5-1972

Model for Predicting Simultaneous Distribution of Salt and Water in Soils

Satish C. Gupta

Utah State University

Recommended Citation

Gupta, Satish C., "Model for Predicting Simultaneous Distribution of Salt and Water in Soils" (1972). *All Graduate Theses and Dissertations*. 3776.
https://digitalcommons.usu.edu/etd/3776

MODEL FOR PREDICTING SIMULTANEOUS DISTRIBUTION OF SALT AND WATER IN SOILS

by

Satish C. Gupta

A dissertation submitted in partial fulfillment
of the requirements for the degree

of

DOCTOR OF PHILOSOPHY

in

Soil Science and Biometeorology

(Soil Physics)

Approved:

[redacted]

UTAH STATE UNIVERSITY
Logan, Utah

1972

ACKNOWLEDGEMENTS

I wish to express my sincere thanks to Dr. R. J. Hanks for his help and unfailing guidance throughout the course of this investigation. His valuable suggestions and constructive criticism during the preparation of this dissertation have been of immense value.

I am thankfull to Dr. J. J. Jurinak and Dr. L. G. King for their reviewing and making suggestions for amending this manuscript. Thanks are also extended to Dr. R. L. Smith and Dr. H. B. Peterson for serving on my graduate committee.

I am grateful to Mrs. G. J. Watumull, Chairman of the Distribution Committee, Watumull Foundation, Honolulu, Hawaii for the award of the scholarship to meet my termination expenses at the conclusion of my studies. Others who helped me in various capacities include Mr. Noli Baldazo, Mr. James Bauder, and Mr. Ray Cartee.

To my family in India, I express my sincere appreciation for their help and encouragement during this period.

Satish C. Gupta

Satish C. Gupta

TABLE OF CONTENTS

Page

LIST OF TABLES

Table Page

LIST OF FIGURES

Figure Page

LIST OF FIGURES (Continued)

NOTATION

$A(z)$	Plant root extraction function
a	Activity of ions
B	Specific moisture capacity. Slope of water content-suction curve.
c	Concentrations of the solute in the solutions, also Henry's Law constant.
c_n	Concentration of solute in the nth layer.
c^o	Initial salt concentration in the solution.
c_o	Total salt concentration in the solution.
D	Dispersion coefficient (cm^2/hr).
d	Distance from the soil surface (cm).
E	Equilibrium concentration of ions in the exchangeable phase.
E^o	Initial concentration of ions in the exchangeable phase.
E_T	Exchange capacity (eq/g).
f	Function symbol.
f'	Derivative of the function f.
G	Gravitational head (cm).
g	Function symbol.
H	Hydraulic head (cm).
h	Pressure head (cm).
I	Ionic strength.
i	Subscript for depth increment.
j	Superscript for time increment.
K	Equilibrium exchange constant, also hydraulic conductivity (cm/hr).

NOTATION (Continued)

Ksp	Solubility product constant.
$K_{[CaSO_4]}$	Dissociation constant for $CaSO_4$ ion pairs.
$K_{[MgSO_4]}$	Dissociation constant for $MgSO_4$ ion pairs.
K_{Ca-Mg}	Ca-Mg exchange coefficient.
K_{Ca-Na}	Ca-Na exchange coefficient.
k	Rate constant.
N	Total number of plates in the column.
n	Number of plates in a column up to point z.
r	Equilibrium parameter $(\frac{1}{K})$, dimensionless.
S	Sink or source term.
s	Column capacity parameter, dimensionless.
t	Time (hr).
Δt	Time increment (hr).
t'	Number of units of leaching solution.
v	Volume of the solution fed to the column.
$\bar{v}$	Average interstitial flow velocity (cm/hr).
u	Bulk packed volume of the column up to point z (cm^3).
W	Water content by weight (%).
X	Symbol for cation exchanger.
x, x_1, x_2	Symbols for the change in initial concentration to get equilibrium concentration.
y, y_1	Symbols for the change in initial concentration to get equilibrium concentration.
Z	Valence of the ions.
Z,ZE	Modified solubility product constants for calcite.

NOTATION (Continued)

z	Depth of column (cm).
Δz	Depth increment (cm).
θ	Water content by volume (fraction).
θS_i	Pore volume at any depth.
α	Void fraction or pore fraction.
ρ	Density of the soil (g/cm^3).
ρ_o	Density of the solution (g/cm^3).
Δ	Plate height (cm).
T	Solution capacity parameter, dimensionless.
ϕ	Cation exchange capacity per unit length of the exchanger.
β	Ratio of gm of soil to liter of solution (g/liter).

ABSTRACT

Model for Predicting Simultaneous Distribution of Salt and Water in Soils

by

Satish C. Gupta, Doctor of Philosophy

Utah State University, 1972

Major Professor: Dr. R. J. Hanks
Department: Soil Science and Biometeorology

Knowledge of water and salt movement in soils is necessary for development of a management scheme for controlling the quality of irrigation return flow. A computer model was developed to predict the distribution of water and salts in the root zone under varying initial and boundary conditions. The model consists of water flow and salt flow sub-models. The water flow sub-model considers the numerical approximation of the general water flow equation with modification for water loss by evapotranspiration (and thus root extraction). The salt flow sub-model considers the mass flow of salts, chemical exchange, precipitation or dissolution of $CaCO_3$, $CaSO_4$, and formation of undissociated Ca and Mg sulphate.

The model was tested under laboratory and field conditions by comparing predicted values with experimental measurements. Satisfactory agreement was noted for the water content distribution in almost all the experiments. The model yielded approximately correct values of total salt distribution in the field and one of the column experiments. The agreement between the measured and predicted values for the two other column experiments was poor. The poor agreement seems to result from the irregular dissolution of the applied powdered salts. The distribution of individual ions was not accurately predicted by the model. The disagreement between the predicted and measured values was large at high salt concentration. Complex ion formation, insufficient description of exchange and activity coefficients at high salt concentration are suggested for this lack of agreement. Further development and field testing of the model are needed.

(112 pages)

INTRODUCTION

Public awareness of environment degradation has created an urgent need for re-evaluation of management techniques in various industries including agriculture. It has been claimed that return flow from various irrigation projects is one of the major contributors to the quality deterioration of streams. Government agencies have given high priorities to the problem of water quality of irrigation return flow and possible means for its control. A project was initiated on the Hullinger Farm near Vernal, Utah in 1970, to develop and field test a scheme to predict and control the quality of irrigation return flow. In this scheme it is necessary that the process of simultaneous transfer of salts and water in soils be understood. The dissertation of this writer involved this part of the project.

The transport of chemical substances through a porous medium in either liquid or vapor depends upon the combined action of diffusion and mass flow. However, chemical interactions such as adsorption, fixation, precipitation, and breakdown or decay adds to the complexity in transport processes. One of the simple systems which is not affected by the above chemical effects is the transport of non-adsorbed salts like chloride and nitrate. Bresler and Hanks (1969) have successfully built a computer model to describe the movement of these salts in the soil profile, under varying boundary conditions. Since a great number of solutes react with the soil it is necessary to deal with this problem to represent more closely the real situation.

Fortunately, in recent years, with the wide spread use of digital computers and better understanding of chemical processes in soils, there are methods available which show promise of being capable of handling the flow of interacting ions in soils.

The purpose of this study was to develop and field test a model for predicting the concentration of adsorbed ionic species in soils under unsaturated flow with root extraction. The following specific chemical processes are considered.

1. Precipitation or dissolution of gypsum, calcite.
2. Formation of undissociated Ca and Mg sulphate.
3. Interaction between ions in solution and solid phase.

The ionic species considered are Ca^{++}, Mg^{++}, Na^{+}, Cl^{-}, HCO_3^{-}, and $SO_4^{=}$.

LITERATURE REVIEW

Column Chromatography

Most of the models developed for tracing salt disturibution in soils are based on the laws of conservation of mass. They state that the amount of salt added by water applied to the soil layers, minus the amount leached out and the amount absorbed by plants is equal to the net increment (positive or negative) of salts in the soil layer.

Any attempt to gather information on the vertical transport of different ions or salt solutions through the soil results in a mass of chromatographic theories. Two different approaches can be defined in the literature. The first one is based on the kinetic process called the "rate theory" (DeVault, 1943; Hiester and Vermeulen, 1952; and Lapidus and Amundson, 1952). The second one is the plate theory of Glueckauf (1949), Thornthwaite, Mather, and Nakamusa (1960), Dutt et al. (1971, and Bresler (1967) in which the height of a plate in the column is the unit of calculation. Historical development of the two different schools of thought will be reviewed separately in the following sections.

Rate theory

One of the simplest rate theories is that of DeVault (1943). It is also described as the equilibrium chromatography. It requires that the penetrating solution move through the porous medium at such a rate that a dynamic equilibrium between the ions in solution and adsorbed phase shall be maintained. The theory starts with a material balance over a cross sectional layer of the column of thickness dz:

$$\frac{\partial c}{\partial z} + \alpha \frac{\partial c}{\partial v} + \frac{\partial E}{\partial v} = 0 \qquad [1]$$

where c is the concentration of solute in the solution phase, E is the concentration of solute in the solid phase, z is the distance from the top of the column, α is the pore or void fraction of the column and v is the volume of the solution fed to the column. Under saturated flow the general solution of this equation is

$$z = g(c) + \frac{v}{\alpha + \phi f'(c)} \qquad [2]$$

where ϕ is the amount of adsorber per unit of length, f'(c) is the derivative of f(c) with respect to c, f(c) is the adsorption isotherm defined in such a way that $E = \phi f(c)$ and g(c) is any function determined by the initial distribution of solute through the column.

Rible and Davis (1955) applied this theory with some success to predict ion distribution in soils. The theory is less involved mathematically but is limited in application to soil because of the assumption of instantaneous equilibrium and negligible channeling.

Hiester and Vermeulen (1952) started with another material balance equation

$$-\left(\frac{\partial c}{\partial u}\right)_v = \left(\frac{\partial E}{\partial v}\right)_u + \alpha\left(\frac{\partial c}{\partial v}\right)_u \qquad [3]$$

where u is the bulk packed volume of the column ($u\alpha$ = void volume) up to point z. Their work was the extension of work started by Thomas (1944) who took account of the rate of exchange by second order kinetics. The starting point is

$$A^+ + BX \rightarrow B^+ + AX \qquad [4]$$

and the rate equation being

$$\frac{\partial E}{\partial t} = k\ [c(E_T - E) - \frac{E}{K}(c_o - c)] \qquad [5]$$

where A^+, B^+ are cations and X is the exchanger, E_T is cation exchange capacity, c_o is the total cation concentration in solution, k is the specific rate factor, and K is the equilibrium constant. They further defined dimensionless parameters, solution capacity parameter T, column capacity parameter s, and equilibrium parameter r, to reduce equation [3] to

$$-\left[\frac{\partial(E/E_T)}{\partial T}\right]_s = \left[\frac{\partial(c/c_o)}{\partial s}\right]_T \qquad [6]$$

and equation [5]

$$\left[\frac{\partial(E/E_T)}{\partial T}\right]_s = \left[\frac{c}{c_o}\left(1 - \frac{E}{E_T}\right) - r\,\frac{E}{E_T}\left(1 - \frac{c}{c_o}\right)\right] \qquad [7]$$

Hiester and Vermeulen (1952) have provided the graphical and numerical solution to the equation [6] and [7] in terms of parameter T, s, and r.

Bower, Gardner, and Goertzen (1957) tested this theory in the soil system. They found a reasonably good agreement between the theoretical and experimental values for the distribution of dissolved and exchangeable ions in the soil solumn as a function of depth and volume of solution applied. Gardner and Brooks (1957) distinguished between immobile and mobile salt moving with the same velocity as the leaching front. They adopted and tested the theory of Hiester and Vermeulen (1952) in laboratory column and field plots of Pachappa sandy loam. Agreement between the predicted and experimental values was found to be satisfactory.

The model of Hiester and Vermeulen differs from the proceeding model of DeVault in that rate dependent processes are considered in lieu of the assumption of equilibrium. However, both the models ignore the dispersion of salts.

The third model that is based on kinetics is by Lapidus and Amundson (1952). They have developed a model which takes into account the dispersion in addition to the mass flow. Previous work of Nielsen and Biggar (1962) has shown this model as the most satisfactory of all models investigated for predicting the spreading of a non-interacting solute, in porous media, where spreading results from diffusion and dispersion. When exchange is also considered the material balance over a layer dz is,

$$D \frac{\partial^2 c}{\partial z^2} = \bar{v} \frac{\partial c}{\partial z} + \frac{\partial c}{\partial t} + \frac{1}{\alpha} \frac{\partial E}{\partial t} \qquad [8]$$

where D is the dispersion coefficient. Depending upon the boundary conditions the equation can be solved analytically (Nielsen and Biggar, 1962) or numerically (Lai, 1970). Some of the assumptions implied in the above model are that the velocity profile can be represented by an average $\bar{v}$, the diffusion coefficient is constant, equilibrium between the two phases is established and there exists some relationship between the ions in solution and the exchanger. A comparative study of three models, DeVault (1943), Hiester and Vermeulen (1952), and Lapidus and Amundson (1952) was reported by Biggar and Nielsen (1963) using Oakley sand. They concluded that all the theories were generally inadequate to describe the experimental values. The lack of agreement was attributed to the inadequate description of exchange, the use of the average value of the flow velocity and the diffusion coefficient.

Plate theory

In the plate theories the column is regarded as being divided into a large number of segments or plates. Within each plate the concentration is considered to be uniform both in sorbent and liquid phases, the two concentrations being assumed to be at equilibrium. It is immaterial whether an exchange process, diffusion process, or any other process is envisaged as the main dispersion process. It is also implied that there is only one unit of length to which this definition applies. If the height of the plate is too long, the concentration may not be regarded as uniform and if it is too short no equilibrium is possible between the two concentrations.

One of the plate theories that has been extensively tested in the soil system is that of Glueckauf (1949). The starting equation is,

$$\left(\frac{\partial f(c)}{\partial v}\right)_z + \left(\frac{\partial c}{\partial z}\right)_v - \frac{\Delta}{2}\left(\frac{\partial^2 c}{\partial z^2}\right)_v = 0 \qquad [9]$$

where Δ is the plate height. In 1956, van der Molen applied this theory to the desalinization of soils under the influence of Dutch climate (mean annual precipitation about 70 cm). The solution of equation [9] for a homogeneous saline profile at large values of N and in the case of a linear adsorption isotherm, may be represented by

$$c = \frac{c_o}{2} \operatorname{erfc} \frac{p - 1}{\sqrt{2\ p}} \sqrt{N} \qquad [10]$$

where N is the number of depths above a distance z, $p = \frac{v}{\alpha \rho d}$,

$\text{erfc } n = 1 - \frac{2}{\pi} \int_o^n e^{-u^2} du$. ρ is the density of the soil, and d is the distance from the soil surface. Some general agreement was found in theoretical and observed values. Dyer (1965) studied the distribution of chloride and nitrate ions in adjacent irrigated and non-irrigated areas and observed a close fit of theoretical values with the observed ones.

Finally, there are two other very practical theories that have nevertheless retained the characteristics of chromatographic transport. Both the theories consider the fixed plate height. Thornthwaite et al. (1960) and Frissel and Poelstra (1964) have described the transport of strontium through soils. Their method is based on Martin and Synge (1941) theory except that the plate height is fixed and it is assumed that 0.1 part of Sr in each layer is leached downward to the next layer, for every unit of the leaching solution added to the soil. If at the beginning of leaching only one layer is loaded, the concentration in the nth layer c_n is found from

$$c_n = \frac{t'!}{(t' - n + 1)!\,(n - 1)!}\, 0.1^{(n - 1)} 0.9^{(t' - n + 1)}\, c_o \qquad [11]$$

where c_o is the total concentration in the first layer and t' is the number of leaching cycles.

The other approach which has received wide spread attention is by Dutt (1963) and his co-workers. He has used his method for calculating the quality of water percolating through soil containing gypsum. The concentration of salts at any depth and time is given by

$$c_i^j = c_{i-1}^j \left(\frac{\theta S_i - \theta_i^o}{\theta S_i}\right) + c_i^{j-1}\left(\frac{\theta_i^o}{\theta S_i}\right) \qquad [12]$$

where i and j are depth and time, respectively. θ is the moisture content and θS_i is pore volume at any depth. c_i^j is then corrected for solubility of minerals and exchange with the soil.

The advantage of this type of approach is that it is possible to introduce such factors as solubility of minerals, etc. Since exchange constants are used it means no linear adsorption isotherm is necessary. The main drawbacks of Dutt (1963) model are that the process is discontinuous and unknown dispersion is present even when physical dispersion is ignored in the model.

Review of the different models applied to the soil for describing the movement of salt are discussed by Frissel et al. (1967) and Biggar and Nielsen (1963). For the most part previous investigators have used constant flow velocities. A notable exception is the work of Bresler and Hanks (1969) who describe the numerical technique for simultaneous flow of water and salt in unsaturated soils and allow for time dependent velocities. This work was essentially a combination of Bresler (1967) model for salt flow, and Hanks and Bower (1962) model for water flow. The model starts with a material balance equation

$$\left[\frac{\partial(\theta c)}{\partial t}\right]_z = \left[\frac{\partial}{\partial z}\left(\theta D \frac{\partial c}{\partial z}\right) - \frac{\partial(\bar{v}c)}{\partial z} + S\right]_z \qquad [13]$$

where $\bar{v}$ is the volumetric flux of water given by Darcy's law, t is the time, S is the sink or source term due to the solubility of mineral or exchange between solid and solution phase. Equation [12] is similar to the equation given by Lapidus and Amundson (1952). The present model of Bresler and Hanks (1969) contains the important features of rate as well as plate theory. The plate height is variable with depth but is constant with time. The model ignored the dispersion and sink or source term. However, a critical examination of the numerical method indicates a tendency for the concentration profile to spread for non-interacting salts rather than have a sharp profile, thus indicating a "built in" dispersion in numerical approximation like Dutt (1963). The model has been tested in the laboratory and gave values which agreed well with the experimental results. The theoretical development of this model and its modifications are described in the next section.

THEORETICAL CONSIDERATIONS

The present model is essentially the combination of the model for water and salt flow by Bresler and Hanks (1969) and Dutt et al. (1971) models for solubility of minerals and exchange between the solution and solid phase. The essential features of both models are discussed in the following paragraphs. One dimensional flow is considered in the model.

Water Flow Model

The basic water flow equation for one dimension is taken as

$$\frac{\partial \theta}{\partial t} = - \frac{\partial \bar{v}}{\partial z} + A(z) \qquad [14]$$

where θ is the water content and $A(z)$ is the plant root extraction function. The theoretical development of $A(z)$ have been discussed by Nimah (1972) and will not be discussed in the present derivation ($A(z) = 0$). The volumetric flux of water $\bar{v}$ is given by Darcy's law

$$\bar{v} = - K(\theta) \left(\frac{\partial H}{\partial z}\right) \qquad [15]$$

where $K(\theta)$ is unsaturated hydraulic conductivity and H is the hydraulic head defined as

$$H = h + z \qquad [16]$$

where h is the pressure head. A numerical solution of equation [14] is given by Hanks and Bower (1962) and a review of solutions by

Freeze (1969). The numeric form of equation [14] is

$$\frac{\theta_i^{j} - \theta_i^{j-1}}{\Delta t} = \frac{\left(h_{i-1}^{j-1} + h_{i-1}^{j} + 2G - h_i^{j-1} - h_i^{j}\right) K_{i-1/2}^{j-1/2}}{2(\Delta z_i)^2} - \frac{\left(h_i^{j-1} + h_i^{j} + 2G - h_{i+1}^{j-1} - h_{i+1}^{j}\right) K_{i+1/2}^{j-1/2}}{2(\Delta z_i)^2} \qquad [17]$$

where G is the gravitational term. $G = \Delta z_i$ for vertical infiltration down, $G = -\Delta z_i$ for vertical infiltration up and $G = 0$ for horizonal infiltration. Δz_i is variable in the present model. The derivation of equation [17] assumes a unique relationship between pressure head, h, and water content, θ. If the assumption holds then it is possible to write a relationship between θ and h,

$$\frac{\theta_i^{j} - \theta_i^{j-1}}{\Delta t} \approx \frac{\left(h_i^{j} - h_i^{j-1}\right)}{\Delta t} B_i^{j-1/2} \qquad [18]$$

where B is the specific moisture capacity defined as

$$B_i^{j-1/2} = \left(\frac{\partial \theta}{\partial h}\right)_i^{j-1/2} . \qquad [19]$$

Substitution of equation [18] reduces equation [17] to

$$\frac{h_i^{j} - h_i^{j-1}}{t} = \frac{\left(h_{i-1}^{j-1} + h_{i-1}^{j} + 2G - h_i^{j-1} - h_i^{j}\right) K_{i-1/2}^{j-1/2}}{2(\Delta z_i)^2 B_i^{j-1/2}} - \frac{\left(h_i^{j-1} + h_i^{j} + 2G - h_{i+1}^{j-1} - h_{i+1}^{j}\right) K_{i+1/2}^{j-1/2}}{2(\Delta z_i)^2 B_i^{j-1/2}} . \qquad [20]$$

An equation similar to equation [20] can be written for each depth increment involving unkown of $h^j_{i(i = 1,2,3,\cdots\cdots, n)}$. The boundary condition supplies the value of h^j_o and h^j_{n+1}. Equation [20] can also be expressed as

$$-AA_i \, h^j_{i-1} + BB_i \, h^j_i - CC \, h^j_{i+1} = DD_i \qquad [21]$$

where

$$AA_i = \frac{\Delta t \, K^{j-1/2}_{i-1/2}}{2(\Delta z_i)^2 B^{j-1/2}_i}$$

$$BB_i = 1 + \frac{K^{j-1/2}_{i-1/2} \, \Delta t}{2(\Delta z_i)^2 B^{j-1/2}_i} + \frac{K^{j-1/2}_{i+1/2} \, \Delta t}{2(\Delta z_i) \, B^{j-1/2}_i}$$

$$CC_i = \frac{\Delta t \, K^{j-1/2}_{i+1/2}}{2(\Delta z_i)^2 B^{j-1/2}_i}$$

$$DD_i = h^{j-1}_i + \frac{K^{j-1/2}_{i-1/2} \, \Delta t}{2(\Delta z_i)^2 B^{j-1/2}_i} \left(h^{j-1}_{i-1} + 2G - h^{j-1}_i\right)$$

$$- \frac{K^{j-1/2}_{i+1/2} \, \Delta t}{2(\Delta z_i)^2 B^{j-1/2}_i} \left(h^{j-1}_i + 2G - h^{j-1}_{i+1}\right)$$

when boundary conditions are substituted, n equations result in tridiagonal matrix

$$\begin{bmatrix} BB_1 & -CC_1 & 0 & & \\ -AA_2 & BB_2 & -CC_2 & & \\ & -AA_3 & BB_3 & -CC_3 & \\ & \cdots & \cdots & \cdots & \\ & & \cdots & \cdots & \cdots \\ & & & \cdots & \cdots \\ & & & -AA_n & BB_n \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \\ h_3 \\ \cdot \\ \cdot \\ \cdot \\ h_n \end{bmatrix} = \begin{bmatrix} DD_1 \\ DD_2 \\ DD_3 \\ \cdot \\ \cdot \\ \cdot \\ DD_n \end{bmatrix} . \qquad [22]$$

Equation [22] is solved for h_i^j by the regular techniques of solving tridiagonal matrix (Carnahan, Luther, and Wilkes, 1969). The water content, θ, is estimated from the relationship between θ and h.

