1986

Modeling of Soil Water Flow and Root Uptake

V. Rasiah

MODELING OF SOIL WATER FLOW AND ROOT UPTAKE

BY

V. RASIAH

A thesis submitted

in partial fulfillment of the requirements for the

the degree Doctor of Philosophy, Major in

Agronomy, South Dakota

State University

December 1986

MODELING OF SOIL WATER FLOW AND ROOT UPTAKE

This thesis is approved as a creditable and independent investigation for the degree, Doctor of Philosophy, and is acceptable as meeting the thesis requirements for this degree. Acceptance of this thesis does not imply that the conclusions reached by the candidate are necessarily the conclusions of the major department.

Dr. R. A. Kohl
Major Advisor

Date

Dr. C. G. Carlson
Thesis Advisor

Date

[redacted]

Head, Plant Science Department.

ACKNOWLEDGEMENTS

The author wishes to express his sincere appreciation to Dr. R. A. Kohl, Associate Professor of Plant Science, for advice, guidance and assistance given while serving as my major advisor throughout the graduate program. Special appreciation is extended to Dr. C. G. Carlson, Assistant Professor of Plant Science, under whose supervision this study was carried out. The amount of time he unselfishly spent with me in correcting the computer programs used in this study is greatly appreciated. Appreciation is also extended to other members of my graduate committee; Dr. M. L. Horton, Department chairman, Dr. G. H. Nielsen and Dr. Han. Kim for their valuable suggestions.

The author is grateful to the Plant Science Department for providing a graduate research assistantship during the completion of this program of study.

Special appreciation is also expressed to my wife and children for their patience and sacrifice, so that I could complete this thesis.

MODELING OF SOIL WATER FLOW AND ROOT UPTAKE

Abstract

Velupillai. Rasiah

Under the supervision of Dr. C. G. Carlson.

The soil water pressure head, h, versus soil water content, θ, and the hydraulic conductivity, K, versus θ, relationships appear as functional coefficients in the non-linear partial differential water flow model. Before the flow equation can be used to simulate the flow of water through soils, the h versus θ and K versus θ relationships must be established. This requires the estimation of the parameters that describe the h versus θ and K versus θ functional relationships.

In-situ water retention and hydraulic conductivity measurements were determined from the knowledge of initial and boundary conditions and water content profiles during drainage. This information obtained in the greenhouse was used to estimate the parameters of the non-linear h(θ) and K(θ) empirical functions. The estimates were obtained through the first and second order least square best fit procedures for the logarithmically linearized h(θ) and K(θ) functions. The estimates, when combined with the flow model, SWATRE, estimated soil moisture content profile, θ, which did not agree well with the observed data.

In the second method, the flow model was linearized using the Taylor series expansion. The same parameters mentioned above were estimated using two iterative procedures, Marquardt (1964) and Taylor. The simulations, θ, for the fitted estimates from both procedures, agreed well with the observed data. The convergence of the estimates in Marguardt's maximum neighborhood method of iterative fitting was more stable than that in the Taylor method. Marquardt's method converged more slowly.

Similar procedures were followed for fitting the root uptake function parameters. The parameters in the root uptake function, estimated and fitted individually for each compartment, produced better solutions than when single function parameters were defined for the whole profile. To obtain a satisfactory solution from the flow model, including root uptake, the parameters in the $h(\theta)$ and $K(\theta)$ functions were estimated for the range of θ in which the root water uptake took place.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF SYMBOLS USED

A = area (cm^2)

b = parameter in the soil water pressure head function

c = parameter in the soil water pressure head function

C(h) = water capacity function

ETP = potential evapotranspiration (cm/day)

Et = actual evapotranspiration (cm/day)

f(a,b) = function of the variables a and b

H = hydraulic head (cm of water)

h = soil water pressure head (cm of water)

he = air entry potential (cm of water)

h(θ) = soil water pressure head function

K = hydraulic conductivity (cm/day)

Ks = saturated hydraulic conductivity (cm/day)

K(θ) = hydraulic conductivity function

L = depth or length (cm)

p = parameter in the root water uptake function, S(h,L)

q = parameter in the root water uptake function, S(h,L)

Q = quantity of water (cm)

R = coefficient of determination

RWU = root water uptake (cm/day)

S(h,L) = root water uptake function

t = time in days

z = height above or below soil surface

θ = volumetric water content (cm^3 of water/cm^3 of soil)

θs = saturation volumetric water content (cm^3 of water/cm^3 of soil)

θr = residual wetness

θest = estimated volumetric water content

θobs = observed volumetric water content

ρ = density of the material (g/cm^3)

SS = least sum squares

INTRODUCTION

The general laws of fluid motion govern the flow of water through porous media like soils. Mathematically these laws are stated as: (1) the equation of continuity (2) the equation of state, and (3) the dynamical equation of motion. Combining these 3 equations for liquid phase flow in the vertical direction results in a non-linear partial differential model in which time, t, and position in space, z, are the independent variables. The dependent variable is volumetric water content, θ, or soil water pressure head, h. The functional coefficients in the flow model are h versus θ and hydraulic conductivity, K, versus θ relationships.

A solution exists for the flow model at $t > 0$, provided the (a) h versus θ and (b) K versus θ relationships are established for the particular situation. The emprical equations that describe the h versus θ and K versus θ relationships are non-linear. Because of the strong non-linearity in it's terms, the flow model is difficult, if not impossible, to solve analytically. Thus the first objective in this study was to solve the flow model numerically for specific initial and boundary conditions.

Because the h versus θ and K versus θ relationships appear as functional coefficients in the flow model, the

accuracy of the model solution or the agreement of the model solution with the experimental data is largely determined by the parameter estimates that describe the functional relationships. Thus the second objective in this study was to estimate the parameters in the $h(\theta)$ and $K(\theta)$ functions so that the model simulation agrees well with observed data.

Theoretically, a well defined root water uptake function, when included in the flow model, should accurately describe flow along with root uptake. Therefore, the third objective in this study was to modify and solve the flow model along with root uptake. To obtain simulations that would agree with the observed data the parameters in the $K(\theta)$, $h(\theta)$ and the root uptake function were estimated and fitted into the flow model.

THEORY

Flow through porous media like soil is limited by numerous constrictions or "necks", and occasional "dead end" spaces. Therefore, the actual geometry and flow pattern is too complicated to be described in detail. For this reason the detail flow pattern is often ignored and the conducting body is treated as though it were a uniform medium with the flow spread out over the entire cross section. Henri Darcy (1831) enunciated a law to satisfy the above condition for steady state flow. This law states that the flow rate, Q, is directly proportional to the difference in hydraulic head, H, area of cross section, A, and inversely proportional to the length, L, of the soil column. This is mathematically expressed as,

$$Q \propto \frac{A \Delta H}{L}$$

or

$$Q = \frac{K A \Delta H}{L} \qquad (1)$$

where the proportionality constant K is called the hydraulic coductivity of the material. Rearranging equation (1) would produces either,

$$\frac{Q}{A} = K \frac{\Delta H}{L}$$

or

$$q = K \frac{\Delta H}{L} \qquad (2)$$

where q is the Darcian flux and $\Delta H/L$ is the hydraulic gradient.

Mathematically Darcy's law is similar to linear transport equations in classical physics, including Ohm's law. This law states that the current I or the flow rate of electricity is proportional to the electric potential gradient, E,

$$I = \frac{E}{R}$$

where, $R = s \frac{L}{A}$,and $s = 1/Ke$

$$I = Ke \frac{E A}{L} \qquad (3)$$

The subcript,

R is the electric resistance,

s is the specific resistance,

Ke is the electrical conductivity of the material,

A is the area of cross section,and

L is the length of the material.

Equation 3 is similar to equation (2).

If the flow is unsteady or the soil is nonuniform, both the hydraulic gradient and the conductivity of the material are variables. Therefore, the localized gradient, flux, and conducitvity values rather than the overall values of the system must be considered. This requires a more generalized expression of Darcy's law. Slitcher (1899) generalized Darcy's law to satisfy the above conditions using a three dimensional macroscopic differential equation of type,

$$q = -K \nabla H \qquad (4)$$

where ∇ is the operator 'del' of the gradient of the hydraulic head, H, in three-dimensional space. For a one dimensional system, equation (4) takes the form,

$$q = - K \frac{\partial H}{\partial x} \qquad (5)$$

Bernoulli's theorem for pure water states that the total hydraulic potential, H, is the sum of the gravity, z, pressure, h, and velocity, v,heads.

$$H = z + h + v$$

If salts are present in the water, then the pressure due to osmotic head is also added. H is now called the total hydraulic head. However, the order of magnitude of the velocity and osmotic heads are small compared to the other components and are usually neglected. Thus the total head is assumed to be,

$$H = z + h \tag{6}$$

The law of conservation of mass applied to a noncompressible fluid in an unsteady condition states that the difference between inflow and outflow in a unit soil volume is equal to the change in volumetric water content, θ. For a dynamic system with flow in one direction, this is mathematically expressed as,

$$\text{Inflow} - \text{Outflow} = [g_z \Delta x \Delta y] - \{[g_z + (\partial g_z / \partial z)\, \Delta z]\, \Delta x \Delta y\}$$

$$\text{Inflow} - \text{Outflow} = - \left\{ \frac{\partial g_z}{\partial z} \right\} \Delta x \Delta y \Delta z \tag{7}$$

where Δx, Δy and Δz are directional components (cm) and g is the flux term (cm/day) in the z direction.

For a general case which includes compressible fluids, equation (7) needs to be multiplied by the fluid density, ρ (g/cm^3), to yield

$$\text{Inflow} - \text{Outflow} = - \rho \left\{ \frac{\partial g_z}{\partial z} \right\} \Delta x \Delta y \Delta z \tag{8}$$

When the flow is considered in three dimensional space equation (8) becomes,

$$\text{Inflow} - \text{Outflow} = -\rho \left\{ \frac{\partial g}{\partial x} + \frac{\partial g}{\partial y} + \frac{\partial g}{\partial z} \right\} \Delta x \, \Delta y \, \Delta z \qquad (9)$$

For a time dependent situation equation (8) becomes,

$$\text{Inflow} - \text{Outflow} = -\rho \left\{ \frac{\partial \theta}{\partial t} \right\} \Delta x \, \Delta y \, \Delta z \qquad (10)$$

where θ is the volumetric water content. Combining equations (9) and (10) yields,

$$\frac{\partial \theta}{\partial t} = -\rho \left\{ \frac{\partial g}{\partial x} + \frac{\partial g}{\partial y} + \frac{\partial g}{\partial z} \right\} \qquad (11)$$

For the flow in the vertical direction, z, and the density of water as 1 g/cm^3, equation (11) becomes,

$$\frac{\partial \theta}{\partial t} = \frac{\partial g}{\partial z} \qquad (12)$$

Substituting for flux **g** in equation (12) yields,

$$\frac{\partial \theta}{\partial t} = -\frac{\partial (-K \, \partial H / \partial z)}{\partial z} \qquad (13)$$

Substituting the components of H in equation (13) produces,

$$\frac{\partial \theta}{\partial t} = \frac{\partial(-K \, \partial(h + z)/ \partial z)}{\partial z} \quad (14)$$

Equation (14) was first presented by Richards (1931). Manipulation of equation (14) would produce the form

$$\frac{\partial \theta}{\partial t} = \frac{\partial K(\partial h/\partial z + 1))}{\partial z} \quad (15)$$

The variables h and θ in equation (15) could be reduced to one by multiplying and dividing the left hand side of the equation by ∂h,

$$\frac{\partial h}{\partial h}\frac{\partial \theta}{\partial t} = \frac{\partial K \, (\partial h/\partial z + 1))}{\partial z} \quad (16)$$

Redefining $\partial O/\partial h$ as C(h), equation (16) becomes,

$$\frac{\partial h}{\partial t} = \frac{1}{C(h)}\left(\frac{\partial K \, (\partial h/\partial z + 1))}{\partial z}\right. \quad (17)$$

where C(h) is the water capacity of the soil (slope of the water retention curve). Equation (17) is called the pressure head form of the flow equation in the vertical direction.

Equation (17) needs to be modified with a root extraction sink term, S, to accurately represent the flow in soils with growing plants. Thus equation (17) becomes,

$$\frac{\partial h}{\partial t} = \frac{1}{C(h)} \left\{ \frac{\partial (K (\partial h/\partial z + 1))}{\partial z} \right\} - S \qquad (18)$$

Solutions to the one dimensional flow equation of the type 17 requires a knowledge of the relationship between, (a) soil water pressure head, h, and volumetric water content, θ, and (b) hydraulic conductivity, K, and θ or h. As yet, no satisfactory theory exists for the prediction of the h versus θ relationship from basic soil properties. However, several empirical equations have been proposed which apparently describe the h versus θ relationship. Therefore, for a specific soil, the h versus θ relationship must be determined from experimental data. The prediction of K from basic or easily obtainable soil properties is not possible. Therefore, the K versus θ relationship must also be described from experimental data. However, the measurements of K values at low soil moisture contents is difficult, if not impossible. As a result several investigators have recently explored the possibilty of predicting K from pore size distribution data for a particular soil.

Solutions to equation (18) requires that the root water uptake function, S, be defined along with h versus θ and K versus θ relationships. The soil-root- water-

atmosphere continuum is too complex to describe the root water uptake function by a universal equation. However, several empirical equations have been developed during the recent past, that apparently describe the root water uptake. Therefore, to describe the root water uptake for a specific soil and a specific crop, the relationship has to be obtained from experimental data.

LITERATURE REVIEW

The subject of water flow in soils has received considerable and detailed study over the past three or four decades. Solutions to the theoretical flow equation (17) for practical field situations have been a major concern of the physical scientists working in soil-water phenomena. There are three known methods to solve the non-linear differential equations : (a) analytical, (b) electrical analog, and (c) numerical methods.

ANALYTICAL METHOD :

In order to obtain analytical solutions to the non-linear partial differential equation (17) certain assumptions are necessary. First by assuming $K(\theta)$ to be a constant and neglecting $\partial K/\partial z$ in equation (17), the resulting flow is horizontal. Second, by allowing K to be a variable and neglecting $\partial K/\partial z$ the flow will still be in the horizontal direction. Vertical flows do not follow the above assumptions.

