

$$H(\theta + d\theta) = H(\theta) + \frac{\partial H}{\partial \theta} \cdot d\theta = 0. \quad (3.20)$$

The derivative of H in Equation (3.19) with respect to  $\theta$

$$\frac{\partial H}{\partial \theta} = 1 - \frac{\partial \theta}{\partial \theta}, \quad (3.21a)$$

is finite-differenced between iterations m and m-1 as

$$\frac{\partial H}{\partial \theta} = 1 - \left( \frac{\theta^m - \theta^{m-1}}{\theta^m - \theta^{m-1}} \right). \quad (3.21b)$$

The correction  $d^* \theta$  is solved from Equation (3.20) such that

$$d^* \theta = \frac{-H}{\partial H / \partial^* \theta} \quad (3.22)$$

Upon substitution of Equations (3.19), (3.21) and (3.22) into (3.4), an improved estimate of water content is obtained by

$${}^* \theta^{m+1}(\text{new guess}) = {}^* \theta^m(\text{old guess}) - \frac{({}^* \theta^m - \theta^m)}{[1 - (\frac{\theta^m - \theta^{m-1}}{{}^* \theta^m - {}^* \theta^{m-1}})]} \quad (3.23)$$

where the notation  ${}^* \theta^{m+1} = {}^* \theta_i^{k+1, m+1}$  and  $\theta^m = \theta_i^{k+1, m}$ . The following algorithm is used to compute the water content in subroutine WATER. A schematic diagram for the scheme is given in Figure 3.3.

- 1) Make an initial estimate of the water content for time level (k+1) by linear extrapolation from the previous time step, using Equation (2.10).
- 2) Compute the surface water flux,  $q_0^{k+1}$  by means of the Golden Section Search routine if a fourth type boundary condition is specified on the upper surface (Section 3.4).
- 3) Compute the plant surface potential,  $\psi_{ps}^{k+1/2}$ , using the Newton-Raphson scheme given in Section 3.2.
- 4) Evaluate the tri-diagonal matrix coefficients using  $q_0^{k+1}$ ,  ${}^* \theta_i^{k+1}$ , and  $\psi_{ps}^{k+1/2}$  in Equations (2.1) to (2.9). Solve the tri-diagonal matrix by the Thomas algorithm and compute  $\theta_i^{k+1}$ .
- 5) If any of the newly computed values of  $\theta_i^{k+1}$  violate the feasibility conditions of Equation (1.4), set them to the limiting value.
  - If  $\theta_i^{k+1} < \theta_d$ , set  $\theta_i^{k+1} = \theta_d$ ,  $i = 1, \dots, n$ . (3.24a)
  - If  $\theta_i^{k+1} > \theta_s$ , set  $\theta_i^{k+1} = \theta_s$ ,  $i = 1, \dots, n$ . (3.24b)
- 6) Compare the estimated and computed values of water content by means of Equation (2.12).
- 7) If a satisfactory degree of convergence is obtained in step 6) at all nodes, the water content algorithm ends and the program proceeds to the next time step or to the Golden Section Search routine to find an improved estimate of the surface flux if the upper boundary condition is described by a flux type.

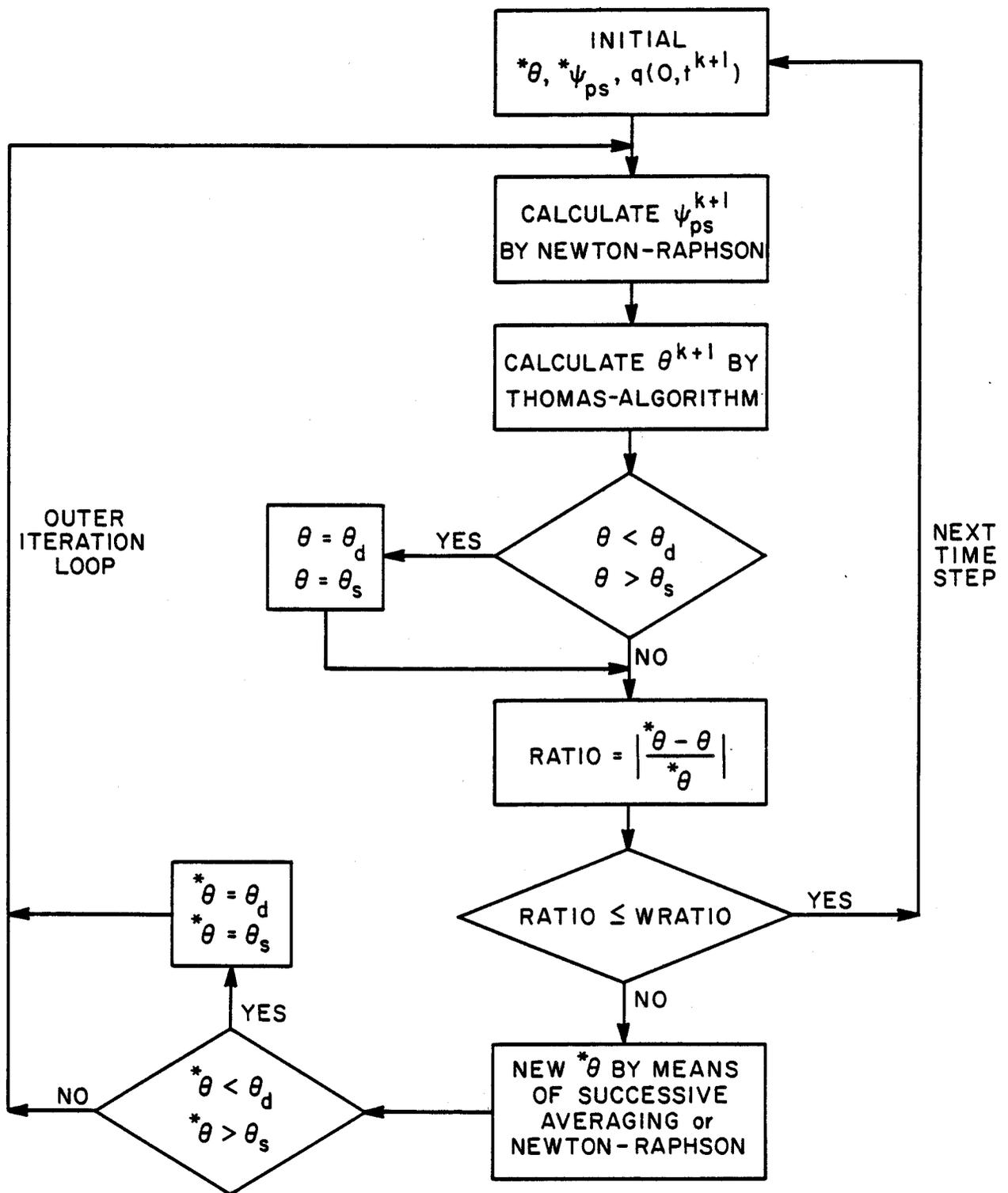


Figure 3.3. Flow chart of the method of iteration used to calculate the water content

- 8) If a satisfactory degree of convergence is not obtained in Step 6), a new estimate of  $\theta_i^{k+1}$  is made. During the first three iterations, a new estimate of water content is made by means of the successive averaging scheme given by Equation (2.11). Proceed to Step 9) at the end of each of the first three iterations. After the fourth or successive iterations, a new estimate of water content is made by means of the Newton-Raphson scheme of Equation (3.23).
- 9) If the new estimates of water content from Step 8) violate the feasibility conditions of Equation (1.4), set them to the limiting value.

$$\text{If } \theta_i^{k+1} < \theta_d, \text{ set } \theta_i^{k+1} = \theta_d, \quad i = 1, \dots, n. \quad (3.25a)$$

$$\text{If } \theta_i^{k+1} > \theta_s, \text{ set } \theta_i^{k+1} = \theta_s, \quad i = 1, \dots, n. \quad (3.25b)$$

Return to Step 3).