Salt Flow Model

The rate of flow of salts at any plane in the direction of flow may be given by the equation [12]

$$\left[\frac{\partial(\theta c)}{\partial t}\right]_z = \left[\frac{\partial}{\partial z}\ \left(\theta D\,\frac{\partial c}{\partial z}\right) - \frac{\partial(\bar{v}c)}{\partial z} + S\right]_z \ .$$

The first term on the right, in the above equation, represents the contribution from diffusion to the flow of solute and the second term represents the contribution from viscous flow. S is the sink or source term due to solubility of minerals and exchange of ions in solution with solid phase. Each component of equation [12] is discussed separately.

Mass flow of salts

If the dispersion is absent and no sink or source exists, the flow of salt is due to the mass flow of water expressed as

$$\left[\frac{\partial(\theta c)}{\partial t}\right]_z = -\left[\frac{\partial(\bar{v}c)}{\partial z}\right]_z \ . \qquad [23]$$

Numerical approximation of equation [23] leads to

$$\frac{\left(\theta_i^j c_i^j - c_i^{j-1}\,\theta_i^{j-1}\right)}{\Delta t} = -\,\frac{\left(\bar{v}_i^{j-1/2} c_i^{j-1/2} - \bar{v}_{i-1}^{j-1/2} c_{i-1}^{j-1/2}\right)}{\Delta z} \qquad [24]$$

with the approximation, $c_i^{j-1/2} = c_i^{j-1}$ and $c_{i-1}^{j-1/2} = c_{i-1}^{j-1}$, equation [24] reduces to

$$c_i^j = \left[\left(\bar{v}_{i-1}^{j-1/2} c_{i-1}^{j-1} - \bar{v}_i^{j-1/2} c_i^{j-1} \right) \frac{\Delta t}{\Delta z} + c_i^{j-1} \theta_i^{j-1} \right] \Big/ \theta_i^j \ . \qquad [25]$$

Equation [25] and its modification are used to compute the mass flow of salts due to water.

Dispersion of salts

If there is no dispersion, there should be piston flow of salts and sharp boundary in the salt distribution should exist at the wetting front. Since the numerical approximation involves the mixing of solutions and then averaging over a new water content (equation [25]) a diffuse salt boundary exists at the wetting front. Although in the present model dispersion is ignored explictly, the mixing of salt indicates a "built in" dispersion in the numerical method of salt flow.

Sink or source term

The concentration of salts at each depth is modified due to the chemical reactions like precipitation or dissolution of minerals and exchange between ions in solution and soil matrix. Both these processes contribute to the source or sink term in equation [12].

Dissolution or precipitation of gypsum. A slightly soluble salt often present or added to the soil is gypsum. An equation relating gypsum to other constituents in soil is

$$CaSO_4 \cdot 2H_2O \rightleftarrows Ca^{++} + SO_4^{=} + 2H_2O \ . \qquad [26]$$

The solubility of gypsum is described by the solubility product constant concept

$$Ksp = a_{Ca}\ a_{SO_4} = c_{Ca} c_{SO_4}\ \gamma^2 = 2.4 \times 10^{-5} \qquad [27]$$

where Ksp is the solubility product constant, a is the activity of the ions designated, γ is the activity coefficients of divalent ions ($\gamma_{Ca} = \gamma_{SO_4}$), and c is the equilibrium concentration of ions designated which are defined further as follows.

Let x moles per liter of Ca^{++} and $SO_4^{=}$ that dissolve or precipitate and c^o_{Ca}, $c^o_{SO_4}$ are the initial molar concentration of Ca^{++} and $SO_4^{=}$, respectively. Then the change in relative composition of Ca^{++} and $SO_4^{=}$ is

$$c_{Ca} = c^o_{Ca} + x \qquad [28]$$

$$c_{SO_4} = c^o_{SO_4} + x\ . \qquad [29]$$

Combining equation [28] and [29] with equation [27], results in equation of the form

$$x^2 + Bx + C = 0 \qquad [30]$$

where

$$B = c^o_{Ca} + c^o_{SO_4}$$

$$C = c^o_{Ca}\ c^o_{SO_4} - Ksp/\gamma^2\ .$$

Equation [30] can be solved for x.

Undissociated Ca and Mg sulphate. In addition to the dissolution or precipitation of gypsum, the $CaSO_4$ - Ca^{++}, $SO_4^{=}$ - H_2O system involves the formation of undissociated $CaSO_4$. The dissociation constant $K_{[CaSO_4^o]}$ of ion-pair is defined as

$$K_{[CaSO_4^o]} = \frac{c_{Ca}\, c_{SO_4} \gamma^2}{c_{CaSO_4^o} \gamma} \qquad [31]$$

where $c_{CaSO_4^o}$ is the molar concentration of the ion-pairs and γ for ion-pairs is taken as unity.

Let x_1 be the moles per liter of Ca^{++} and $SO_4^{=}$ which forms undissociated $CaSO_4$. If the initial concentration of $CaSO_4^o$ ion-pair is $c^o_{CaSO_4^o}$ then the change in concentration will be

$$c_{Ca} = c^o_{Ca} - x_1 \qquad [32]$$

$$c_{SO_4} = c^o_{SO_4} - x_1 \qquad [33]$$

$$c_{CaSO_4^o} = c^o_{CaSO_4^o} + x_1 \qquad [34]$$

when equation [32], [33], and [34] are combined with equation [31], rearrangement yields an equation of the form

$$Ax_1^2 + Bx_1 + C = 0. \qquad [35]$$

The chemistry of undissociated $MgSO_4$ is similar to $CaSO_4$ and results in an equation similar to equation [35], where

$$A = \gamma^2$$

$$B = -\left(K_{[CaSO_4^o] \text{ or } [MgSO_4^o]} + \gamma^2\, c^o_{Ca \text{ or } Mg} + \gamma^2\, c^o_{SO_4}\right)$$

$$C = \gamma^2\, c^{o}_{\text{Ca or Mg}}\, c^{o}_{SO_4} - K_{[CaSO_4^o]\text{ or }[MgSO_4^o]}\, c^{o}_{CaSO_4^o\text{ or }MgSO_4^o} .$$

Equation [35] can be solved for x_1. When the system contains gypsum, the undissociated $CaSO_4$ becomes constant

$$c_{CaSO_4^o} = \frac{Ksp}{K_{[CaSO_4^o]}} \quad . \qquad [36]$$

Dissolution or precipitation of lime. An equation relating to the dissociation of lime in water with its constituent is shown as

$$CaCO_3 \rightleftarrows Ca^{++} + CO_3^{=} \qquad [37]$$

and the solubility of calcite is usually described by the solubility product constant Ksp;

$$Ksp = a_{Ca}\, a_{CO_3} \qquad [38]$$

where a is the activity of ions designated by the subscript. Since $CO_3^{=}$ concentration is a function of partial pressure, and HCO_3 concentration is usually the predominant form in which CO_2 occurs in soil water systems, it is more convenient to consider the following reactions.

$$H_2CO_3 + CaCO_3 \rightleftarrows Ca^{++} + 2HCO_3^{-} \qquad [39]$$

$$K = \frac{a_{Ca}\, a^{2}_{HCO_3}}{a_{H_2CO_3}} . \qquad [40]$$

If an equilibrium system is under constant pressure of CO_2 and if the activity coefficient of non-charged species (H_2CO_3) is unity, equation [40] becomes

$$Z = K\ c_{H_2CO_3} = a_{Ca}\ a^2_{HCO_3} \qquad [41]$$

$$ZE = \frac{Z}{\gamma_{Ca}\ \gamma^2_{HCO_3}} = c_{Ca}\ c^2_{HCO_3} \qquad [42]$$

where γ is the activity of associate ion.

It has been pointed out by Olsen and Watanbe (1959) that the solubility of $CaCO_3$ in the soil is different from pure calcite, and the H_2CO_3 content in the soil solution is variable at different moisture contents. This in turn means that the value of Z, in the soil, varies with water content. A comparison of equation [38] with [41] and [42] shows Z and ZE to be equivalent to the solubility product constant. Dutt et al. (1971) determined the following relationship between Z and water content.

$$\log Z = -\ 1.68 \log W - 4.46 \qquad [43]$$

where W is water content by weight expressed as percent. The same relation is used in the present model. ZE is then estimated from equation [42].

Using the same argument as in the case of solubility of gypsum that x_2 is the moles per liter of Ca^{++} that dissolves or precipitates, then the equilibrium concentration of Ca^{++} and HCO_3^- is

$$c_{Ca} = c^o_{Ca} + x_2 \qquad [44]$$

$$c_{HCO_3} = c^o_{HCO_3} + 2x_2\ . \qquad [45]$$

Substituting equation [44] and [45] in equation [42] results in a cubic equation

$$A\ x_2^3 + B\ x_2^2 + C\ x_2 + D = 0 \qquad [46]$$

where

$$A = 4$$

$$B = 4\left(c^o_{Ca} + c^o_{HCO_3}\right)$$

$$C = \left(c^{o^2}_{HCO_3} + 4\ c^o_{Ca}\ c^o_{HCO_3}\right)$$

$$D = \left(c^o_{HCO_3} \cdot c^o_{Ca} - ZE\right).$$

Equation [46] can be solved for x_2 by Newton Raphson iteration method.

Cation exchange. An equation that describes Ca-Mg exchange is

$$\frac{a_{Ca}}{a_{Mg}} = K_{Ca\text{-}Mg}\frac{E_{Ca}}{E_{Mg}} \qquad [47]$$

where $K_{Ca\text{-}Mg}$ is the exchange coefficient for Ca and Mg. Let y moles of Mg^{++} per gm of soil go into solution or are adsorbed. Let the initial concentration of Ca^{++} and Mg^{++} be c^o_{Ca} and c^o_{Mg} moles/liter in the solution phase and E^o_{Ca}, E^o_{Mg} be moles/gm adsorbed on the soil matrix. The change in the relative composition of Ca^{++} and Mg^{++} from the interaction of solution and adsorbed phase is then

$$E_{Ca} = E^o_{Ca} - y \qquad [48]$$

$$E_{Mg} = E^o_{Mg} + y \qquad [49]$$

$$c_{Ca} = c^o_{Ca} + \beta y \qquad [50]$$

$$c_{Mg} = c^o_{Mg} - \beta y \qquad [51]$$

where β is the ratio of gm of soil to liter of solution. Combining equation [48] to [51] with equation [47] results in quadratic expression

$$Ay^2 + By + C = 0 \qquad [52]$$

where

$$A = \beta \left(1 - K_{Ca-Mg}\right)$$

$$B = \beta \left(E^o_{Mg} + K_{Ca-Mg} E^o_{Ca}\right) + c^o_{Ca} + K_{Ca-Mg} c^o_{Mg}$$

$$C = c^o_{Ca} E^o_{Mg} - K_{Ca-Mg} c^o_{Mg} E^o_{Mg} .$$

Equation [52] can be solved for y.

Gapon's equation was used to describe the non-symmetrical exchange between Ca and Na

$$\frac{\sqrt{a_{Ca}}}{a_{Na}} = K_{Ca-Na} \frac{E_{Ca}}{E_{Na}} . \qquad [53]$$

Using the same reasoning for calculating the equilibrium concentration as in the case of Ca-Mg exchange, equation [53] reduces to

$$Ay_1^4 + By_1^3 + Cy_1^2 + Dy_1 + E = 0 \qquad [54]$$

where y_1 is the change in concentration required to reach equilibrium from initial concentration, and

$$A = -4\ K_{Ca-Na}\ \beta^2$$

$$B = 4\beta\left(\gamma_{1/2} + 2\ K^2_{Ca-Na}\ E^o_{Ca}\ \beta + K^2_{Ca-Na} c^o_{Na}\right)$$

where $\gamma_{1/2}$ is the ratio of activity coefficent of Ca to Na,

$$C = 4\gamma_{1/2}\left(c^{o}_{Ca} + E^{o}_{Na}\beta\right) - 4K^{2}_{Ca-Na}\beta\, E^{o}_{Ca}\left(\beta E^{o}_{Ca} + 2c^{o}_{Na}\right)$$

$$- K^{2}_{Ca-Na}\, c^{o^{2}}_{Na}$$

$$D = E^{o}_{Na}\,\gamma_{1/2}\left(4c^{o}_{Ca} + E_{Na}\beta\right) + 2K^{2}_{Ca-Na}E^{o}_{Ca}c^{o}_{Na}\left(2\beta E^{o}_{Na} + c^{o}_{Na}\right)$$

$$E = E^{o^{2}}_{Na}c^{o}_{Ca}\gamma_{1/2} - K^{2}_{Ca-Na}c^{o^{2}}_{Na}E^{o^{2}}_{Ca} \quad .$$

Equations [30], [35], [46], [52], and [54] are used to calculate the equilibrium concentrations.

MATERIALS AND METHODS

The applicability of the theoretical model was tested in the laboratory as well as in the field experiment.

Laboratory Experiment

In the laboratory the experiment was done using a lucite column packed with air dry soil. The soil used in the experiment was obtained from the Hullinger Farm near Vernal, Utah. The farm is located west of the airport, about 1 and 1/2 mile south of 5th East and Main Streets.

Column set up

The column consisted of 12 stacked rings with an inner diameter of 10.4 cm and an outer diameter of 11.4 cm. The top ring was 8.5 cm high, whereas the other 11 rings were 5.1 cm high. The rings were interlocked by a groove and projection arrangement coated with petroleum gel to prevent leakage of water from the column. The whole column was bolted together by three brass rods. The bottom ring had a plate at the bottom with an outlet at its center to collect the effluent. To avoid sealing the outlet with soil, it was covered with a screen and a filter paper.

Packing of the column

In order to avoid layering of soil in the column while packing, the following procedure was adopted: Two sieves of 4 mm and 2 mm size were placed one above the other at the top of the column. Air dried, sieved soil is passed through the 4 mm and then onto the 2 mm sieve at such a rate that sieves were not blocked. The column was filled to a height of about 61 cm. The soil was leveled at the surface by hand. The uniformity in the packing was checked with the density probe (Davidson et al., 1963).

Column experiment

Three different cases of initial and boundary conditions were considered.

Case #1. "Sprinkler irrigation" condition with a layer of salt at the soil surface. $CaCl_2 \cdot 2H_2O$ salt was applied at the rate of (4547.2 kg/ha) before wetting with the irrigation water. The soil was wetted by simulated sprinkler irrigation (0.57 cm/hr). The soil was leached until the wetting front nearly reached the bottom of the column (35.6 hrs). The column was then segmented. Each segment was weighed to estimate the bulk density. Portions of the soil from each segment were used to extract soil solution and to determine the water content. Exchangeable cations were determined from the other portion of the soil left in each segment. The chemical composition of irrigation water and soil is reported in Tables 1 and 2, respectively.

Table 1. Chemical composition of irrigation water

EC	µmhos/cm at 25 C	864
Ca^{++}	me/l	3.16
Mg^{++}	me/l	3.88
Na^{+}	me/l	1.6
Cl^{-}	me/l	0.17
HCO_3^{-}	me/l	0.17
$SO_4^{=}$	me/l	8.3
$CaSO_4$ ion-pair	me/l	0.84
$MgSO_4$ ion-pair	me/l	1.02

Table 2. Initial conditions for column experiments

	Case #1	Case #2 and #3
Calcium (me/l)	15.83	15.0
Magnesium (me/l)	11.31	9.87
Sodium (me/l)	1.67	1.49
Sulphate (me/l)	26.80	24.78
Chloride (me/l)	0.75	0.30
Bicarbonate (me/l)	1.26	1.28
Exchange capacity (me/100 gm)	11.0	14.0
Gypsum (gm/100 gm)	0.0	0.5
Water content (fraction)	0.0175	0.0175

Case #2. "Rain" condition with a layer of salt at the soil surface. The salts applied were $CaCl_2 \cdot 2H_2O$ (1993.6 kg/ha), $MgCl_2 \cdot 6H_2O$ (3225.6 kg/ha), and NaCl (1523.6 kg/ha). The chemical composition of the soil used in this case is given in Table 2. The soil was wetted with distilled water by simulated rain (0.58 cm/hr) for 37.6 hours at which time the wetting front was nearly at the bottom of the column. The column was then segmented and analysed by the same procedure as in case #1.

Case #3. "Irrigation-evaporation-irrigation" with a layer of salt at each irrigation. Before wetting $CaCl_2 \cdot 2H_2O$ salt was applied at the rate of 4547.2 kg/ha. The soil was wetted for 35.4 hours by simulated sprinkler irrigation (0.59 cm/hr). The same soil was used as in case #2. The irrigation water applied had the same composition as in case #1. A water table was created at the end of infiltration and evaporation was allowed @0.095 cm/hr for 75.8 hours. The chemical composition of water of the water table was the same as that in the irrigation water. Evaporation was then continued without a water table and with the bottom outlet plugged for another 196.8 hours @0.0304 cm/hour. At the end of evaporation the soil was wetted by simulated irrigation (0.78 cm/hr for 23.7 hours) with a layer of salt at the soil surface. The salt applied was NaCl (3427.2 kg/ha). During infiltration the bottom outlet was unplugged. At the end of the last irrigation, the column was segmented and analysed by the same procedure as in cases #1 and #2.

Physical properties of the soil

In order to test the applicability of the computer model it is required to have appropriate data of the hydraulic properties of the soil. These properties are hydraulic conductivity-water content (Figure 1) and pressure head-water content (Figure 2) relationships. The data reported by Andrade (1971) for the given soil was used in this study.

Chemical analysis

Electrical conductivity of the soil solution was measured with a Beckman Model RC-19 conductivity bridge using a 2 ml pipet cell with a cell constant of one. Measurements were taken at room temperature and corrected to 25 C.

Chloride concentration was determined potentiometrically using a silver billet electrode and a saturated calomel electrode in conjunction with a corning model 12 expanded scale pH meter.

The solution extract was diluted with lanthanum oxide in concentrated HCl and the concentration of calcium, magnesium, and sodium was analysed by atomic adsorption spectophotometer (Perkin Elmer Model - 303).

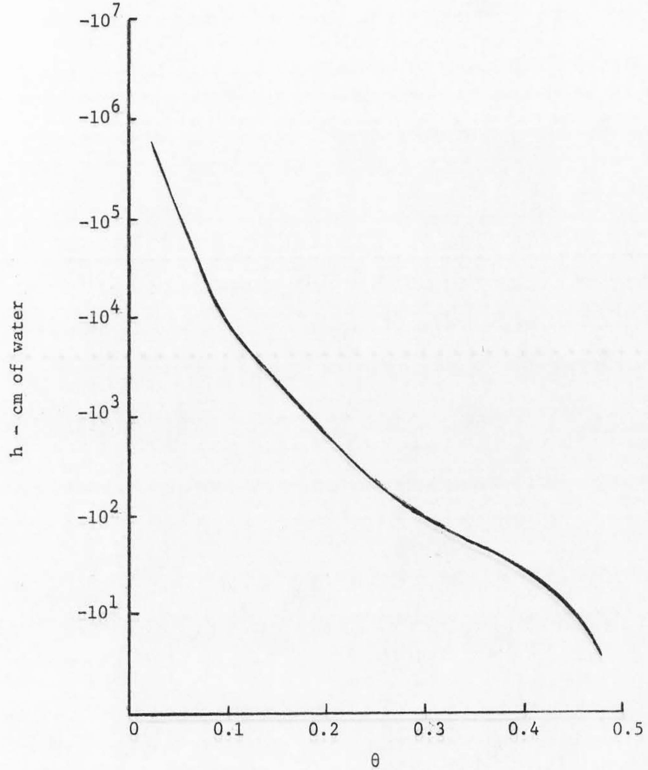

Figure 1. Pressure head-water content relationship for Mesa sandy loam.

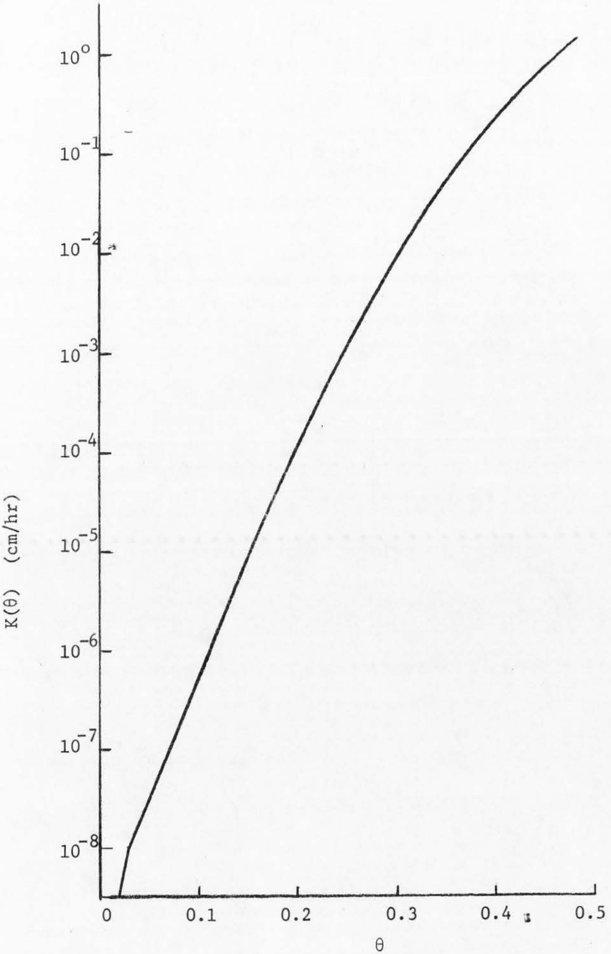

Figure 2. Hydraulic conductivity-water content relationship for Mesa sandy loam.

