COMPUTER ESTIMATES OF NATURAL RECHARGE FROM SOIL MOISTURE DATA HIGH PLAINS OF COLORADO

by

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COMPUTER ESTIMATES OF NATURAL RECHARGE FROM SOIL MOISTURE DATA - HIGH PLAINS OF COLORADO

Completion Report

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by

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LIST OF SYMBOLS

Symbol	Description	Dimension
C	Infiltration rate	L/T
C_1	Constant in the mathematical model	L^2/T
C_2	Constant in the Mathematical model	L/T
C_3	Constant in the mathematical model	L^2/T
C_4	Slope of the Linear relationship of C_3 in space, z	L/T
C_{45}	Constant in the mathematical model	L/T
C_5	Slope of the linear portion of hydraulic conductivity function	L/T
C_6	Constant in the mathematical model	1/T
C_7	Constant in the mathematical model	1/T
C_8	Vertical intercept of the linear relation between $K(\theta)$ and θ	L/T
d_c	Depth of control volume	L
$D(\theta)$	Soil water diffusivity as a function of θ	L^2/T
e	Random error	1/T
ε	Mathematical expectation	-
F	Soil water flux	L/T
g	Acceleration due to gravity	L/T^2
	Aquifer saturated thickness	L
h	Capillary pressure head	L

LIST OF SYMBOLS (Cont'd)

Symbol	Description	Dimension
H	Number of Spatial grids	none
H	Water table elevation above datum	L
H*	Total hydraulic head	L
i	Subscript refers to n	-
j	Subscript refers to n, H	-
K	Hydraulic conductivity	L/T
K(θ)	Hydraulic conductivity as a function of θ	L/T
K(h)	Hydraulic conductivity as a function of capillary pressure head	L/T
K_s	Saturated hydraulic conductivity	L/T
ℓ_n	Naperian logarithm	-
$\bar{m}$	Estimated values of coefficients of the mathematical model	varies
n	Subscript, number of observations	none
N	Number of coefficients of the mathematical model	none
p_b	Bubbling pressure	F/L^2
p_c	Capillary pressure	F/L^2
q	Darcy's flux	L/T
r	Recharge	L
R	Recharge	L/T
S_y	Specific yield	none

LIST OF SYMBOLS (Cont'd)

Symbol	Description	Dimension
s	Saturation	none
s_r	Residual saturation	none
t	Superscript, time	T
T	Transpose	-
T	Time	T
x	Spatial coordinate	L
x	Observed value in the linear model	varies
x	Matrix form of the observations in the linear model	varies
y	Random variable in the linear model	1/T
Y	Random variable in the linear model in matrix form	1/T
z	Vertical coordinate	L
α	Slope of the linear portion of the soil water characteristic curve	L
β	Intercept of the linear relation of the soil water characteristic curve	L
γ	Coefficient with stochastic model	none
δ	Coefficient in the stochastic model	none
θ	Moisture content	none
Θ	Moisture content	none
λ	Random component of water table elevation at x	L

LIST OF SYMBOLS (Cont'd)

Symbol	Description	Dimension
μ	Random component of water table elevation $x+\Delta x$	L
ρ	Density of soil water	M/L^3
σ^2	Variance	varies
ϕ	Porosity	none
ψ	Random component of water table elevation at $x-\Delta x$	L
Ω	Random component of recharge values	L
∇	Gradient operator	1/L
Δs	Change in storage	L^3
Δt	Discrete time step	T
Δx	Discrete space step	L
Δz	Discrete space step	L
∂	Partial differential operator	none
$\hat{}$	Refers to either scaled values of variables or estimated values of variables	-
-	Refers to vector and average	-

ABSTRACT

The research described briefly in this completion report has shown that transient soil moisture data observed at vertical positions at one station can be used as descriptors of natural groundwater recharge to evaluate its time distribution at that station. Hydraulic properties of the soil and initial and boundary conditions must be known before applying the mathematical model developed in this study to other locations.

The model developed in this study assumed that the moisture content of unsaturated soil below the zone of influence of evapotranspiration varies in the linear range of the soil water characteristic curve. The parameters of the model characterize the hydraulic properties of the soil and their spatial variability. They were estimated by a linear statistical model. The mathematical model was solved by a Finite-Difference technique adopting the Crank-Nicholson scheme.