A powerful method in mathematics used to solve equations of type 17 is the use of perturbation. However, this method is applicable only when the degree of non-linearity associated with the non-linear term is small. In such cases, the original non-linear equation

is first separated into one part with a linear equation that has an exact solution. The second part has the non-linear term plus all additional terms that are difficult to solve. The part with the linear equation can be solved easily, thus providing a zero-order or generating solution, which is then employed in some way with the non-linear term to produce the first order correction term. Next, the first order correction term is combined with the generating solution to yield a first order corrected solution which would be an approximate solution to the original non-linear equation. If the degree of non-linearity is not very small, the procedure is repeated to obtain a second order correction term. This term is then combined with the first order corrected solution to provide a second order corrected solution. However, the repeated application of this procedure produces great mathematical difficulties without assuring an increase in accuracy. Moreover, the evaluation of the error is very difficult. Therefore, this procedure is seldom used for practical situations.

ELECTRICAL METHOD :

The similarity between Darcy's law and Ohm's law allows the use of electrical analogs or models to obtain

solutions to the flow equation. Using electrical analogs Childs (1950) worked out a series of solutions for the flow equation. However, this method is applicable only to uniform soil profiles. Luthin (1953), and Bouwer and Little (1959) used modified electrical analogs to solve the flow equation in non-uniform profiles. However, the analog was limited to the specific geometry of the profile for which it was constructed. Nevertheless, electrical analogs are fairly simple to build and could be used to solve problems that cannot be solved analytically.

NUMERICAL METHOD :

Because of the aforementioned difficulties in using analytical and/or electrical analog methods to solve the flow equation, many researchers have turned to numerical methods. With the availability of computers, numerical methods are now widely used to obtain solutions to flow equations. In the numerical procedure, the differential equation is transformed to a "finite difference" form, which later is solved as a system of equations. The finite difference method consists of replacing each of the derivatives in the differential equation by an appropriate difference quotient approximation. These quotients are obtained by using Taylor expansion. The

function is expanded about a point "x", first in the forward direction and then in the backward direction as follows:

$$f(x + \Delta x) = f(x) + \frac{\Delta x\, df}{dx} + \frac{(\Delta x)^2\, d^2f}{2!\, dx^2} \quad \ldots\ldots \quad (19)$$

$$f(x - \Delta x) = f(x) - \frac{\Delta x\, df}{dx} + \frac{(\Delta x)^2\, d^2f}{2!\, dx^2} \quad \ldots\ldots \quad (20)$$

Subtracting equation (20) from 19, truncating both after the third term, and solving for df/dx, will yield:

$$\frac{df}{dx} = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\,\Delta x} \quad (21)$$

The term on the right hand side of the equation is called the central difference approximation. By using a very similar analysis, truncating all the terms to the right of the third term, d^2f/dx^2 can be solved by adding equations (19) and (20) :

$$\frac{d^2f}{dx^2} = \frac{f(x+\Delta x) + f(x-\Delta x) - 2f(x)}{(\Delta x)^2} \quad (22)$$

Truncation errors are introduced in equations (21) and (22) when the terms in the series beyond the second order (the third term) are dropped.

Richtmyer et al.(1967) describe 14 implicit finite

difference methods for the heat flow problem. They concluded the general equation for finite differences as:

$$\frac{df}{dx} = \frac{f_j^{n+1} - f_j^n}{x} \tag{23}$$

$$\frac{d^2f}{dx^2} = \alpha\frac{(f_{j+1}^n - 2f_j^n + f_{j-1}^n)}{(x)^2} + (1-\alpha)\frac{(f_{j+1}^{n+1} - 2f_j^{n+1} + f_{j-1}^{n+1})}{(x)^2} \tag{24}$$

Crank and Nickelson (1947) obtained numerical solutions for equations of type (24) by setting $\alpha = 1/2$. The equation is explicit when $\alpha = 0$. and f_j^n may be found directly in terms of the known values of f_j^n. However, when $\alpha \neq 0$, a system of linear equations is developed to obtain the values of f_j^{n+1}, and the system is called implicit.

Klute (1952), using the Boltzman's transformation technique, numerically solved the flow equation for horizontal flow:

$$\frac{\partial\theta}{\partial t} = \frac{\partial(\partial\theta)}{\partial x(\partial x)} \tag{25}$$

In the Boltzman's transformation procedure the partial differential equation is first transformed into a differential equation, which is later converted to a solvable form. However, Klute's method requires a

uniform medium with uniform initial moisture content in the profile. Staple and Lehane (1954), Day and Luthin (1956) and Gardner (1959) also utilized Boltzman's transformation to obtain solutions for the horizontal flow equation. Philip (1957), using Boltzman's method, numerically solved the flow equation in the vertical direction in uniform profiles.

Hanks and Bowers (1962) were the first to numerically estimate the solutions for vertical flow in layered soils with nonuniform initial moisture contents. They used the Crank-Nickelson finite difference approach. The flow equation was linearized with predictive values for K(h) and C(h). The critical part of the solution depends on the choice of values for K,C and Δt. They suggested a method for determining t, with,

$$\Delta t^{j+1/2} = \frac{Q}{I^{j-1/2}} \qquad (26)$$

where,

Δt^{j+1} is the next time period

Q a constant for water entering the soil

$I^{j-1/2}$ infiltration rate from the previous time.

K(θ) was estimated using predictive terms for θ, with,

$$\theta_i^{j+1} = (\theta_i^{j} - \theta_i^{j-1})b + \theta_i^{j} \qquad (27)$$

where b =0.7 or $\Delta t^{i+1} / t^{i+.33}$ whichever is greater. They report excellent agreement when compared with solutions obtained by Phillip (1957) or Scot (1962).

There are several other reports using the finite difference method of solutions for vertical flow. Haverkamp (1977) compared six of them in terms of execution time, accuracy, and programming consideration. He concluded that the (a) h-based explicit models require more computer time than the implicit models, (b) implicit schemes with implicit or explicit evaluation of K(θ), and C(h) functions appear to have the widest range of applicability both for unsaturated and saturated conditions.

The above mentioned models do not have a root sink term to accurately describe the flow interacting with root water uptake. Nimmah and Hanks (1973) added a sink term A(z,t) or root water uptake function to the flow equation (17) and solved the model numerically. Feddes et al. (1978) and Hoogland et al. (1981) proposed another model for the root water uptake function to numerically solve the flow equation with a root sink. The problem is defining a universally acceptable root water uptake function. Thus, as indicated earlier, the

solution to the flow equation depends not only in defining the h versus θ and K versus θ functions but also the root water uptake function.

SOIL WATER PRESSURE HEAD, h, VERSUS SOIL WATER CONTENT, θ, RELATIONSHIP :

The functional relationship between soil water pressure head, h, and volumetric soil water content, θ, is usually described by a plot of h versus θ. The curve obtained is called the soil moisture retention curve (Childs, 1950) or soil moisture characteristic curve. However, the curve obtained for a specific soil is not unique. This is because the curve obtained through the wetting cycle will differ from that obtained in the drying cycle. The curve obtained through the wetting cycle is called the sorption curve and that from the drying cycle is the desorption curve. The dependence of the h versus θ curve upon the direction and history of the process is called hysteresis. The two complete characteristic curves, from saturation to dryness and vice versa, are called the main branches of the hysteristic curve. The desorption curve for partially wetted soil or the sorption curve of a partially dry soil follows intermediate curves called scanning curves. Because of the complexity involved, the

hysteresis phenomena is often neglected, and the soil moisture characteristic curve is often represented by the desorption curve.

The absorbtion and pore-geometry effects are often too complex to describe the h versus θ relations from basic soil properties. Therefore, several empirical relationships have been proposed. Visser's (1966) relationship for h versus θ is,

$$h(\theta) = a(f - \theta)^{b} / \theta^{c} \qquad (28)$$

where, f is the porosity of the soil, and a, b and c are empirical constants to be estimated from the best fit of experimental data. Brooks and Corey (1964) proposed another equation,

$$\left[\frac{h_e}{h}\right]^{\lambda} = \left[\frac{\theta - \theta_r}{\theta_s - \theta_r}\right] \qquad (29)$$

where,

h_e is the air entry potential

λ is the pore-size distribution index

θ_r is the residual wetness considered to be confined to the small pores

θ_s is saturation wetness.

Gardner et al. (1970) suggested a simplified relationship,

$$h = a\ \theta^{-b} \qquad (30)$$

Here a and b are emprical constants. Campbell's (1974) equation for this relationship is

$$h = h\ (\theta / \theta_s)^{-b} \qquad (31)$$

Here b is an emprical constant. This relationship is valid provided the log h versus log (θ/θ_s) plot produces a linear graph. Haverkamp et al. (1977) developed another equation for h versus θ relationship,

$$\theta = \frac{(\theta_s + \theta_r)}{a + |h|^n} + \theta_r \qquad (32)$$

Here a and b are emprical constants. Van Genuchten's (1979) equation for h(θ) function is,

$$\frac{(\theta - \theta_r)}{(\theta_s - \theta_r)} = \left\{ \frac{1}{1 + \alpha |h|^n} \right\}^m \qquad (33)$$

The parameters m,n, and α depends on the shape of the h versus θ curve. It is evident from the foregoing equations that the empirical relationships are non-linear.

HYDRAULIC CONDUCTIVITY, K, VERSUS SOIL WATER CONTENT, θ, RELATIONSHIP :

In-situ K versus θ determinations are time

consuming and expensive. Therefore, several investigators have developed empirical equations from water retention data (Brooks and Corey, 1964; Green and Corey, 1971; Marshall, 1958;Millington and Quirk, 1961; Campbell, 1974; and Van Genuchten, 1979). However, if the K(θ) function is to be defined from the h(θ) function, in-situ data is preferred to define the h(θ) function rather than data from core samples. The discussion on K(θ) emprical relationship is restricted to the latter two models, Campbell's and Van Genuchten's equations. Campbell's equation is

$$K(\theta) = K_s \left\{ \frac{\theta}{\theta_s} \right\}^{2b+3} \tag{34}$$

Van Genuchten's equation is

$$K(\theta) = \left[\frac{\theta - \theta_r}{\theta_s - \theta_r} \right]^{1/2} \left\{ 1 - \left[\frac{\theta - \theta_r}{\theta_s - \theta_r} \right]^{1/m} + 1 - \left[\frac{\theta - \theta_r}{\theta_s - \theta_r} \right]^{1/m} \right\}^{2} \tag{35}$$

The parameters b and m are obtained from the respective h(θ) functions. Van Genuchten's equation is used to calculate the relative K(θ) values, whereas Campbell's equation is for actual K(θ) values. It should also be noticed that Van Genuchten's equation is considerably more complex.

PARAMETER ESTIMATION :

Solutions to the non-linear partial differential equation (14) require the definition of the $h(\theta)$ and $K(\theta)$ relationships. If Campbell's or Van Genuchten's equations are assumed to describe relationships, the parameters which describe the relationships must be found. Results found when solving the model are largely determined by the parameters that describe the functional relationships of $h(\theta)$ and $K(\theta)$.

The parameters are usually estimated by the least squares sum, SS, procedure, using experimental data. The SS procedure requires that the function be linear. The most obvious method of linearization is by logarithmic transformation. However, the estimates obtained for the transformed equations need not strictly represent the least squares solution for the original equation. On the other hand, the function may be linearized by expanding it as a Taylor series. The parameters are then iteratively estimated until a desired minimum SS is achieved. The minimum SS could also be traced by following the path of steepest-descent or Marquardt's (1963) compromise method.

The convergence with the Taylor expansion method is fast, but divergence is common. The convergence with the steepest-descent method is consistent but is

agonizingly slow. Marguardt's algorithm makes use of the good qualities of both methods and is a hybrid.

Since Marquardt's method combines Taylor and the steepest-descent methods a brief description of it is included. Let the parameters B1,B2....Bk, be fitted to a model,Y.

$$Y = f(B1,B2....Bk) \tag{36}$$

where B's are population values of k parameters. The problem is to compute those estimates of the parameters which will give the minimum sum, SS. Using the principle of least squares sum, we have:

$$SS = \Sigma (Yo - Ye)^2$$

where Yo and Ye are observed and predicted solutions for the population parameter values and estimates respectively. Definig Ye as a function of the estimates and expanding f(B1,B2...) as a Taylor series, we have:

$$f(b + et) = f(b)_i + \sum \frac{\partial f_i}{\partial b_i} (et) \tag{37}$$

where the converged value of b's being the least squares estimate for B's. The vector, e, is a small correction term to the estimate b, and t refers to Taylor series estimation. The et now appears linearly and can be found by setting the $\partial ss/\partial et = 0$ for all et. Thus et is found by solving,

$$A\ et = G$$

where A and G are kxk and kx1 matrices. (38)

The A and G matrices are computed as follows:

$$A^{[kxk]} = P^T P \quad (39)$$

where, $P = \{\partial f/\partial b_j\}$, $j = 1,2,...k$ (40)

and P^T is the transpose of P matrix. Where T denotes the matrix transposition.

$$G^{[kx1]} = \{\Sigma [Yo - Ye]\ \partial f/\partial b_j\} \quad (41)$$

In the steepest descent method the trial vector e is designated as eg and moves in the negative gradient of SS,

$$eg = -\{\partial ss/\partial b1,\ \partial ss/\partial b2,....\} \quad (42)$$

or

$$eg = G$$

In Marguardt's method an optimum interpolation is carried out between Taylor series and Steepest-descent methods, the interpolation being based upon the maximum neighborhood in which the truncated Taylor series gives an adequate representation of the non-linear model.

ROOT WATER UPTAKE :

During the last two to three decades a fair amount of information has appeared in the literature that

describes root water uptake by crops grown under different environmental conditions. Gardner (1966) defined the root water uptake or the sink, S, as a function of soil water pressure head, h, root water pressure head, h_r, hydraulic conductivity, K, and rooting depth, L. However, the proportionality constant, B(z), that describe the functional relationship in Gardner's equation, equation (43) is a function of either root surface area, a, or root mass, m,

$$S(h) = K(h - h_r - L)\, B(z) \qquad (43)$$

where, $B(z) = c(m \text{ or } a)$

Nimmah and Hanks (1973) improved equation (43) by adding a term for the influence of soil salts in the soil water. Although the potential evapotranspiration, ETP, is a major factor in dertermining the sink, it was not included in the above sink functions. Feddes et al. (1978), in trying to include ETP as a variable in determining the sink, proposed another model,

$$S(h) = \frac{\alpha(h)\ ETP}{L} \qquad (44)$$

where $\alpha(h)$ is a water shortage factor in the soil.