The algorithm to solve the water flow equation is the same, regardless of whether the problem is solved in terms of  $\theta$  (volumetric water content),  $\psi$  (matric potential) or  $F$  (diffusivity potential).

### 3.4 Algorithm to Compute the Surface Flux of Water

To solve the flow equation based on water content with a flux type boundary condition (4th type) on the upper surface, one must specify the potential flux,  $R(0,t)$ . Water infiltrates the soil as fast as supplied as long as the rate of supply to the surface is smaller than the rate of infiltrability. Hillel (1971) calls this flux condition as being "flux-controlled". When the rate of supply exceeds the rate of infiltration, it determines the rate of infiltration. Hillel (1971) refers to this flux condition as being "profile-controlled". The same terminology is used to describe water flux during evaporation.

When the surface flux is flux-controlled, the actual flux equals the potential flux

$$q_0^{k+1} = R(0, t^{k+1}). \quad (3.26)$$

The solution to the water flow equation under this condition is straightforward. Substitute Equation (3.26) into the right side of the boundary

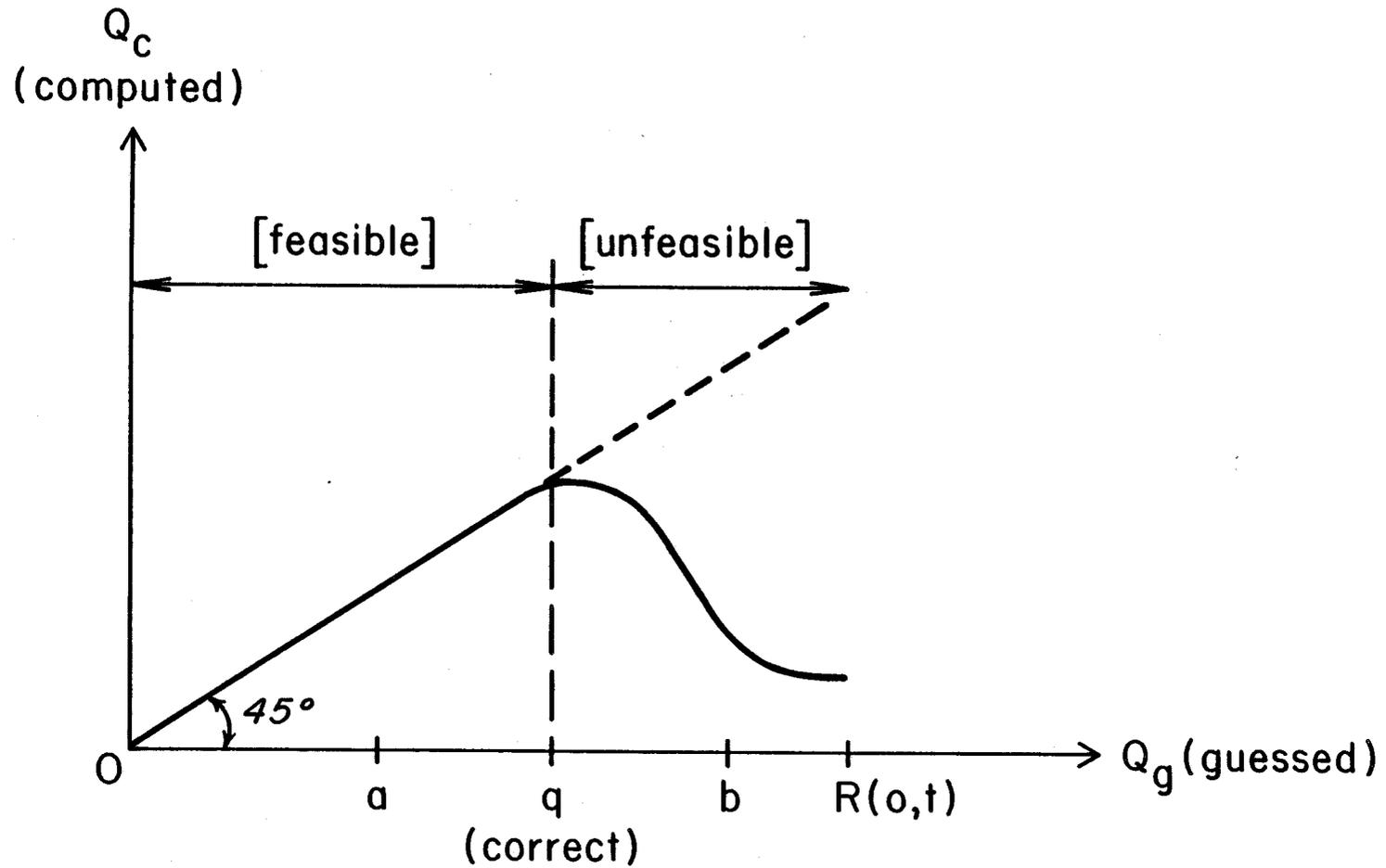


Figure 3.4. Conceptual diagram of the method used to determine convergence of the iterator for calculating the flux of water at the soil surface.

condition of Equation (2.6c). When the surface flux becomes profile-controlled, the magnitude of the actual flux is less than that of the potential flux, thus

$$|q_0^{k+1}| < |R(0, t^{k+1})|. \quad (3.27)$$

The actual flux is not known beforehand and an iterative algorithm must be used to find it. The solution to this problem is not trivial, but it has received little attention. In fact, Neuman et al. (1975) seem to be the only authors who attempted to describe this problem with any degree of completeness.

Two major difficulties are encountered in solving the profile-controlled problem. These are defining an appropriate criterion that indicates when the correct flux has been found by an iteration scheme and finding an iterator scheme that is not time consuming. The actual surface flux is subject to the condition that its magnitude be as large as possible but not greater than the potential flux according to Equation (3.27). In addition, the resulting water content profile must not violate the air-dry and saturation limits given by Equation (1.4).

Figure 3.4 shows schematically a method for determining the actual surface flux. Figure 3.4 is constructed by plotting the guessed values of flux versus the computed values of flux. In the feasible range, the guessed and the computed values of flux are equal. In the unfeasible range, the guessed and the computed values of flux differ. The latter condition occurs only when a computed value of water content in one or both of the two top nodes is unfeasible and is set to either an air-dry or saturated value.

The iteration scheme used to find the correct surface flux is that of the Golden Section Search method.