The model was verified with an analytical solution and the agreement for the case of homogeneous soil was very good. Field data collected during a drainage cycle were used to verify the model for non-homogeneous soil. The verification was also found to be satisfactory in the latter case.

The model was then applied to estimate recharge rates from data collected by the USGS and ARS at the Great Plains Field Experiment Station near Akron, Colorado. Estimated monthly recharge rates varied from a low of 0.02 inches to a high of 1.42 inches. Comparison of the Akron recharge estimates with other data indicates the values were acceptable. An average annual recharge of 4 inches was computed for the Akron site. This result was compatible with the observed rise in the local water table of 3 feet during the same time period.
KEY WORDS: *Natural recharge, *transient soil moisture, *groundwater, *mathematical model, finite-difference solution, Newton-like method, hydraulic properties of soil.

FOREWORD

The initial attempts to develop a statistical model for predicting the areal and time distribution of natural recharge were discontinued because of insufficient data. A review of literature during the first year indicated that development of a first-order Markov model could be used. Data collected by the USGS and ARS at the Akron, Colorado Great Plains Experiment Station were obtained and graphs of soil moisture distributions with depth, water table fluctuations, and precipitation periods were prepared. However, upon analysis of these data it was determined there were insufficient data points and the time between measurements was too long to allow development of the Markov model.

A mathematical model was developed which utilizes soil moisture data measured at various times and depths for a single location to estimate the natural recharge. Model parameters were estimated statistically from the observed data. The technique was checked against both an analytical solution and field data reported in the literature. The model was then applied to estimate recharge rates for data collected at the Great Plains Field Experiment Station. Details of how this was accomplished are described in the following pages.

1. RESEARCH OBJECTIVES

The original proposal, dated March 1972, envisioned the determination of recharge as a function of soil type, topography and geology including identification of system parameters characterized by natural features such as topography and plant cover given the input (precipitation series) and output (recharge series) to the system. More specifically, the objectives of the proposal included the following:

1. Develop techniques for evaluating the areal and time distribution of natural recharge.

2. Define procedures for estimating the quantity of water available for artificial recharge on the High Plains.

3. Evaluate the use of soils maps for selecting artificial recharge sites.

II. INTRODUCTION AND APPROACH TO THE PROBLEM

2.0 Background.

Recharge of groundwater, defined as the amount of water reaching the water table, is the principal mechanism for replenishing the underground water reservoir. There are, theoretically, two approaches in modeling a natural process like groundwater recharge: (i) deterministic and (ii) probabilistic or stochastic. Whatever the approach, the descriptors of the phenomenon are the same. Rainfall is the principal causal factor for recharge resulting in occurrence and movement of moisture in the soil water system (Fig. 1) and fluctuation of water table elevations. Soil moisture content and water table elevations are known descriptors of recharge. Water table flucturations are caused not only by recharge but also by external pumping, barometric pressure variations and deep seepage from irrigation. It is difficult to identify the causative factor or factors. In research efforts to determine the natural recharge, it is usually assumed that the aquifer is in dynamic equilibrium and fluctuations of the water table due to other causes are absent. A time series analysis of groundwater levels was made under the above ideal conditions by Ericksson (1970) and his conclusion was that water levels in a linear aquifer obey Markov's law. Later investigation by Gelhar (1974) agreed with this finding.

2.1 Stochastic Approach.

During the initial period of this research study, a stochastic model was developed using water table as the descriptor of recharge. Appendix A describes the assumptions and development of the model. The stochastic model required water level and pumping time series data for long periods of time but these data were not available. Further, the status of dynamic equilibrium did not exist after large scale groundwater