The information available on root water uptake patterns suggest that the water uptake rate per unit

root length is generally small at the top of the profile and increases with depth (Arya et al. 1973, and Allmaras et al. 1975). However, the total uptake from deeper layers appears to depend on the environmental demand, the depth of rooting, root density, and soil water pressure head (Willatt and Taylor 1978). There is also evidence to suggest that there is upward flow from layers below the root zone (Feddes et al. 1978, and Van Bavel 1976). In addition, root water uptake rates vary with time of day (Parsons and Kramer 1974) and environmental demand of the plant(Brouwer 1953). It is also reported that as the soil dries through the growing season, the zone of maximum uptake moves from shallower to deeper depths (Reicosky et al 1973, Willatt 1975). From the foregoing it is evident that the root water uptake process is complex. However, oversimplification of the water uptake process would lead to poor simulation capability. Therefore a compromise has to be reached.

Hoogland et al. (1981) modified Feddes et al. (1978) model to satisfy some of the above conditions. Their model is

$$S(h) = \alpha(h)\ Smax \qquad (45)$$

where, $$Smax = (p - qL) \qquad (46)$$

The term (p-qL) accounts for the decrease in uptake with

depth at maximum pressure head. They defined this as the Smax. function. In this function L could be the entire rooting profile and not necessarily the rooting depth. Although this model is very crude to describe all the variables of root water uptake, it has the advantage that it could be used with the least amount of information on root data.

MATERIALS AND METHODS

EXPERIMENTAL ARRANGEMENT :

The experiments were conducted in the Plant Science Department greenhouse at South Dakota State Universaity, Brookings, SD. Five steel cylindrical tanks, 1.5 m height and 0.91 m internal diameter were placed 0.45 m apart with their closed bottoms resting on the floor. These tanks, when filled with the soil, served as non-weighing type lysimeters. A drainage outlet was made on the side of the tank, about 0.3E-1 m above the closed bottom. The internal diameter of the outlet was 0.45E-1 m . A cylindrical pipe 0.5E-1 m length and diameter equal to that of the drainage outlet was welded onto the outlet such that the pipe is outside the tank. A piece of glass wool was inserted into the pipe before the tank was filled with soil to reduce clogging by fine soil material. The pipe was closed by a rubber stopper with a glass tube 0.3E-2 m diameter through it, to carry the drainage water. A vertical, transparent PVC tube was attatched to the glass tube to indicate the water table level in the tank.

SOIL COLUMN PACKING :

A neutron access tube 1.6 m long, with the sealed end resting on the bottom of the tank was positioned at

the center of the tank before the tank was filled with soil. The open end of the tube was kept closed during column packing so that neither soil nor water would enter. Volumetric water content, θ, was monitored in this tube by the neutron scattering method.

The tanks were filled with top soil from the top 0.10 m of a silt loam soil. The air dried soil was passed through a 0.1E-1 m screen. Packing and settling was accomplished as follows. A galvanized steel cylinder 0.60 m in height and having an external diameter equal to the internal diameter of the tank was placed tightly inside the open end of the tank. This created an additional 0.45 m height above the top of the tank. The tanks were filled with the soil to a depth of 1.85 to 1.90 m. The drainage outlets were closed. The columns were then saturated with water and allowed to settle under gravity. When no further settling was observed the drainage outlet was opened. The columns were allowed to drain and dry for several days. The galvanized ring was removed and the process of wetting and drying repeated several time. After three cycles of wetting and drying, no additional settling was observed. The final column height was kept at 1.45 m by removing any excess soil.

For rooting depth observation in the columns a

mini-rhizotron (Bohm et al. 1978) was constructed. This consisted of a bottom sealed pyrex glass tube internal diameter 0.4E-1 m, and 1.0 m length. The glass tube was positioned at 70 degrees to the surface of the soil with 0.90 m of the tube in the soil column. The portion of the tube above the soil surface was covered on the outside by aluminum foil to reduce light entering the tube. The roots visible adjacent to glass tube were observed by using an oval shaped pocket mirror glued on to a thin steel rod. A 3-volt bulb focused close to the mirror provided sufficient light inside the tube for root observation. Normally the roots can be observed with the naked eye to 1 m depth. The rooting depths observed are approximate, used only as a guide in determining the root water uptake depth.

The bulk density, saturation water content (θs) and drainable porosity determinations were made from settled column number 5. Although the profile was assumed to be uniform with respect to bulk density, the calculated soil densities suggest it was not (Table 2).

SOIL WATER CONTENT, θ, AND SOIL WATER PRESSURE HEAD, h, MEASUREMENTS :

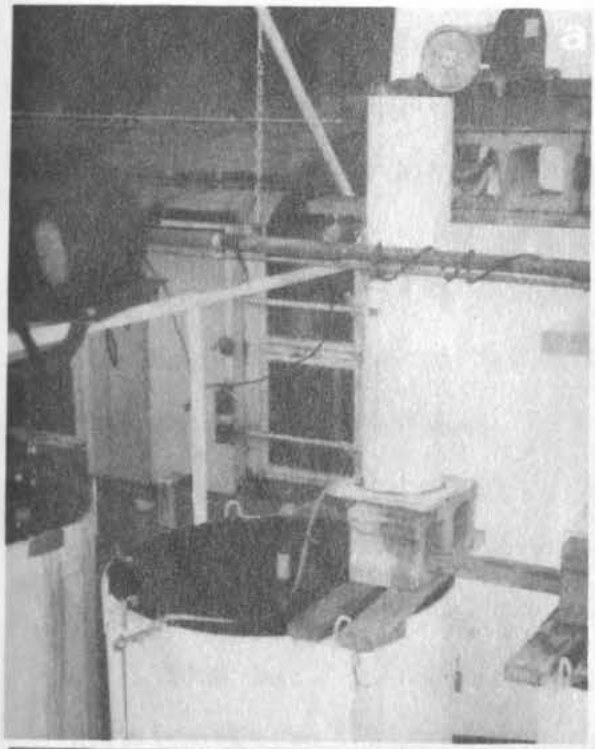
The volumetric water content measurements in the soil columns, exclusive of the top 0.15 m were monitored

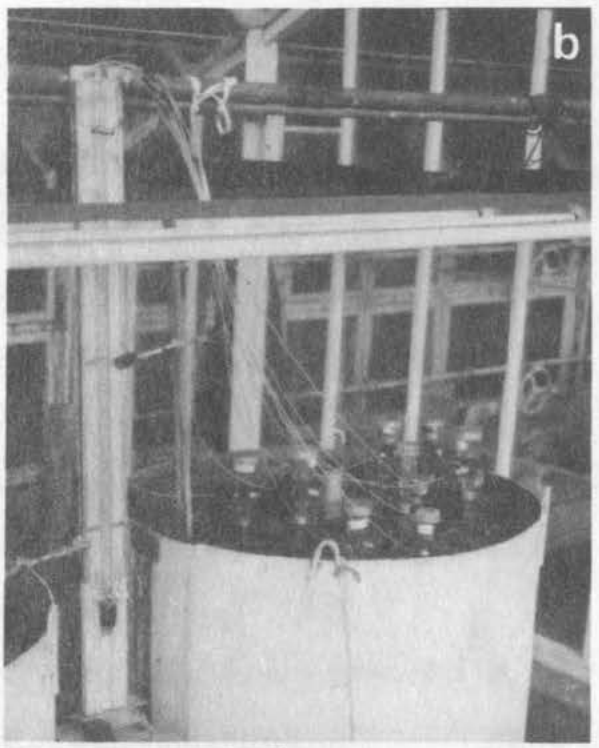
Figure 1. Lysimeter arrangement.

a = Drainage experiment showing the stage recorder.

b = Mercury manometer tensiometer.

c = Vacuum gauge tensiometers.


a


b


c

by neutron scattering for every 0.15 m increment depth. Two different instrument were used throughout the study. Both were calibrated against soil samples from column 5. The R^2 values for the calibrations are 0.97 and 0.98 respectively. During the last run, soil samples from the top 0.15 m were taken for gravimetric moisture content determination.

The neutron readings were taken once in every third day during the first and second run and once every five to seven days during the last run.

The soil water pressure head, h, was measured with tensiometers. Nine tensiometers were installed in each column so that the center of the ceramic cup was approximately at the predetermined nodal points of 0.08, 0.24, 0.40,....and 1.36 m. The neutron counts were also taken at these nodes. Two types of tensiometers, mercury manometer and vacuum gauge, were used to measure h. Column 1 had the mercury type and columns 2 and 3 had the vacuum type gauges. All vacuum gauge tensiometers were checked for accuracy against a standard gauge. A few drops of copper carbonate solution was added to the tensiometers to reduce algal growth. The range of these tensiometers is within 0 to - 650 cm of water.

Tensiometer readings were taken at the same time as

neutron readings. Air entry is a common problem with the tensiometers. This was kept at a minimum by removing the air bubbles on the day prior to the observation. However, very small air entrapment in the mercury tensiometers was unavoidable. Malfunctioning tensiometers were replaced with tested ones as soon as the malfunctioning was detected.

The tensiometer neutron probe data were first used to establish the h versus θ relationship. The data was fitted to Campbell's (1974) emprical equations.

HYDRAULIC CONDUCTIVITY, K, DETERMINATION :

Saturated steady state flow requires that a (a) constant head be maintained above the soil surface, (b) the water input equal the output and (c) the outflow be maintained at a constant outflow elevation.

The instrument arrangement for saturated hydraulic conductivity, Ks, measurement consisted of a (a) stage recorder (b) water source, a cylinder of water, to feed the soil column and (c) a small water float valve to control the water level (Figure 1). The water source, a PVC cylinder 1 m height and 0.19 m internal diameter, was kept at about 0.40 m above the surface of the soil column. The float in the cylinder was attached to the stage recorder which registered the amount of water leaving the source. The water leaving the cylinder

through a small outlet was carried to the soil column by a small PVC pipe which had a control float valve at the end. The control float valve maintained a constant depth of water 0.7E-1 above the soil column. The drainage from the soil column was collected in a container at a constant out flow elevation, 0.30 m above bottom of the column.

The determination of unsaturated K is more difficult than that of the Ks determination. For unsaturated K determinations the water supply was eliminated. The drainage outlet was opened and the drainage volume collected. Neutron readings for θ were taken at regular intervals. Equation (2) was used in the calculation of unsaturated K with the assumption that the hydraulic gradient in equation (2) to be unity.

The data collected in the unsaturated K determination could also be used to cross check the neutron probe calibration. The total change in θ in the soil column monitored by the neutron probe during a specific time period was equal to the drainage collected in that period.

CROP MANAGEMENT :

Corsoy/79 soybeans were grown in the lysimeters throughout the study. Seeds were sown in 0.15 m rows. The plant population was thinned to 55 to 60 seedlings

per column at ten days after planting, DAP. The plant population around 30 DAP was maintained between 26 to 28. This would represent the plant density per unit area found in the field.

Two columns were planted simultaneously at each run. Another pair was planted two weeks later. Each pair of columns was planted three times, making a total of six runs. The beans were removed at 110 to 120 DAP. The column 5 was kept as a standby.

SOIL WATER MANAGEMENT :

The soil water content in the top 0.45 m of the profile was allowed to be depleted to about - 650 cm of water during the first 60 DAP. A known amount of water was added to the column, when the h at 0.45 m reached - 650 cm of water. Any drainage that occured was collected. Sixty days after planting irrigation was withdrawn from one of the soil columns in a run to allow root water uptake from lower sections of the soil column.

GREEN HOUSE TEMPERATURE :

Although the influence of temperature in water flow is recognized, it is not taken into consideration in this study to avoid complexity in the flow equation. The fall, winter and spring temperatures in the green

house were maintained between 20 to 23 °C. The daytime summer temperatures inside the green house varied from 20 to 40 °C.

BOUNDARY CONDITIONS IN THE LYSIMETERS :

Equation 17 was solved subject to defined boundary conditions, - L < Z < 0 and t > 0. Here Z, distance ,positive above the soil surface, L,depth of soil profile and Z=0, at the surface. The flow through the soil columns was simulated for the following initial and boundary conditions:

$$\theta(z,0) = 0.36 \qquad -1.44 \text{ m} < z < 0$$

$$Q(0,t) = 0 \qquad 0 < t < 5d$$

$$\partial h/\partial z = 1. \qquad z = -1.44 \text{ m}$$

Here $\theta(z,0)$ the soil moisture content at the begining; $Q(0,t)$, the outflow at the surface at any time; z depth of the soil column, negative down; t, time in days, where the initial and final times are 0 and 5 respectively.

Although no fixed time interval can be specified for successive monitoring of profile water content, it would seem reasonable to assume larger t values for slow draining profiles.

The SWATRE flow model (Belman et al. 1981), used in the present study, has seven alternate lower boundary conditions. However, only two of them are selected in

this study,

1. the constant water table level and
2. zero flux at the bottom of an unsaturated zone.

The upper boundary condition, the potential evapotranspiration , ETP, can be calculated by three alternate methods in the model. However, ETP is set equal to the actual evapotranspiration in this study. The actual evapotranspiration in this study is calculated from the soil column water balance.

During a specific time period both boundary conditions are assumed to be constant in the model but could be varied between periods.

RESULTS AND DISCUSSION

I. FITTING THE FLOW MODEL PARAMETERS :

The Richard's flow equation, equation (14), describes the flow of water through soils. Solution to this equation requires that the relationship between h versus θ and K versus θ be known or established because both h versus θ and K versus θ appear as functional coefficients in the flow equation. The parameters that describe the functional relationship between h versus θ and K versus θ thus become the flow model parameters. Their estimation was carried out as follows. First, empirical equations were assumed to describe the functional relationships. Campbell's (1974) equations (31) and (34) were selected in this study to describe the h versus θ and K versus θ relationships.

In order to obtain good agreement between solutions from the flow equation and observed data the parameters must be estimated for the particular soil profile. The estimates can be obtained from experimental data provided the assumed empirical equations are linear. If the empirical equations are non-linear, the equations must be linearized before the estimations can be made.