- 1) The initial interval of uncertainty in finding the actual flux is defined as  $[a_0, b_0]$  where

$$a_0 = 0,$$

$$b_0 = R(0, t^{k+1}),$$

with intermediate test points

$$x_0 = a_0 + .328(b_0 - a_0),$$

$$x'_0 = a_0 + .618(b_0 - a_0),$$

and the initial guess of the surface flux given as

$$Q_g = b_0 = R(0, t^{k+1}).$$

- 2) Make an initial guess of the water content,  ${}^* \theta_i^{k+1}$ , for time level (k+1) by linear extrapolation from the previous time step using Equation (2.10).
- 3) Substitute  $Q_g$  and  ${}^* \theta_i^{k+1}$  into the coefficients of the finite-difference equations 2.1, 2.6c, and 2.8c, where  $q_0^{k+1} = Q_g$ .
- 4) Solve the resulting tri-diagonal matrix of Step 3) by the Thomas algorithm.
- 5) Holding  $Q_g$  fixed, iterate on the values of water content  ${}^* \theta_i^{k+1}$  by means of the successive averaging and the Newton-Raphson techniques until  ${}^* \theta_i^{k+1}$  and  $\theta_i^{k+1}$  converge. The water content is always restricted between air-dry and saturation, as in Equation (3.25). This last step must be completed before proceeding to Step 6).
- 6) Compute the surface flux by solving for  $Q_c$  from the backward-difference expression of Equation (2.6c) using the  $\theta_i^{k+1}$  values from step 5),

$$Q_c = \frac{(\theta_1^{k+1} - \theta_1^k)}{\Delta t^{k+1}} (z_2 - z_1) - D({}^* \theta_{1+1/2}^{k+1}) \frac{\{\theta_2^{k+1} - \theta_1^{k+1}\}}{(z_2 - z_1)} + K({}^* \theta_{1+1/2}^{k+1}) \cdot \text{GRAV}, \quad (3.28)$$

where  $\theta_i^{k+1}$  are the most recently computed values of water content and  ${}^* \theta_i^{k+1}$  are the most recently guessed values of water content.

- 7) If  $Q_g \neq Q_c$  or if in step 5), the computed water content of one of the top three nodes is either greater than saturation or less than air-dry (i.e., the computer program sets MQFAIL = I, where I is the node that failed), then the magnitude of  $Q_g$  is too large and must be reduced. The new interval of uncertainty is chosen as  $[a_{m+1}, b_{m+1}]$  such that

$$\begin{aligned} a_{m+1} &= a_m, \\ b_{m+1} &= x'_m, \\ x'_{m+1} &= x'_m, \end{aligned}$$

$$x_{m+1} = a_{m+1} + .328(b_{m+1} - a_{m+1}).$$

In other words, the upper limit is moved to a lower value and the new flux guess is taken as

$$Q_g = x_{m+1}.$$

Go to Step 9).

- 8) If  $Q_g = Q_c$ , the guessed flux is in the feasible range but it might not be as large as possible.  $Q_g$  should be increased in magnitude. This is described in the following steps. The new interval of uncertainty is chosen as  $[a_{m+1}, b_{m+1}]$  such that

$$a_{m+1} = x_m,$$

$$b_{m+1} = b_m,$$

$$x_{m+1} = x'_m,$$

$$x'_{m+1} = a_{m+1} + .618(b_{m+1} - a_{m+1}).$$

In other words, the lower limit is moved to a higher value and the new flux guess is taken as

$$Q_g = x'_{m+1}.$$

- 9) After each iteration, plot the guessed flux  $Q_g$  versus its computed value,  $Q_c$ , according to Figure 3.4. This step is not actually done by the computer program but the user may wish to do this as a conceptual aid in understanding this routine. The correct flux lies at the point of bifurcation or separation in the conceptual diagram of Figure 3.4. The correct flux is the flux with the largest feasible flux. Since an iteration scheme is being used to find the correct flux, the final solution will only be known to lie within some specified interval of uncertainty, given by

$$\left| \frac{b_{m+1} - a_{m+1}}{Q_g} \right| \leq \text{QRATIO}. \quad (3.29)$$

If Equation (3.29) is not satisfied, return to Step 3). Iteration is continued until Equation (3.29) is satisfied. The convergence criteria, QRATIO, is a ratio specified in parameter card #4. Typically, one would set QRATIO = .01 (one percent).

In subroutine WATER, the variables used in steps 1) through 9) above are defined as:

$$\begin{aligned}
 a_{m+1} &= \text{QGAk}, \\
 x_{m+1} &= \text{QGTK}, \\
 x'_{m+1} &= \text{QGTKP}, \\
 b_{m+1} &= \text{QGBK}, \\
 Q_c &= \text{QC}, \\
 Q_g &= \text{QG}, \\
 R(0, t^{k+1}) &= \text{QP}.
 \end{aligned}$$

The iteration scheme using the Golden Section Search of Steps 1) through 9) can fail to converge, depending on the magnitude of the potential flux, the diffusivity function, the size of the time step, or the size of the space step. The most sensitive step is that of the initial guess of water content,  $\theta_i^{k+1}$ , in Step 2) and the subsequent water content guesses during the first few flux iterations. If too large a change is made in guessing  $\theta_i^{k+1}$ , the program will fail to converge and  $Q_g \neq Q_c$ . It is not possible to know if this condition (i.e.,  $Q_g \neq Q_c$ ) is caused by an incorrect estimate of the flux guess or by a too large change.

#### 3.4.1 Modifications of the Golden Section Search Method

Through trial and error, a method was found which is effective in eliminating the various "starting" problems associated with the Golden Section Search. This method is used to start the first four flux iterations. From the fifth flux iteration on, the regular Golden Section Search is followed.

The modified iteration scheme consists of Steps 1) through 6) as described above. Then a different procedure is followed.

7a) At the end of the first flux iteration of Step 6), feasibility is checked.

- i) If  $Q_g$  is feasible and if  $\theta_1^{k+1}$ ,  $\theta_2^{k+1}$ ,  $\theta_3^{k+1}$  are feasible, then set

$$a_{m+1} = Q_g$$

$$b_{m+1} = b_m,$$

and the program proceeds to step iii).

ii) If either  $Q_g$ ,  $\theta_1^{k+1}$ ,  $\theta_2^{k+1}$  or  $\theta_3^{k+1}$  is unfeasible, then set

$$a_{m+1} = a_m,$$

$$b_{m+1} = Q_g,$$

$$Q_g = Q_g.$$

Return to Step 3) of the Golden Section Search.

iii) The next guess for the flux is given as

$$Q_g = a_{m+1} + .328(b_{m+1} - a_{m+1}).$$

Return to Step 3) of the Golden Section Search.

8a) At the end of the second flux iteration of Step 6), feasibility is checked.

iv) If  $Q_g$  is feasible and if  $\theta_1^{k+1}$ ,  $\theta_2^{k+1}$ ,  $\theta_3^{k+1}$  are feasible, then set

$$a_{m+1} = Q_g,$$

$$b_{m+1} = b_m,$$

$$x_{m+1} = a_{m+1} + .328(b_{m+1} - a_{m+1}),$$

$$x'_{m+1} = a_{m+1} + .618(b_{m+1} - a_{m+1}),$$

and the program proceeds to step vi).

v) If either  $Q_g$ ,  $\theta_1^{k+1}$ ,  $\theta_2^{k+1}$  or  $\theta_3^{k+1}$  is unfeasible, then set

$$a_{m+1} = a_m,$$

$$b_{m+1} = b_m,$$

$$x_{m+1} = a_{m+1} + .1(b_{m+1} - a_{m+1}),$$

$$x'_{m+1} = a_{m+1} + .2(b_{m+1} - a_{m+1}),$$

and the program proceeds to Step 6

vi) The next estimate of the flux is given as

$$Q_g = x'_{m+1}.$$

Return to Step 3) of the Golden Section Search.

9a) At the end of the third flux iteration of Step 6), set

$$a_{m+1} = a_m,$$

$$b_{m+1} = b_m,$$

$$x_{m+1} = x_m,$$

$$x'_{m+1} = x'_m,$$

$$Q_g = x_{m+1}.$$

Return to Step 3) of the Golden Section Search.

10a) At the end of the fourth flux iteration of Step 6), return to steps 7) through 9). On the fifth and subsequent iteration, follow Steps 1) through 9) of the Golden Section Search until convergence is reached, as specified by Equation (3.29).