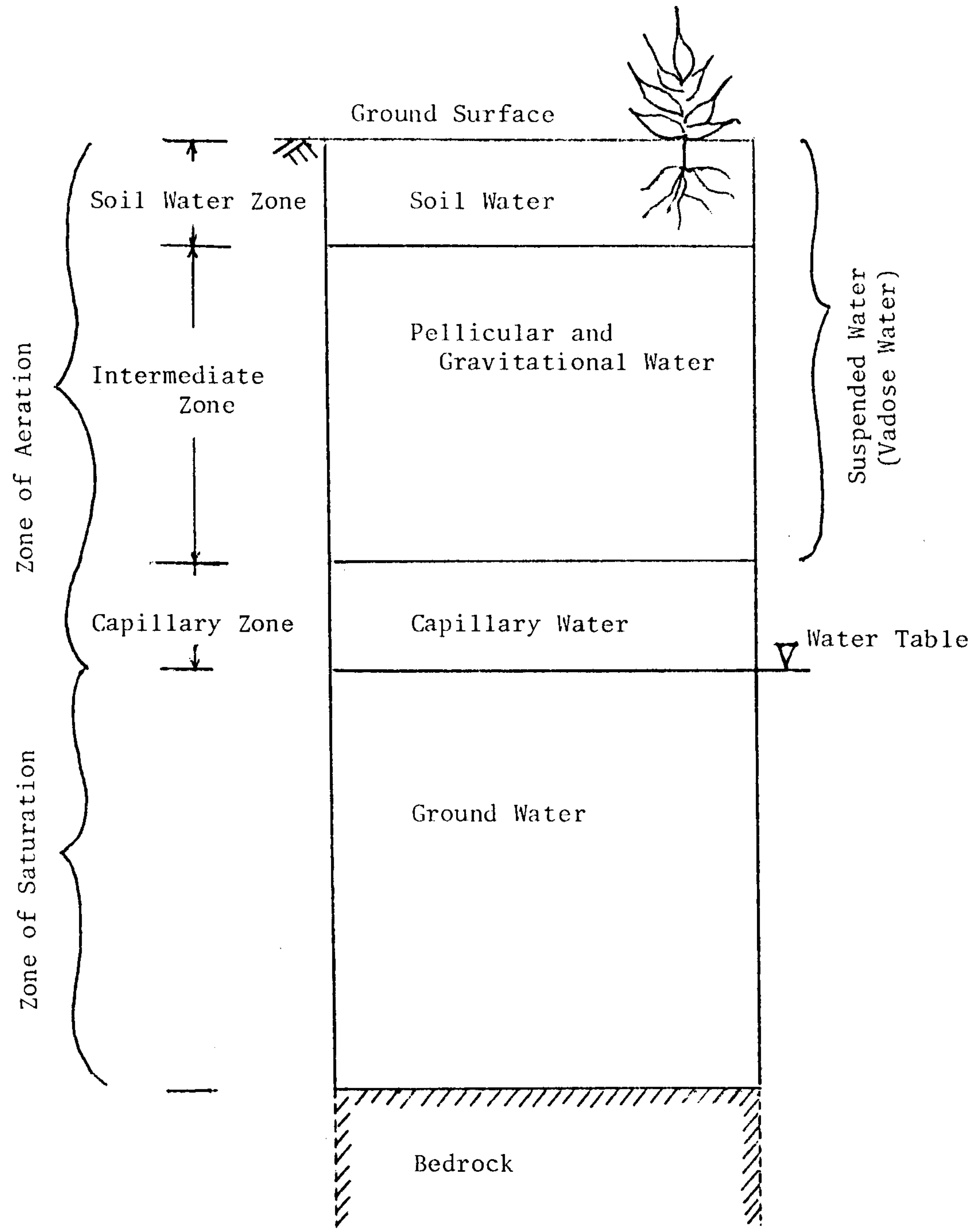

Figure 1. Classification of subsurface water system. (Todd, D. K. 1960)

development began in the High Plains of Colorado (Fig. 2). The data available for calculating pumpage were not sufficient to identify the influence of pumping on water table elevations. For these reasons, it was necessary to abandon the method which estimates natural recharge rates from data on water table fluctuations.

2.2 Deterministic Approach.

As indicated above, moisture content in the soil is the next best descriptor of recharge. Chien (1972) adapted moisture content as a stochastic variable and developed a Markov model for moisture movement. However, Markov models are applicable only when the process is described by a linear differential equation. The Richards' equation describing the flow of water with moisture content Θ, as the variable is highly non-linear and as such, the Markov model is not applicable to the process. Development of a linear stochastic model was therefore, not possible without proper transformation of the variable Θ which would linearize the Richards' equation.