There are two approaches by which the non-linear equations can be linearized. The linearization can be carried out by using logarithmic transformations. The

parameters can then be estimated from experimental data using the traditional least squares best fit, LSBF, procedure. Or the linearization can be carried out by the Taylor series expansion. In this procedure, the flow equation solution is defined as an objective function of the parameters to be fitted to the flow model. The objecitve function is then expanded as a Taylor series. The parameters in the expanded series are then iteratively estimated by changing the estimates at each iteration and solving the flow equation until the solution obtained agrees with the observed data. In this study, the objective function is θest which is estimated by the flow model, SWATRE. The parameters to be estimated are b, he and Ks from Campbell's equations (31) and (34). The parameter, b, a term that describes the pore geometry in soils is identical both in equations (31) and (34). The parameter he in equation (34) is called the air entry potential and Ks is the saturated hydraulic conductivity.

The data required for the LSBF parameter estimates in Campbell's equations are h, θ, and K. The tensiometer and neutron meter readings collected throughout the experimental period provided the data for h and θ, respectively. The data for the K versus θ relationship was obtained from the drainage experiments.

The K value was computed by using equation (2). The hydraulic gradient in equation (2) was assumed to be unity. However, this assumption is not valid because the depth, L, is constant whereas H changed with changes in θ. The LSBF estimation results are discussed in Method 1 A and B.

The iterative estimation and fitting using Taylor expansion and Marquardt's (1964) methods is discussed in Method 2 A and B.

The computer program, SWATRE (Belmans et al. 1983), for the Richard's flow equation is in Fortran code. This program was used to obtain the solution of θest.

METHOD 1A. FIRST ORDER LEAST SQUARES BEST FIT :

Logarithmic linearization of Campbell's equations, equations (31) and (34), would produce

$$\log h(\theta) = -b \log(\theta/\theta s) + \log(he) \qquad (47)$$

$$\log K(\theta) = (2b+3) \log(\theta/\theta s) + \log Ks. \qquad (48).$$

For simplicity the antilog of log(he) is renamed as c. The parameters b, Ks and c in equations (47) and (48) are estimated, through the first order LSBF procedure.

Theoretically, one would anticipate that the LSBF of equations (47) and (48) would produce identical values of b because it is a term that accounts for pore geometry in both equations. Also the intercept, Ks, from the LSBF of equation (48) should be approximately

equal to the experimentally determined value from the drainage experiments.

The LSBF estimates for b were 5.81 and 7.17 for equations (47) and (48) respectively. The R^2 value for the best fit was 0.81 and 0.79 for equations (47) and (48) respectively. The transformed intercept of equation (48) was 78.4, whereas the calculated Darcy's Ks's ranged from 6.0 to 34.9, with a mean of 8.4. Thus we are not only faced with the problem of selecting a value for b, but also for Ks.

While fitting equation (48) we assumed unit hydraulic gradient in the calculation of unsaturated hydraulic conductivities, K. However, this assumption is not valid for reasons mentioned elsewhere. So, we may disregard the b estimate from the LSBF of equation (48). Further, if we select the b estimate from the LSBF of equation (48), then the question araises as to what value should be used for c. Also the R value for the LSBF of equation (47) is slightly greater than that of equation (48). For these reasons, we selected the estimates from the LSBF of equation (47).

Using the selected estimates for b and c, and Ks as 8.4, the θ profile in the draining column 3 was simulated by the SWATRE flow model. The simulation along with the observation is shown in figure 2, for the

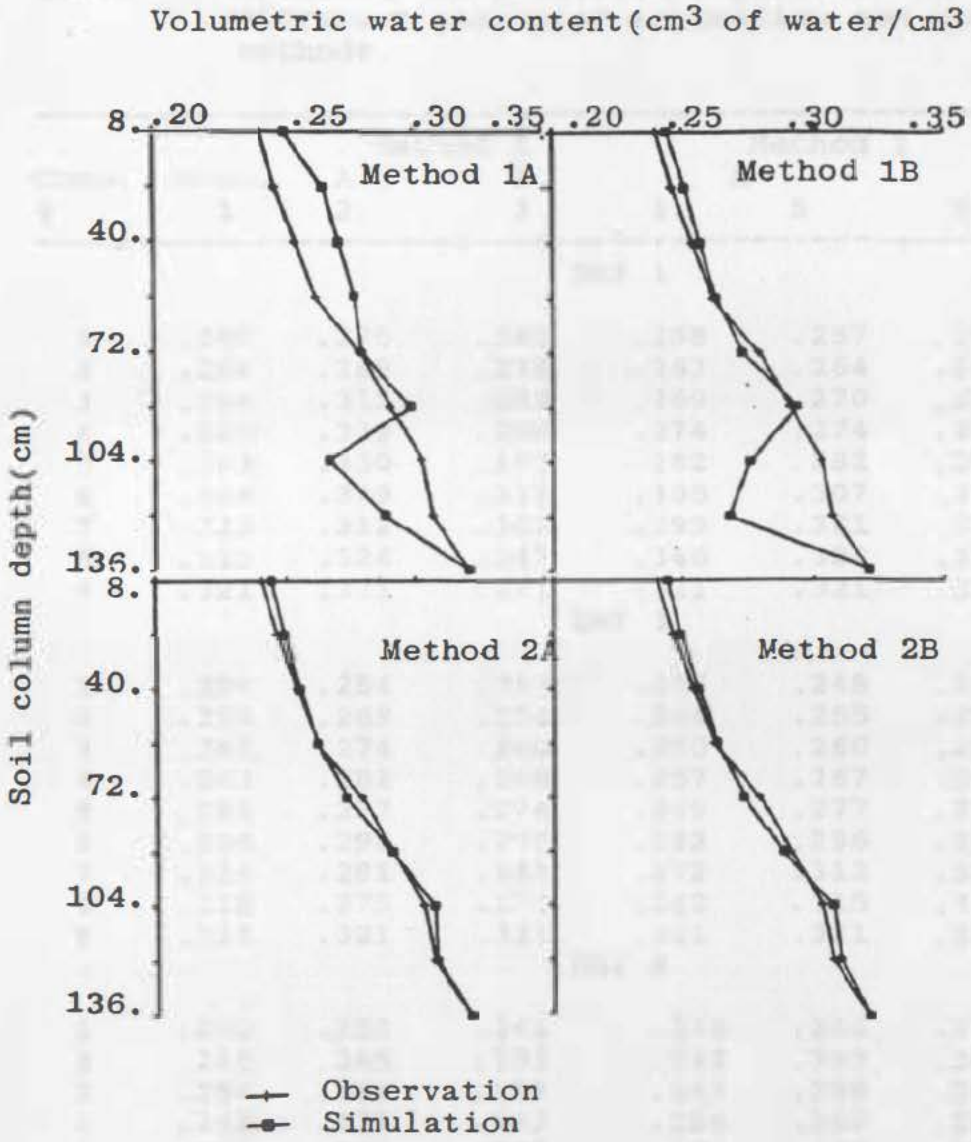


Figure 2. Observed and simulated moisture profiles for the parameter estimates in the different estimation methods.

Table 1. Observed and predicted θ profiles in the different parameter estimation and optimization methods.

Comp. #	Obsn.	Method 1 A	Method 1 B	Method 2 A	Method 2 A	Method 2 B	Method 2 B
	1	2	3	4	5	6	7
				DAY 1			
1	.260	.275	.263	.258	.257	.259	.259
2	.264	.289	.276	.263	.264	.265	.265
3	.264	.313	.282	.269	.270	.272	.271
4	.280	.339	.288	.274	.274	.280	.278
5	.283	.330	.292	.282	.282	.292	.288
6	.304	.329	.312	.305	.307	.316	.311
7	.323	.312	.302	.299	.321	.325	.323
8	.322	.326	.347	.346	.328	.325	.328
9	.321	.321	.321	.321	.321	.321	.321
				DAY 3			
1	.250	.254	.247	.237	.248	.245	.246
2	.252	.269	.254	.244	.255	.250	.251
3	.261	.274	.260	.250	.260	.257	.257
4	.263	.282	.265	.257	.267	.265	.265
5	.280	.287	.276	.269	.277	.276	.275
6	.296	.298	.297	.292	.296	.292	.291
7	.319	.281	.283	.272	.312	.309	.309
8	.318	.275	.273	.262	.315	.313	.313
9	.321	.321	.321	.321	.321	.321	.321
				DAY 5			
1	.240	.250	.244	.235	.244	.243	.244
2	.246	.265	.251	.242	.249	.249	.249
3	.254	.271	.257	.247	.255	.255	.256
4	.262	.277	.263	.256	.262	.263	.263
5	.279	.280	.273	.267	.273	.274	.273
6	.291	.299	.294	.289	.291	.289	.288
7	.307	.289	.276	.266	.307	.308	.307
8	.303	.267	.268	.256	.308	.311	.310
9	.321	.321	.321	.321	.321	.321	.321

Copm # = Compartment number
Obsn = Observed θ.

Table 2. Bulk density (g/cm^3), saturation θ_s and drainable porosity in the soil columns.

Compartment number	Bulk density	Saturation θs	Drainable porosity
1	1.04	.420	.249
2	1.11	.385	.221
3	1.10	.382	.220
4	1.12	.378	.222
5	1.12	.370	.200
6	1.13	.365	.218
7	1.14	.360	.213
8	1.14	.360	.213
9	1.15	.356	.211

data presented in table 1, columns 3 and 2, respectively. The agreement between them is very poor. This indicates that the estimates have failed to simulate the flow satisfactorily. This may be due to the fact that the estimates obtained for the transformed equation need not strictly represent the approximation for the original equation.

The simulated θ increased with depth to 0.96 m (Table 1 and Figure 2). An abrupt decrease in θ between 0.96 and 1.12 m depth suggests that there is a change in the uniformity in the soil column, at least with respect to hydraulic properties. The tendency for the bulk density to increase with depth and the decrease in the saturation θ with depth (Table 2) lends support to the fact that the soil column may not be uniform with respect to hydraulic properties. Therefore, we decided to treat the soil column as a two layered profile. The layer boundary was chosen at 0.96 m. The top 0.96 m of the column is the first layer, and 0.96 to 1.44 m the second layer.

The failure of the first order LSBF parameter estimates to satisfactorily simulate solutions for the flow equation suggested that better estimates might be obtained through the second order procedure.

METHOD 1B . SECOND ORDER LEAST SQUARES BEST FIT :

The soil column is now treated as two layered, having six parameters for estimation, three for each layer. However, the estimation was carried out only for 4 parameters, b1,b2,c1 and c2. For the other two parameters, Ks1 and Ks2 we assumed that the experimentally determined values were dependable. Using the second order LSBF procedure the parameters were estimated independently for each layer.

The estimates for b and c, for layers one and two were, 6.41 and 5.23 and 4.19 and 2.49 respectively. The R^2 value for the best fit was 0.98 for both layers. The SWATRE θ simulation for these estimates is shown in figure 2 for the data in table 1, column 4. It is obvious that the agreement improved compared to that in method 1A, but was still not satisfactory.

In the previous two parameter estimation methods we assumed that the Ks values calculated from experimental data are more dependable. However, the estimates for b and c obtained either in method 1, A or B, along with the observed Ks values failed to simulate the θ profile that agrees with the observation. The estimate for Ks as a parameter in equation (48) is 78.4, whereas we took the mean observed value, 8.4, for the θv simulation in method 1A. The θ simulation in method 1B, was obtained with Ks values of 34.9 and 8.4 for layers one and two,

respectively. The estimates in method 1B overpredict the θ profile in the upper section of the column on the first day and underpredict it on days 3 and 5 at most of the nodes (Table 1, column 4). The overpredicting tendency at relatively high soil wetness suggests that the assigned Ks value for the top layer is low for drainage near saturation. Thus we decided to resimulate θ with the Ks estimate from equation (48) for the top layer along with the estimates for b and c from method 1B. The simulation is shown in Table 1,column 5. The agreement with the observed data is still poor and the model, in general, underpredicts the θ profile. The foregoing observations suggest that we may have to estimate a different Ks value along with other parameters to better describe the flow in the particular situation. The fact that Ks is a parameter in equation (34) lends support to the above decision. Since the estimates obtained through the logarithmic linearization failed to simulate the θ profile satisfactorily, we decided to fit the parameters using Taylor expansion and Marguardt's methods.

METHOD 2A. TAYLOR EXPANSION METHOD :

In this method, as mentioned earlier, we define the objective function as θest. For the two layered soil column the objective function is defined as follows:

$$\theta est = f(b1,b2,c1,c2,Ks1,Ks2) \quad (49)$$

Using Taylor series procedure to linearize the objective function, we have:

$$\begin{aligned} f(b1,c1,Ks1,b2,c2,Ks2) = {} & f(\bar{b1},\bar{c1},\bar{Ks1},\bar{b2},\bar{c2},\bar{Ks2}) \\ & + f'(\bar{b1}...)(b1-\bar{b1}) + f'(\bar{c1}...) \\ & (c1-\bar{c1}) + f'(\bar{Ks1}...)(Ks1-\bar{Ks1}) \\ & + f'(\bar{b2}..)(b2-\bar{b2}) + f'(\bar{c2}..) \\ & (c2-\bar{c2}) + f'(\bar{Ks2}..)(Ks2-\bar{Ks2}) \end{aligned} \quad (50)$$

The terms beyond the first order were dropped from the series. The initial estimates for $\bar{b1}$,$\bar{b2}$,$\bar{c1}$ and $\bar{c2}$ were obtained from method 1B, and $\bar{Ks1}$ and $\bar{Ks2}$ were obtained from experimental data. The derivatives in the series were approximated by the difference quotient technique. For example, the derivative with respect to b1 is:

$$f'(b1..) = \frac{f(b1.. + .1) - f(b1.. - .1)}{.20} \quad (51)$$

The derivatives for the other parameters were approximated in a similar way. The value of 0.10 which is added to or subtracted from a parameter was found by trial and error such that the difference between the θest for f(b1 + .1) and f(b1 - .1) was minimum.