### 3.4.2 Mini-Iterator

The Golden Section Search scheme involving Steps 1) through 9) and Steps 7a) through 10a) as described here is very accurate. But it is very time consuming, particularly if the number of spatial nodes is large. The top 10 nodes usually have the most influence in the determination of the magnitude of the surface flux. It was determined by trial and error that a sliding scale approach may be used. In the start of each new time step, the flux iterator algorithm uses only the first 10 nodes at the top of the soil column to evaluate the water content. After each additional flux iteration, only the top (10 + IWORST) nodes are used. IWORST is the node at which the largest difference occurred between computed and guessed values of water content. The location of the spatial nodes does not change during this procedure, only the number of nodes at which the water content is being evaluated. The Golden Section Search is accelerated by the following steps, which are shown schematically in Figure 3.5.

- a) Set  $NMINI = \min|10, n|$ , and the index of iteration  $m = 0$  and make an initial guess of water content,  $\theta_i^{*k+1, m=0}$ .
- b) Use the Golden Section Search scheme described previously in Steps 1) through 9) and Steps 7a) through 10a), but solve the flow equation based on water content using only the top  $NMINI$

spatial nodes. At node NMINI, specify a first type boundary condition such that  $\theta(NMINI)$  is held fixed to its guess during the water content iteration:

$$\theta_{NMINI}^{k+1,m+1} = \theta_{NMINI}^{*k+1,m}$$

The program continues to iterate until all NMINI water content values,  $\theta_i^{*k+1,m}$ , converge and the surface flux iterator converges. At the end of each iteration, set  $m = m+1$ .

- c) Using the NMINI values of water content and the flux computed in Step b as an initial guess, solve the water flow equation using all  $n$  nodes. The proper lower boundary condition must be used. The initial guess is taken as

$$\theta_i^{*k+1,m+1} = \theta_i^{*k+1,m} \quad i=1, \dots, NMINI,$$

obtained from step b, and

$$\theta_i^{*k+1,m+1} = \theta_1^{*k+1,m=0} \quad i=NMINI+1, \dots, n$$

where the RHS of the above expression is the most recent guessed value, from Equation (2.10) or Step e).

- d) If the computed and guessed values of water content and flux agree in Step c), the program has converged for this time step.  
 e) If the computed and guessed values of water content and flux do not agree in Step c), then set

$$\theta_i^{*k+1,m+1} = \theta_i^{k+1,m} \quad i=1, \dots, n$$

as obtained from Step c, and

$$NMINI = \min\{I WORST + 10, n\}.$$

Return to Step b, using the new value of NMINI, and

$$\theta_i^{*k+1,m+1}$$

Step b) is called the "mini-iterator" and Step c) the "maxi-iterator." Under most conditions, this method will require 1 to 20 mini iterations and 1 to 3 maxi iterations per time step. If the maxi-iterator is used by itself as indicated in the original Golden Section Search scheme, 1 to 20 iterations per time step are needed. Hence, the mini-maxi approach reduces the computational time by at least an order of magnitude, assuming

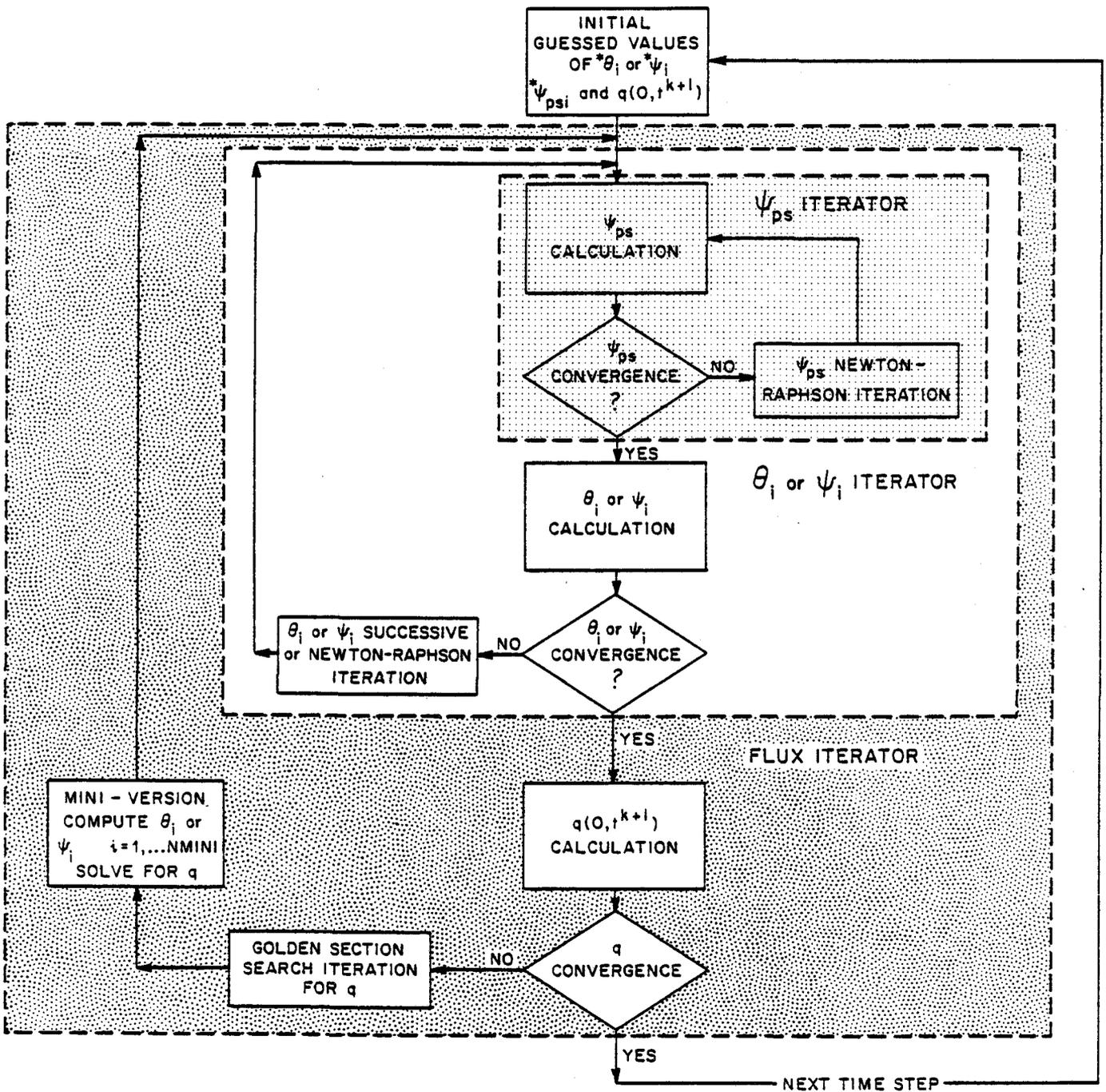


Figure 3.5. Flow chart of the method of iteration used in the calculation of the water flux at the soil surface.

a problem involving 100 nodes is being solved, or to state it another way, 10 mini-iterations require approximately the same computational time as one maxi-iteration.

Initial examination might suggest that the mini-iterator would give very poor results since it only solves the flow equation based on water content at the top NMINI nodes and it specifies an arbitrary lower boundary condition. However, in practice, the mini-iterator works very well. The mini-iterator is only used to decide if a guessed flux value is either feasible or unfeasible. Only the top several nodes are needed to make this decision. Once the Golden Section Search routine locates a possible flux solution, the maxi-iterator is used to correctly determine the water content of all nodes. The mini-iterator does most of the work, and is also the quickest. The mini-iterator provides a "coarse adjustment" and the maxi-iterator gives a "fine adjustment" to the Golden Section Search technique.