In view of the above, CSU researchers used moisture content Θ as the descriptor of natural recharge and developed the deterministic model using the principle of continuity and Darcy's law.

2.3 Recharge Studies on the High Plains of Colorado.

The Central Great Plains Field Station operated by the Agricultural Research Service of the U. S. D. A. was selected as the study area not only because of its location on the Northern High Plains, but also because of the availability of data for use with the model. The Central Great Plains Field Station research facilities are located 4 miles east of Akron, Colorado (Fig. 3). Exploratory studies on subsurface water movement have been conducted at that Station by USGS and ARS personal since July 1969. Moisture data from studies of 16 separate wells representing

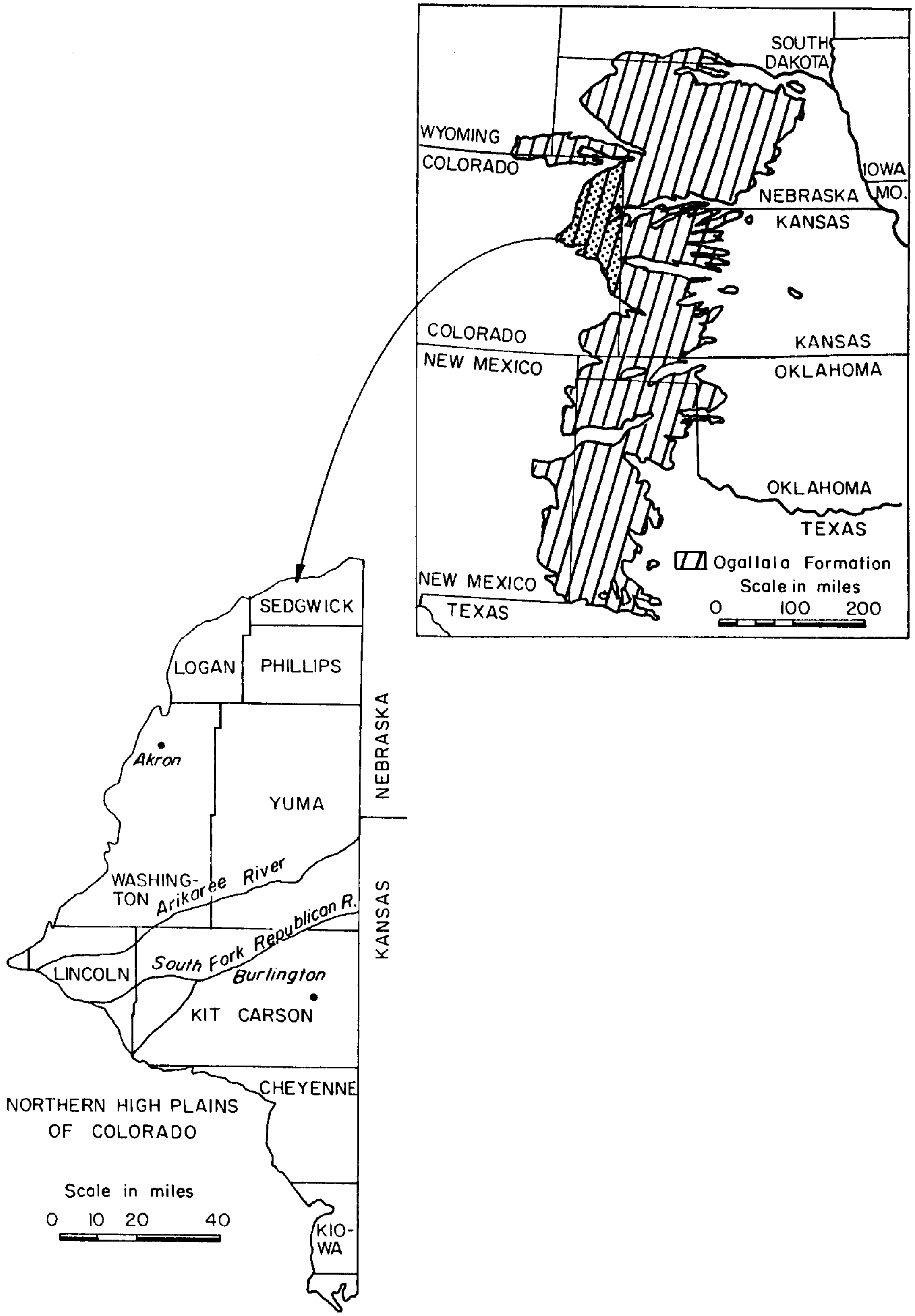

Figure 2. Boundaries of the Northern High Plains of Colorado and Ogallala Formation (Adapted from Special Report 39, Texas Tech, 1970).