Bicarbonate ion concentration in the irrigation water was calculated using the relationship

$$H_2O + CO_2 \underset{\leftarrow}{\overset{K}{\rightarrow}} H^+ + HCO_3^- \qquad [55]$$

$$K = \frac{a_H \, a_{HCO_3}}{cP_{CO_2}} \qquad [56]$$

where a is the activity of the ions designated, $a = m\gamma$, m is the molality and γ is the activity coefficient. At the reference state $\gamma_{CO_2} = a_{H_2O} = 1$ in pure water. Thus, CO_2 can be replaced by $m_{CO_2} = cP_{CO_2}$, where c is Henry's law constant (0.0344 at 25 C), P_{CO_2} is partial pressure of CO_2 in atmosphere (3×10^{-4}) and $K = 4.45 \times 10^{-7}$.

Bicarbonate ions concentration in the soil solution was estimated from the relationship given by equation [38] and

$$HCO_3 \underset{\leftarrow}{\overset{K}{\rightarrow}} H^+ + CO_3^= \qquad [57]$$

$$K = \frac{a_H \, a_{CO_3}}{a_{HCO_3}} \qquad [58]$$

where $K = 4.69 \times 10^{-11}$. Details of this method are given by Olsen and Watanbe (1959). These concentrations were just an approximation to start with and were corrected by subroutine EXCH to bring into equilibrium with the system.

The concentration of sulphate ions was estimated from the difference of total salts and the summation of chloride and bicarbonate ions.

For the analysis of exchangeable cations, 5 to 7 gms of wet soil sample was washed with 150 ml of 95 percent ethanol in a leaching funnel until free of chloride. Exchangeable calcium and magnesium were extracted by leaching with 100 ml of 1N sodium acetate at pH 8.2. A similar procedure was followed for exchangeable sodium except that it was extracted with 1N ammonium acetate (pH 7.0). Analysis of cations was made as described previously.

Because of the insufficient amount of solution, collected in the field experiments for chemical analysis, soil samples were collected and saturation paste prepared (Richards, 1954). The saturation extracts were analysed as described previously.

Exchange constant

Exchange constants are defined by equation [47] and [53]. Their values were determined from the known concentration of ions in the solution and exchangeable phase. Although their names implies a constant value, they vary with the total salt concentration in the present system. It would be more appropriate to define them as exchange coefficient rather than exchange constant. Figures 3 and 4 are the plot of these coefficients with total salt concentration. Exchange coefficients for case #1 are given by Figures 3 a and 4a, while for case #2 and #3, their values are given in Figures 3b and 4b.

Field Experiment

The field experiment was conducted on the Hullinger Farm near Vernal, Utah. The soil type was Mesa sandy loam. Tensiometer, salinity sensors, and four probe units were installed in the center of the plot

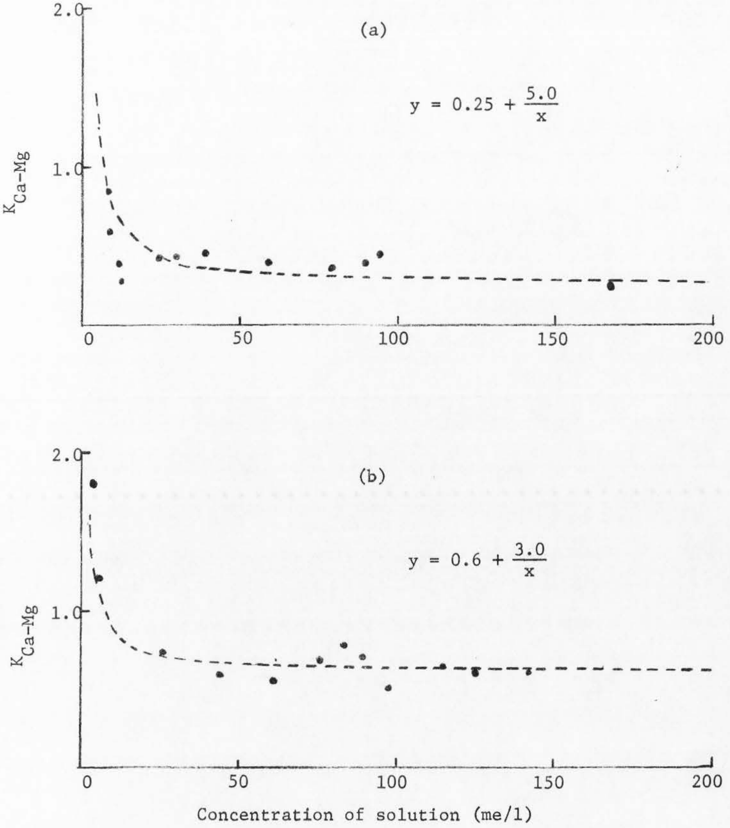

Figure 3. Variation of Ca-Mg exchange coefficient with solution concentration a) surface soil, b) sub soil.

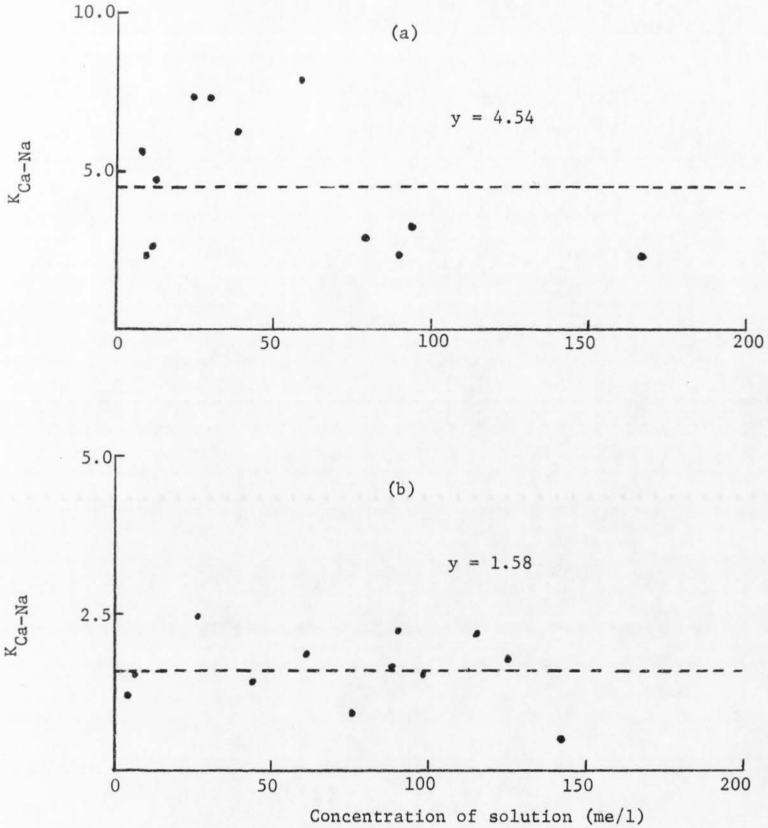

Figure 4. Variation of Ca-Na exchange coefficient with solution concentration a) surface soil, b) sub soil.

at 15, 45, 75, 105, and 165 cm depth at site A, and, 15, 45, 75, 135, and 165 cm depths at site B. Duplicate tensiometer cups were also installed at the given depths to obtain soil solution samples. To facilitate the collection of reasonable amounts of soil solution for electrical conductivity (EC) measurements, suction was applied on the solution cups for 8 to 12 hours depending upon the moisture content of the soil. Soil samples were collected for chemical analyses at three different times during the experiment. Samples were taken at 30 cm intervals to a depth of 120 cm. Alfalfa was the major crop grown. Sprinklers were used as means of irrigation. $CaCl_2 \cdot 2H_2O$ (4390.4 kg/ha) and NaCl (3561.6 kg/ha) were applied before the first and second irrigation cycles. Initial and boundary conditions to the above experiment are given in Tables 3 and 4, respectively. Chemical composition of irrigation water was reported in Table 1. Soil moisture distribution was determined by the neutron probe and water loss by evapotranspiration was estimated from the lysimeter data.

Computer Model

The computer model of Dutt et al. (1971) for solubility of minerals and exchange between ions in solution and soil was combined with the salt and water transport model of Bresler and Hanks (1969). The resultant model consists of a main program and five sub programs. The sub programs are designated as: (1) PLOT, (2) EXCH, (3) EQEXCH, (4) SALT, and (5) ACOF.

Main program

Figure 5 is the flow chart for the main program. The main program has several major responsibilities. First it reads the initial and

Table 3. Initial conditions for field experiments

Depth	Water Content	Calcium	Magnesium	Sodium	Sulphate	Chloride	Bicarbonate	Gypsum
(cm)	(θ)	(me/l)	(me/l)	(me/l)	(me/l)	(me/l)	(me/l)	(gm/100 gm)
0 - 30	0.2347	36.0	14.31	5.04	44.25	10.35	0.75	0.0
30 - 55	0.2446	25.75	14.19	4.22	34.08	9.16	0.92	0.5
55 - 100	0.2764	27.25	16.29	7.13	44.05	5.67	0.95	0.5
100 - 115	0.3053	35.10	19.95	4.91	57.84	1.30	0.82	0.5
115 - 165	0.3661	32.0	16.25	4.39	50.54	1.26	0.83	0.5

Table 4. Boundary condition in the field experiment for soil water flow

Time (hrs)	Flux at the Surface (10^2 x cm/hr)	ET Flux (10^1 x cm/hr)	Comment
24.0	-0.300	-0.300	
16.0	0.0064	0.0	Irrigation
8.0	0.00	0.00	
24.0	-0.211	-0.211	
120.0	-0.187	-0.187	
72.0	-0.135	-0.135	
60.0	-0.219	-0.219	
15.0	0.0062	0.0	Irrigation
69.0	-0.224	-0.224	
2.0	0.0037	0.0	Rain
70.0	-0.190	-0.190	
24.0	0.0021	0.0	Rain
24.0	-0.226	-0.226	
24.0	0.005	0.0	Rain
24.0	-0.227	-0.227	
24.0	-0.198	-0.198	
27.0	-0.191	-01.91	

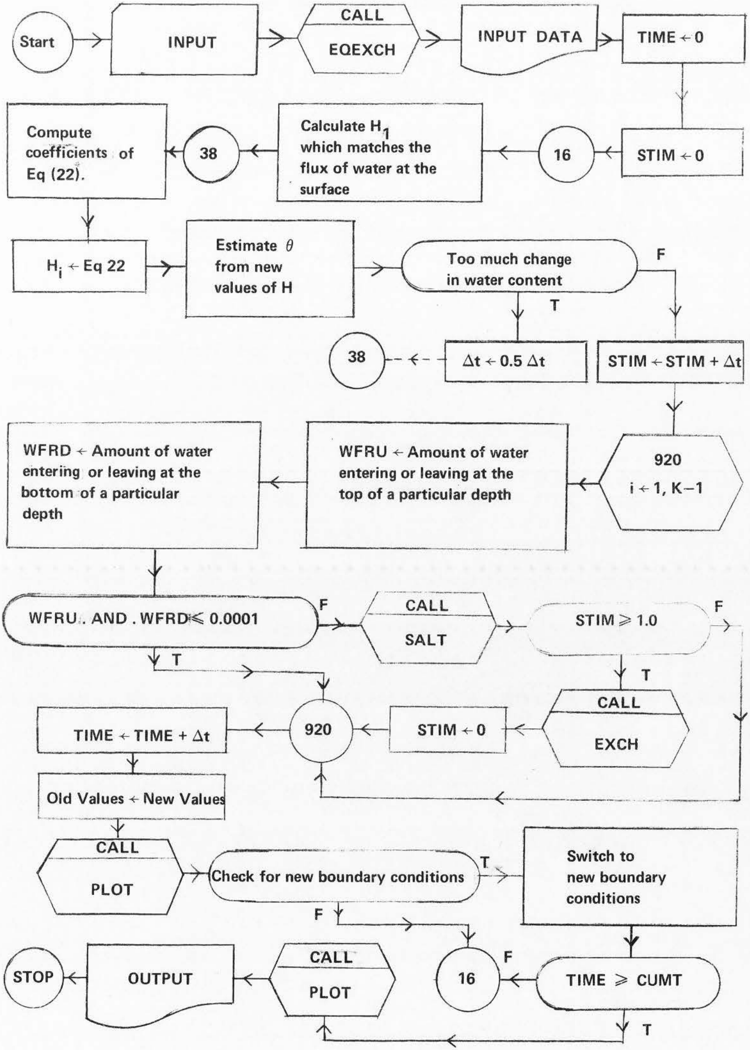

Figure 5. Flow diagram for MAIN.

boundary conditions. The initial conditions in this experiment include the concentration of salts applied on the soil surface at the beginning of the experiment. Since the salts were applied in the powder form rather than in solution, it was assumed that they were soluble at the given water content of the soil. The program then calls for subroutine EQEXCH. This subroutine calculates $CaSO_4$, $MgSO_4$ ion-pairs and equilibrium concentration of exchangeable ions. The input and transformed data are then printed to provide the user with a record. Concurrently, the main program calls for subroutine PLOT which plots the water and salt content with depth. After setting various counters and initializing certain values the program computes the new values of pressure head and water content.

The routine then executes a large outer loop for the number of depths in a profile. Within this loop the routine checks for the amount of water leaving or entering the top or bottom of a soil segment at a particular depth. If the amount of moisture flow is not negligible subroutine SALT is called which computes the flow of salts due to mass flow of water. A check is then made to call the subroutine EXCH. The check insures that changes in concentration of ions due to solubility of minerals and exchange are calculated every hour rather than every Δt. No great difference was noted in the predicted values when subroutine EXCH was called each Δt. The counter for this check is initialized to zero after each call for subroutine EXCH.

Then the program increments the time counter with Δt and initializes the old values with the recently computed values of the variables used in salt and water flow. The routine then calls for subroutine PLOT and prints the output.

A check is then made for the new boundary conditions and cumulative time for which the program is allowed to run. If the time equals the cumulative time then it stops after the subroutine PLOT is called and the needed output information is printed. Otherwise, it goes back to statement 16 and executes for the next Δt increment.

Input data. The input data needed are as follows.

1. Hydraulic conductivity-water content and pressure head-water content tabular data covering the range of water content to be encountered during the period of interest (basic soil property).

2. Air dry and saturated soil water contents (basic soil data).

3. Root distribution with depth (active roots for adsorbing water) for the period. At present the model has no provisions for changing this with time (basic plant property).

4. Plant water potential below which the plant wilts and the actual transpiration will be less than potential transpiration (basic plant property).

5. Activity coefficient-ionic strength tabular data covering the range of ionic strength encountered in the system.

6. Water content-depth tabular data at the beginning (initial conditions).

7. Chemical composition depth tabular data at the beginning (initial conditions). This involves the knowledge of the chemical analysis of the important chemical species. At present it considers Ca, Mg, Na cations and Cl, SO_4, and HCO_3 anions.

8. Potential transpiration and potential evaporation rate or portential irrigation or rainfall rate as a function of time for the period (boundary conditions).

9. Chemical composition of the irrigation or rain water (boundary conditions).

10. Presence or absence of a water table at the bottom of the soil (boundary condition).

Output data. The type of output data that is available is almost infinite. Consequently, a selection of the desired data is made from the following.

1. Soil water content and pressure head *vs* depth and time during the period.

2. Chemical composition of the soil solution *vs* depth and time during the period.

3. Estimated evaporation and transpiration as a function of time.

4. Water flow into the water table or up from the water table as a function of time.

5. Chemical composition of the water going into the water table or up from the water table as a function of time.

6. Estimated plant water potential as a function of time.

Subroutine PLOT

This subroutine plots the salt and water content with depth.

Subroutine EXCH

Figure 6 is the flow chart for this subroutine. The subroutine is called in the main program approximately every hour or at each Δt if Δt is greater or equal to one hour. This implies that in a time of one hour equilibrium is established between the ions in the solution and solid phase. Adjustment in the concentration of different ions due

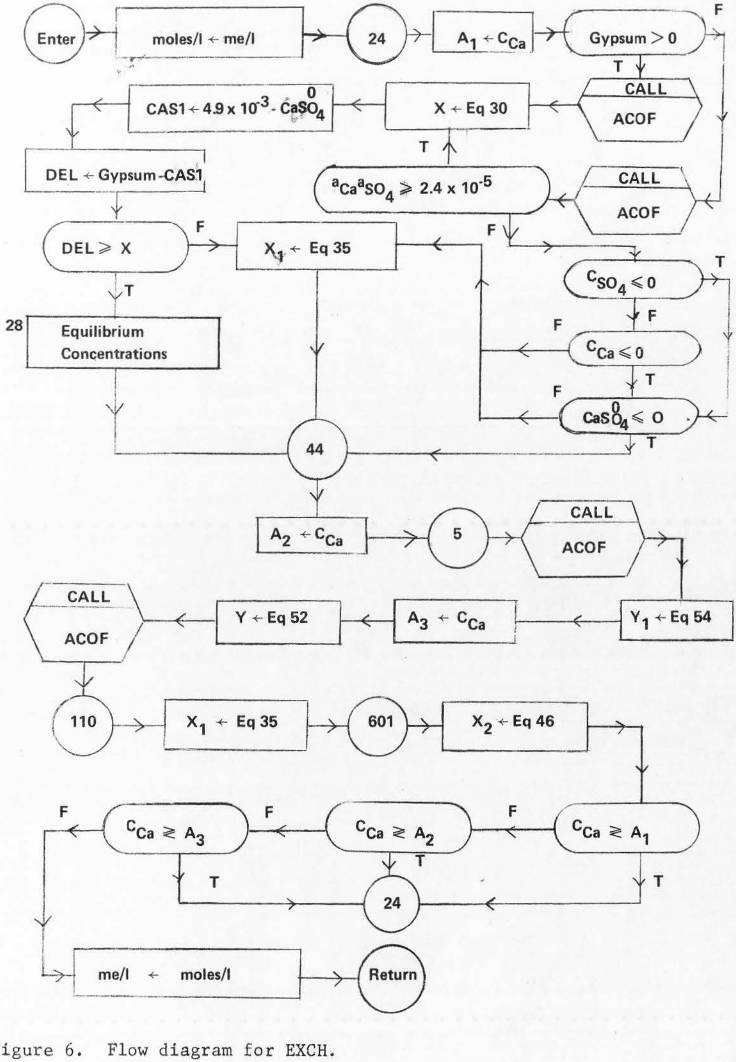

Figure 6. Flow diagram for EXCH.

to solubility of minerals and exchange with soil particles is made in this subroutine. The adjusted concentrations are then returned to the main program.

Subroutine EQEXCH

Since the concentration of exchangeable cations are necessary to predict changes in soil solute composition, and, reliable analytical methods are not available when excess calcium carbonate is present, an improved method for their calculation is necessary. This subroutine calculates exchangeable ions from initial soil analysis. It also calculates the concentration of Ca^{++}, Mg^{++}, $SO_4^=$, $CaSO_4$ ion-pair and $MgSO_4$ ion-pair from their total analysis. Theory underlying this subroutine is discussed in the following sections.

Sulphate occurs in basic solution in more than one form. In addition to free sulphate ion, there are two forms which have been shown to be of importance in base saturated soil-water systems; these are undissociated, soluble $CaSO_4$ (Dutt, 1964) and $MgSO_4$ (Tanji and Doneen, 1966). Thus the total sulphate in solution is

$$^{c}TSO_4 = {^{c}SO_4} + {^{c}CaSO_4} + {^{c}MgSO_4}. \qquad [59]$$

Similarly, the total calcium, ^{c}TCa and magnesium ^{c}TMg is

$$^{c}TCa = {^{c}Ca} + {^{c}CaSO_4} \qquad [60]$$

$$^{c}TMg = {^{c}Mg} + {^{c}MgSO_4}. \qquad [61]$$

The thermodynamic equilibrium constant for equilibrium between the undissociated species in solution and the appropriate ions is

$$K_{[CaSO_4^o]} = \frac{a_{Ca}\ a_{SO_4}}{a_{CaSO_4^o}} \qquad [62]$$

and

$$K_{[MgSO_4^o]} = \frac{a_{Mg}\ a_{SO_4}}{a_{MgSO_4^o}}. \qquad [63]$$

Combining equation [60] and [62], we get

$$c_{CaSO_4^o} = \frac{\gamma_{SO_4}\ \gamma_{Ca}\ c_{TCa}\ c_{SO_4}}{K_{[CaSO_4^o]} + \gamma_{Ca}\ \gamma_{SO_4}\ c_{SO_4}} \qquad [64]$$

and similarly combining equation [61] with [63] we get

$$c_{MgSO_4^o} = \frac{\gamma_{SO_4}\ \gamma_{Mg}\ c_{TMg}\ c_{SO_4}}{K_{[MgSO_4^o]} + \gamma_{Mg}\ \gamma_{SO_4}\ c_{SO_4}}\ . \qquad [65]$$

Combining equation [59] with [64] and [65] result in a cubic equation

$$A\ x^3 + B\ x^2 + C\ x + D = 0 \qquad [66]$$

where

$$x = c_{SO_4}$$

$$A = \gamma_2^4 = \left(\gamma_{Ca}\ \gamma_{SO_4}\right)^2 = \left(\gamma_{Mg}\ \gamma_{SO_4}\right)^2$$

$$B = \gamma_2^2\left((K_{[CaSO_4^o]} + K_{[MgSO_4^o]}) + \gamma_2^2\,(c_{TMg} + c_{TMg} - c_{TSO_4})\right)$$

$$C = K_{[CaSO_4^o]}\ K_{[MgSO_4^o]} + \gamma_2^2\Big[c_{TMg}K_{[CaSO_4^o]} + c_{TCa}\ K_{[MgSO_4^o]}$$

$$- c_{TSO_4}\ K_{[CaSO_4^o]} + K_{[MgSO_4^o]}\Big]$$

$$D = c_{TSO_4}\ K_{[MgSO_4^o]}\ K_{[CaSO_4^o]}.$$

Equation [66] is solved by Newton Raphson method for c_{SO_4}. Concentration of Ca^{++}, Mg^{++} are calculated using equations [60], [61], [64], and [65].