By substituting equation (51) into (50), equation (50) into (49) and equation (49) into (52) to compute the deviation sum squares, SS, we have:

$$SS = \Sigma[\theta obs - \theta est]^2 \quad (52)$$

The optimum values for the parameters are found when the SS in equation (52) is minimum. Taking the partial dervative of the SS in equation (52) with respect to each one of the parameters and setting $\partial ss/\partial bi$ equal to zero, would produce six equations with six unknowns, the parameter estimates. This system of equations was then solved by the Gauss elimination method with complete pivoting. The estimates thus obtained were used in an iterative procedure to minimize the SS such that the mean minimum deviation tolerance was less than or equal to 0.10E-2. The mean minimum deviation, was computed as follows:

$$\text{Tolerance} = \Sigma [\theta obs - \theta est]^2 / n \qquad (53)$$

where n is the number of observations and 0est is the model simulation.

A brief description of the modeling procedures developed in this study for the Taylor expansion method of fitting the parameters to the flow equation is appropriate now.

COMPUTER PROGRAMMING :

All the programs used in this study are in Fortran code. The principle, the procedures, the inputs required and the outputs from the programs are described briefly below.

The SWATRE flow model is described elsewhere

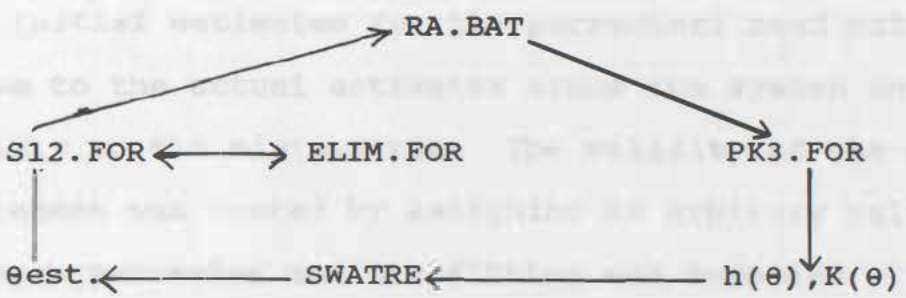
(Belmans et al, 1981). However, a brief description of the h(θ) and K(θ) table of values required as an input by this program needs special attention. This input table should contain h and K values for every 0.01 increment in θ from 0.05 to 0.36. This table of values is used in the computation of the solution. The maximum θ is the mean saturation θ in the soil column. The minimum is an arbitrary minimum θ that would be expected in the soil columns.

The program PK3.FOR computes the h and K table of values using Campbell's equations (31) and (34). The inputs required are the initial estimates for b1,b2,c1,c2,Ks1 and Ks2 and the saturation θ. The program will first compute h and K for the initial estimates for every 0.01 increment in θ from 0.05 to 0.36. Next, it will add 0.10 to the first estimate while keeping the other estimates unchanged and repeat the computation. Then it will subtract 0.10 from the original estimate of the first parameter and repeat the computation. The computation will be repeated for the other 5 estimates. Since there are 6 parameters there will be 12 such tables of values plus one for the initial estimates.

These tables of values are entered one at a time to the SWATRE model to simulate the corresponding θest. A

total of 13 θest will be simulated.

The program named S12.FOR, for Taylor series linearization of equations (50) and (51) require 13 sets of θest, θobs and the initial estimates as input. The program first computes the solutions for equations (51) and (52). Using the computed values it will generate the coefficients for a 6x7 matrix. A subroutine for the Gauss elimination method of solution for a system of linear algebraic equations, ELIM.FOR, takes the matrix coefficients and solve them for the parameters. The calculated SS was used to compute the minimum deviation by using equation (52). If the mean deviation is greater than the tolerance, the process is repeated for the new set of estimates obtained in ELIM.FOR. The above programs are executed by the batch file program, RA.BATCH. The programming is schematically shown below.



Although a tolerance limit was set to terminate the iterations, the iterations could also be terminated either when the SS repeated or the parameter estimates are very close. In this study, the SS repeated after

six iterations (Table 3). We assumed the function converged to solutions in the seventh iteration. The SS repeated in the seventh and eighth iterations. Frequent divergence and oscillations were observed throughout the iterations (Table 3). The computed mean minimum deviation, 0.64E-3, is less than the tolerance limit, 0.10E-2. The estimates in column 7 or 8 of table 3 could be used to describe h(θ) and K(θ) functions. The θ simulation for the estimates in table 3,column 7 is shown in figure 2 for the data in table 1,column 6. The simulated θ profile correlated well with the observed data. However, it should be noted that the estimate for Ks1, 85.60, is greater than the observed value, 34.9. Dane et al. (1983) reported that the fitted Ks estimates could vary by one order of magnitude.

Initial estimates for the parameters need not be close to the actual estimates since the system converges rapidly to the minimum sum. The validity of the above statement was tested by assigning an arbitary value of 5 to each parameter and the fitting was repeated. The results are presented in table 4. The function appeared to have coverged in the tenth iteration. Although the SS at convergence is greater than that obtained previouly (Table 3 and 4), the mean deviation, 0.93E-3,

Table 3. Parameter estimates and the sum squares during the iterations in method 2A, Taylor expansion method.

Iteration number	b1	b2	c1	c2	Ks1	Ks2	SS
			Parameter values.				
1	6.41	4.59	5.23	2.49	34.90	8.40	.737E-2
2	5.88	7.19	8.38	5.60	57.36	11.00	.500E-3
3	6.00	9.23	9.56	5.42	77.04	14.36	.370E-3
4	6.13	10.99	7.93	2.69	79.75	20.64	.380E-3
5	6.34	11.53	8.04	3.91	101.66	23.68	.290E-3
6	6.66	10.87	4.42	1.81	69.98	20.83	.420E-3
7	6.50	10.46	6.30	2.73	85.61	19.61	.300E-3
8	6.15	12.43	7.68	2.71	82.14	28.25	.300E-3
9	6.39	15.23	6.40	0.99	82.05	46.77	.510E-3
10	6.77	14.44	6.26	1.47	112.63	46.67	.290E-3
11	6.97	18.53	4.92	0.20	112.48	95.16	.780E-3

The procedure failed after 11 iterations generating negative values for c2.

Table 4. Parameter estimates and the sum squares during the iterations in Taylor expansion method for an initial guess to the parameters.

Iteration number	b1	b2	c1	c2	Ks1	Ks2	SS
			Parameter values				
1	5.00	5.00	5.00	5.00	5.00	5.00	.145E-1
2	3.67	7.67	12.16	10.86	6.73	8.87	.851E-2
3	5.68	13.10	3.33	2.26	15.60	23.36	.478E-2
4	5.57	11.83	4.96	1.82	20.17	25.82	.234E-2
5	6.12	13.32	4.99	2.06	28.69	31.53	.182E-2
6	6.25	13.18	8.58	1.99	41.33	34.51	.161E-2
7	5.75	11.86	9.85	2.61	45.39	40.63	.125E-2
8	6.04	13.50	9.68	2.51	60.98	31.11	.890E-3
9	5.96	14.19	11.84	3.64	80.28	23.97	.750E-3
10	6.30	14.60	8.96	2.30	80.59	29.54	.650E-3

The procedure failed after 10 iterations generating negative values for c2.

is less than the tolerance limit. The SS decreased progressively during the iterations (Table 4) unlike the oscillations found earlier (Table 3). The θ simulation for the converged estimates is as good as the previous one (Table 1,column 6 and 7). This raises the question as to whether or not we need initial estimates from experimental data to fit the parameters. Although a definite answer is not possible at present, it should be noted that the values from experimental data suggested the order-of-magnitude values for the estimates.

METHOD 2B. MARGUARDT'S METHOD :

The theory for Marguardt's (1963) algorithm is discussed in the literature review. A brief description of the programs, principles, inputs required and outputs from the programs is appropriate.

The first step in the alogorithm is Taylor series computations which are similar to those in method 2A. The program PK3.FOR is used to generate 13 tables of values for h(θ) and K(θ). These tables of values are used to simulate 13 sets of θvest.

The program S15.FOR, using the 13 sets of θest and initial estimates will compute the partial, P matrix (equation 40) and the independent vector matrix, G (equation 41). The computed matrices are passed on to program MAR.FOR.

The subroutine TRANS.FOR in MAR.FOR takes the transpose of P and passes the transpose to another subroutine TRANSP.FOR. This subroutine converts the P-transpose and the independent vector to a 6x7 matrix. The matrix coefficients are then passed to the program, STEEP.FOR.

The program STEEP.FOR performs the steepest descent method (equation 42) computations and produces 2 sets of trial vectors, equation (42). The trial vectors are passed to the progarm NPARA.FOR, which computes 2 new sets of estimates by adding the trial vectors to the initial estimates. The h and K table of values for the 2 new sets of estimates are generated by the program PK.FOR. These tables of values are then supplied to the SWATRE model to simulate the corresponding θest.

The three sets of parameter estimates, the initial and the two new sets, the corresponding θest, and the θobs are passed on to the program SUM.FOR. This program computes the SS (equation 52) for each set of 0est versus θobs. It selects the minimum sum of the three. The minimum mean deviation computed (equation 53) is compared with the tolerance, 0.10E-2. If the mean deviation is less than or equal to tolerance then the programming is terminated; otherwise it proceeds through another iteration. The programs are executed by the

Table 5. Parameter estimates and sum squares during the iterations for Marguardt's method.

Iteration number	b1	b2	c1	c2	Ks1	Ks2	SS
			Parameter values				
1	6.49	7.96	5.75	2.64	46.88	9.60	.200E-2
2	6.41	11.56	4.96	0.78	45.37	15.19	.219E-2
3	6.90	12.13	5.23	1.82	52.24	13.36	.143E-2
4	7.04	13.08	4.71	0.99	66.79	15.42	.195E-2
5	5.83	9.38	6.90	2.57	37.76	10.06	.173E-2
6	6.56	10.78	8.03	3.82	62.29	10.69	.106E-2
7	5.87	12.69	9.80	3.42	57.83	16.19	.752E-3
8	6.02	14.69	10.13	2.51	69.57	26.82	.739E-3
9	6.42	13.12	8.82	2.92	91.92	16.53	.593E-3
10	6.58	13.83	8.56	2.84	113.07	17.68	.580E-3
11	6.4	13.88	9.22	2.90	110.90	20.92	.565E-3
12	6.79	13.76	7.30	2.50	100.67	15.52	.691E-3
13	6.77	14.00	7.38	2.44	98.68	19.95	.552E-3
14	6.74	12.92	7.11	2.40	101.57	15.03	.694E-3
15	6.73	13.11	7.56	2.60	101.91	16.59	.514E-3
16	6.75	13.01	7.54	2.66	102.84	17.84	.525E-3
17	6.73	12.97	7.53	2.61	100.18	18.09	.521E-3
18	6.73	12.94	7.51	2.58	98.90	17.94	.522E-3
19	6.73	12.98	7.52	2.59	98.69	17.95	.519E-3

modified batch file program, RA.BAT.

The function converged to solutions after 19 iterations (Table 5). The SS at convergence is 0.519E-3. The corresponding mean deviation is 0.844E-3, which is less than the tolerance limit. The θ simulation for the converged estimates is shown in figure 2 for the data in table 1,column 8. The agreement with the obseved data is good indicating the converged estimates fit the flow model well.

COMPARISON OF THE ESTIMATION PROCEDURES :

The minimum SS, 0.29E-3, during the fitting procedures was obtained with the Taylor expansion method, method 2A, with the initial estimates from experimental data. However, the frequent divergence (Table 3) found during the iterations in this method suggests it is difficult to come to a conclusion. Nevertheless, when the function does converge it converges to solutions faster than Marguardt's method. Although the convergence in Marguardt's procedure is slower, the diverging tendency was eliminated. The estimates near convergence remained relatively stable for changes in SS, in the range, 0.514E-3 to 0.525E-3 (Table 5,row 15 through 19). For similar changes in SS the changes in the estimates in method 2A are high (Table 3, column 6,7 &8).

The θ simulations for the converged estimates from both methods 2A and 2B agreed well with the observed data, indicating that these estimates fit the flow model well. However, the stability of the estimates near convergence in Marguardt's procedure suggests that the estiamtes obtained in this procedure are better than those obtained in method 2A. Therefore, the estimates obtained in method 2B are selected to describe the h(θ) and K(θ) functions. Soil water pressure head, h, versus the soil moisture, θ, relationship for the converged estimates in Marguardt's procedure along with the observations are shown in figure 3. Although the data points suggests hysteresis, the simulated curve is assumed to be unique.

The first and second order LSBF estimates failed to describe the flow satisfacotrily. The high R^2 value, 0.98, obtained in method 1B suggests that 98% of the variability in the h(θ) and K(θ) functions is explained by θ. However, the simulated θ profile was not satifactory. This is anticipated because the estimates for the original non-linear equations (31) and (34) could differ siginificantly from that obtained for the logarithmically transformed linear equations (47) and (48).