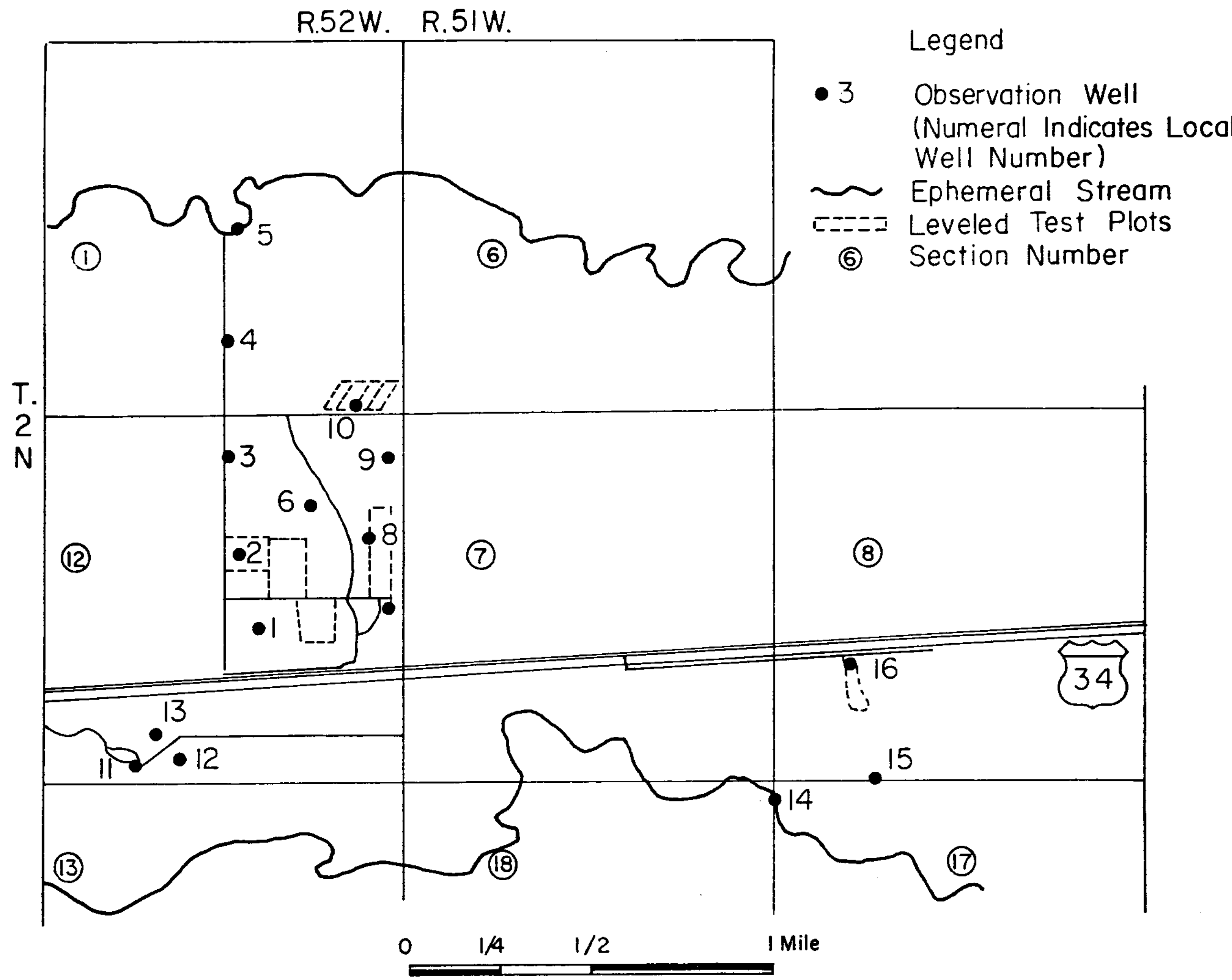

Figure 3. Sketch of Central Great Plains Field Station located 4 miles east of Akron, Colorado showing the locations of sixteen observation wells (Hofstra, 1970).

several different topographic and vegetative areas and collected at 16 different time periods over a five-year span (1969-74) were utilized.