### 3.5 Algorithm to Compute the

#### Liquid Phase Solute Concentration

In the absence of any source/sink terms, the solute displacement Equation (1.34) is linear and no iteration scheme is needed to obtain the liquid phase solute concentration,  $c_i^{k+1}$ . However, if there is a source/sink term,  $G$ , the solute displacement equation becomes non-linear if  $G$  is a non-linear function of  $c_i^{k+1/2}$  (Section 1.5). Since the magnitude of the source/sink function is normally small in comparison to that of dispersion and convection, the procedure adopted here is to approximate the  $G$  term and treat the solute displacement equation as if it is linear. The computer program uses a guessed value of concentration,  $c_i^{*k+1}$ , in the evaluation of the  $G$  term. The program guesses  $c_i^{*k+1}$  using a linear extrapolation such that

$$c_i^{*k+1} = c_i^k + \text{ACLRAT}\left(\frac{\Delta t^{k+1}}{\Delta t^k}\right)(c_i^k - c_i^{k-1}) \quad i=1, \dots, n. \quad (3.30)$$

Substitute  $*c_i^{k+1/2}$  from Equation (3.31) into Table 1.5 to evaluate GCOEF. The source/sink term  $G(i)$  is defined

$$*S_i^{k+1/2} = (*S_i^{k+1/2} + S_i^k)/2 \quad (3.31a)$$

$$*c_i^{k+1/2} = (*c_i^{k+1} + c_i^k)/2 \quad (3.31b)$$

$$\text{Passive: } G_i^{k+1/2} = \text{GCOEF} (*c_i^{k+1/2}, *S_i^{k+1/2}) \cdot A_i^{k+1/2} \quad (3.32a)$$

$$\text{Active: } G_i^{k+1/2} = \text{GCOEF} (*c_i^{k+1/2}, *S_i^{k+1/2}) \quad (3.32b)$$

at the  $(k+1/2)$  time step by substituting Equation (3.31) into Equation (1.54) to get Equation (3.32). The resulting tri-diagonal matrix of Equations (2.25), (2.29) and (2.30) is solved by the Thomas algorithm for the  $n$  values of  $c_i^{k+1}$ . The program will not iterate on  $c_i^{k+1}$ , even if this value is not identical to the guessed value  $*c_i^{k+1}$ . Since the numerical contribution of  $G(i)$  is small, the guessed value is not much different from the computed one and this approximation gives good results.

However, a slight modification is made to update the guessed value of  $*c_i^{k+1}$  when a sorption model is included in the solute displacement equation (Section 3.6).

### 3.6 Algorithm to Compute the Sorbed or Solid Phase Solute Concentration

When specifying a sorption term in Equation (1.34), the solute displacement equation becomes a function of the two dependent variables,  $c_i^{k+1}$  and  $S_i^{k+1}$ . The liquid phase of solute at time level  $(k+1)$  and node  $i$  is defined by variable  $c_i^{k+1}$  and the sorbed phase by variable  $S_i^{k+1}$ . For each of the space nodes, one must specify two equations, namely the transport equation of Equation (1.34) and the sorption model (Tables 1.3 and 1.4). Typically, one would solve these  $2n$  equations simultaneously. An alternative method is to use an iterative algorithm where one of the dependent variables,  $*S_i^{k+1}$ , is assumed to be known for a given time level and the remaining variable,  $c_i^{k+1}$ , is then obtained by the Thomas

algorithm as in Section 3.5. An iterative procedure is used to improve on the guessed value of  $S_i^{k+1}$  and the procedure is repeated until reaching a specified convergence criterion. No iteration is required when using a linear equilibrium sorption term (e.g., JSORB=1). The iteration algorithm is as follows:

- 1) Make an initial guess of  $S_i^{k+1}$ , using the linear extrapolation technique, where

$$S_i^{k+1} = S_i^k + \text{ACLRAT} \left( \frac{\Delta t^{k+1}}{\Delta t^k} \right) (S_i^k - S_i^{k-1}) \quad i=2, \dots, n-1 \quad (3.33)$$

assuming that there is no sorption at Nodes 1 and n.

- 2) If there is a source/sink term, the coefficient GCOEF(i) is evaluated using an approximated value of concentration,  $c_i^{k+1}$ , obtained by a linear extrapolation technique as given by Equation (3.30). The source/sink term,  $G_i^{k+1/2}$ , is then determined using Equations (3.31) and (3.32) with GCOEF evaluated at  $c_i^{k+1/2}$  and  $S_i^{k+1/2}$ .

- 3) The sorption term is obtained by finite-difference methods such that

$$\left( \frac{\partial S}{\partial t} \right)_i = \frac{S_i^{k+1} - S_i^k}{\Delta t^{k+1}} \quad i=2, \dots, n-1 \quad (3.34)$$

where  $S_i^{k+1}$  is the most recently guessed value of sorption at node i.  $S_i^k$  is the computed value of sorption at node i, time level (k). There is no sorption allowed at Nodes 1 and n.

- 4) Substitute the value of G(i) from Step 2 and  $(\partial S / \partial t)_i$  from Step 3) into Equation (2.25).
- 5) Specify the upper and lower boundary conditions for the solute equation, using Equations (2.29) and (2.30).
- 6) Evaluate the tri-diagonal matrix of coefficients of Equation (2.25) and solve for  $c_i^{k+1}$ ,  $i = 1, \dots, n$  by the Thomas algorithm.
- 7) Use the computed values of  $c_i^{k+1}$  to recalculate the solid phase solute concentration  $S_i^{k+1}$  as follows:
  - 1) If sorption is modeled as an equilibrium process, backward-difference the sorption model at (i,k+1) and solve for  $S_i^{k+1}$  (Table 2.4) where  $c_i^{k+1}$  is taken from Step 6).

- ii) If sorption is modeled as a non-equilibrium process, finite-difference the model by a centered-in-time Crank-Nicolson scheme at  $(i, k+1/2)$  and solve for  $S_i^{k+1}$  (Table 2.5) where  $c_i^{k+1}$  is taken from Step 6).

8) The routine converges for this time step when

$$\max \left| \frac{S_i^{*k+1} - S_i^{k+1}}{S_i^{*k+1}} \right| \leq \text{SRATIO} \quad i=2, \dots, n-1 \quad (3.35)$$

where SRATIO is the convergence criterion, specified as a ratio. A one percent criterion is set by specifying SRATIO = .01.

- 9) If a satisfactory degree of convergence is not obtained in Step 8), new estimates of  $S_i^{*k+1}$  and  $c_i^{*k+1}$  are made. An improved estimate of the concentration of solute in the liquid phase is made by setting the estimated value equal to that of the most recently computed value

$$c_i^{*k+1} = c_i^{k+1} \quad i = 1, \dots, n. \quad (3.36)$$

Note that  $c_i^{*k+1}$  is only used to evaluate the source/sink term  $G(i)$ . A new estimate of  $S_i^{*k+1}$  is made as follows:

- i) During the first three iterations of a given time step, a successive averaging scheme is used to improve the estimate

$$S_i^{*k+1} = (S_i^{*k+1} + S_i^{k+1})/2 \quad i = 2, \dots, n-1. \quad (3.37)$$

- ii) On the fourth and additional iterations, a Newton-Raphson scheme is used. The optimization function  $H$  is defined as the difference between the computed  $S_i^{k+1}$  and guessed  $S_i^{*k+1}$  values of sorption at node  $i$ .

$$H_i = S_i^{*k+1} - S_i^{k+1} \quad i = 2, \dots, n-1. \quad (3.38)$$

The objective is to iterate on  $S_i^{*k+1}$  until  $H_i$  goes to zero for each node. The procedure is the same as that given for water content in Equations (3.20) through (3.23).