Equations [47] and [53] are used to describe Ca-Mg and Ca-Na exchange in this model. If calcium, magnesium, and sodium are the only cations in the soil then

$$E_T = E_{Ca} + E_{Mg} + E_{Na} \qquad [67]$$

where E_T is the cation exchange capacity. Combining equations [47], and [53] with [67] results in

$$E_{Ca} = \frac{E_T}{\left(\frac{a_{Na}}{K_{Na-Ca}\sqrt{a_{Ca}}} + \frac{K_{Ca-Mg}\, a_{Mg}}{a_{Ca}} + 1 \right)} \quad . \qquad [68]$$

Exchangeable cation concentrations are calculated using equations [53], [67], and [68].

Figure 7 is the flow chart for this subroutine. This subroutine is called only once at the start in the main program.

Subroutine SALT

The subroutine calculates the changes in salt concentration due to mass flow of water. The mass flow of salt is computed by equation [23].

Subroutine ACOF

This subroutine is called in both subroutines EQEXCH and EXCH. It calculates the activity coefficients of monovalents and divalent ions. In the dilute solution activity coefficient of ions can be adequately described by a modified form of Debye Hückel law for mixed electrolytes

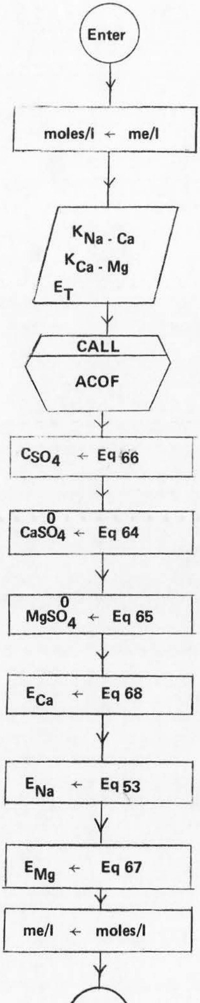

Figure 7. Flow diagram for EQEXCH.

$$\log \gamma_i = - \frac{0.509\ Z_i^2 \sqrt{I}}{1 + \sqrt{I}} \qquad [69]$$

where

$$I = \frac{1}{\rho_o} \frac{1}{2} \sum_{i=1}^{n} c_i Z_i^2 \qquad [70]$$

where i is the ion species of interest, n is the total number of ion species in solution, Z is the valence, and ρ_o is density of the solution ($\rho_o = 1$).

In concentrated salt solution as used in the present experiments, table values (Robinson and Stokes, 1955) of activity coefficients are used. Activity coefficients of individual ions are calculated from the mean molal activity coefficient of salts using the following relationship

$$\gamma_{Ca} = \frac{\gamma_{\pm}^3\ CaCl_2}{\gamma_{\pm}^2 KCl} \qquad [71]$$

$$\gamma_{Na} = \frac{\gamma_{\pm}^2\ NaCl}{\gamma_{\pm} KCl} . \qquad [72]$$

As a first approximation, it is assumed

$$\gamma_{Ca^{++}} = \gamma_{Mg^{++}} = \gamma_{SO_4^{=}} \qquad [73]$$

$$\gamma_{Na^{+}} = \gamma_{HCO_3^{-}} . \qquad [74]$$

This subroutine looks up the table value of divalent or monovalent ion activity coefficient corresponding to a given ionic (I) strength.

RESULTS AND DISCUSSION

To test the applicability of the model predicted values are compared with the experimental measurements. Results of each case are discussed separately.

Column Experiment

Case #1

Figure 8a is the plot of experimental and predicted soil moisture distribution after 35.6 hours of infiltration. Total salt distribution curves corresponding to the soil moisture distribution are given in Figure 8b. Figure 8a shows that the predicted water content is slightly higher than the measured values at depths greater than 40 cm and vice versa at depths below 40 cm. These differences are due to the hydraulic parameters used in this model which were determined for an undisturbed soil while in the column the soil was loosely packed.

Observed and predicted total salt concentration (Figure 8b) have the same distribution pattern. The depth at which the maximum concentration occurs is almost the same in both cases. The concentration of salt in the upper 18 cm had the same total concentration as that of the irrigation water. However, below 18 cm there are some differences between the measured and predicted values. The predicted concentrations are less than the measured values between 18 and 33 cm while below 33 cm, the reverse is true. These differences are hard to explain with the present state of information. One of the reasons for high predicted salt concentrations below 40 cm is the low predicted water content. However, the agreement is considered good enough for most purposes.

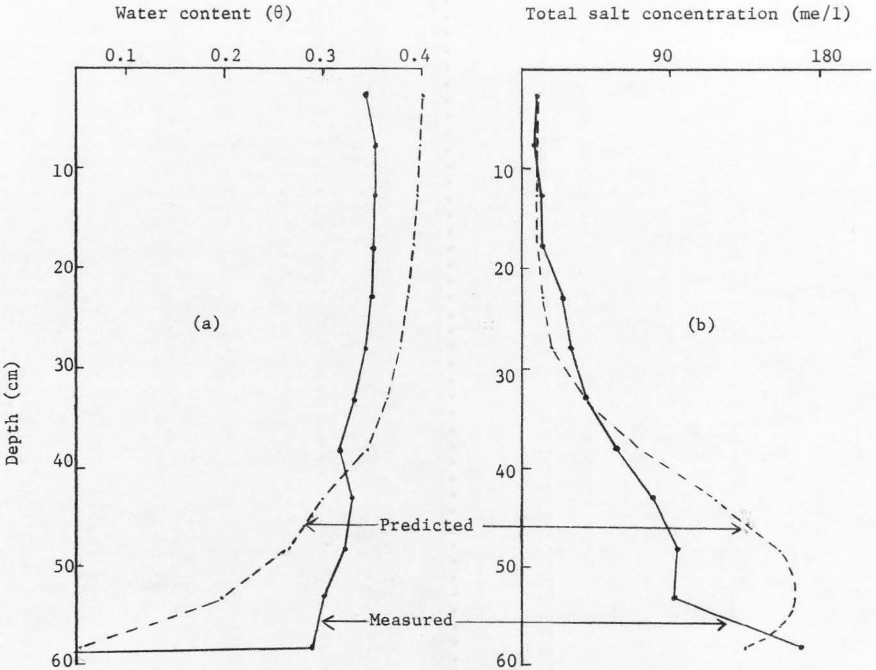

Figure 8. Comparison of predicted and measured a) water content, b) total salt concentration for condition of case #1.

The comparison of the experimental and predicted concentrations of individual ions comprising the total salts is plotted in Figure 9. Since the sulphate and bicarbonate ion concentrations were calculated and not measured the plot for these ions are not drawn. Calcium and magnesium includes the corresponding ions and ion-pairs. Ion-pairs of sodium ions are assumed to be the same as the total sodium concentration.

In general both the cations and anions followed the same distribution as that of total salts. The concentration of each ion increased with depth and maximum concentration occurred at about 58 cm. Predicted concentration of calcium, magnesium, and sodium seemed to be in close correspondence with the experimental values at low salt concentration. However, there is a significant difference between computed and measured cation concentrations at total salt concentration greater than 45 me/l. This lack of agreement seems to result from the inadequate description of the cation exchange process at the higher salt concentrations. Since measured and predicted total salts distribution are in reasonable agreement, it is expected that the cations comprising the total salts also follows the same trend. This, however, is not ture. The predicted calcium concentration is about 1 and 1/2 to 2 times greater than its measured concentration below 30 cm depth while the predicted magnesium and sodium concentrations are less than the measured values. Since relative concentration of each cation is controlled by the exchange coefficient, the above differences seems to be due to inadequate information concerning exchange coefficients.

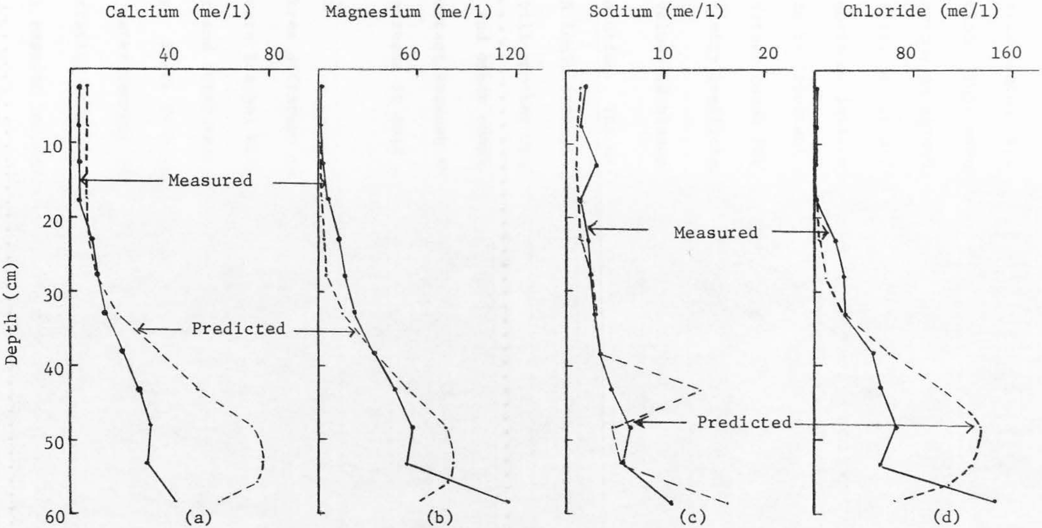

Figure 9. Comparison of predicted and measured ion concentration profiles for conditions of case #1.

It has been assumed in this study that a given exchange coefficient-total salt concentration relationship holds at all levels of salt concentration. This assumption is not necessarily true as discussed in the previous paragraph. Since concentration of each cation at the end of infiltration is affected by the composition of solution in the early hours of infiltration, the correct values of exchange coefficients seems to be important at high salt concentrations in soils.

Another cause for disagreement may be the assumption involving the activity coefficients. It has been assumed that $\gamma_{Ca} = \gamma_{Mg} = \gamma_{SO_4}$. Table values (Robinson and Stokes, 1955) indicate $\gamma_{SO_4} < \gamma_{Ca} < \gamma_{Mg}$ in pure solution. The difference between their values is quite prominent at high ionic strength.

Still another cause for disagreement may be that Na_2SO_4, $CaCO_3$, $MgCO_3$, and other complex ion formations are not considered. This may be important because there is an increase in complex ion formation with increase in salt concentration.

Case #2

Three different salts ($CaCl_2$, $MgCl_2$, and NaCl) having a common anion were leached with distilled water. Figure 10 shows the water content and total salt distribution at the end of 37.6 hours of infiltration. There is a good agreement between the observed and the predicted water content distributions. However, the measured total salt concentration is quite different than the predicted values. There is not any regular increase with depth of the measured total salts. There is no well defined depth at which maximum concentrations of total salts occurs. The zig-zag distribution of total salts indicates that there

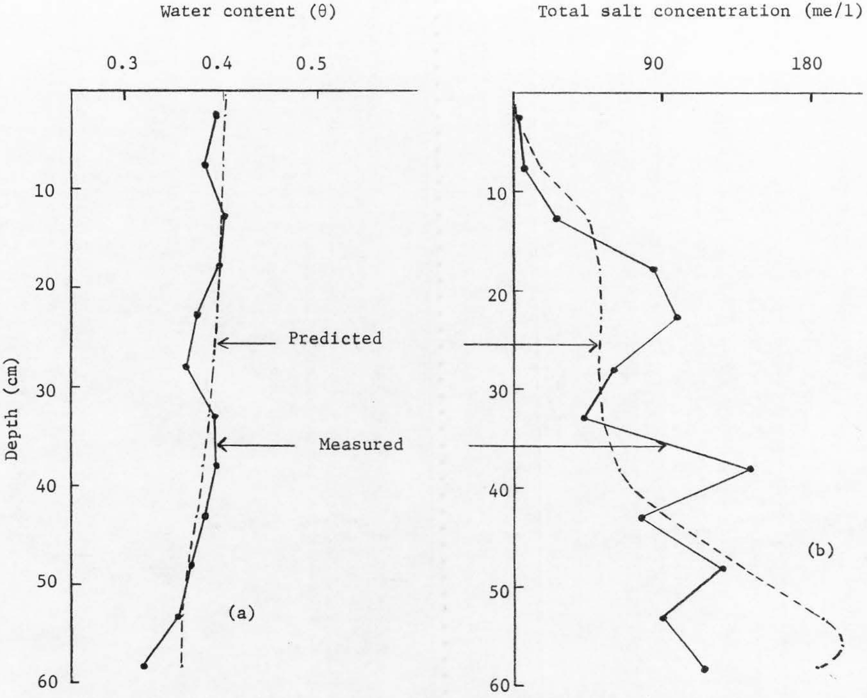

Figure 10. Comparison of predicted and measured a) water content and b) total salt concentration profiles for conditions of case #2.

may have been alternate addition of salty and non-salty water at the surface. It is postulated that this kind of behavior results from the assumption that all the salts are soluble at initial soil water content. Since the salts were applied in the powder form, it seems that some of the salts were not solublized after the first wetting. Because the water was applied in drops and manually checked for its uniform application at the surface, it is believed that these salts eventually became dissolved at irregular time intervals and led to this type of distribution. There may also be analysis problems or errors unaccounted for.

Figure 11 gives the distribution of individual ions. Measured concentration of almost all the ions follows the same general distribution of total salts. There is a poor agreement between the measured and computed values for all the ions. The model at its present stage does not predict this kind of distribution.

Case #3

This is the case where wetting-drying-wetting cycle was followed. Figure 12 shows the soil moisture and total salt distribution at the end of the experiment. Agreement between measured and predicted water content is reasonable considering the assumption that hydraulic properties used were for an undisturbed sample. Measured total salts distribution indicated the presence of two peaks at about 12 and 52 cm depths, while the model predicted a single depth (38 cm) at which maximum concentration occurred. Since enough water was applied at the second irrigation, it is expected that all the salts would have moved to the bottom of the column at the end of the second infiltration. As sodium ions (Figure 13c) are the major component contributing to the peak in

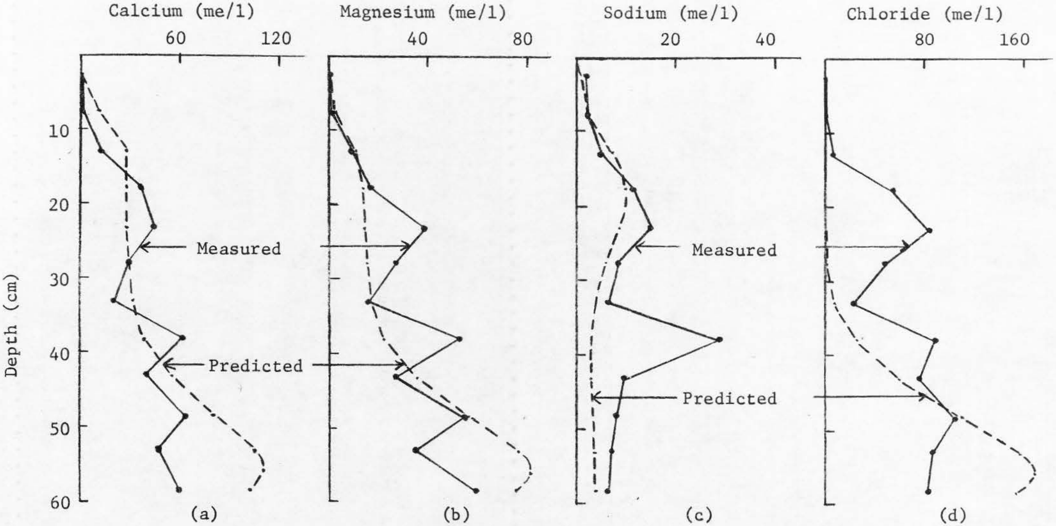

Figure 11. Comparison of predicted and measured ion concentration profiles for conditions of case #2.

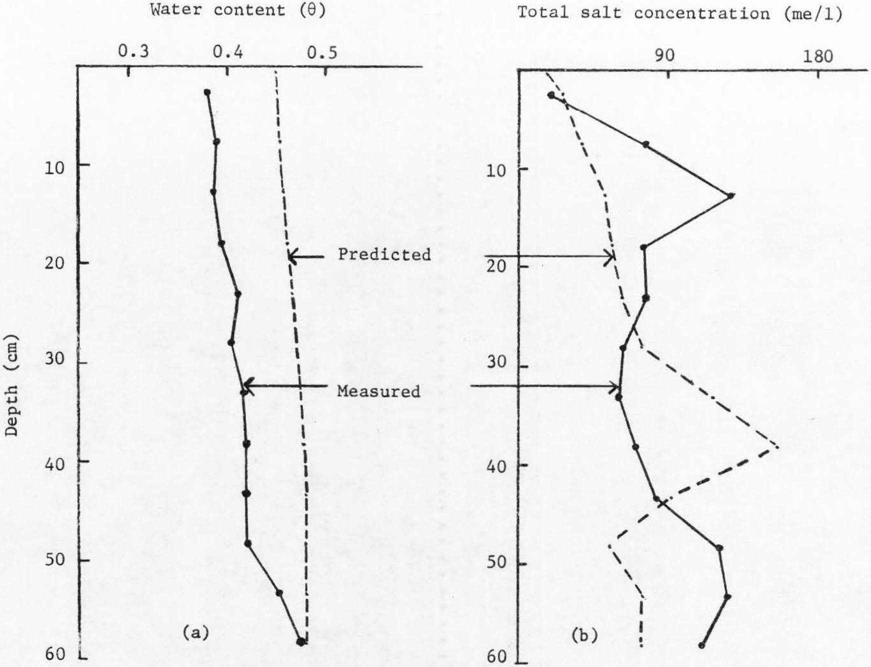

Figure 12. Comparison of measured and predicted a) water content and b) total salt concentration profiles of case #3.

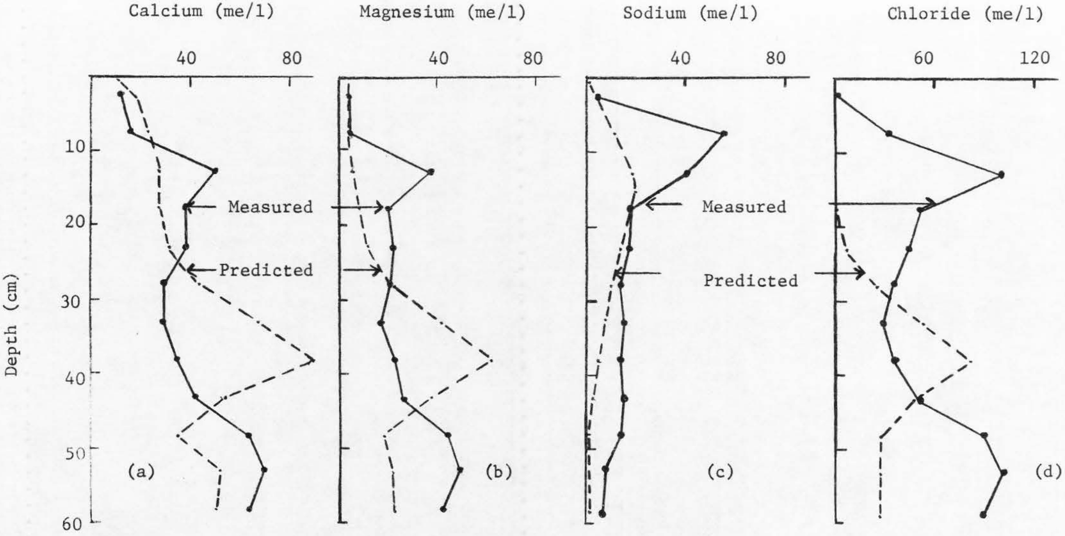

Figure 13. Comparison of predicted and measured ion concentrations profiles for conditions of case #3.

total salt concentration, at 12 cm depth, it seems that all the NaCl salt added before the second irrigation apparently did not dissolve immediately after irrigation, as is assumed in the model. Crystals left undissolved eventually became solublized at some later time in the irrigation cycle and led to the peak in total salt and other ions at the 12 cm depth.

Figure 13, the plot of individual ions, shows the same distribution pattern as that of total salts. Measured chloride ion distribution also supports the postulation discussed in the last paragraph.

Field Experiment

The model was tested under field conditions at Hullinger Farm near Vernal, Utah. Water movement and, thus, the salt movement due to the presence of roots was also considered. In order to avoid the complexity arising due to layered soil, the soil profile was assumed to have uniform properties throughout. Presence of gypsum was considered in the initial conditions below 30 cm depth. The model was tested over a period of two drying and wetting cycles. Hysteresis in the hydraulic properties was ignored. Comparison of the predicted and measured values was made at three different times in the cycle. Since no measurements of individual ions were made on the solution samples at field water content, an approximate method was used to arrive at the concentrations from the saturation extraction analysis. The method involves the assumption that the individual ion concentration changes in the same proportion with changing water content as does the electrical conductivity of the solution. This assumption may not be exactly valid for complex ions and ions which react with the soils. Since chloride ions do not interact with the soil, it is expected that the given assumption holds good for chloride.

Figure 14 is the plot of water content distribution at three different times during the cycle. There is a good correspondence between the measured and predicted values on the first (Figure 14a) and the third (Figure 14c) samplings. Although, the predicted water content does not agree too well with the measured values on the second sampling (Figure 14b) both distribution follows the same trend.