Previous estimates of recharge on the High Plains of Colorado were made by Weist (1960), Cardwell and Jenkins (1963), McGovern (1964), Boettcher (1966), Reddell (1967) and Luckey et al. (1973). Longenbaugh (1966) studied the feasibility of artificial recharge at the Arikaree River site near Cope, Colorado. Reddell used a steady state model and adopted Finite-Difference technique to determine the area distribution of recharge over the entire High Plains area. Results from Reddell's study indicate the natural recharge rates in the Akron study area are one to two inches per year. Recharge rates computed by the technique developed in this study are compared to these values. The applicability of the technique for future periods of time and other locations is discussed.

III. THEORY AND DEVELOPMENT OF A MATHEMATICAL MODEL

3.1 Necessity for a Simulation Model to Determine the Time-Distribution of Natural Recharge.

The occurrence and movement of moisture in a natural soil water system depends in part on the occurrence of precipitation events at that location. Each precipitation event causes changes in the moisture, depending on its amount and time-distribution, soil properties and topography. Figure 4(a) shows the moisture content measured in a hypothetical soil water system at three time levels t_o , t_1 and t_n . The distribution of moisture content at time t_o is the result of all historical storm events and moisture extraction by plants and evaporation which occurred prior to that time. The distributions of moisture content at times t_1 and t_n reflect significant recharge due to a storm which occurred between time t_0 and t_1 . For the purpose of discussion, let us assume that there were no other storms between the time levels t_1 and t_n . During that period of time, however, recharge due to movement of moisture does occur.

One objective of this research is to find a method for evaluating the amount of recharge and its distribution in time. To formulate the problem, a control volume is defined by soil mass of unit cross-sectional area and depth equal to the distance between the lower limit of the zone of influence of evapotranspiration and the upper limit of the capillary zone, figure 4(b). A water molecule passing through the upper boundary of this control volume continues to flow downward and has no chance to move upward; hence, the name gravitational water. The amount of water passing across the lower boundary of this control volume is the recharge that actually reaches the saturated zone.