- 10) Return to Step 2).

The above procedure is further modified in that a "mini-iterator" scheme is also used. At the start of each new time step, the solute iterator algorithm uses only the first 20 nodes at the top of the soil column to evaluate the solute and sorption equations. Obviously, it is not necessary to use this technique if there are fewer than 20 nodes. After each additional solute iteration, only the top (20 + IWORST) nodes are used. IWORST is the node at which the largest difference occurred between computed and guessed values of sorption. At node NMINI = 20 + IWORST, a first type boundary condition is specified, where

$$c_{NMINI}^{k+1,m+1} = * c_{NMINI}^{k+1,m} \quad (3.38a)$$

$$s_{NMINI}^{k+1,m+1} = s_{NMINI}^{k+1,m=0} \quad (3.38b)$$

m is the mth iteration and m=0 refers to the initial guess given by Equation (3.33) at node NMINI. Additional details are given in Section 3.4.2.

### 3.7 Algorithms to Compute the Mass Balances

Program OR-NATURE uses two numerical integration techniques to evaluate integrals. One of these is called piecewise-constant integration, the other is based on a second-order Taylor series expansion (Salvadori and Baron, 1961). A mathematical description of the two is given in Sections 3.7.1 and 3.7.2).

Additional description of the integration techniques used to compute the mass balances of water and solute are given in Vol. IV, Section 7.1.18, keyed points (21) to (23). This discussion includes computer output variables CACCUM, CCMPT, CTRSUM, EVPRTE, FLTRTE, TRNSPR, WACCUM, AND WCMPT. SCMPTE is discussed in Vol. IV, Section 7.5.14, keyed point (3).

#### 3.7.1 Piecewise-Constant Integration

Define H(z) as the dependent variable and z as the independent variable. The piecewise-constant integration of H(z) versus z is

defined as

$$\text{Integral} = \sum_{i=1}^{n-1} H(z_i) \cdot (z_{i+1} - z_i) \quad (3.39)$$

where  $n$  is the total number of increments in variables  $H$  and  $z$ .

### 3.7.2 Integration Based on a Second-Order Taylor Series Expansion

Let  $H(z)$  be the dependent variable and  $z$  the independent variable. Define function  $y$  as the integral of variable  $H$  over the limits of  $x_1$  to  $x$ , so that

$$y(x) = \int_{x_1}^x H(z) dz. \quad (3.40)$$

Take successive derivatives of Equation (3.40) with respect to  $x$

$$\begin{aligned} y' &= H(x) \\ y'' &= H'(x) \\ &\cdot \cdot \cdot \\ y^n &= H^{(n-1)}(x). \end{aligned} \quad (3.41)$$

Substitute Equation (3.41) into the Taylor series expansion of  $y(x+ah)$  about  $x$ :

$$y(x+ah) = y(x) + ahH(x) + \frac{a^2 h^2}{2} H'(x) + \frac{a^3 h^3}{6} H''(x) + \frac{a^4 h^4}{24} H'''(x) + \frac{a^5 h^5}{120} H^{iv}(x), \quad (3.42)$$

where  $h = (x_i - x_{i-1})$  and  $a = (x_{i+1} - x_i)/h$ .

The Taylor series expansion of  $y(x-h)$  about  $x$  becomes

$$y(x-h) = y(x) - hH(x) + \frac{h^2}{2} H'(x) - \frac{h^3}{6} H''(x) + \frac{h^4}{24} H'''(x) - \frac{h^5}{120} H^{iv}(x). \quad (3.43)$$

Integrate Equation 3.40 over the intervals  $(x, x+ah)$  and  $(x-h, x+ah)$ , and define these integrals as  $I_1$  and  $I_2$ , respectively.

$$I_1 = \int_x^{x+ah} H(z) dz = y(x+ah) - y(x) \quad (3.44)$$

$$I_2 = \int_{x-h}^{x+ah} H(z) dz = y(x+ah) - y(x-h). \quad (3.45)$$

For unequal pivotal or integration points, the derivative  $H'(x)$  can be expressed to fourth-order as

$$H'(x) = \frac{1}{ah(1+a)} (-a^2 H_{i-1} - (1-a^2) H_i + H_{i+1}) - \frac{ah^2 H'''}{6} + \frac{a(1-a)h^3 H^{iv}}{24}. \quad (3.46)$$

For unequal pivotal or integration points, the second derivative  $H''(x)$  can be expressed to fourth-order as

$$H''(x) = \frac{2}{ah^2(1+a)} (aH_{i-1} - (1+a)H_i + H_{i+1}) + \frac{(1-a)hH'''}{3} - \frac{(1+a^3)h^2 H^{iv}}{12(1+a)}. \quad (3.47)$$

Substitute Equations 3.42, 3.43, 3.46, and 3.47 into Equations (3.44) and (3.45) to get

$$I_1(i) = H_{i-1} \left[ \frac{-a^2 h}{6(1+a)} \right] + H_i \left[ \frac{3ah+a^2 h}{6} \right] + H_{i+1} \left[ \frac{3ah+2a^2 h}{6(1+a)} \right] \\ + H_i''' \left[ \frac{a^3 h^4 (6-7a)}{24} \right] + H_i^{iv} \left[ \frac{a^3 h^5 (25-9a^2+16a^3)}{720(1+a)} \right]. \quad (3.48)$$

$$I_2(i) = H_{i-1} \left[ \frac{h(2+3a-a^3)}{6(1+a)} \right] + H_i \left[ \frac{h(1+3a+3a^2+a^3)}{6a} \right] + H_{i+1} \left[ \frac{h(2a^3+3a^2-1)}{6a(1+a)} \right] \\ + H_i''' \left[ \frac{h^4 (-7a^4 - 2a^3 + 2a + 7)}{72} \right] + H_i^{iv} \left[ \frac{h^5 (-4a^6 - 9a^5 + 10a^3 - 9a - 4)}{720(1+a)} \right]. \quad (3.49)$$

Equations 3.48 and 3.49 are fourth-order correct, three point integration schemes when the pivotal points  $(x_{i-1}, x_i, x_{i+1})$  are unequally spaced and fifth-order correct when equally spaced ( $a=1$ ). The interval of integration is between  $x_{i-1}$  and  $x_{i+1}$ .

To evaluate the complete integral of  $y$ , where

$$y = \int_{x_1}^{x_n} H(z) dz, \quad (3.50)$$

two cases are considered.