Electrical conductivities of solution at field water content and saturation extract are plotted in Figure 15. The ratio of the two values was used to correct the saturation extract analysis to get ion concentration at field water content. Except the first sampling (Figure 16a), the predicted values closely relate the corrected total salt concentration. Since the saturation extract analysis represented an average of 30 cm depth, the corrected concentrations are represented by histograms. Depth at which the maximum concentration occurs is deeper in measured than in predicted distribution. This may be the result of discontinuity in the measured distribution.

Figures 17, 18, and 19 give the individual cation distribution. Measured calcium concentrations are generally less than the predicted values, while the reverse is true for sodium and magnesium concentrations. These differences seem to result from the assumption that cation concentration changes in the same proportion as does the EC of the solution. Since the preference of exchanger for the ions of higher valence increased with dilution of the solution (Helfferich, 1962) it is expected that the proportionate increase in calcium and magnesium be more than in sodium. The approximation used to get the ion concentration

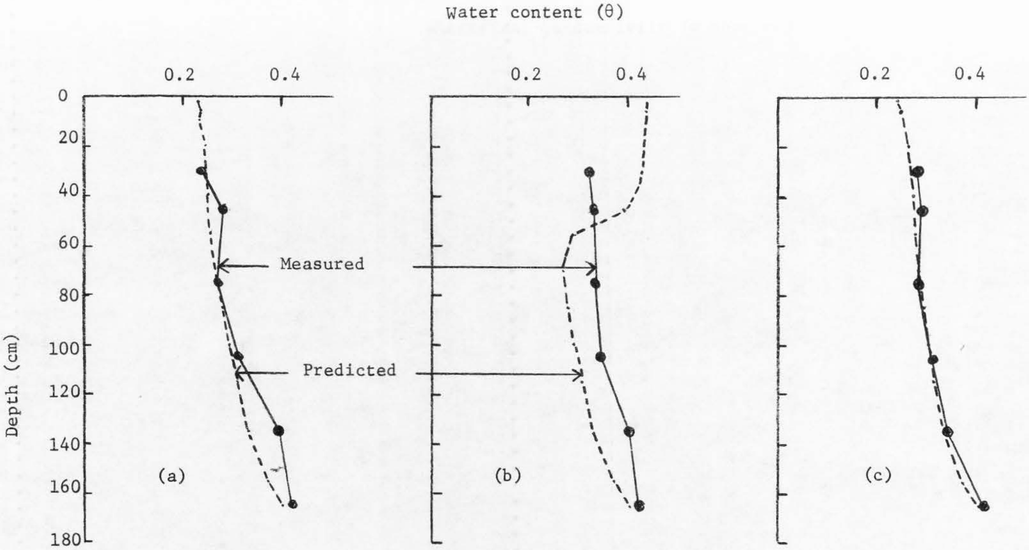

Figure 14. Comparison of predicted and measured water content profiles for alfalfa, a) 324 hrs, b) 339 hrs, and c) 627 hrs.

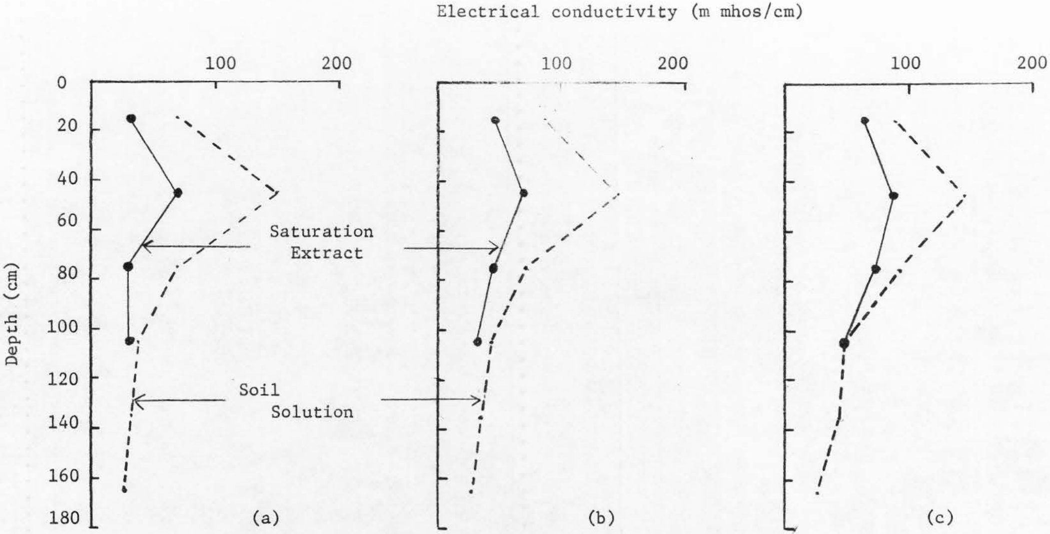

Figure 15. Comparison of saturation extract and soil solution electrical conductivity profiles for alfalfa, a) 324 hrs, b) 339 hrs, and c) 627 hrs.

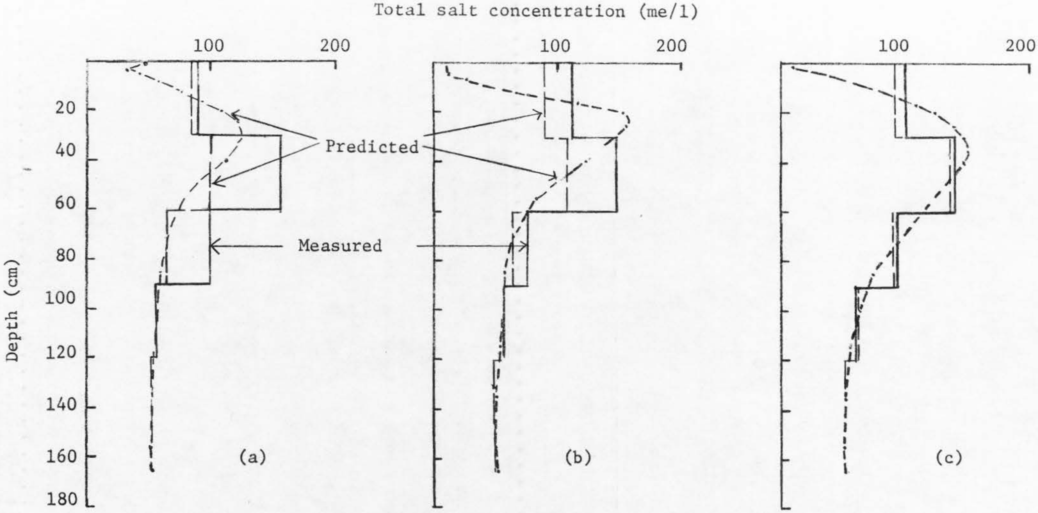

Figure 16. Comparison of predicted and measured total salt concentration profiles for alfalfa, a) 324 hrs, b) 339 hrs, and c) 627 hrs. Both the predicted histogram and continuous curves are shown.

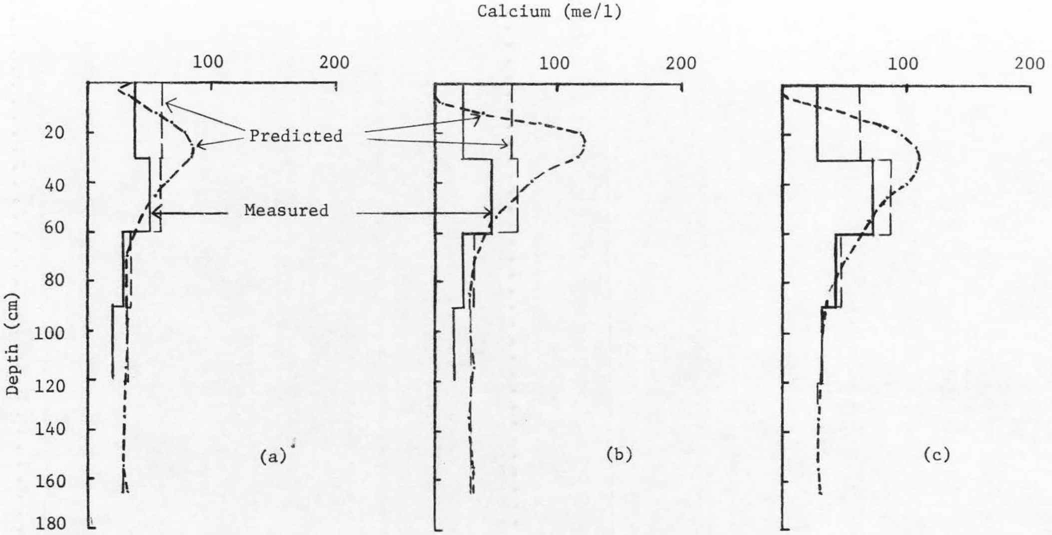

Figure 17. Comparison of predicted and measured calcium concentrations profiles for alfalfa, a) 324 hrs, b) 339 hrs, and c) 627 hrs. Both the predicted histogram and continuous curves are shown.

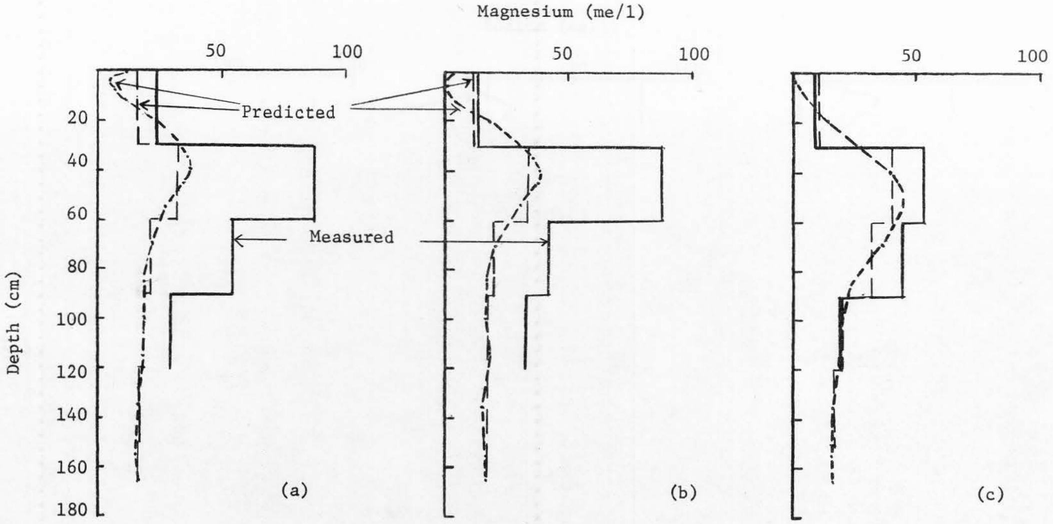

Figure 18. Comparison of predicted and measured magnesium concentration profiles for alfalfa, a) 324 hrs, b) 339 hrs, and c) 627 hrs. Both the predicted and histogram and continuous curves are shown.

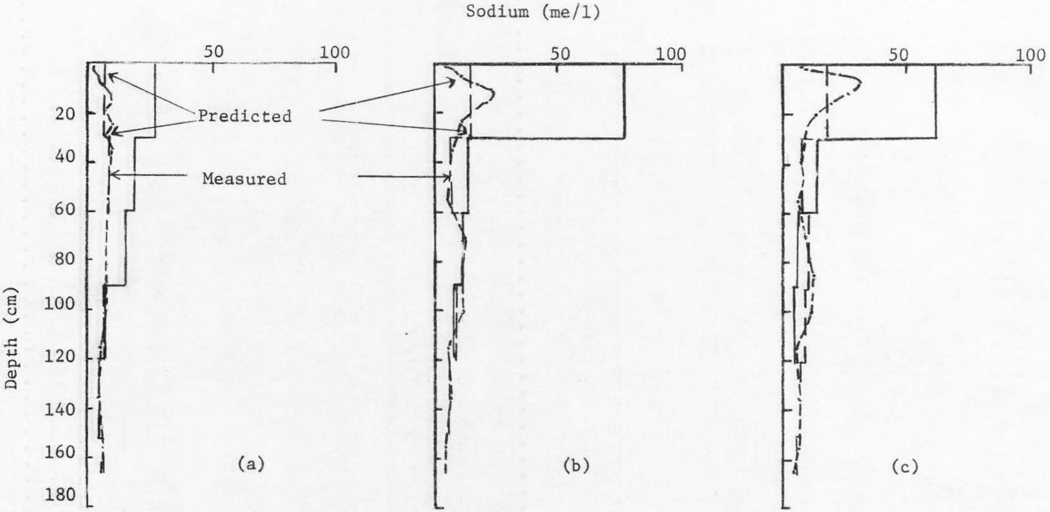

Figure 19. Comparison of predicted and measured sodium concentration profiles for alfalfa, a) 324 hrs, b) 339 hrs, and c) 627 hrs. Both the predicted and histogram and continuous curves are shown.

at field water content, however, assumes the same dilution effect for all the cations.

Sodium concentration measured in the saturation extract is also higher than the computed values while the opposite is true for the magnesium and calcium concentrations. Since the area under total salt curves is about the same for both measured and predicted distribution, the relative concentration of cations depends upon the exchange coefficients as discussed previously in case #1.

Chloride concentrations are plotted in Figure 20. It follows the same distribution as that of total salts. The agreement between the measured and predicted chloride concentration is fair. However, the depth at which the maximum chloride ion concentration occurs is different in both measured and predicted distribution. This lack of agreement seems to be due to the discontinuous nature of measured chloride distribution curve.

Figure 21 gives the depth and salt concentration of the drainage water during this experiment. Since no measurements were made only computed values are plotted. It shows the capability of this model to provide this kind of information, which is useful in devising a scheme for quality control of irrigation return flow.

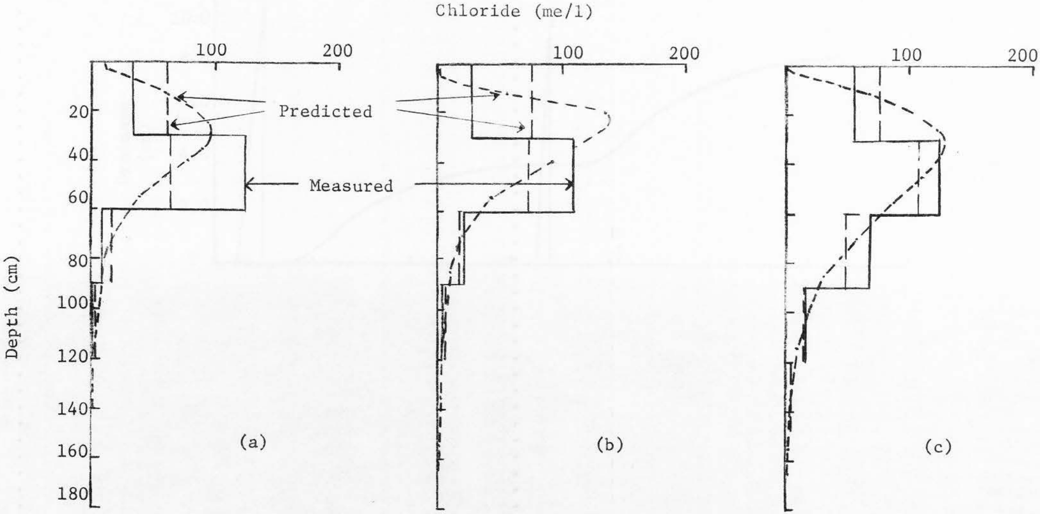

Figure 20. Comparison of predicted and measured chloride concentration profiles for alfalfa, a) 324 hrs, b) 339 hrs, and c) 627 hrs. Both the predicted histogram and continuous curves are shown.

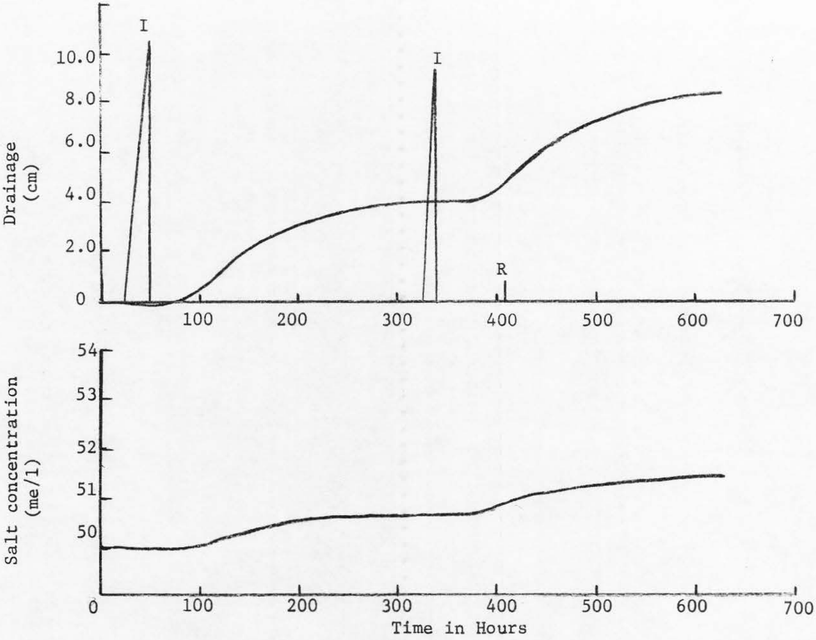

Figure 21. Predicted drainage and salt concentration of the drainage water over a period of 627 hrs.

SUMMARY AND CONCLUSIONS

A model was developed to describe the simultaneous flow of water and salts in soils under varying initial and boundary conditions. Water and thus the salt movement due to plant roots extraction was also considered. To predict the distribution of adsorbed ionic species, correction due to sink or source term was made in their concentration. Specific chemical processes contributing to sink or source term in the model are:

1. Dissolution or precipitation of gypsum and lime.
2. Formation of undissociated Ca and Mg sulphate.
3. Exchange between cations in solution and the soil matrix.

The principles of solubility product and equilibrium exchange were used. The solutes considered were Ca^{++}, Mg^{++}, Na^{+}, and Cl^{-}. The model was tested under field and laboratory conditions. In the laboratory three cases with different initial and boundary conditions were studied. In the field the experiment was conducted with alfalfa as the major crop.

Tensiometer, salinity sensors, four probe units, and solution cups were installed in the center of the plots. Two wetting and drying cycles were followed. Measurements of water content and salt concentrations were made three times in the experiment. Experimental measurements were then compared with the predicted values.

There was a close correspondence between the measured and predicted water content in all experiments. However, predicted total salt concentration agreed fairly well with the measured values only in the field and one of the column experiments. Chloride ions followed the same distribution pattern as that of total salts in the above experiments. Predicted calcium concentration was higher than the measured values while the opposite was true for predicted magnesium and sodium concentration. It is postulated that these differences results because of (1) insufficient description of the exchange and activity coefficients at high salt concentrations, (2) and other complex ion formation not included in the model at the present time.

In two laboratory experiments there was a poor agreement between the predicted and measured total salt concentration. The lack of agreement seems to result from the assumption involved in the present model or some reasons unknown at the present time. Since the salts were applied in the powder form they were assumed to be soluble at the initial water content. It was concluded that this assumption is one of the reasons for the apparent differences in the predicted and measured values. Different ion concentrations in these experiments followed the same distribution as the total salts.

The investigation regarding the applicability of model suggests that more tests are needed. It does appear to yield approximately correct values for total salt but individual species are not as accurately described.

SUGGESTIONS FOR FURTHER RESEARCH

Probably no research has ever been conducted that did not bring up more questions than were answered. This one is no exception. Since the model was not tested under a variety of initial and boundary conditions for salt flow, it should be further investigated in the field and laboratory to determine its suitability. In addition, there appears to be at least six related areas where more investigation is needed to improve and test this model. They are:

1. What is the effect of "built in" dispersion in numerical methods on the salt flow?

2. How do the activity coefficients of different ionic species vary at high salt concentration in soil solutions?

3. How do the exchange coefficients behave in the mixed salt solutions at high salt concentrations?

4. What is the correction due to other complex ion formations at high salt concentrations?

5. Because it was felt in this study that powdered salt does not dissolve immediately after wetting under unsaturated flow conditions, it is suggested that salt solutions rather than salt crystals should be used. This may be a problem in the field and needs further consideration.

6. The extraction of a sufficient amount of solution for chemical analysis, under field condition was difficult. Further research on the methods of solution extraction is desirable.

LITERATURE CITED

Andrade, R. B. 1971. The influence of bulk density on the hydraulic conductivity and water content-matric suction relations of two soils. Unpublished MS thesis. Utah State University Library, Logan, Utah. 49 p.

Biggar, J. W., and D. R. Nielsen. 1963. Micible displacement, V. Exchange processes. Soil Sci. Soc. Amer. Proc. 27:623-627.

Biggar, J. W., and D. R. Nielsen. 1967. Micible displacement and leaching phenomenon, p. 254-274. In Irrigation of Agricultural Lands. Amer. Soc. Agron., Madison, Wisconsin.

Bower, C. A., W. R. Gardner, and J. O. Goertzen. 1957. Dynamics of cation exchange in soil columns. Soil Sci. Soc. Amer. Proc. 21: 20-24.

Bresler, E. 1967. A model for tracing salt distribution in the soil profile. Soil Sci. 104:227-233.

Bresler, E., and R. J. Hanks. 1969. Numerical method of estimating simultaneous flow of water and salts in unsaturated soils. Soil Sci. Soc. Amer. Proc. 33:827-832.

Carnahan, B., H. A. Luther, and J. O. Wilkes. 1969. Applied numerical methods. John Wiley and Sons, Inc., New York. 604 p.

Davidson, J. M., J. W. Biggar, and D. R. Nielsen. 1963. Gamma radiation attenuation for measuring bulk density and transient water flow in porous media. J. Geophys. Res. 68:4777-4783.

DeVault, D. 1943. The theory of chromatography. J. Amer. Chem. Soc. 65:532-540.