The progressive improvement in the agreement

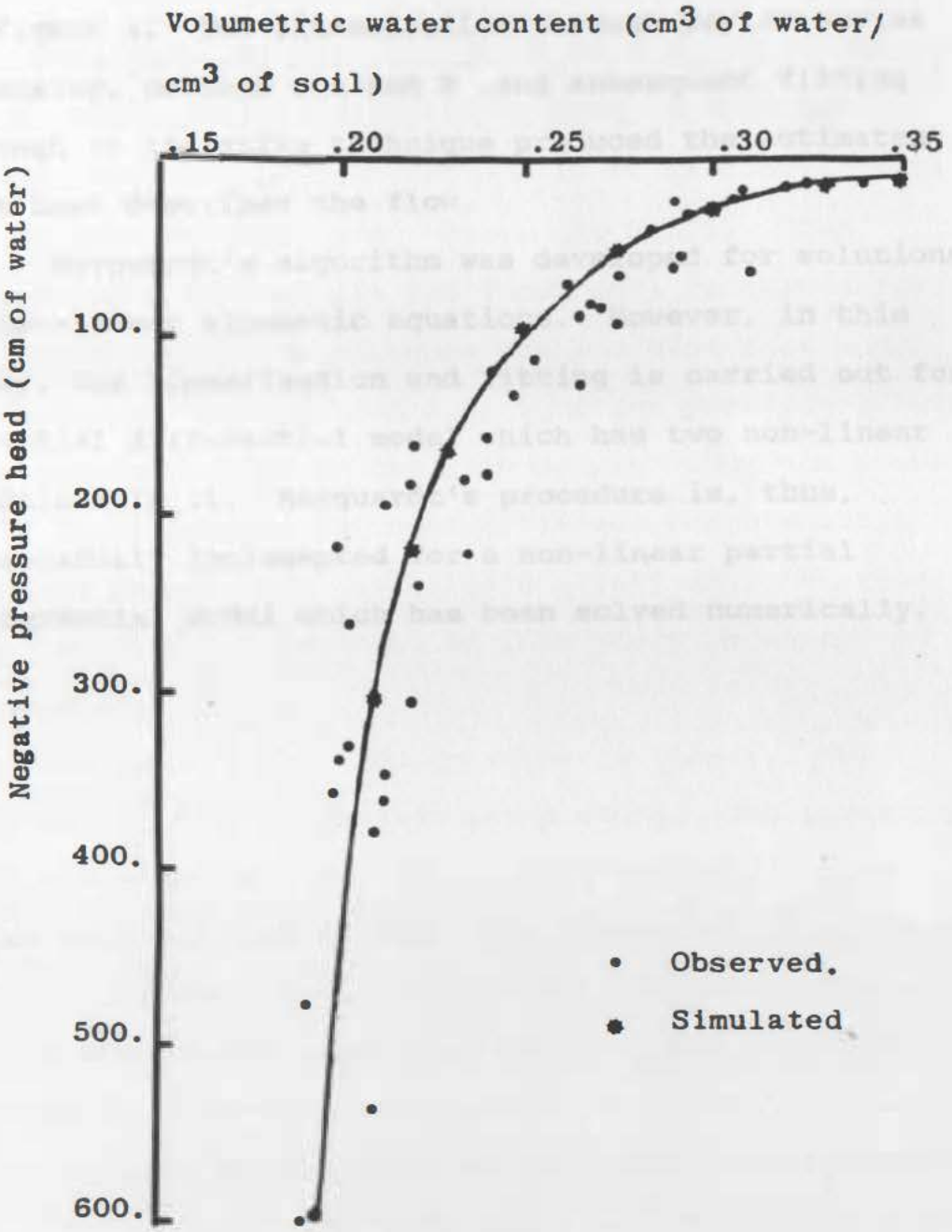


Figure 3. Soil moisture characteristic curve.

between the observed θ values and simulations is shown in figure 2. The linearization through Taylor series expansion, methods 2 A and B ,and subsequent fitting through an iterative technique produced the estimates that best described the flow.

Marguardt's algorithm was developed for solutions to non-linear algebraic equations. However, in this study, the linearization and fitting is carried out for a partial differential model which has two non-linear functions in it. Marguardt's procedure is, thus, successfully implemented for a non-linear partial differential model which has been solved numerically.

II. MODELING ROOT UPTAKE

Equation (18), the Richard's flow equation modified to describe the flow of water along with root water uptake, RWU, has three functions in it as coefficients. The 3 functions are, $h(\theta)$, $K(\theta)$, and $S(h,L)$. The parameters that describe the functional relationships in these 3 functions thus become the modified flow model parameters. The $h(\theta)$ and $K(\theta)$ function parameters have already been fitted to the flow model. Thus the problem now is to determine the best estimates for the $S(h,L)$ function parameters. Hoogland's (1980) RWU function, equation (45), is selected in this study to describe root uptake.

Hooglands (1980) RWU function is linear. The parameters in this equation are p and q. The parameter p is a term associated with root density and uptake rates per unit root length. The parameter q describes the rate of decrease in uptake with respect to depth, L.

There are two approaches by which the parameters in the RWU function can be estimated and fitted to the flow model. Since the RWU function is linear, the parameters can be estimated from experimental data through the LSBF procedure and put into the flow model. On the other hand, because the modified flow model is non-linear the parameters can be fitted directly to the flow model by

using the Taylor series linearization technique.

In order to fit the parameters through the LSBF procedure we need information on maximum RWU at different depths in the soil column. Soil water depletions are usually equated to RWU. Equating soil water depletions to RWU is not always valid, because the fluxes within the rooting profile and that just below the root zone are disregarded in RWU computation. Assuming uptake to be equal to depletion could be misleading in situations where the root zone is just above the water table and/or when part of the profile is quite wet. Parameter estimation using experimental results and soil water depletions is discussed in method 1.

In fitting the parmeters to the flow model through the Taylor series linearization technique, the estimated volumetric water content, θest, was defined as an objective function of the parameters to be fitted. The fitting procedure is discussed in method 2.

METHOD 1. LEAST SQUARES BEST FIT :

The LSBF of the maximum uptake from the soil column compartments versus the uptake depth produced, 0.21E-1, and -0.73E-05 as the estimates for p and q respectively. The R^2 value for the LSBF is 0.09.

The above estimates were fitted to the flow model

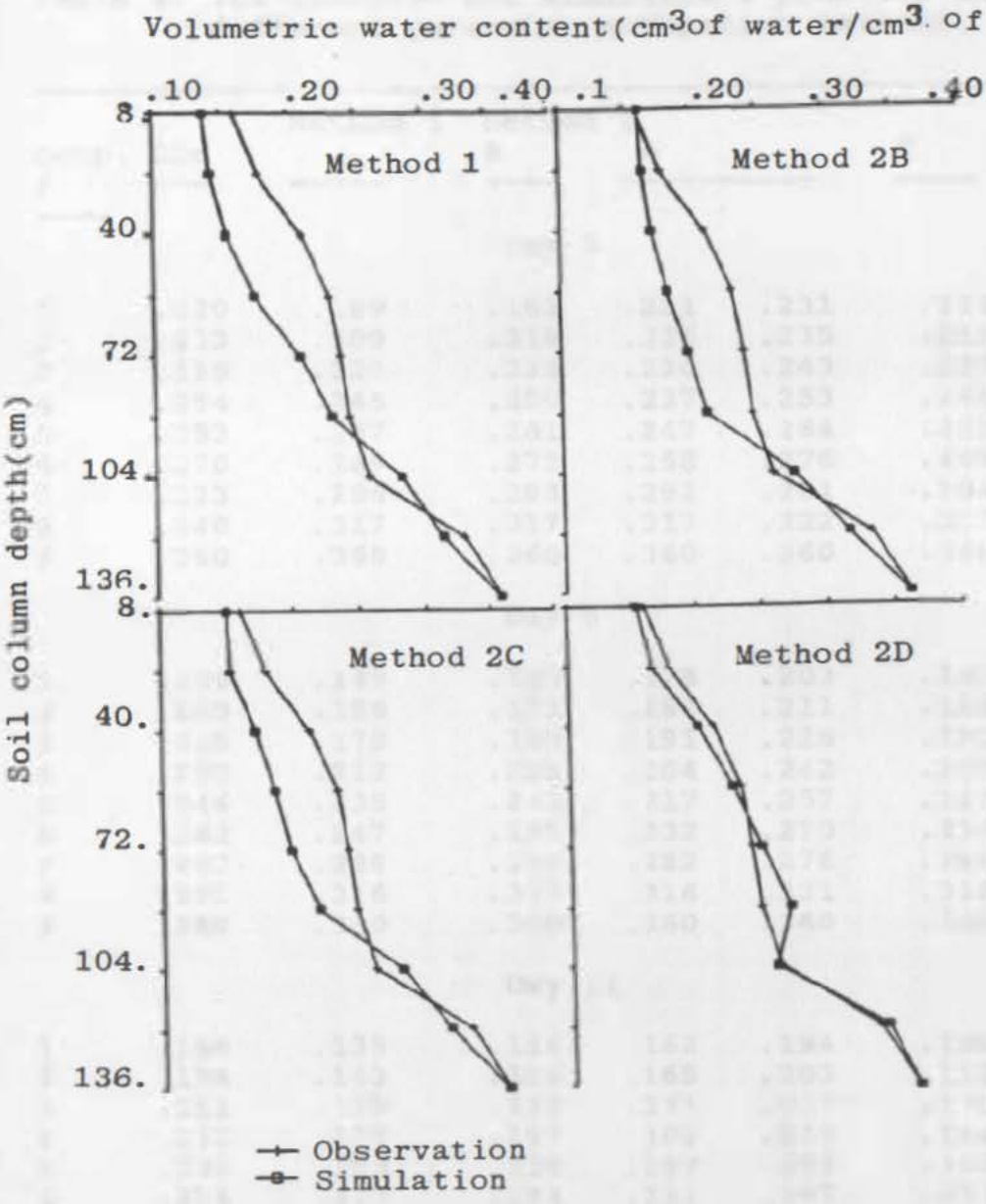


Figure 4. Observed and simulated moisture profiles for the parameter estimates in the different estimation methods.

Table 6. The Observed and simulated θ profiles for the different parameter estimation methods.

comp. #	Obs	Method 1	Method 2 A	Method 2 B	Method 2 C	Method 2 D
			Day 3			
1	.220	.189	.163	.221	.231	.211	.213
2	.233	.209	.219	.225	.235	.215	.217
3	.235	.229	.238	.230	.243	.227	.231
4	.254	.245	.250	.237	.253	.240	.245
5	.253	.257	.261	.247	.264	.253	.260
6	.270	.269	.273	.258	.276	.265	.276
7	.323	.296	.298	.292	.281	.294	.260
8	.340	.317	.317	.317	.322	.317	.338
9	.360	.360	.360	.360	.360	.360	.360
			Day 8			
1	.180	.149	.120	.178	.203	.163	.167
2	.189	.158	.133	.183	.211	.166	.175
3	.218	.178	.188	.191	.226	.192	.209
4	.232	.212	.228	.204	.242	.209	.232
5	.246	.235	.243	.217	.257	.222	.250
6	.262	.247	.255	.232	.270	.239	.270
7	.267	.288	.290	.282	.278	.286	.258
8	.351	.316	.317	.316	.321	.316	.338
9	.360	.360	.360	.360	.360	.360	.360
			Day 11			
1	.160	.138	.116	.162	.194	.150	.155
2	.178	.143	.116	.165	.203	.152	.165
3	.211	.155	.132	.171	.217	.170	.199
4	.231	.175	.197	.182	.237	.184	.225
5	.239	.209	.230	.197	.253	.196	.246
6	.245	.232	.244	.211	.267	.217	.267
7	.259	.284	.287	.275	.275	.279	.256
8	.332	.316	.316	.316	.321	.316	.338
9	.360	.360	.360	.360	.360	.360	.360

Obs = Observed θ profile
Comp.# = Compartment number
= Number.

Table 7. Observed and simulated data on evapotranspiration, Et (cm/day), and root water uptake depths (m).

Step #	Et Obsd. *	Et Pred. *	Depth of root water uptake Observed	Predicted
1	.85	.85	.64 - 1.28	.48 - .80
2	.85	.85	.64 - 1.28	.32 - .64
3	.85	.85	.64 - 1.28	.96 - 1.14
4	.85	.85	.64 - 1.28	.80 - 1.14
5	.85	.85	.64 - 1.28	.80 - .96

* Et Obsd. = Calculated Evapotranspiration.

* Et Pred. = Evapotranspiration predicted.

Step # = Step number.

to simulate the θ profile and root uptake. At the beginning of the simulation, July 28, 1985, the beans were 63 days old. The θ simulation along with the observed data on specific days during a 11 day period are shown in figure 4 for the data in table 6, columns 2 and 3. The simulated θ profile did not agree very well with the observed data. Belman et al. (1983), the model developers, recognized this weakness but did not attempt to correct it.

The evapotranspiration, Et, was accurately predicted by the model (Table 7). The uptake depth predicted by the model ranged from 0.48 to 0.80 m, but the observed soil water depletion depths ranged from 0.64 to 1.28 m (Table 7). The observed rooting depth was 0.96 m.

The inabilty of the model to accurately predict the θ profile for the estimates is attributed to the following reasons. First, the low R^2 value obtained for the LSBF suggests that either the RWU function was inadequately described and/or more experimental data is reqiured to improve the R^2 value. Second, the magnitude of the slope, q, suggests that the independent variable, depth, is not a strong variable in the RWU function. Third, the soil water redistribution may be quite significant and must be considered in the fitting

Table 8. The mean observed root water uptake (cm^3 of water/cm^3 of soil/day) in the soil columns.

Compt.#	Column I	Column II	Column III	Column IV
1	.015	.013	.020	.018
2	.016	.020	.022	.027
3	.014	.018	.016	.020
4	.017	.012	.014	.013
5	.014	.016	.019	.016
6	.016	.019	.017	.014
7	.012	-	.011	-
8	.011	-	.011	-
9	-	-	-	-

Compt.# = Compartment number.

procedures.

Reicosky et al. (1972) and Allmaras et al. (1975) reported that the maximum uptake from a unit soil compartment was independent of it's location for depths less than about a meter provided the root density was not limiting. The experimental data from this study lends support to the above findings (Table 8). Exclusive of one or two extreme data, the uptake from the soil compartments is similar but not equal. The magnitude of the slope, q, for the variable, L, obtained in this study also tends to suggests that the RWU function is not strongly dependent on the variable, L. Belman et al. (1983) and Mahey et al. (1984) set the slope, q, in the RWU function equal to zero for uptake computations. The foregoing observations suggests that the RWU function is not strongly dependent on depth.

METHOD 2A. TAYLOR EXPANSION METHOD :

The principles and procedures used in fitting the RWU function parameters are very similar to those used in section I, method 2A. Now the objective function is defined as:

$$\theta est = f(p,q). \qquad (57)$$

The optimum values for the parameters are found when the deviation sum of squares, SS, is a minimum,

$$SS = \Sigma [\ \theta obs - \theta est\ ]^2 \qquad (58)$$

Using the Taylor series expansion procedure to linearize the objective function, f(p,q), we have:

$$f(p,q) = f(p,q) + f'(\bar{p}..)(p - \bar{p}) + f'(\bar{q}..)(q - \bar{q}) \quad ...(59)$$

The terms beyond the first order were dropped from the series. Substituting equations (58) in (57) and taking the partial derivative of the SS with respect to each one of the parameters would produce a system of equations. Setting $\partial ss/\partial p$ and $\partial ss/\partial q$ equal to zero, would produce two equations with two unknowns. These equations were then solved simultaneously for the unknowns. The SS was minimized through an iterative technique by continuously changing the estimates and fitting to the flow model. A set of programs in Fortran code was written to estimate and fit the parameters. The programming principles and procedures are very similar to those described in section I, method 1A.