If the number of pivotal points,  $n$ , is odd, Equation (3.50) is evaluated as

$$y = \sum_{j=1}^{(n-1)/2} I_2(i), i=2j. \quad (3.51)$$

If the number of pivotal points,  $n$ , is even, Equation 3.50 is evaluated as

$$y = I_1(n-1) + \sum_{j=1}^{(n-2)/2} I_2(i), i=2j. \quad (3.52)$$

#### 4. LITERATURE CITED

- Aoki, M. 1971. Introduction to Optimization Techniques. The Macmillan Company, New York. 335 p.
- Bear, J. 1972. Dynamics of Fluids in Porous Media. American Elsevier Publishing Company, Inc. 765 p.
- Boast, C. W. 1973. Modeling the movement of chemicals in soils by water. Soil Science 115:224-230.
- Braester, C. 1972. Vertical infiltration at constant flux at the soil surface. Second Annual Report. Project No. A10-SWC-77, Hydrodynamics and Hydraulics Laboratory. Technion, Haifa, Israel.
- Bresler, E. 1973. Simultaneous transport of solutes and water under transient unsaturated flow conditions. Water Resources Research 9:975-986.
- Cowan, I. R. 1965. Transport of water in the soil-plant-atmosphere system. Journal of Applied Ecology 2:221-239.
- Dutt, G. R., M. J. Shaffer, and W. J. Moore. 1972. Computer Simulation Model of Dynamic Bio-Physicochemical Processes in Soils. Agricultural Experiment Station, The University of Arizona, Tucson. Technical Bulletin 196.
- Enfield, C. G., C. C. Harlin Jr., and B. E. Bledsoe. 1976. Comparison of five kinetic models for orthophosphate reactions in mineral soils. Soil Science Society of America Journal 40:243-249.
- Farnum, P. 1977. Post-planting water relations of container-grown seedlings: A mathematical model using finite elements. Ph.D. Dissertation, University of Washington. 307 p.
- Farnum, P., and G. F. Carey. 1981. Moisture transport in a soil-plant system: a mathematical model and finite element analysis. Advances in Water Resources 4:67-76.
- Feddes, R. A. and P. E. Rijtema. 1972. Water withdrawal by plant roots. Journal of Hydrology 17:33-59.
- Feddes, R. A., E. Bresler, and S. P. Neuman. 1974. Field test of a modified numerical model for water uptake by root systems. Water Resources Research 10:1199-1206.

- Finlayson, B. A. 1977. Water movement in desiccated soils.  
p. 3.91-3.106. In W. G. Gray, G. F. Pinder and C. A. Brebbia  
(eds.) Finite Elements in Water Resources, Proceedings of the First  
International Conference on Finite Elements in Water Resources,  
held at Princeton University, July, 1976. Pentech Press, London.
- Finlayson, B. A., and R. W. Nelson. 1977. A Preliminary Investigation  
into the Theory and Techniques of Modeling the Natural Moisture  
Movement in Unsaturated Sediments. Report BCSR-40, BCS Richland,  
Inc., Scientific Consulting and Programming Department, September,  
1977. 133 p.
- Frissel, M. J. 1978. Cycling of Mineral Nutrients in Agricultural  
Ecosystems. Elsevier Scientific Publishing Co., Amsterdam. 356 p.
- Frissel, M. J., and P. Poelstra. 1967. Chromatographic transport  
through soils. I. Theoretical evaluations. Plant and Soil  
26:285-302.
- Frissel, M. J., P. Poelstra, and P. Reiniger. 1970. Chromatographic  
transport through soils. III. A simulation model for the evalua-  
tion of the apparent diffusion coefficient in undisturbed soils  
with tritiated water. Plant and Soil 33:161-176.
- Gardner, W. R. 1960. Dynamic aspects of water availability to plants.  
Soil Science 89:63-73.
- Gardner, W. R. 1964. Relation of root distribution to water uptake and  
availability. Agronomy Journal 56:41-45.
- Gardner, W. R. 1965. Movement of nitrogen in soil. Agronomy Monograph  
10:550-572.
- Gessel, S. P. and D. W. Cole. 1965. Influence of removal of forest  
cover on movement of water and associated elements through soil.  
Journal of American Water Works Association 57:1301-1310.
- Graham-Bryce, I. J. 1963. Effect of moisture content and soil type on  
self-diffusion of  $^{86}\text{Rb}$  in soils. Journal of Agricultural Science  
60:239-244.
- Gupta, S. P. and R. A. Greenkorn. 1973. Dispersion during flow in  
porous media with bilinear adsorption. Water Resources Research  
9:1357-1368.

- Hanks, R. J. and S. A. Bowers. 1969. Numerical solution of the moisture flow equation for infiltration into layered soils. *Soil Science Society of America Proceedings* 26:530-534.
- Hillel, D. 1971. *Soil and Water. Physical Principles and Processes.* Academic Press, New York. 288 p.
- Huck, M. G., B. Klepper, and H. M. Taylor. 1970. Diurnal variations in root diameter. *Plant Physiology* 45:529-530.
- Jacoby, S. L. S., J. S. Kowalik, and J. T. Pizzo. 1972. *Iterative Methods for Nonlinear Optimization Problems.* Prentice-Hill, Inc. Englewood Cliffs, New Jersey. 274 p.
- Johnson, N. M., G. E. Likens, F. H. Bormann, and R. S. Pierce. 1968. Rate of chemical weathering of silicate minerals in New Hampshire. *Geochimica et Cosmochimica Acta* 32:531-545.
- Keller, H. M. 1970. Der Chemismus kleiner Bäche in teilweise bewaldeten Einzugsgebieten in der Flyschzone eines Voralpentales. *Schweizerische Anstalt für das Forstliche Versuchswesen. Mitteilungen* 46:113-155.
- Lai, S. H. and J. J. Jurinak. 1971. Numerical approximation of cation exchange in miscible displacement through soil columns. *Soil Science Society of America Proceedings* 35:894-899.
- Lapidus, L. and N. R. Amundson. 1952. Mathematics of adsorption in beds. VI. The effect of longitudinal diffusion in ion exchange and chromatographic columns. *Journal of Physical Chemistry* 56:984-988.
- Leenheer, J. A. and J. L. Ahlrichs. 1971. A kinetic and equilibrium study of the adsorption of carbaryl and parathion upon soil organic matter surfaces. *Soil Science Society of America Proceedings* 35:700-705.
- Lindstrom, F. T., R. Haque, and W. R. Coshov. 1970. Adsorption from solution. III. A new model for the kinetics of adsorption-desorption processes. *Journal of Physical Chemistry* 74:495-502.
- Lindstrom, F. T. and L. Boersma. 1970. Theory of chemical transport with simultaneous sorption in a water saturated porous medium. *Soil Science* 110:1-9.
- Lindstrom, F. T. and L. Boersma. 1971. A theory on the mass transport of previously distributed chemicals in a water saturated sorbing porous medium. *Soil Science* 111:192-199.

- Lindstrom, F. T., L. Boersma, and D. Stockard. 1971. A theory on the mass transport of previously distributed chemicals in a water saturated sorbing porous medium: Isothermal cases. *Soil Science* 112:291-300.
- Molz, F. J. and I. Remson. 1971. Application of an extraction term model to the study of moisture flow to plant roots. *Agronomy Journal* 63:72-77.
- Molz, F. J. 1981. Models of water transport in the soil-plant system: a review. *Water Resources Research* 17:1245-1260.
- Neuman, S. P., R. A. Feddes, and E. Bresler. 1975. Finite element analysis of two-dimensional flow in soils considering water uptake by roots: I. Theory. *Soil Science Society of America Proceedings* 39:224-230.
- Nimah, M. N. and R. J. Hanks. 1973. Model for estimating soil water, plant, and atmospheric interrelations: I. Description and sensitivity. *Soil Science Society of America Proceedings* 37:522-527.
- Nye, P. H. and P. B. Tinker. 1977. *Solute Movement in the Soil-Root System*. University of California Press, Berkeley. 342 p.
- Penman, H. L. 1948. Natural evaporation from open water, bare soil and grass. *Proceedings of the Royal Society A* 193:120-145.
- Philip, J. R. 1955. Numerical solution of equations of the diffusion type with diffusivity concentration-dependent. *Transactions of the Faraday Society* 51:885-892.
- Philip, J. R. 1957. Numerical solution of equations of the diffusion type with diffusivity concentration-dependent. II. *Australian Journal of Physics* 10:29-42.
- Philip, J. R. 1969. Theory of infiltration. p. 216-291. In V. T. Chow (ed.) *Advances in Hydroscience*, Vol. 5. Academic Press, New York, N.Y.
- Remson, I., G. Hornberger, and F. Molz. 1971. *Numerical Methods in Sub-surface Hydrology*. Wiley-Interscience. 389 p.
- Rubin, J. and R. Steinhardt. 1963. Soil water relations during rain infiltration: I. Theory. *Soil Science Society of America Proceedings* 27:246-251.