Dutt, G. R. 1963. Developments of a computer program for calculating the ionic composition of percolating waters. Dept. Irrigation, Univ. of Calif. Davis. Contribution No. 50. 35 p.

Dutt, G. R. 1964. Effect of small amount of gypsum in soils on the solutes in effluents. Soil Sci. Soc. Amer. Proc. 28:754-757.

Dutt, G. R., T. C. Tucker, M. J. Shaffer, and W. J. Moore. 1971. Predicting nitrate content of agricultural drain water. Dept. of Agriculture Chemistry and Soils. Univ. of Arizona, Tuscon. 101 p.

Dyer, K. L. 1965. Interpretation of chloride and nitrate ion distribution pattern in adjacent irrigated and non-irrigated Panoche soils. Soil Sci. Soc. Amer. Proc. 29:170-176.

Freeze, R. A. 1969. The mechanism of natural ground water recharge and discharge. I. One dimensional vertical, unsteady, unsaturated flow above a recharging or discharging ground water flow system. Water Resour. Res., 5:153-171.

Frissel, M. J., and P. Poelstra. 1964. A theoretical approach to the movement of strontium through soils. Soil Science 98:274-277.

Frissel, M. J., and P. Poelstra. 1967. Chromatographic transport through soils. I. Theoretical evaluations. Plant and Soils 26:285-302.

Gardner, W. R., and R. H. Brooks. 1957. A descriptive theory of leaching. Soil Science 83:295-304.

Glueckauf, E. 1949. Theory of chromatography. PVI. J. Chem. Soc. 3280-3285.

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

Helfferich, F. 1962. Ion exchange. McGraw-Hill Book Company, Inc. 624 p.

Hiester, N. K., and T. Vermeulen. 1952. Saturation performance of ion-exchange and adsorption columns. Chem. Eng. Progress. 48:505-516.

Lai, S. 1970. Cation exchange and transport in soil columns undergoing micible displacement. Unpublished PhD dissertation. Utah State University Library, Logan, Utah. 128 p.

Lapidus, L., and N. R. Amundson. 1952. Mathematics of adsorption in beds. VI. The effect of logitudinal diffusion in ion exchange and chromatographic columns. J. Phy. Chem. 56:984-988.

Martin, A. J. P., and R. L. M. Synge. 1941. A theory of chromatography. Biochem. J. 35:1358-1364.

Molen, W. H. van der. 1956. Desalinization of saline soils as a column process. Soil Sci. 8:19-27.

Nielsen, D. R., and J. W. Biggar. 1962. Micible displacement: III Theoretical considerations. Soil Sci. Soc. Amer. Proc. 26:216-221.

Nimah, M. 1972. Model for estimating soil water flow, water content, evapotranspiration, and root extraction. Unpublished PhD dissertation. Utah State University Library, Logan, Utah. 131 p.

Olsen, S. R., and F. S. Watanbe. 1959. Solubility of calcium carbonate in calcarious soils. Soil Science 88:123-129.

Rible, J. M., and L. E. Davis. 1955. Ion exchange in soil columns. Soil Science 79:41-47

Richards,L. A. 1954. Diagnosis and improvement of saline and alkali soils. USDA Agriculture Handbook, No. 60. 160 p.

Robinson, R. A., and R. H. Stokes. 1955. Electrolyte solutions. Academic Press Inc., New York. 512 p.

Tanji, K. K., and L. D. Doneen. 1966. Predictions on the solubility of gypsum in aqueous solutions. Water Resour. Res. 2:543-548.

Thomas, H. C. 1944. Heterogenous ion exchange in a flowing system. J. Amer. Chem. Soc. 66:1664-1666.

Thornthwaite, C. W., J. R. Mather, and J. K. Nakamura. 1960. Movement of radioactive strontium in soils. Sci. 131:1015-1019.

APPENDICES

Appendix A. Tables

Table 5. Measured bulk density, water content, electrical conductivity, and ion concentration profiles for conditions of case #1

Depth	Bulk Density	Water Content	EC	Total Salts	Calcium	Magnesium	Sodium	Chloride
(cm)		(θ)	(μmhos)	(me/1)	(me/1)	(me/1)	(me/1)	(me/1)
0 - 5.1	1.15	0.346	866	9.3	4.4	2.9	2.0	0.6
5.1 - 10.2	1.16	0.353	744	8.5	4.3	2.6	1.7	0.3
10.2 - 15.2	1.20	0.353	852	11.9	4.4	4.4	3.2	0.3
15.2 - 20.3	1.19	0.350	1100	12.4	4.6	6.0	1.7	1.5
20.3 - 25.4	1.19	0.348	2410	24.4	9.0	13.1	2.3	16.1
25.4 - 30.5	1.21	0.340	3162	29.8	10.9	16.5	2.5	23.6
30.5 - 35.6	1.17	0.331	3448	38.8	14.1	21.8	2.9	24.6
35.6 - 40.6	1.14	0.332	5440	58.8	21.0	34.4	3.4	46.7
40.6 - 45.7	1.17	0.326	6000	79.1	27.5	46.9	4.7	52.9
45.7 - 50.8	1.14	0.322	7190	94.2	31.5	56.3	6.5	64.3
50.8 - 55.9	1.15	0.300	6524	90.2	30.6	53.8	5.8	52.6
55.9 - 61.0	1.15	0.281	13840	167.3	41.9	114.9	10.5	144.0

Table 6. Measured bulk density, water content, electrical conductivity, and ion concentration profiles for conditions of case #2

Depth	Bulk Density	Water Content	EC	Total Salts	Calcium	Magnesium	Sodium	Chloride
(cm)		(θ)	(μmhos)	(me/1)	(me/1)	(me/1)	(me/1)	(me/1)
0 - 5.1	1.10	0.397	379	4.4	1.6	0.6	2.2	0.2
5.1 - 10.2	1.12	0.386	552	6.4	2.6	1.1	2.7	0.3
10.2 - 15.2	1.15	0.405	1894	26.2	12.3	8.9	5.0	7.3
15.2 - 20.3	1.15	0.40	6612	84.3	36.3	26.7	11.4	54.3
20.3 - 25.4	1.15	0.377	8064	98.2	45.0	38.3	14.9	82.5
25.4 - 30.5	1.10	0.267	6480	61.2	29.4	23.5	8.3	47.5
30.5 - 35.6	1.22	0.396	4836	43.6	20.6	16.4	6.6	22.0
35.6 - 40.6	1.18	0.397	12031	142.2	61.9	52.1	28.3	87.8
40.6 - 45.7	1.15	0.385	8252	75.9	39.4	26.7	9.9	68.0
45.7 - 50.8	1.12	0.370	10186	125.0	62.5	54.2	8.3	104.0
50.8 - 55.9	1.13	0.359	9590	90.1	47.4	35.4	7.3	86.5
55.9 - 61.0	1.13	0.324	9230	115.3	59.1	49.6	6.6	81.8

Table 7. Measured bulk density, water content, electrical conductivity, and ion concentration profiles for conditions of case #3

Depth (cm)	Bulk Density	Water Content (θ)	EC (µmhos)	Total Salts (me/l)	Calcium (me/l)	Magnesium (me/l)	Sodium (me/l)	Chloride (me/l)
0 - 5.1	1.11	0.376	1408	20.8	12.2	4.0	4.6	2.9
5.1 - 10.2	1.13	0.388	6090	77.0	16.5	5.7	54.8	33.5
10.2 - 15.2	1.12	0.376	11040	128.2	50.0	36.9	41.3	100.4
15.2 - 20.3	1.16	0.394	7372	76.5	38.5	20.0	18.0	52.2
20.3 - 25.4	1.16	0.412	6532	78.0	38.0	22.4	17.6	43.9
25.4 - 30.5	1.16	0.404	5745	63.2	29.3	20.2	13.7	34.5
30.5 - 35.6	1.18	0.416	5320	61.4	29.5	17.1	14.8	29.0
35.6 - 40.6	1.16	0.419	6128	70.9	34.5	22.4	14.1	35.7
40.6 - 45.7	1.14	0.418	7380	83.0	42.0	26.3	14.7	49.9
45.7 - 50.8	1.17	0.419	10653	121.9	63.5	44.3	13.8	89.2
50.8 - 55.9	1.17	0.451	11610	126.4	70.0	48.9	7.5	101.1
55.9 - 61.0	1.16	0.473	9379	111.4	63.5	42.0	6.4	89.5

Table 8. Chemical analysis of saturation extract for field experiment

Depth	EC	Total Salts	Calcium	Magnesium	Sodium	Chloride
(cm)	(μmhos)	(me/1)	(me/1)	(me/1)	(me/1)	(me/1)
			(a) 324 hours			
0 - 30	3281	42.9	18.5	11.3	13.1	16.2
30 - 60	6952	72.9	32.4	41.1	8.4	57.6
60 - 90	2941	41.4	12.8	22.4	6.3	3.7
90 - 120	3178	46.0	16.3	23.9	5.9	0.4
			(b) 329 hours			
0 - 30	4571	59.1	12.3	6.9	40.0	14.1
30 - 60	6996	70.6	22.5	41.7	6.4	51.9
60 - 90	4562	48.1	14.9	26.5	6.6	13.8
90 - 120	3670	47.9	14.3	27.2	6.4	2.5
			(c) 627 hours			
0 - 30	6468	73.0	21.1	6.7	45.2	40.2
30 - 60	8981	88.6	46.7	33.2	8.7	78.1
60 - 90	7260	73.6	34.1	34.8	4.8	53.3
90 - 120	4462	52.8	30.6	17.7	4.6	16.4

Table 9. Water content (θ) profiles for field experiment

Depth	Time				
	24 hrs	40 hrs	324 hrs	339 hrs	627 hrs
(cm)					
30	0.20	0.32	0.24	0.32	0.28
45	0.24	0.32	0.28	0.33	0.29
75	0.25	0.32	0.27	0.33	0.28
105	0.29	0.33	0.31	0.34	0.31
135	0.38	0.40	0.39	0.40	0.39
165	0.41	0.42	0.42	0.42	0.41

Table 10. Electrical conductivity (μmhos) profiles at the field water content

Depth	Time					
	24 hrs	48 hrs	76 hrs	324 hrs	327 hrs	627 hrs
(cm)						
15	-	4082	3740	6915	8747	8883
45	3369	33657	32422	15070	14745	14350
75	4068	4252	13877	7032	7175	9285
105	3111	6686	6382	3930	4410	4756
135	3426	3279	3012	3372	3594	4373
165	2671	2820	2765	2654	2700	2622