The increment and decrement in the parameters p and q, to compute the corresponding derivatives were generated by the program, AB1.FOR. The generated values were entered one at a time into the input file of the SWATRE model to simulate the corresponding θ profile. There were five θ sets. The program S16.FOR reads the 5 θ sets, the initial estimates, and then proceeds to compute the SS and the new estimates. The process was repeated until the desired minimum SS was achieved. The

minimum SS was set, such that the mean θ deviation tolerance was < ± 0.10E-2. The SS computed at each iteration will indicate whether the function is converging or diverging.

Unfortunately, the procedure failed after two iterations in this study, generating positive values for the parameter, q. The positive estimates for q mean a negative root uptake. The partially optimized estimates for p and q are 0.61E-1 and -0.21E-2, respectively. The θ simulation for these estimates is shown in figure 4 for the data in table 6 column 4. The agreement between the simulated and observed θ is still poor. The simulated water depletion depth ranged from 0.32 to 0.64 m (Table 7).

Failure to simultaneously fit the parameters p and q in method 2A and the lesser dependence of the RWU function on uptake depth, as indicated earlier, suggests that the consideration of depth may be dropped from the RWU function. Therefore, we decided to fit only the parameter , p, to the flow model.

METHOD 2B. FITTING THE PARAMETER p :

The principles and procedures used here are very similar to those used in section II, method 2A, the Taylor series expansion and iterative fitting. The objective function, θest, is a function of only one

parameter, p. The programs AB2.FOR and S17.FOR are modifications of AB1.FOR and S16.FOR, respectively, to estimate and fit the parameter, p. The function converged at the fifth iteration with monotonously decreasing SS (Table 9). The p estimate at convergence was 0.10E-1. The θ simulation for this estimate is shown in figure 4 for the data in table 6 column 5. It is obvious that the agreement between the observed and simulated θ profiles improved compared to those in method 2A, but still are not satisfactory. It appears that the converged estimate doesn't describe the RWU satisfactorily. This may be due to the fact that when we dropped the parameter, q, from the RWU function we assumed that the parameter, p, was independent of depth. In other words we say that Smax, equation (46),is independent of depth. However, this might not be true. The experimental data on soil water depletion (Table 7) from this study did not support the hypothesis that the Smax is independent of depth. The maximum RWU from the various compartments in the soil columns are similar but not equal. In other words, p varied with depth. Therefore, we hypothesized that individual p values should be defined for each individual compartment.

METHOD 2C. FITTING p(i) PARAMETERS :

Soil water depletion was observed from only eight

Table 9. Parameter,p, estimates during the iterations in method 2B.

Iteration number	Parameter estimate	Sum squares SS.
1	.21E-01	.3173E-01
2	.78E-02	.1917E-01
3	.95E-02	.1872E-01
4	.10E-01	.1860E-01
5	.10E-01	.1860E-01

diverging tendency. The initial b,k,and c estimates were from section I, method 2B. The RWU function parameters were from section II, method 2C.

The function converged to solutions after 21 iterations. The estimates and the SS for the last four iterations are presented in table 12. The SS remained unchanged after twenty one iterations. The mean deviation was 0.2E-2. The simulated θ profile agreed well with the observed data (Figure 4). The predicted depth of uptake ranged from 0.80 to 0.96 m (Table 7). The θ underpredicting tendency was greatly reduced (Table 6,column 8). However, the agreement between observed and predicted θ profile was not as close as that obtained in the drainage run. This is anticipated because of the complex nature of the root uptake process, which, in this study, was approximated by only two variables. However, the results obtained with a simple uptake function is better than the earlier complex models (Nimmah and Hanks, 1973).

Does the RWU function parameters have to be fitted for all the compartments individually? The question may be now asked whether the refitted estimates for the h(θ) and K(θ) functions along with the p-estimate in section II, method 2B would satisfactorily describe the uptake. In order to check the above statement the θ profile was

Table 10. Parameter p(i) estimates during the iterations in method 2C.

Parameter	Iteration number					
p(i)	1	2	3	4	5	6
	Parameter valuse					
p(1)	.30E-1	.57E-2	.12E-1	.14E-1	.14E-1	.13E-1
p(2)	.20E-1	.17E-1	.19E-1	.19E-1	.19E-1	.19E-1
p(3)	.10E-1	.91E-2	.11E-1	.11E-1	.11E-1	.11E-1
p(4)	.80E-2	.13E-2	.11E-1	.99E-2	.98E-2	.99E-2
p(5)	.80E-2	.76E-2	.14E-1	.17E-1	.17E-1	.17E-1
p(6)	.80E-2	.17E-1	.78E-2	.79E-2	.79E-2	.79E-2
p(7)	.30E-2	.79E-2	.84E-2	.10E-1	.11E-1	.11E-1
p(8)	.10E-1	.25E-1	.32E-1	.47E-1	.50E-1	.52E-1
SS	.247E-2	.253E-2	.450E-3	.180E-3	.140E-3	.140E-3

compartments in the soil columns. The estimation and fitting was therefore carried out for 8 p's. Using the same principles and procedures used in section II, method 2B, we define the objective function, 0est now as,

$$\theta est = f[p1,p2,.....p8] \quad (59)$$

The flow model SWATRE, AB2.FOR, and S17.FOR, were modified to handle eight p parameters. The function converged to solutions in the sixth iteration (Table 10). The θ simulation for the converged estimates is shown in figure 4 for the data in table 6 column 7. The agreement between the observed and simulated θ profiles showed improvement, but still was not satisfactory. The mean deviation caluculated from the minimum SS suggests that it should be $<\pm$ 0.10E-2. However, the difference between the observed and predicted θ at some nodes differs by one order of magnitude (Table 6), particularly in the upper sections of the column.

At relaively high soil water content, during the first three days, the flow model underpredicted the θ profile at the first 4 nodes in methods 1 and 2 (Table 6). A similar trend was observed during the whole simulation period at the other nodes too but not at node 7, where it overpredicted. Since the model predicted

the Et accurately the differences between the θ profiles was attributed to the fluxes upward from the saturated zone. The mean observed flux during this period was 0.24 cm/day, whereas the model prediction was 0.09, 0.07, 0.13 and 0.11 cm/day respectively in method 1 and 2A, 2B, and 2C. This suggests that the h(θ) an K(θ) functions were not describing the flow along with root uptake.

When the parameters for the h(θ) and K(θ) functions were originally fitted, it was during a five day drainage cycle beginning with profile saturation (Table 1). However, the RWU function parameters were fitted in a drier soil (Table 6). Thus it appears that the parameters in the h(θ) and K(θ) functions fitted for a wet soil were not working well in the drier end. Therefore, we decided to refit the parameters in the h(θ) and K(θ) functions in the θv range in which uptake took place. To minimize the complexity in programming we kept the p(i) parameters obtained in method 2C unchanged while refitting the h(θ) and K(θ) function parameters.

METHOD 2D . FITTING THE b, Ks, AND c PARAMETERS :

The programs developed in section I, method 2B (Marquardt's method) were used to fit the parameters. The Taylor series procedure was avoided because of it's

Table 11. Root water uptake (1/day) in the soil compartments

Com. #	Observed depln.	Predicted uptake Mehtod 1	Method 2 A	B	C	D
		Day 3				
1	.10E-1	.22E-1	.32E-1	.10E-1	.13E-1	.13E-1
2	.20E-2	.23E-1	.21E-1	.10E-1	.19E-1	.19E-1
3	.00E-0	.88E-2	-	.10E-1	.11E-1	.11E-1
4	.10E-2	-	-	.10E-1	.97E-2	.97E-2
5	-	-	-	.10E-1	.63E-2	.63E-2
6	-	-	-	.31E-2	-	-
		Day 8				
1	.10E-1	.49E-2	.42E-2	.75E-2	.54E-2	.60E-2
2	.88E-2	.76E-2	.11E-1	.88E-2	.88E-2	.12E-1
3	.34E-2	.18E-1	.38E-1	.10E-1	.11E-1	.11E-1
4	.44E-2	.23E-1	-	.10E-1	.97E-2	.97E-2
5	.14E-2	-	-	.10E-1	.17E-1	.15E-1
6	.16E-2	-	-	.69E-2	.12E-2	-
7	.11E-1	-	-	-	-	-
		Day 11				
1	.11E-1	.29E-2	.00E+0	.40E-2	.32E-2	.36E-2
2	.59E-2	.39E-2	.00E+0	.45E-2	.48E-2	.72E-2
3	.37E-2	.69E-2	.15E-1	.58E-2	.60E-2	.11E-1
4	.55E-2	.17E-1	.39E-1	.87E-2	.90E-2	.97E-2
5	.37E-2	.23E-2	-	.10E-1	.17E-2	.17E-1
6	.80E-2	-	-	.10E-1	.79E-2	.46E-2
7	.40E-2	-	-	.10E-1	.48E-2	-
8	.69E-2	-	-	-	-	-

Com. # = Compartment number
Depln = Depletion

Table 12. Parameter b,k, and c estimates during the root water uptake modeling iterations in mehtod 2D.

Iteration nummber	Parameter estimates b1	b2	k1	k2	c1	c2	Sum square SS
1	6.62	13.42	99.88	10.08	7.49	2.73	.672E-2
2	6.45	13.67	101.99	7.30	7.49	2.76	.579E-2
3	6.83	7.04	104.78	37.75	7.59	6.07	.431E-2
4	8.81	7.36	111.48	19.32	7.72	6.52	.270E-2

* The sum squares remained uchanged at .270E-2 .

simulated for these estimates. The agreement between the observed and simulated θ profiles was very poor (Table 6, column 6), confirming that the p-parameters have to be fitted for each compartment individually.

ROOT UPTAKE DISTRIBUTION :

Although the observed soil water depletion distribution need not strictly represent root uptake distribution, it does provides some information regarding the depth and distribution of uptake. During the first three days, at relatively higher soil water content, the uptake distribution was apparently masked by the fluxes in the rooting profile (Table 11, column 2). The total uptake computed from soil water depletion data during this period, exclusive of the flux from the water table, was about 0.13 cm/day, but the actual Et was 0.85 cm/day. However, at relatively lower soil water content, on day 11, the masking was greatly reduced. The results from the uptake for the first 3 days lends support to the fact that uptake and redistribution occur simultaneosly.

The soil water depletion depths in time indicate that the uptake depth increased with time (Table 11, column 2). Disregarding the first 3 days of observation, the depletion depth during the simulation period ranged from 1.12 to 1.28 m. The observed rooting

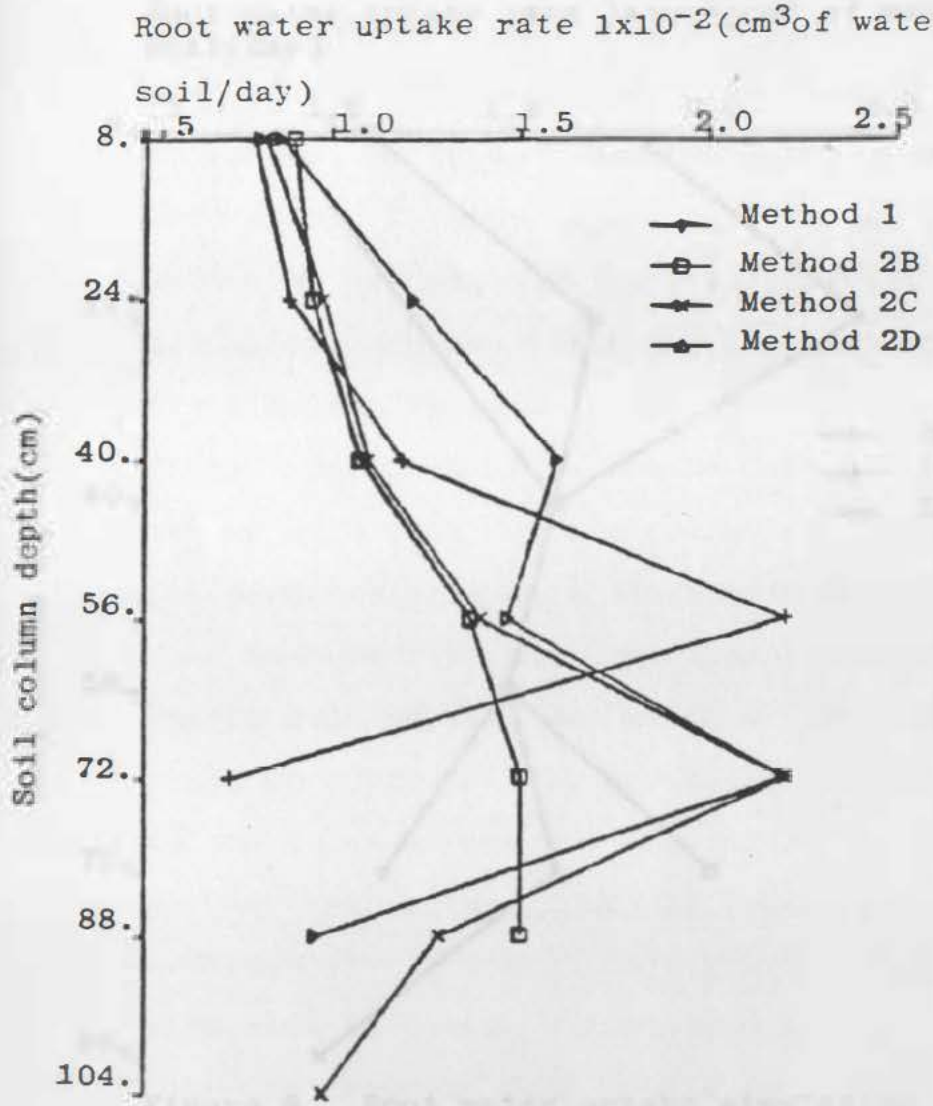


Figure 5. Root water uptake simulations for the parameter estimates in the different estimation methods.