- Salvadori, M. G. and M. L. Baron. 1961. Numerical methods in Fortran, p. 67-70. Prentice Hall Inc., Englewood Cliffs, N.J. 302 p.
- Shampine, L. F. and R. C. Allen. 1973. Numerical Computing: An Introduction. W.B. Saunders Co., Philadelphia. 258 p.
- Tanji, K. K. 1970. A computer analysis on the leaching of boron from stratified soil columns. Soil Science 110:44-51.
- Taylor, S. A. and G. L. Ashcroft. 1972. Physical Edaphology. W. H. Freeman and Company, San Francisco. 533 p.
- Taylor, H. M. and B. Klepper. 1974. Water relations of cotton. I. Root growth and water use as related to top growth and soil water content. Agronomy Journal 66:584-588.
- Taylor, H. M. and B. Klepper. 1975. Water uptake by cotton root systems: An examination of assumptions in the single root model. Soil Science 120:57-67.
- Ungs, M. J., R. W. Cleary, L. Boersma, and S. Yingjajaval. 1977. The quantitative description of transfer of water and chemical through soils. p. 109-137. In R. C. Loehr (ed.): Land as a Waste Management Alternative. Ann Arbor Science Publishers, Inc., Michigan.
- Ungs, M. J., L. Boersma, and Suntaree Akkratanakul. 1982. Effect of temperature on nutritional requirements of plants. Agricultural Experiment Station, Technical Bulletin 142, Oregon State University, Corvallis, Oregon. 32 p.
- van Genuchten, M. Th., J. M. Davidson, and P. J. Wierenga. 1974. An evaluation of kinetic and equilibrium equations for the prediction of pesticide movement through porous media. Soil Science Society of America Proceedings 38:29-35.
- van Genuchten, M. Th., and R. W. Cleary. 1979. Movement of solutes in soil: computer-simulated and laboratory results. p. 349-386. In G. H. Bolt (ed.) Soil Chemistry B. Physico-Chemical Models. Elsevier Scientific Publishing Company, New York. 479 p.
- van Genuchten, M. Th., and W. J. Alves. 1982. Analytical solutions of the one-dimensional convective-dispersive solute transport equation. U.S. Department of Agriculture, Technical Bulletin 1661. 149 p.

- Vauclin, M., R. Haverkamp, and G. Vachaud. 1979. Résolution numérique d'une équation de diffusion non-linéaire. Presses Universitaires de Grenoble, France. 183 p.
- Von Rosenberg, D. U. 1969. Methods for the Numerical Solution of Partial Differential Equations. American Elsevier Publishing Co., Inc., New York. 128 p.
- Warrick, A. W., J. W. Biggar, and D. R. Nielsen. 1971. Simultaneous solute and water transfer for an unsaturated soil. Water Resources Research 7:1216-1225.
- Whisler, F. D., A. Klute, and R. J. Millington. 1968. Analysis of steady-state evapotranspiration from a soil column. Soil Science Society of America Proceedings 32:167-174.
- Yingjajaval, S. 1979. Diffusion and Surface Reaction Processes of Adsorption on Surfaces of Soil Particles in Unsaturated Soils. Ph.D. Thesis. Oregon State University, Corvallis, OR 97331. 130 p.
- Yule, D. F. and W. R. Gardner. 1978. Longitudinal and transverse dispersion coefficients in unsaturated Plainfield sand. Water Resources Research 14:582-588.

## 5. LIST OF SYMBOLS

<u>Bracket Notations</u>	<u>Physical Unit</u>
[1]	unitless
[°K]	absolute temperature (Kelvin scale)
[L]	gross length (e.g., 1 cm of soil)
$[L_p]$	potential (e.g., 1 millibar) $[M/L/T^2]$
$[L_r]$	root length (e.g., 1 cm of root)
$[L_w]$	fluid length (e.g., 1 cm of water)
[M]	mass (e.g., 1 gram)
[T]	time (e.g., 1 second)

The unit potential shown here is not a unique physical unit. It can be obtained by setting  $[L_p] = [Energy/L^3] = [M/L/T^2]$ .

### English Letter Symbols

$A(z, \theta, \psi_{ps})$	rate of water uptake by roots as a function of soil water content and plant water potential at soil surface	$[L_w^3/L^3/T]$
c	solute concentration in solution	$[M/L_w^3]$
CNVRSN	converts units of potential to units of pressure head	$[L/L_p]$
$c_{st}$	stomatal correction factor	[unitless]
D	soil water diffusivity defined as $D = K(d\psi/d\theta)CNVRSN$	$[L^2/T]$
$D_{sz}$	apparent solute dispersion coefficient	$[L^2/T]$
F	diffusivity potential as defined by $F(\theta) = \int_{\theta'_d=\theta}^{\theta} D(\theta')d\theta'$	$[L_w^3/L/T]$
f(t)	liquid phase solute flux at a boundary	$[M/L^2/T]$

S	local concentration of solute in the sorbed or solid phase	$[M/L^3]$
$T_r$	actual transpiration rate	$[L_w^3/L^2/T]$
$T_{cr}$	rate of solute uptake by root system	$[M/L^2/T]$
t	time	[T]
v	magnitude of the pore-water velocity, $v =  q_z/\theta $	$[L/T]$
z	spatial coordinate, positive downwards	[L]
$z_{max}$	position of the lower boundary	[L]

#### Greek Letter Symbols

$\theta$	volumetric water content	$[L_w^3/L^3]$
$\psi$	matric potential of soil water	$[L_p]$
$\psi_{ps}$	potential of the water in xylem of the plant at the soil surface	$[L_p]$
$\psi_r$	potential of water in xylem vessels of the roots	$[L_p]$
$\psi_{wilt}$	potential of water in the plant cells at which permanent wilting occurs	$[L_p]$

#### Subscripts

d	water content when soil is air-dried
i	spatial node index
0	initial condition
s	water content when soil is saturated

#### Superscripts

k	current time index
*	indicates that the variable is an estimated value

g	acceleration from gravity	$[L/T^2]$
G(z,t, $\theta$ ,c,S)	solute source/sink term	$[M/L^3/T]$
GRAV	coefficient of gravity, having a value of either zero or one	[unitless]
K	hydraulic conductivity of the soil	$[L_w^3/L^2/T]$
K <sub>r</sub>	hydraulic conductivity of root cortex	$[L_w^3/L^2/T]$
K <sub>sys</sub>	hydraulic conductivity through the soil-root system	$[L_w^3/L^2/T]$
n	total number of spatial nodes	
q(0,t)	actual flux across soil surface	$[L_w^3/L^2/T]$
q <sub>ps</sub>	potential transpiration demand	$[L_w^3/L^2/T]$
q <sub>z</sub>	volumetric or Darcian flux	$[L_w^3/L^2/T]$
R(0,t)	potential flux of soil water at soil surface defined as flux which satisfies evaporative demand	$[L_w^3/L^2/T]$
RAF	root absorption function	$[1/L^2]$
RHS	right hand side	
RPF	friction loss incurred by the water flowing through the root xylem from the site of absorption to the soil surface level	[L]
R <sub>a</sub>	root uptake activity as determined by soil water content and solute concentration	[unitless]
R <sub>cyl</sub>	radius of the cylinder of soil through which water is moving to the root	[L]
R <sub>d</sub>	length of roots per unit soil volume	$[L_r/L^3]$
R <sub>r</sub>	radius of root	$[L_r]$
R <sub>stele</sub>	radius of the root stele	$[L_r]$