Appendix B. FORTRAN Program

```
C       PROGRAM-SOIL WATER,SALT,FLOW WITH PLANT UPTAKE
C       PROGRAM OF SEP. 25, 1971
C       HWET IS PRESSURE OF HIGHEST POSSIBLE WATER CONTENT
C       V IS BOUNDARY CONDITIONS AT TOP AND TIMES CONDITIONS APPLY
C       DETT IS TIME INCREMENT TO START WITH AND LOWEST TO USE
C       CONQ IS SMALLEST WATERCONTENT CHANGE ALLOWED EACH COMPUTATION
C       GRAVY IS GRAVITY COMPONENT USUALLY THE SAME AS DELX
C       DELW IS WATER CONTENT DIFFERENCE CORRESPONDING TO TABLE INCREMENTS
C       T IS WATER CONTENT TABLE  HAS EQUAL SPACED INCREMENTS
C       TIME IS CUMULATIVE TIME AT START OF COMPUTATION
C       TT IS 1.0 FOR LAASONEN AND 0.5 FOR CRANK NICHOLSON
C       CUMT IS TIME AT END OF COMPUTATION
C       TAA=1. FOR ZERO FLUX AT BOTTOM,TAA=0 FOR H(KK) CONSTANT          A
C         FROM G(I) OR H(I)=G(I)
C       CTM IS LOWEST VALUE OF DELT PERMITTED--IF AS LOW STOPS
C       HDRY IS PRESSURE OF LOWEST POSSIBLE WATER CONTENT
C       PP IS PRESSURE TABLE(WETTING)STARTING WITH LOWEST PRESSURE
C       D IS CONDUCTIVITY TABLE STARTING WITH LOWEST WATER CONTENT VALUE
C       QQ SAME AS ABOVE EXCEPT STARTS FROM WETTING
C       C IS WATER CAPACITY AS A FUNCTION OF DEPTH  BEGINNING AT TOP
C       DELX IS DEPTH INCREMENT
C       W IS WATER CONTENT  AS A FUNCTION OF DEPTH  BEGINNING AT TOP
C       H IS WATER PRESSURE AS A FUNCTION OF DEPTH  BEGINNING AT TOP
C       WATL IS LOWEST POSSIBLE WATER CONTENT
C       WATH IS HIGHEST POSSIBLE WATER CONTENT
C       CB IS A CONSTANT TO MULTIPLY D ARRAY BY--USUALLY 1.0
C       K IS NO. OF DELX INCREMENTS,MM NO. OF TIMES H+W PRINTED,KIT NO.OF   A  12
C-----START HERE FOR A NEW PROGRAM                                          A  13
C       MI IS TO PRINT H,W ARRAYS EACH ITER.,IER NO. OF V ELEMENTS          A  14
C       HROOT IS THE ACTUAL ROOT WATER POTENTIAL
C       BB REPRESENTS PLANT UPTAKE ADDITIONS
C       HLOW IS THE MINIMUM ROOT POTENTIAL ALLOWED
C       HHI IS THE MAXIMIM  ROOT POTENTIAL ALLOWED
C       ET IS THE POTENTIAL EVAPOTRANSPIRATION,ALWAYS NEGATIVE
C       WFDD IS THE WATER FLOW RATE AT THE SURFACE
C       ETPL IS THE POTENTIAL TRANSPIRATION,ALWAYS NEGATIVE
C       SUMS--SALT CONCENTRATION GOING OUT
C       TET IS THE BOUNDARY POTENTIAL ET,ALWAYS NEGATIVE,LTV ARRAY
C       DD,H,G,Y,W,RDF,A,SE,SS,SD ARRAYS ARE OF SAME DIMENSION AT LEAST =KK
C       P,D,T,ARE OF EQUAL DIMENSIONS,ARE EQUAL TO 60 AT MOST
C       SF,TET,V ARRAYS ARE OF SAME DIMEMSION AT LEAST =IER
C       CS=CALCIUM,MS=MAGNESIUM,SN=SODIUM,CL=CHLORIDE,SU=SULPHATE,HC=BICARBONATE
C       CE,ME,EN,ARE EXCHANGBLE CALCIUM,MAGNESIUM,SODIUM
C       CAL,CAS,ARE CALCITE,
C       CAL,CAS,ARE CALCITE AND GYPSUM,CSO,MGSO,ARE ION PAIRS
C       CSG,MSO,SNO,CLO,HCO,SUO,CSX,MGSX,ARE OLD CONCENTRATIOS
C       AM,AC,SAM,SAC,ARE TABLES OF IONIC-STRENGTH ACTIVITY COEFFICIENT OF
C       CALCIUM AND SODIUM IONS
C       TCA,TMG,ARE TOTALCONCERATIONS(CATIONS+ION-PAIRS)
        DIMENSION CF(35),MF(35),SNF(35),SUF(35),CSOF(35),MGSF(35),CLF(35)
        DIMENSION HCF(35)
        DIMENSION DD(25),H(25),G(25),Y(25),W(25),RDF(25),A(25),SE(25)
        DIMENSION SS(25),SD(25),C(25),B(25),E(25),F(25)
        DIMENSION SF(65),TET(65),V(65)
        DIMENSION P(50),D(50),T(50)
        DIMENSION CS(27),MS(27),SN(27),SU(27),CL(27),HC(27),CE(26),ME(26)
        DIMENSION EN(26),CAS(27),CSO(27),MGSX(27),TMG(27)
```

```
      DIMENSION CSG(27),MSO(27),SNO(27),CLO(27),HCO(27),SUO(27),CSX(27)
      DIMENSION AM(27),AC(27),SAM(26),SAC(26)
      DIMENSION TCA(26)
      DIMENSION CAL(27),MGSO(27)
      REAL MF,MGSF
      REAL MGSO,MGSX,MSP
      REAL MSO
      REAL MS,ME,MFA,MSA
      WRITE(6,8765)
 8765 FORMAT(1H1,25X,'****************************************************
     *************')
      WRITE(6,8766)
 8766 FORMAT(1H ,34X,'CROP ALFALFA..ROOT DEPTH IS (2) FEET.')
      WRITE(6,9999)
 9999 FORMAT(1H ,25X,'DATA ARE FROM 3/8/1971 TO11/9/1971 CROP ALFALFA, E
     1=0.10ET')
      WRITE(6,8767)
 8767 FORMAT(1H ,25X,'****************************************************
     *************')
      READ 163, ML                                                      A   9
      LMM=0                                                             A  11
1     LMM=LMM+1                                                         A  10
      READ 163, K,MM,IER,NB,ND
      KK=K+1                                                            A  18
      READ 165,(DD(I),I=1,KK)
      READ(5,165) (TET(I),I=1,IER)
      READ(5,165) (RDF(I),I=1,KK)
      KC=1
      ET=TET(1)
      LL=MM                                                             A  19
      READ(5,165)(P(I),I=1,ND)
      READ(5,165)(D(I),I=1,ND)
      READ 165, (W(I),I=1,KK)                                           A  25
      READ 165, (V(I),I=1,IER)                                          A  26
      READ 165, DELX,DETT,GRAVY,CONQ,DELW,TIME
      READ 165, TT,CUMT,TAA,HLOW,HHI,RRES
      READ 165, HDRY,HWET,WATL,WATH,CB
C     BOUNDRY CONDITIONS FOR SALT FLOW
      READ 165,(SF(I),I=1,IER)
      READ(5,165)(CF(I),I=1,IER)
      READ(5,165)(MF(I),I=1,IER)
      READ(5,165)(SNF(I),I=1,IER)
      READ(5,165)(SUF(I),I=1,IER)
      READ(5,165)(CLF(I),I=1,IER)
      READ(5,165)(HCF(I),I=1,IER)
      READ(5,165)(CSOF(I),I=1,IER)
      READ(5,165)(MGSF(I),I=1,IER)
      WRITE(6,166)(CF(I),I=1,IER)
      WRITE(6,166)(MF(I),I=1,IER)
      WRITE(6,166)(SNF(I),I=1,IER)
      WRITE(6,166)(SUF(I),I=1,IER)
      WRITE(6,166)(CLF(I),I=1,IER)
      WRITE(6,166)(HCF(I),I=1,IER)
      WRITE(6,166)(CSOF(I),I=1,IER)
      WRITE(6,166)(MGSF(I),I=1,IER)
      READ(5,165)AM
      READ(5,165)AC
      READ(5,165)SAM
      READ(5,165)SAC
      WRITE(6,166)(AM(I),AC(I),I=1,27)
      WRITE(6,166)(SAM(I),SAC(I),I=1,26)
```

```
C       INTIAL CONDITIONS FOR SALT FLOW
        READ(5.165)(CS(I).I=1.KK)
        READ(5.165)(MS(I).I=1.KK)
        READ(5.165)(SN(I).I=1.KK)
        READ(5.165)(SU(I).I=1.KK)
        READ(5.165)(CL(I).I=1.KK)
        READ(5.165)(HC(I).I=1.KK)
        READ(5.165)(CAL(I).I=1.KK)
        READ(5.165)(CAS(I).I=1.KK)
        WRITE(6.166)(CS(I).I=1.KK)
        WRITE(6.166)(MS(I).I=1.KK)
        WRITE(6.166)(SN(I).I=1.KK)
        WRITE(6.166)(SU(I).I=1.KK)
        WRITE(6.166)(CL(I).I=1.KK)
        WRITE(6.166)(HC(I).I=1.KK)
        WRITE(6.166)(CAL(I).I=1.KK)
        WRITE(6.166)(CAS(I).I=1.KK)
        WRITE (6.169)
        WRITE (6.163) K.MM.IER.NB.ND
        SMAX=WATH•400.
        P(1)=P(1)•1.0E+03
        T(1)=0.0                                                            A   38
        STIM=0.0
        DO 900 I=2.ND
        T(I)=DELW+T(I-1)
  900   P(I)=P(I)•1.0E+03
C--------------------------------------------------------------------------------
        DO 600 I=2.KK
        CSA=CS(I)
        MSA=MS(I)
        SNA=SN(I)
        SUA=SU(I)
        CLA=CL(I)
        HCA=HC(I)
        SEA=CS(I)+MS(I)+SN(I)
        CALL EQEXCH(CSA.MSA.SNA.CLA.SUA.HCA.CEA.MEA.ENA.CSP.MSP.SEA.AM.AC.
       QSAM.SAC)
        CS(I)=CSA
        MS(I)=MSA
        SN(I)=SNA
        SU(I)=SUA
        CL(I)=CLA
        HC(I)=HCA
        CE(I)=CEA
        ME(I)=MEA
        EN(I)=ENA
        CSO(I)=CSP
        MGSO(I)=MSP
        SE(I)=SEA
        WRITE(6.166)CS(I).MS(I).SN(I).CL(I).SU(I).HC(I ).CE(I).ME(I).EN(I).
       GCSO(I).MGSO(I)
  600   CONTINUE
        CS(2)=2590.9588
        CL(2)=2590.9588
  825   WRITE(6.911)
        DO 910 I=1.KK
  910   WRITE(6.166)(CS(I).MS(I).SN(I).SU(I).CL(I).HC(I).CE(I).ME(I).EN(I)
       1.CAS(I).CSO(I))
        WRITE(6.166)MGSO
C--------------------------------------------------------------------------------
        SE(1)=SF(1)
```

```
          CS(1)=CF(1)
          MS(1)=MF(1)
          SN(1)=SNF(1)
          SU(1)=SUF(1)
          CL(1)=CLF(1)
          HC(1)=HCF(1)
          CSO(1)=CSOF(1)
          MGSO(1)=MGSF(1)
          CWFLX=0.0
          EOR=V(1)                                                      A  74
          DELT=DETT
          TM=1.0-TT                                                     A  76
          TBB=1.0-TAA                                                   A  77
          YMAX=WATH                                                     A  82
          DO 14 I=1,KK
          SS(I)=SE(I)
          SD(I)=SE(I)*W(I)
14        Y(I)=W(I)                                                     A  87
          PIT=0.0                                                       A  89
          DO 15 I=2,K
     15 PIT=W(I)*(DD(I+1)-DD(I-1))/2.+PIT
          WRITE (6,170)
          TW=D(1)
          D(1)=(D(1)*(P(2)-P(1)))*CB                                    A  39
          J=(W(1)-T(1))/DELW+1.0
          H(1)=(P(J+1)-P(J))*(W(1)-T(J))/DELW+P(J)
          G(1)=H(1)
          C(1)=DELW/(P(J+1)-P(J))
          WRITE ( 6,166) T(1),P(1),TW,D(1),C(1),DD(1),W(1),H(1),RDF(1 ),SF(1)
          DO 3 I=2,KK
          TW=D(I)
          D(I)=D(I)*(P(I)-P(I-1))*CB+D(I-1)                             A  41
          J=(W(I)-T(1))/DELW+1.0
          H(I)=(P(J+1)-P(J))*(W(I)-T(J))/DELW+P(J)
          C(I)=DELW/(P(J+1)-P(J))
          G(I)=H(I)                                                     A  86
          WRITE ( 6,166) T(I),P(I),TW,D(I),C(I),DD(I),W(I),H(I),RDF(I),SF(I)
3         CONTINUE
          N=KK+1
          DO 2 I=N,ND
          TW=D(I)
          D(I)=D(I)*(P(I)-P(I-1))*CB+D(I-1)
C         ------------------------------------------------------------------
2         WRITE (6,166) T(I),P(I),TW,D(I)
C         D IS NOW DIFFUSIVITY TIMES DELW NOT CONDUCTIVITY
          WRITE (6,179)
          DO 5 I=2,IER,2
5         WRITE (6,166) V(I),V(I-1),TET(I-1),SF(I-1)
          WRITE (6,180)
          WRITE (6,166) DELX,DETT,GRAVY,CONQ,DELW,TIME
          WRITE (6,181)
          WRITE (6,166) TT,CUMT,TAA,HLOW,HHI,RRES
          WRITE (6,172)
          WRITE (6,166) HDRY,HWET,WATL,WATH,CB
C         ------------------------------------------------------------------
          KCK=1                                                         A  93
          HROOT=G(2)
          RUNOF=0.0                                                     A  95
          CUMS=0.0                                                      A  96
          CUMB=0.0                                                      A  97
          CUMM=0.0                                                      A  98
```

```
      SUMA=0.0
      CALL PLOT (KK,WATH,W,DD,SMAX,SD)
      WRITE(6,166) TIME
C----COMPUTATION OF CONDUCTIVITY (B) AND WATER CAPACITY (C)
16    TOP=WATH
      BOT=WATL
      HKP=H(1)
      WKP=W(1)
      IF (EOR-0.0) 17,19,18
17    W(1)=WATL
      H(1)=HDRY
      GO TO 19
18    W(1)=WATH
      H(1)=HWET
19    TWW=(W(1)+Y(1))*0.5
      J=(TWW-T(1))/DELW+1.0
      BB=(TWW-T(J))/DELW
      DIFFA=(D(J+1)-D(J))*BB+D(J)
      HI=(P(J+1)-P(J))*BB+P(J)
      DO 37 I=1,K
      TW=(W(I+1)+Y(I+1))*0.5
      J=(TW -T(1))/DELW+1.0
      BB=(TW-T(J))/DELW
      DIFFB=(D(J+1)-D(J))*BB+D(J)
      GI=(P(J+1)-P(J))*BB+P(J)
  219 IF(HI-GI)20,32,20
20    B(I)=(DIFFA-DIFFB)/(HI-GI)
      IF (I-1) 21,21,33
21    IF (EOR-0.0) 22,33,22
   22 ER=(B(1)*(H(1)*TT-H(2)*TT-G(2)*TM+G(1)*TM+DD(2)))/DD(2)
      IF (ABS(1.1*EOR-ER)-ABS(0.1*EOR)) 236,236,23
23    IF(KCK.EQ.1) GO TO 220
      IF(KCK-10) 305,236,236
  236 H(1)=(EOR*DD(2)/B(1)+H(2)*TT-G(1)*TM+G(2)*TM-DD(2))/TT
      IF(H(1).LT.HDRY) H(1)=HDRY
      IF (H(1).GT.HWET) H(1)=HWET
      GO TO 33
220   H(1)=HKP
      W(1)=WKP
      KCK=KCK+1
      GO TO 19
305   KCK=KCK+1
      IF (ER-EOR) 24,33,26
24    IF (W(1)-WATH) 25,33,33
25    BOT=W(1)
      W(1)=(W(1)+TOP)*0.5
      GO TO 28
26    IF (W(1)-WATL) 33,33,27
27    TOP=W(1)
      W(1)=(W(1)+BOT)*0.5
   28 J=(W(1)-T(1))/DELW+1.0
      BB=(W(1)-T(J))/DELW
      IF(EOR-0.0)30,33,30
30    H(1)=(P(J+1)-P(J))*BB+P(J)
  218 TWW=(W(1)+Y(1))*0.5
      J=(TWW-T(1))/DELW+1.0
      BB=(TWW-T(J))/DELW
      DIFFA=(D(J+1)-D(J))*BB+D(J)
      HI=(P(J+1)-P(J))*BB+P(J)
      GO TO 219
32    B(I)=(D(J+1)-D(J))/(P(J+1)-P(J))
```

```
      IF (I-1) 33,21,33                                              A 143
33    TWW=TW                                                         A 144
      HI=GI                                                          A 145
      DIFFA=DIFFB                                                    A 146
      TW=(W(I+1)+Y(I+1))*0.5                                         A 147
      J=(TW -T(1))/DELW+1.0
35    C(I+1)=DELW/(P(J+1)-P(J))                                      A 151
37    CONTINUE                                                       A 154
      KCK=1
      IF(EOR.GT.0.0.AND.ET.GE.0.0) GO TO 6666
      IF(EOR.GT.0.0.AND.ET.LT.0.0) GO TO 5555
 6666 ETPL=ET-EOR
      IF(ET.GE.0.0) GO TO 39
      IF(ETPL-0.0) 365,39,39
 5555 ETPL=ET
365   HHOLD=HROOT
      HROOT=HLOW                                                     BB
      SINK=0.0
      DO 250 I=2,K
  250 E(I)=G(I)-0.5715*SE(I)-DD(I)*RRES
      DO 420 I=2,K
      IF(HROOT-E(I).GT.0.0) GO TO 420
      SINK=B(I)*RDF(I)*(HROOT-E(I))+SINK
 420  CONTINUE
      IF(SINK-ETPL.GT.0.0) GO TO 402
      HROOT=HHOLD
410   HROOT=1.2*HROOT
      SINK=0.0
      DO 421 I=2,K
      IF(HROOT-E(I).GT.0.0) GO TO 421
      SINK=B(I)*RDF(I)*(HROOT-E(I))+SINK
 421  CONTINUE
      IF(SINK-ETPL)411,402,410
 411  HRLO=HROOT
      HROOT=HHOLD
      LCOUNT=0
412   HROOT=0.8*HROOT
      LCOUNT=LCOUNT+1
      IF(LCOUNT.EQ.5) GO TO 490
      SINK=0.0
      DO 422 I=2,K
      IF(HROOT-E(I).GT.0.0) GO TO 422
      SINK=B(I)*RDF(I)*(HROOT-E(I))+SINK
 422  CONTINUE
      IF(SINK-ETPL)412,402,413
 413  HRHI=HROOT
      GO TO 491
  490 HRHI=HHI
491   LCOUNT=0
      HROOT=HHOLD
405   SINK=0.0                                                       BB
      DO 400 I=2,K                                                   BB
      IF(HROOT-E(I).GT.0.0) GO TO 400
      SINK=B(I)*RDF(I)*(HROOT-E(I))+SINK
400   CONTINUE                                                       BB
      LCOUNT=LCOUNT+1                                                BB
      IF(LCOUNT.EQ.20) GO TO 402
      IF(ABS(SINK-ETPL)-0.002)402,402,401
401   IF(SINK-ETPL)403,402,404                                       BB
403   HRLO=HROOT                                                     BB
      HROOT=0.5*(HROOT+HRHI)                                         BB
```

```
      GO TO 405                                                          BB
 404  HRHI=HROOT
      HROOT=0.5*(HROOT+HRLO)                                             BB
      GO TO 405                                                          BB
   39 DO 251 I=2.K
      SINK=0.0
  251 A(I)=0.0
      GO TO 38
C     ---------------------------------------------------------------
C     A IS THE DEL WATER/DELT CAUSED BY PLANT EXTRACTION
 402  DO 406 I=2.K
      IF(HROOT-E(I).GT.0.0) GO TO 407
      A(I)=B(I)*(HROOT-E(I))*2.0*RDF(I)/(DD(I+1)-DD(I-1))
      GO TO 406
 407  A(I)=0.0
406   CONTINUE
C     ---------------------------------------------------------------
C----COMPUTATION OF TRIDIAGONAL MATRIX MAIN BODY                         A 158
38    DO 42 I=2.K                                                        B 159
      POT=(DD(I+1)-DD(I-1))/(2.0*DELT)                                   B 160
      DLXA=(DD(I)-DD(I-1))                                               B 161
      DLXB=(DD(I+1)-DD(I))                                               B 162
      BB=C(I)*POT/TT+B(I)/DLXB+B(I-1)/DLXA                               B 1621
      DA=(C(I)*POT*G(I)+(B(I)/DLXB)*(TM*(G(I+1)-G(I))-DLXB)+(B(I-1)/DLXA B 1622
     1)*(TM*(G(I-1)-G(I))+DLXA)+A(I)*(DD(I+1)-DD(I-1))*0.5)/TT
      IF(I-2)390.390.40
  390 IF(H(1).GE.HWET.OR.H(1).LE.HDRY) GO TO 394
      DA=DA-((B(I-1)/DLXA)*(TM*(G(I-1)-G(I))+DLXA))/TT+EOR/TT
      BB=BB-B(I-1)/DLXA
      GO TO 393
  394 DA=DA+H(I-1)*B(I-1)/DLXA
  393 F(I)=DA/BB
      E(I)=(B(I)/DLXB)/BB                                                B 1661
      GO TO 42                                                           A 167
40    IF (I-K) 41.43.43                                                  A 168
41    E(I)=(B(I)/DLXB)/(BB-(B(I-1)/DLXA)*E(I-1))                         B 169
      F(I)=(DA+(B(I-1)/DLXA)*F(I-1))/(BB-(B(I-1)/DLXA)*E(I-1))           B 170
  42  CONTINUE
43    BB=BB-TAA*B(I)/DLXB                                                B 172
      DA=DA+TAA*(B(I)/DLXB)*((G(I)-G(I+1))*TM+DLXB)/TT+TBB*B(I)/DLXB*H(  B 173
     1KK)                                                                B 174
      H(I)=(DA+(B(I-1)/DLXA)*F(I-1))/(BB-(B(I-1)/DLXA)*E(I-1))           B 1741
44    I=I-1                                                              A 175
      H(I)=E(I)*H(I+1)+F(I)                                              A 176
      IF (I-2) 45.45.44                                                  A 177
45    IF(TAA-1.0)47.46.46
46    H(KK)=H(K)+DD(KK)-DD(K)                                            B 178
47    DO 60 I=2.KK
300   IF (H(I)-HWET-DD(I)) 60.60.55
55    H(I)=HWET+DD(I)
60    CONTINUE                                                           A 197
C----COMPUTATION OF WATER CONTENTS AS A FUNCTION OF PRESSURES JUST COMP  A 199
      IF(H(1).GE.HWET.OR.H(1).LE.HDRY) GO TO 1005
      WFDD=EOR
      H(1)=(EOR*DD(2)/B(1)+H(2)*TT-G(1)*TM+G(2)*TM-DD(2))/TT
      GO TO 134
 1005 WFDD=B(1)*((H(1)-H(2))*TT+(G(1)-G(2))*TM+DD(2))/DD(2)              B 189
 134  I=1
 62   IF (H(I)-G(I)) 65.116.65
65    NHI=54                                                             A 206
      NLO=1                                                              A 207
```

```
      J=25
66    IF (H(I)-P(J)) 67,72,68
67    NHI=J
      GO TO 69
68    NLO=J
69    JT=J
      J=(NHI-NLO)/2+NLO
      IF (J-JT) 66,70,66
70    IF (H(I)-P(J)) 71,72,72
71    J=J-1
72    WAT=(H(I)-P(J))*DELW/(P(J+1)-P(J))+T(J)
      W(I)=WAT
      GO TO 117
116   W(I)=Y(I)
  117 DO 268 I=2,KK
268   W(I)=C(I)*(H(I)-G(I))+Y(I)
      GO TO 269
269   SUM3=0.0
      SUM2=0.0
      SUM1=0.0
      DO 131 I=2,K
      SUM1=W(I)+SUM1
      SUM2=Y(I)+SUM2
      IF (ABS(SUM1-SUM2)-ABS(SUM3)) 131,131,130
130   SUM3=SUM1-SUM2
131   CONTINUE
      IF (ABS(SUM3)-ABS(CONQ))63,63,132
 132  IF(DELT-DETT*0.1)63,63,133
  133 DELT=0.5*DELT
      GO TO 38
   63 SUM1=0.0
      SUM2=0.0
      DO 800 I=2,K
      SUM1=W(I)*(DD(I+1)-DD(I-1))/2.+SUM1
  800 SUM2=Y(I)*(DD(I+1)-DD(I-1))/2.+SUM2
      CWF=SUM1-PIT
      WFRDD=(SUM1-SUM2)/DELT
      WFUU=B(NB)*((H(NB)-H(NB+1))*TT+(G(NB)-G(NB+1))*TM+DD(NB+1)-DD(NB))