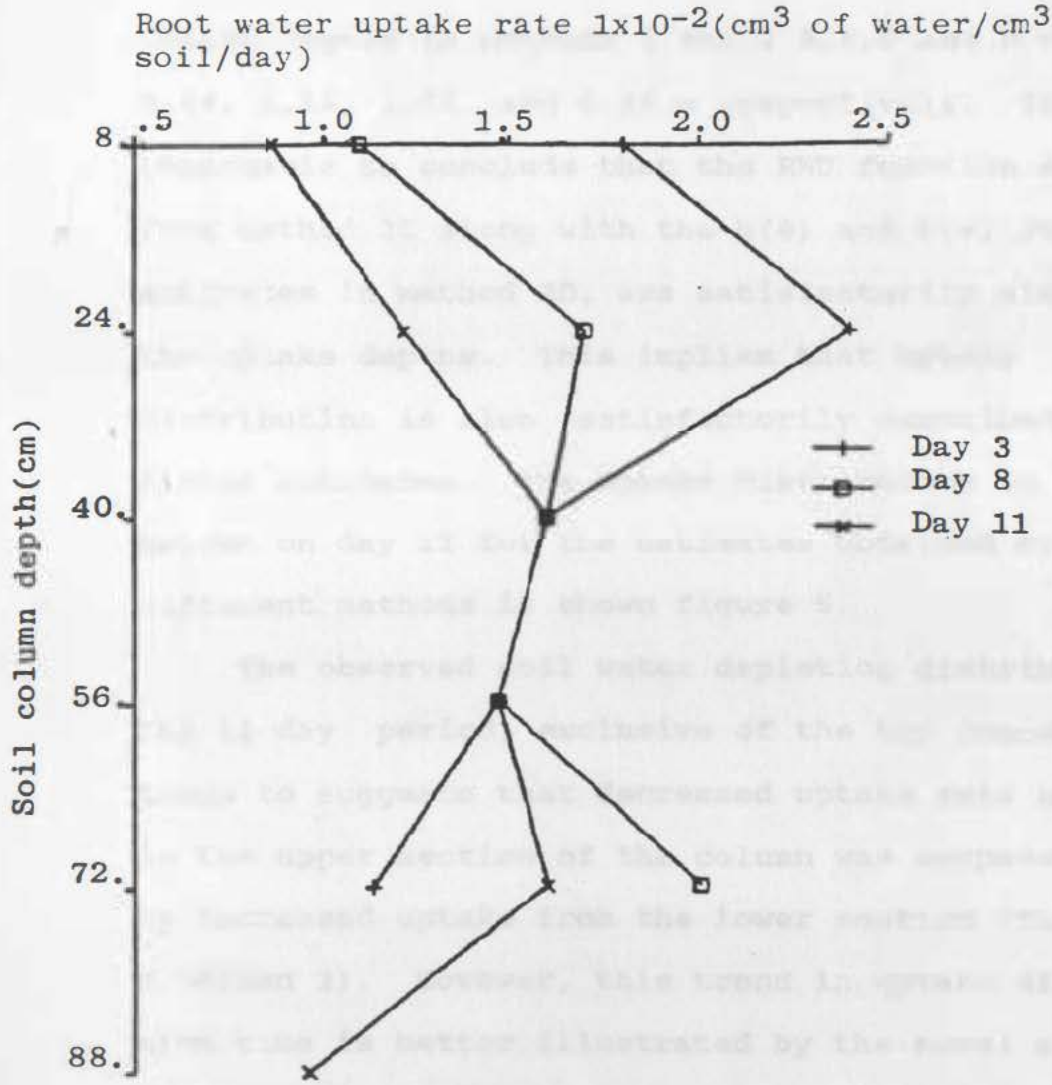


Figure 6. Root water uptake simulation in time and space for the parameter estimates in method 2D.

depth during this period was 0.96 m. The simulated uptake depths in methods 1 and 2 A,B,C and D were 0.80, 0.64, 1.14, 1.14, and 0.96 m respectively. Thus, it is reasonable to conclude that the RWU function estimates from method 2C along with the $h(\theta)$ and $K(\theta)$ function estimates in method 2D, are satisfactorily simulating the uptake depths. This implies that uptake distribution is also satisfactorily described by the fitted estimates. The uptake distribution in the soil column on day 11 for the estimates obtained by the different methods is shown figure 5.

The observed soil water depletion distribution for the 11 day period, exclusive of the top compartment tends to suggests that decreased uptake rate with time in the upper section of the column was compensated for by increased uptake from the lower section (Table 6,column 2). However, this trend in uptake distribution with time is better illustrated by the model simulation than the observed data (Table 11, columns 2, and 7, and figure 6). Thus, we conclude that a properly defined RWU function with it's parameters fitted to the flow model will describe the uptake distribution satisfactorily.

MODEL VERIFICATION :

The question now araises as to whether the refitted

Table 13. The θ simulation for the drainage run and for a low Et rate, obtained with the new parameter estimates for b,k,and c.

comp. #	Obsd.θ For drainage	Simul.θ	Obsd.θ For Et =.45	Simul.θ
	Day 1		Day 7	
1	.260	.258	.150	.160
2	.264	.263	.193	.193
3	.264	.269	.232	.230
4	.280	.275	.263	.250
5	.283	.283	.272	.266
6	.304	.297	.286	.283
7	.323	.309	.317	.318
8	.322	.314	.360	.360
9	.321	.321	.360	.360
	Day3		Day 14	
1	.250	.244	.140	.158
2	.252	.254	.190	.190
3	.261	.260	.242	.230
4	.263	.267	.264	.254
5	.280	.267	.281	.266
6	.296	.277	.301	.283
7	.319	.288	.334	.318
8	.318	.298	.360	.360
9	.321	.312	.360	.360
	Day 5		Day 23	
1	.240	.243	.140	.156
2	.246	.247	.193	.188
3	.254	.252	.235	.229
4	.262	.258	.261	.249
5	.279	.265	.278	.265
6	.291	.276	.279	.282
7	.307	.286	.324	.318
8	.303	.297	.360	.360
9	.321	.312	.360	.360

Comp # = Compartment number
Obsd θ = Observed θ
Simul θ = Simulated θ

h(θ) and K(θ) function estimates obtained in method 2D would satisfactorily describe the saturated flow and the root uptake for any other Et rate. The simulated θ profile for the same drainage period in section I agreed with the observed data (Table 13). However, the agreement is not as good as that obtained with the estimates in the drainage run. The θ at nodes 6 and 7 is slightly underpredicted by the new estimates. This is anticipated, because the new Ks2 estimate is greater than that obtained in section II, method 2D.

Root uptake and θ profiles were simulated for the beans transpiring at 0.45 cm/d. At the begining of the simulation, January 3, 1986, the beans were 53 days old. The simulated θ profile agreed well with the observed data (Table 13). However, the slight underpredicting tendency in the θ continued to be observed at lower Et rates also.

SUMMARY AND CONCLUSION

The Fortran coded program, SWATRE, was used in this study to numerically solve the Richards' flow equation for two lower and two upper boundary conditions. The model solution, soil water content (θ), was validated against measured 0 from green house experiments. The validation required that the parameters which describe the soil water pressure head, h, versus the soil water content, θ, and the hydraulic conductivity ,K, versus θ relationships should be fitted to the flow model. The non-linearity associated with the h(θ) and K(θ) empirical functions required that the equations be linearized before the estimations could be carried out.

The h(θ) and K(θ) functions were first linearized by using a logarithmic transformation. The estimates from the first order least squares best fit, LSBF, procedure when fitted to the flow model, produced very poor solutions. The second order LSBF estimates produced solutions better than those obtained with the first order, but were not satisfactory. We concluded that the estimates obtained from the logarithmically linearized functions were not satisfactory.

In the second method of linearization we defined the flow model solution, θ, as an objective function of the parameters in the h(θ) and K(θ) emiprical equations.

The objective function was then expanded as a Taylor series. The parameters in the expanded series were estimated and fitted to the flow model through two iterative techniques, Marquardt's and Taylor methods. The fitted estimates produced solutions that agreed well with observed data. The estimates near convergence in Marguardt's method were more stable than those in the Taylor method. Although frequent divergence was observed with the Taylor method of estimation the function converged to a solution faster than Marquardt's method. This is the first study that utilizes Taylor and Marquardt's methods to fit the parameters in the flow model.

The programs developed in this study for the estimation of parameters in the h(θ) and K(θ) functions could be used to develop more reliable h versus θ curves for field conditions. The capability of the SWATRE flow model is now enhanced through the programs developed in this study.

In order to solve the flow equation along with root water uptake, we used similar procedures to estimate and fit the root uptake function parameters to the flow model. Here too, the LSBF procedure estimates failed to simulate satisfactory solutions. The estimates obtained through the Taylor series linearization and subsequent

iterative fitting procedure produced satisfactory solutions.

A single uptake function defined to describe the uptake from the whole profile failed to simulate satisfactory solutions. Instead, independent functions defined for individual soil compartments simulated better solutions. However, to obtain satisfactory uptake simulations from the flow model, the parameters in the $h(\theta)$ and $K(\theta)$ functions should be estimated and fitted for the moisture regime in which the root water uptake place.

The programs developed in this study could be modified to include solute transport in the flow model. The thermodynamic constants of solute transport could be estimated in a similar manner to those utilized for the parameter estimation in this study. This is an area the weed scientists, the pollution control agencies and plant nutrient specialists could consider.

Although the mathematical models would saisfactorily describe a dynamic system, they are no cure-all.

LITERATURE CITED

Allmaras, R.R., W.W. Nelson, and W.B. Voorhees. 1975. Soybean and corn rooting in Southern Minnesota. II. Root distribution and related water flow. Soil Sci. Soc. Am. Proc. 39:771-777.

Belmans, C.J., J.G. Wesseling, and R.A. Feddes. 1983. Simulation model of the water balance of a cropped soil: SWATRE. J. Hydrol. 63:271-276.

Bohm, W. Ecological Studies. Analysis and Sysnthesis Vol. 33. pp.39-41. Springer- Verlag Berlin Heideberg N.Y. 1979.

Boltzman, L. 1894. Ann. Physik, Leipzig 53: 959-962.

Bouwer, H., and W.C. Little. 1959. A unifying numerical solution of two-dimensional flow problem in porous media with an electrical resistance network. Soil Sci. Soc. Am. Proc. 23:90-96.

Brooks, R.H., and A.T. Corey. 1964. Hydraulic properties of porous media. Colorado State University. Hydrlogy paper No.3.

Campbell, G.S. 1974. A simple method for determining unsaturated conductivity from moisture retention data. Soil Sci. 117(6):311-314.

Childs, E.C., and N.C. George. 1950. The permeability of porous material. Proc. Royal Soc. A:201:392-405.

Crank, J., and P. Nicolson. 1947. A practical method for numerical evaluation of solutions to partial differential equations of the heat conduction type. Proc. Cambridge Phil. Soc. 32:50-67.

Dane, J.H., and S. Hruska. 1983. In-situ determination of soil hydraulic properties during drinage. Soil Sci. Soc. Am. J. 47:619-624.

Day, R.R., and Luthin. 1956. A numerical solution of the differential equation of flow for a vertical drainage problem. Soil Sci. Soc. Am. Proc. 20:443-447.

Feddes, R.A., P.J. Kowalik, and H. Zarandy. 1978.

Simulation of field water use and crop yield. Simulation monographs. Pudoe, Wageningen. 189 p.

Gardner, W.R., D. Hillel, and Y. Benyamini. 1970. Post irrigation movement of soil water: I. Redistribution , Water Resources Res. 6(3), 851-861, II: Simulations redistribution and evaporation. Water resources Res. 6(4) 1148-1153.

Gardner, W.R. 1959. Solution of the flow equation for the drying of soils and other porous media. Soil Sci. Soc. Am. Proc. 23:183-187.

Green, R.E., and J.C. Corey. 1971. Calculation of hydraulic conductivity : A further evaluation of some predictive methods. Soil Sci. Soc. Am. Proc. 35:3-8.

Hanks, R.J., and S.A. Bowers. 1962. Numerical solution of the moisture flow equation for infiltration into layered soils. Soil Sci. Soc. Am. Proc. 26:530-534.

Haverkamp, R., M. Vaculin., J. Touma., and P.J. Wierenga. 1977. A comparison of numerical simulation models for one-dimensional infiltration. Soil Sci. Soc. Am. J. 41:285-293.

Hoogland, J.C., C. Belamans, and R.A. Feddes. 1981. Root water uptake model depending on soil water pressure head and maximum extraction rate. Acta Horticulture No. 119:123-136.

Klute, A. 1952. Some theoretical aspects of the flow of water in unsaturated soils. Soil Sci. Soc. Am. Proc. 16:144-148.

Luthin, N.J. 1953. An elecrtical resistance network solving drainage problem. Soil Sci. 75:259-274.

Mahey, R.K., J. Feyen, and Wyseure. 1984. A numerical analysis of irrigation treatments of Barley with respect to drainage losses and crop response. Transactions of the ASAE: 1805-1816.

Marquardt, W.D., 1963. An algorithm for least squares sum of nonlinear parameters. J. Soc. Indust.

Appl. Math. 11:431-441.

Marshall, T.J. 1958. A relation between permeability and size distribution of pores. J. Soil Sci. 9:1-8.

Millington, R.J., and J.P. Quirk. 1961. Permeability of porous solids. Trans. Faraday Soc. 57:1200-1206.

Nimmah, M.N., and R.J. Hanks. 1973. Model for estimating soil water,plant, and atmospheric interactions. Soil Sci. Soc. Am. Proc. 37:522-527.

Philip, J.R., and D.A. De Vries. 1957. Moisture movement in porous materials under temperature gradients. Trans. Am. Geophy. Un. 38:222-232.

Reicosky, D.C., R.J. Millington, A.Klute, and D.B. Peters 1972. Pattern of water uptake and root distribution of soybeans in the presence of a water table. Agron. J. 64:292-297.

Richards, L.A. 1931. Capillary conduction of liquids through porous mediums. Physics 1:318-333.

Richtmyer, R.D., and K.W. Morton. 1967. Different methods for initial-value problems. Intersceince Publishers, New York.

Scot, E.J., R.J. Hanks, and A. Klute. 1962. A power series solution of the one-dimensional diffusion equation for exponential and linear diffusivity function. USDA, ARS 41-64.

Staple, W.J., and J.J. Lehane. 1954. Movement of moisture in unsaturated soils. Canadian J. Agric. Sci. 34:329-342.

Van Genuchten, M.Th. 1979. A closed form equation for predicting hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. Proc. 35:3-8.

Visser, W.C. 1966. Progress in the knowledge about the effect of soil moisture content on plant production. Inst. Land water management, Wageningen, Netherlands. Tech. Bull. 45.