     1/(DD(NB+1)-DD(NB))
      CUMS=WFDD*DELT+CUMS
      CUMB=WFUU*DELT+CUMB
      SUMA=SUMA+SINK*DELT
      CWFLX=(SUM1-SUM2)
      KB=K-1
C     ------------------------------------------------------------------
      DO 444 I=1,KK
      CSG(I)=CS(I)
      MSO(I)=MS(I)
      SNO(I)=SN(I)
      CLO(I)=CL(I)
      HCO(I)=HC(I)
      SUO(I)=SU(I)
      CSX(I)=CSO(I)
      MGSX(I)=MGSO(I)
 444  CONTINUE
      STIM=STIM+DELT
      KB=K-1
C     MASS FLOW OF DIFFERENT IONIC SPECIES
      DO 920 I=1,KB
      DELX=(DD(I+2)-DD(I))/2.0
      WFRU=(B(I)*((H(I)-H(I+1))*TT+(G(I)-G(I+1))*TM+DD(I+1)-DD(I))*DELT)
```

```
     1/(DD(I+1)-DD(I))
      WFRD=(B(I+1)*((H(I+1)-H(I+2))*TT+(G(I+1)-G(I+2))*TM+DD(I+2)-DD(I+1
     J))*DELT)/(DD(I+2)-DD(I+1))
  254 IF(ABS(WFRU).LT.0.0001.AND.ABS(WFRD).LT.0.0001)GO TO 920
      CL1=CLO(I)
      CL2=CLO(I+1)
      CL3=CLO(I+2)
      CL4=W(I+1)
      CL5=Y(I+1)
      CALL SALT (CL1,CL2,CL3,CL4,CL5,CL6,WFRU,WFRD,DELX,I,EOR)
      CL(I+1)=CL6
      CL1=SUO(I)
      CL2=SUO(I+1)
      CL3=SUO(I+2)
      CALL SALT (CL1,CL2,CL3,CL4,CL5,CL6,WFRU,WFRD,DELX,I,EOR)
      SU(I+1)=CL6
      CL1=HCO(I)
      CL2=HCO(I+1)
      CL3=HCO(I+2)
      CALL SALT (CL1,CL2,CL3,CL4,CL5,CL6,WFRU,WFRD,DELX,I,EOR)
      HC(I+1)=CL6
      CL1=CSG(I)
      CL2=CSG(I+1)
      CL3=CSG(I+2)
      CALL SALT (CL1,CL2,CL3,CL4,CL5,CL6,WFRU,WFRD,DELX,I,EOR)
      CS(I+1)=CL6
      CL1=MSO(I)
      CL2=MSO(I+1)
      CL3=MSO(I+2)
      CALL SALT (CL1,CL2,CL3,CL4,CL5,CL6,WFRU,WFRD,DELX,I,EOR)
      MS(I+1)=CL6
      CL1=SNO(I)
      CL2=SNO(I+1)
      CL3=SNO(I+2)
      CALL SALT (CL1,CL2,CL3,CL4,CL5,CL6,WFRU,WFRD,DELX,I,EOR)
      SN(I+1)=CL6
      CL1=CSX(I)
      CL2=CSX(I+1)
      CL3=CSX(I+2)
      CALL SALT (CL1,CL2,CL3,CL4,CL5,CL6,WFRU,WFRD,DELX,I,EOR)
      CSO(I+1)=CL6
      CL1=MGSX(I)
      CL2=MGSX(I+1)
      CL3=MGSX(I+2)
      CALL SALT (CL1,CL2,CL3,CL4,CL5,CL6,WFRU,WFRD,DELX,I,EOR)
      MGSO(I+1)=CL6
      SE(I+1)=CS(I+1)+MS(I+1)+SN(I+1)+CSO(I+1)+MGSO(I+1)
      TCA(I+1)=CS(I+1)+CSO(I+1)
      TMG(I+1)=MS(I+1)+MGSO(I+1)
      LS=I+1
      IF(STIM.LT.1.0)GO TO 920
  475 WA=W(I+1)
      CSA=CS(I+1)
      MSA=MS(I+1)
      SNA=SN(I+1)
      SUA=SU(I+1)
      CLA=CL(I+1)
      HCA=HC(I+1)
      CEA=CE(I+1)
      MEA=ME(I+1)
      ENA=EN(I+1)
```

```
      CSP=CSO(I+1)
      MSP=MGSO(I+1)
      CAP=CAL(I+1)
      CASA=CAS(I+1)
      SEA=SE(I+1)
      CALL EXCH(CSA,MSA,SNA,SUA,CLA,HCA,CEA,MEA,ENA,CSP,MSP,CASA,CAP,WA,
     KSEA,AM,AC,SAM,SAC)
      CS(I+1)=CSA
      MS(I+1)=MSA
      SN(I+1)=SNA
      SU(I+1)=SUA
      CL(I+1)=CLA
      HC(I+1)=HCA
      CE(I+1)=CEA
      ME(I+1)=MEA
      EN(I+1)=ENA
      CSO(I+1)=CSP
      MGSO(I+1)=MSP
      CAL(I+1)=CAP
      CAS(I+1)=CASA
      SE(I+1)=SEA
      IF(CS(I+1).LT.0.0)CS(I+1)=0.0
      IF(MS(I+1).LT.0.0)MS(I+1)=0.0
      IF(SN(I+1).LT.0.0)SN(I+1)=0.0
      IF(SU(I+1).LT.0.0)SU(I+1)=0.0
      IF(CAS(I+1).LT.0.0)CAS(I+1)=0.0
      IF(CSO(I+1).LT.0.0)CSO(I+1)=0.0
      TCA(I+1)=CS(I+1)+CSO(I+1)
      TMG(I+1)=MS(I+1)+MGSO(I+1)
 920  CONTINUE
      IF(STIM.GE.1.0)STIM=0.0
C-----------------------------------------------------------------------
      DO 704 I=1,KK
704   SD(I)=SE(I)*W(I)                                                  B 345A
706   IF(EOR-0.0)136,136,135
135   RUNOF=(EOR-WFDD)*DELT+RUNOF                                       A 345
136   TIME=TIME+DELT                                                    A 346
      IF (LL-MM) 138,137,137                                            A 347
  137 CALL PLOT (KK,WATH,W,DD,SMAX,SD)
      WRITE (6,166) (H(I),I=1,KK)                                       A 349
      WRITE(6,166)(SE(I),I=1,KK)
      WRITE(6,166)(A(I),I=2,K)
      WRITE(6,911)
      WRITE(6,111)(CS(I),MS(I),SN(I),SU(I),CL(I),HC(I),CE(I),ME(I),EN(I)
     J,CAS(I),SE(I),I=1,LS)
      WRITE(6,2001)
 2001 FORMAT(1H ,2X,'CASO',6X,'MGSO',6X,'CAL',7X,'TCA',7X,'TMG')
      WRITE(6,2000)(CSO(I),MGSO(I),CAL(I),TCA(I),TMG(I),I=1,LS)
      LL=0                                                              A 352
      WRITE (6,184)
  138 WRITE (6,111) TIME,CWF,EOR,HROOT,RUNOF,CUMS,CUMB,SUMA,WFRDD,WFUU,S
     1E(20)
      IF (SUM3-0.0) 139,301,139
  301 DELT=2.0*DELT
      GO TO 145
139   TW=ABS(CONQ*DELT/SUM3)                                            A 357
140   IF (TW-0.1*DETT) 141,142,142                                      A 359
  141 TW=0.1*DETT
      GO TO 144
  142 IF(TW-1000.0*DETT)144,144,143
 143  TW=1000.0*DETT
```

```
   144 IF(TW.GT.2.0*DELT) GO TO 301
       DELT=TW
C----TEST TO SEE IF EVAP OR RAIN INTENSITY (EOR) HAS CHANGED
 145   IF(TIME-V(KC+1))148,147,148
 147   CALL PLOT (KK,WATH,W,DD,SMAX,SD)
       WRITE (6,166) (H(I),I=1,KK)
       WRITE(6,166)(SE(I),I=1,KK)
  2000 FORMAT(SE10.4)
       WRITE(6,911)
       WRITE(6,111)(CS(I),MS(I),SN(I),SU(I),CL(I),HC(I),CE(I),ME(I),EN(I)
      1,CAS(I),SE(I),I=1,KK)
       WRITE(6,2001)
       WRITE(6,2000)(CSO(I),MGSO(I),CAL(I),TCA(I),TMG(I),I=1,KK)
       WRITE (6,166) TIME,CWF,EOR,HROOT,RUNOF,CUMS,CUMB,SUMA,WFRDD,WFUU
C      ------------------------------------------------------------------
       DELT=DETT
       EOR=V(KC+2)
       SE(1)=SF(KC+2)
       ET=TET(KC+2)
       MS(1)=MF(KC+2)
       CS(1)=CF(KC+2)
       SN(1)=SNF(KC+2)
       CL(1)=CLF(KC+2)
       SU(1)=SUF(KC+2)
       CSO(1)=CSOF(KC+2)
       MGSO(1)=MGSF(KC+2)
       HC(1)=HCF(KC+2)
       KC=KC+2
C      ------------------------------------------------------------------
       IF(TIME.LT.324.0.OR.TIME.GE.339.) GO TO 151
       SN(2)=SN(2)+(630.5555/W(2))
       CL(2)=CL(2)+(630.5555/W(2))
       GO TO 151
 148   IF(TIME+DELT-V(KC+1))151,151,149
 149   DELT=V(KC+1)-TIME
 151   LL=LL+1
       IF (TIME-CUMT) 153,152,152
 152   IF (ML-LMM) 162,162,1
 153   Y(1)=(W(1)+Y(1))*0.5
       J=(Y(1)-T(1))/DELW+1.0
       BB=(Y(1)-T(J))/DELW
       IF (EOR-0.0) 155,156,155
 155   G(1)=(P(J+1)-P(J))*BB+P(J)
 156   DO 161 I=2,KK
       J=(W(I)-T(1))/DELW+1.0
       BB=(W(I)-T(J))/DELW
       G(I)=(P(J+1)-P(J))*BB+P(J)
       TW=(W(I)-Y(I))+W(I)
       IF (TW-WATH) 157,157,159
 157   IF (TW-WATL) 158,160,160
 158   TW=WATL
       GO TO 160
 159   TW=WATH
 160   Y(I)=W(I)
       W(I)=TW
       SS(I)=SE(I)
 161   CONTINUE
       SS(1)=SE(1)
       GO TO 16
 162   STOP
 163   FORMAT (20I3)
```

```
165   FORMAT (7E10.4)
166   FORMAT (10E12.5)
 111 FORMAT (11F12.4)
 169 FORMAT(1H ,' K MM IER NB ND')
170   FORMAT (119H   WATER    POTENTIAL   CONDUCTIVITY DIFFUSIVITY
     1C(I)      DEPTH          W-DEPTH       H-DEPTH      RDF-DEPTH   SE-DEPTH)
172   FORMAT (53H   HDRY             HWET           WATL          WATH          CB)
179   FORMAT (54H  TIME END   SOIL FLUX    ET FLUX      SALT CONC.          )
180   FORMAT (66H  DELX            DETT            GRAVY          CONQ          DELW
     1          TIME)
181   FORMAT (66H   TT               CUMT            TAA            HLOW          HHI
     1          RRES)
184   FORMAT (1H ,'  TIME            CWF             EOR            HROOT         RUN
     10F        CUMS           CUMB           TRANS.        WFROD         WFUU
     2SE(20)')
 911  FORMAT(120H       CS             MS              SN              SU            C
     YL         HC             CF              ME              EN          GYPSUM    )
      END


      SUBROUTINE PLOT(N,WMAX,WVALUE,XVALUE,TMAX,TVALUE)
      DIMENSION ALINE(101),WVALUE(25),XVALUF(25),TVALUE(25)
      DATA FILL,AXIS,CHAR,CHAB,SAME/1H ,1H.,1HW,1HS,1H*/
      WRITE (6,7) WMAX,TMAX
      DO 1 J=1,101
1     ALINE(J)=AXIS
      WRITE (6,8) (ALINE(K),K=1,101)
      DO 2 J=1,101
2     ALINE(J)=FILL
      ALINE(1)=AXIS
      DO 4 L=1,N
      J=100.0*(WVALUE(L)/WMAX)+1.5
      JJ=100.0*(TVALUE(L)/TMAX)+1.5
      IF(J.LT.1) J=1
      IF(J.GT.101) J=101
      IF(JJ.LT.1) JJ=1
      IF(JJ.GT.101) JJ=101
      IF (J-JJ)10,11,10
11    ALINE (J)=SAME
      GO TO 12
10    ALINE (J)=CHAR
      ALINE(JJ)=CHAB
   12 WRITE(6,9) XVALUE(L),WVALUE(L),TVALUE(L),(ALINE(K),K=1,101)
      ALINE(JJ)=FILL
      ALINE(J)=FILL
   55 ALINE(1)=AXIS
4     CONTINUE
      DO 5 J=1,101
5     ALINE(J)=AXIS
      WRITE (6,8) (ALINE(K),K=1,101)
      RETURN
    7 FORMAT (24H  X VALUE WVALUE  SVALUE,5X,17H  MAX WAT CONT IS,F7.4,'
     1  MAX SALT CONCENTRATION IS',F9.2,1H )
8     FORMAT (31X,101A1)
   9  FORMAT(1H ,F6.1,F9.4,F8.2,7H          ,101A1)
      END
```

```
      SUBROUTINE EXCH(A,F,S,G,H,HCO3,ET,CT,SAT,CASO,AGSO,XXT,CAL,PW1,SEA
     M,AM,AC,SAM,SAC)
      DIMENSION AM(27),AC(27),SAM(26),SAC(26)
      DOUBLE PRECISION ZZZ
      MH=1
      IG=1
      PW1=PW1*100.0/1.16
      B=100000.0/PW1
      B1=PW1
      A=A/(1000.0*2.0)
      F=F/(1000.0*2.0)
      G=G/(1000.0*2.0)
      S=S/1000.0
      H=H/1000.0
      HCO3=HCO3/1000.
      AGSO=AGSO/(1000.*2.)
      CASO=CASO/(1000.*2.)
C     DA IS K(CA-NA)EXCHANGE COEFFCIENT
      DA=4.5377
      D=0.25+5.0/SEA
      U=SQRT(2.0*(A+F+G)+0.5*(S+H+HCO3))
      IF(U**2.LT.0.003)GO TO 100
      CALL ACOF(AM,AC,SAM,SAC,U,ADI,AMO)
      ASA=ADI*AMO**2.0
      GO TO 101
  100 ASA=EXP(-7.0242*U/(1.0+U))
  101 IF(CAL)1000,602,603
 602  IK=1
      AAA=452.
  604 ZE=AAA/(B1**1.68)
      GO TO 24
  603 IK=2
      ZE=(-1.68*ALOG(B1)-4.46)*2.3
      ZE=EXP(ZE)/ASA
  24  A1=A
      IF(XXT)4,4,26
 4    U=SQRT(2.0*(A+F+G)+0.5*(S+H+HCO3))
      IF(U**2.LT.0.003)GO TO 102
      CALL ACOF(AM,AC,SAM,SAC,U,ADI,AMO)
      AA=ADI**2
      GO TO 103
  102 AA=EXP(-9.366*U/(1.0+U))
  103 IF(2.4E-5-A*G*AA)26,18,18
  26  X=0.0
      U=SQRT(2.0*(A+F+G)+0.5*(S+H+HCO3))
      IF(U**2.LT.0.003)GO TO 104
      CALL ACOF(AM,AC,SAM,SAC,U,ADI,AMO)
      EX=1.0/(ADI**2)
      GO TO 105
  104 EX=EXP((9.366*U)/(1.0+U))
  105 BB=A+G
      CC=A*G-(2.4E-5)*EX
      R=SQRT(BB*BB-4.0*CC)
      X=(-BB+R)/2.0
      CAS1=4.897E-3-CASO
      DEL=R*XXT-CAS1
      IF(DEL-X)27,28,28
  27  X=XXT*B
      XXT=0.0
      CAS1=0.0
      A=A+X
```

```
      G=G+X
      U=SQRT(2.0*(A+F+G)+0.5*(S+H+HCO3))
      IF(U**2.LT.0.003)GO TO 106
      CALL ACOF(AM,AC,SAM,SAC,U,ADI,AMO)
      AA=ADI**2
      GO TO 7
  106 AA=EXP(-9.366*U/(1.+U))
 7    BB=-(4.9E-3+AA*A+AA*G)
      CC=AA*A*G-4.9E-3*CASO
      XXXX=BB*BB-4.0*AA*CC
      IF(XXXX)35,35,36
  35  X1=0.0
      GO TO 37
  36  X1=(-BB-SQRT(XXXX))/(2.0*AA)
  37  CASO=CASO+X1
      A=A-X1
      G=G-X1
      GO TO 44
  18  IF(G)1,1,6
 6    IF(A)1,1,7
 1    IF(CASO)44,44,7
  28  A=A+X
      G=G+X
      XXT=XXT-X/B
      CASO=CASO+CAS1
      XXT=XXT-CAS1/B
  44  A2=A
      IT=1
      IH=1
      MX=1
      IF(S)80,181,80
  181 IF(SAT)80,515,80
  80  IJ=2
  404 IF(SAT-ET)402,403,403
  402 Z=SAT/10.
      Z1=Z
      GO TO 5
  403 Z=ET/10.
      Z1=Z
 5    U=SQRT(2.0*(A+F+G)+0.5*(S+H+HCO3))
      IF(U**2.LT.0.003)GO TO 107
      CALL ACOF(AM,AC,SAM,SAC,U,ADI,AMO)
      EX=ADI/AMO**2
      GO TO 108
  107 EX=EXP((-2.341*U)/(1.0+U))
  108 AA=-4.0*DA*DA*B*B
      BB=4.0*B*(EX+2.0*DA*DA*ET*B+DA*DA*S)
      CC=4.0*EX*(A+SAT*B)-4.0*DA*DA*B*ET*(B*ET+2.0*S)-DA*DA*S*S
      DD=SAT*EX*(4.0*A+SAT*B)+2.0*DA*DA*ET*S*(2.0*B*ET+S)
      EE=SAT*SAT*A*EX-DA*DA*S*S*ET*ET
  81  ZZ=-((((AA*Z+BB)*Z+CC)*Z+DD)*Z+EE)
      ZZZ=(((4.0*AA*Z+3.0*BB)*Z+2.0*CC)*Z+DD)
      ZZ=ZZ/ZZZ
      IF(ZZ-0.0)302,303,302
 303  IF(Z-0.0)302,515,302
  302 ZZZ=ZZ/Z
      Z=Z+ZZ
      IF(IH.GE.5)GO TO 83
      IH=IH+1
      IF(DABS(ZZZ)-0.001)83,83,81
 83   IF(Z.GE.0.0)GO TO 305
```

```
      IF(SAT.LT.ABS(Z*2.0))Z=SAT/2.0
  815 A=A+B*Z
      IF(A)510,510,512
  552 SAT=SAT-2.*Z
  551 ET=ET+Z
  550 S=S+2.*B*Z
  510 A=A-B*Z
      Z=-Z1
      IF(MX.GE.5)GO TO 512
      MX=MX+1
      GO TO 81
  512 S=S-2.0*B*Z
      IF(MX.GE.5)GO TO 513
      MX=MX+1
      IF(S)550,550,513
  513 ET=ET-Z
      IF(MX.GE.5)GO TO 514
      MX=MX+1
      IF(ET)551,551,514
  514 SAT=SAT+2.0*Z
      IF(MX.GE.5)GO TO 515
      MX=MX+1
      IF(SAT)552,552,515
  515 A3=A
      BB=A+B*(CT+D*ET)+D*F
      AA=B*(1.0-D)
      CC=(A*CT-D*F*ET)
      R=SQRT(BB*BB-4.0*AA*CC)
      Y=(-BB+R)/(2.0*AA)
      A=A+B*Y
      F=F-B*Y
      ET=ET-Y
      CT=CT+Y
      IF(G)790,790,791
  791 IF(F)790,790,792
  792 IF(U**2.LT.0.003)GO TO 109
      CALL ACOF(AM,AC,SAM,SAC,U,ADI,AMO)
      AA=ADI**2
      GO TO 110
  109 AA=EXP(-9.366*U/(1.+U))
  110 BB=-(5.9E-3+AA*F+AA*G)
      CC=AA*F*G-5.9E-3*AGSO
      XXXX=BB*BB-4.0*AA+CC
      IF(XXXX)793,793,794
  793 X1=0.0
      GO TO 795
  794 X1=(-BB-SQRT(XXXX))/(2.0*AA)
 795  AGSO=AGSO+X1
      F=F-X1
      G=G-X1
  790 CONTINUE
      GO TO (600,601),IK
  601 AA=4.0
      BB=4.0*HCO3+A
      CC=HCO3**2+4.0*A*HCO3
      DD=A*HCO3**2-ZE
      IF(HCO3-A)61,61,62
  61  Z=-HCO3/4.
      GO TO 650
  62  Z=-A/2.
  650 Z1=Z
```

```
63    ZZ=-(((AA*Z+BB)*Z+CC)*Z+DD)
      ZZZ=((3.0*AA*Z+2.0*BB)*Z+CC)
      IF(ZZ-0.0)300.301.300
301   IF(ZZZ-0.0)300.600.300
300   ZZ=ZZ/ZZZ
      ZZZ=ZZ/Z
      Z=Z+ZZ
      IF(IT.GE.5)GO TO 64
      IT=IT+1
      IF(DABS(ZZZ)-.001)64.64.63
64    A=A+Z
      HCO3=HCO3+2.*Z
      IF(HCO3)752.752.651
752   HCO3=HCO3-2.*Z
      A=A-Z
      Z=-Z1
      GO TO 63
651   IF(A)752.752.753
753   CAL=CAL-Z
600   ZX=A*HCO3**2
      IF(ZX-ZE)606.605.605
605   IK=2
606   DEL=A-A1
      IF(IG.GE.5)GO TO 8
      IG=IG+1
      IF(DEL+1.0E-5)24.48.48
48    IF(DEL-1.0E-5)49.49.24
49    DEL=A-A2
      IF(DEL+1.0E-5)24.50.50
50    IF(DEL-1.0E-5)51.51.24
51    DEL=A-A3
      IF(DEL+1.0E-5)24.52.52
52    IF(DEL-1.0E-5)8.8.24
8     AP=A
1000  CONTINUE
67    CONTINUE
      A=A*1000.0*2.0
      F=F*1000.0*2.0
      S=S*1000.0
      G=G*1000.0*2.0
      H=H*1000.0
      HCO3=HCO3*1000.
      CASO=CASO*1000.0*2.0
      AGSO=AGSO*1000.*2.0
      SEA=A+F+S+CASO+AGSO
      RETURN
      END


      SUBROUTINE EQEXCH(CA.AMG.SOS.CL.SO.HCO3.E5.C5.SA5.CASO.AGSO.SEA.AM
     Y.AC.SAM.SAC)
      DIMENSION AM(27).AC(27).SAM(26).SAC(26)
      CA=CA/(1000.0*2.0)
      AMG=AMG/(1000.0*2.0)
      SOS=SOS/1000.
      SO=SO/(1000.0*2.0)
      CL=CL/1000.
      HCO3=HCO3/1000.0
      EC=0.11E-03
C     DA IS K(NA-CA) OR 1.0/K(CA-NA) EXCHANGE COEFFCIENT
```

```
      DA=0.3115
      D=0.25+5.0/SEA
      CASO=0.0
      U=SQRT(2.0*(CA+AMG+SO)+0.5*(SOS+HCO3+CL))
      AGSO=0.0
      IF(U**2.LT.0.003)GO TO 42
      CALL ACOF(AM,AC,SAM,SAC,U,ADI,AMO)
      ACT2=ADI**2
      GO TO 150
 42   ACT2=EXP(-9.366*U/(1.0+U))
 150  IF(SO)1000,713,712
 712  AA=ACT2*ACT2
      BB=ACT2*(10.8E-3+(ACT2*(AMG+CA-SO)))
      CC=28.91E-6+(ACT2*(AMG*4.9E-3+(CA*5.9E-3)-(SO*10.8E-3)))
      DD=-SO*28.91E-6
 800  Z=SO/2.
 850  Z1=Z
 863  ZZ=-(((AA*Z+BB)*Z+CC)*Z+DD)
      ZZZ=((3.0*AA*Z+2.0*BB)*Z+CC)
      ZZ=ZZ/ZZZ
      ZZZ=ZZ/Z
      Z=Z+ZZ
      IF(ABS(ZZZ)-.001)840,840,863
 840  SOT=SO
      SO=Z
      IF(SO)710,710,711
 710  SO=SOT
      Z=Z1
      GO TO 863
 711  CASX=SO*CA*ACT2/(4.9E-3+ACT2*SO)
      CX=CA-CASX
      AGSX=SO*AMG*ACT2/(5.9E-3+ACT2*SO)
      AMX=AMG-AGSX
      UU=SQRT(2.0*(CX+AMX+SO)+0.5*(SOS+HCO3+CL))
      IF(ABS(UU/U-1.)-1.0E-4)40,40,41
  41  U=UU
      SO=SOT
      GO TO 42
 40   CASO=CASX
      AGSO=AGSX
      CA=CX
      AMG=AMX
 713  ACT1=SQRT(ACT2)
      ACTM=SQRT(ACT1)
      ACTM=SQRT(ACTM)
      CA=CA*2.
      AMG=AMG*2.
C--CA,MG,ARE IN EQUIVALENT/LITER
      E5=EC/((ACTM*SOS/(DA*SQRT(ACT1*CA)))+1.+(D*ACT1*AMG/(ACT1*CA)))
      SA5=ACTM*SOS*E5/(SQRT(ACT1*CA)*DA)
      C5=EC-E5-SA5
      E5=E5/2.
      C5=C5/2.
      CA=CA*1000.0
      AMG=AMG*1000.0
C--CA,MG,ARE IN ME/LITER
      SOS=SOS*1000.0
      CL=CL*1000.0
      SO=SO*1000.0*2.0
      HCO3=HCO3*1000.0
      CASO=CASO*1000.0*2.0
```

```
      AGSO=AGSO*1000.0*2.0
      SEA=CA+AMG+SOS+CASO+AGSO
      WRITE(6,100)CA,AMG,SOS,CL,SO,HCO3,E5,C5,SA5,AGSO,CASO,SEA
  100 FORMAT(12E10.4)
 1000 RETURN
      END


      SUBROUTINE SALT(A,B,C,D,E,F,WFRU,WFRD,DELX,J,EOR)
C     SE AND SS ARE NEW AND OLD CONCENTRATIONS
      DIMENSION SS(3),W(3),SE(3),Y(3)
      I=1
      SS(I)=A
      SS(I+1)=B
      SS(I+2)=C
      W(I+1)=D
      Y(I+1)=E
      IF(J.EQ.1)GO TO 201
      IF(WFRU.GE.0.0.AND.WFRD.GE.0.0)GO TO 205
      IF(WFRU.LE.0.0.AND.WFRD.LE.0.0)GO TO 209
      IF(WFRU.GE.0.0.AND.WFRD.LE.0.0)GO TO 208
      IF(WFRU.LE.0.0.AND.WFRD.GE.0.0)GO TO 210
  205 SE(I+1)=(SS(I+1)*Y(I+1)+(SS(I)*WFRU-SS(I+1)*WFRD)/DELX)/W(I+1)
      GO TO 200
  201 IF(EOR-0.0)203,204,202
 203  IF(WFRD.GT.0.0)GO TO 206
 207  SE(2)=(SS(2)*Y(2)-(SS(3)*WFRD)/DELX)/W(2)
      GO TO 200
  206 SE(2)=(SS(2)*Y(2)-(SS(2)*WFRD)/DELX)/W(2)
      GO TO 200
  204 IF(WFRD.LT.0.0)GO TO 207
      GO TO 206
  202 IF(WFRD.GT.0.0)GO TO 205
  208 SE(I+1)=(SS(I+1)*Y(I+1)+(SS(I)*WFRU-SS(I+2)*WFRD)/DELX)/W(I+1)
      GO TO 200
  209 SE(I+1)=(SS(I+1)*Y(I+1)+(SS(I+1)*WFRU-SS(I+2)*WFRD)/DELX)/W(I+1)
      GO TO 200
  210 SE(I+1)=(SS(I+1)*Y(I+1)+(SS(I+1)*WFRU-SS(I+1)*WFRD)/DELX)/W(I+1)
  200 IF(SE(I+1).LT.0.0)SE(I+1)=SS(I+1)
      F=SE(I+1)
      RETURN
      END


      SUBROUTINE ACOF(AM,AC,SAM,SAC,U,ADI,AMO)
      DIMENSION AM(27),AC(27),SAM(26),SAC(26)
      U=U**2
      IF(U.LE.15.0)GO TO 1
      ADI=587.0
      GO TO 2
  1   DO 751 I=1,27
      IF(U.GT.AM(I))GO TO 751
      AG=U-AM(I-1)
      ADI=AC(I-1)+((AC(I)-AC(I-1))*AG)/(AM(I)-AM(I-1))
      GO TO 2
  751 CONTINUE
  2   IF(U.LE.5.0)GO TO 3
      AMO=1.295
```

```
      GO TO 4
  3   DO 604 I=1,26
      IF(U.GT.SAM(I))GO TO 604
      AG=U-SAM(I-1)
      AMO=SAC(I-1)+((SAC(I)-SAC(I-1))*AG)/(SAM(I)-SAM(I-1))
      GO TO 4
604   CONTINUE
  4   RETURN
      END
```

VITA

Satish Chander Gupta

Candidate for the degree of

Doctor of Philosophy

Dissertation: Model for predicting simultaneous distribution of salt and water in soils

Major Field: Soils and Biometeorology

Biographical Information:

Personal data: Born at Poonch, Jammu India, July 29, 1945; son of Sita Ram and Laj Wanti Gupta.

Education: Received the Bachelor of Science degree from Punjab Agricultural University, Ludhiana, majoring in Soil Science, in 1966; received the Master of Science degree from Punjab Agricultural University, Hissar, majoring in Soil Science, in 1968; completed requirements for the Doctor of Philosophy majoring in Soil Physics, at Utah State University, Logan, Utah in 1972.

Professional Activities: Selected for junior research fellowship 1966-1968 by the Indian Council of Agricultural Research; paper presented: "Influence of water content on electrical conductivity of the soil." Annual meeting of the Western Soil Science Society of America, 1971.

Affiliations: American Society of Agronomy; Soil Science Society of America.