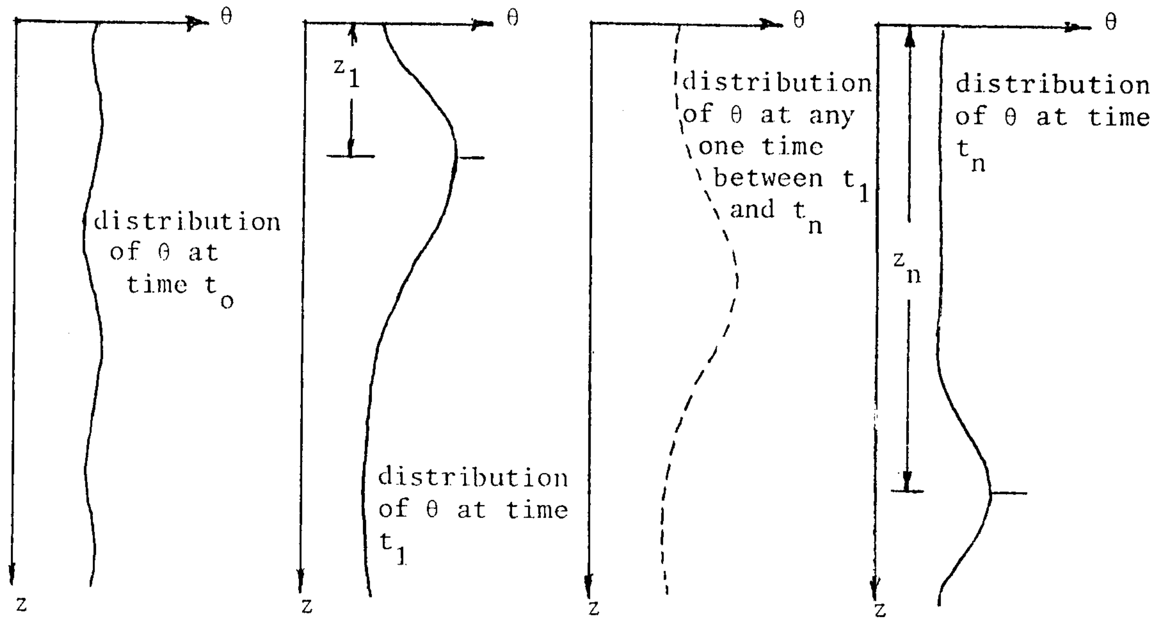

Figure 4(a). Hypothetical distributions of moisture content, θ, after an infiltration event between times t_o and t_n.

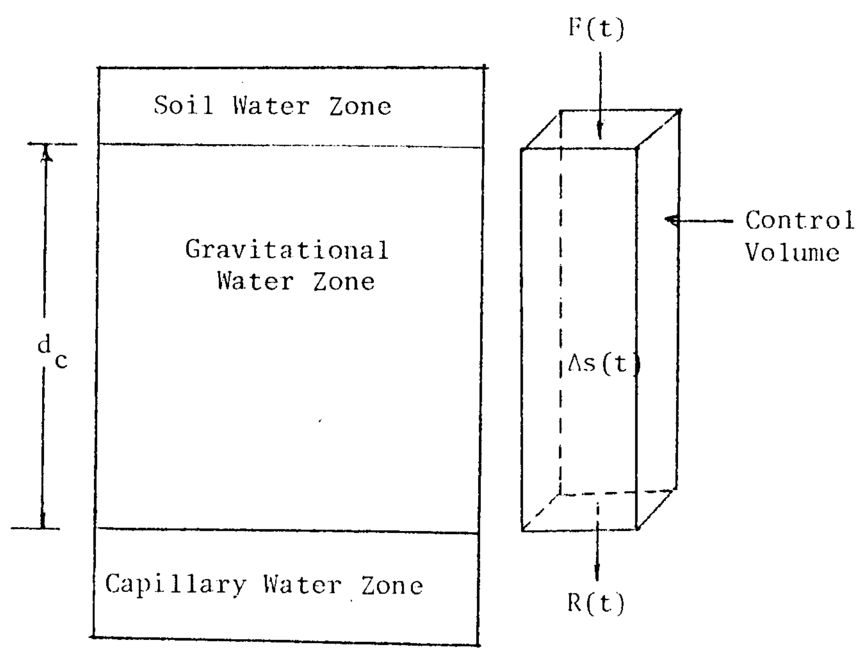

Figure 4(b). Definition sketch for control volume.

The amount of recharge can then be quantified using the principle of continuity. If $F(t)$ is the time-distribution of soil water flux at the upper boundary and $\Delta s(t)$ is the time distribution of change in the storage of soil moisture within the control volume, the time distribution of recharge $R(t)$ is given by

$$R(t) = F(t) - \Delta s(t) \tag{3.1.1}$$

$F(t)$ at the upper boundary can be calculated by Darcy's law. Similarly, $\Delta s(t)$ can be calculated if the distributions of soil moisture at different times are known. We know from observations the distributions of soil moisture at times t_o , t_1 and t_n. We would like to know the distributions of soil moisture at times t_2 , t_3 ,..., t_{n-1} . A simulation model for movement of moisture could be developed to evaluate the moisture distribution.

The control volume has another significance. The precipitation event which occurred between the time period t_o and t_1 , is perceptible from the soil moisture distribution showing an increase in moisture at depth z_1 at time t_1 and an increase at depth z_n at time t_n . The position of this event at any one of the time periods t_2 , t_3 ,..., t_{n-1} could be as shown in figure 4(a) in dotted lines. It is possible, that the time interval t_n-t_1 between the observations of soil moisture may be large and the depth of control volume d_c may be small, in which case, the precipitation and the resulting recharge event may pass the lower boundary of the control volume before it is detected by observation at time t_n . This occurrence should be prevented by carefully selecting the time interval between observations and depth of control volume from the knowledge of the hydraulic conductivity function.

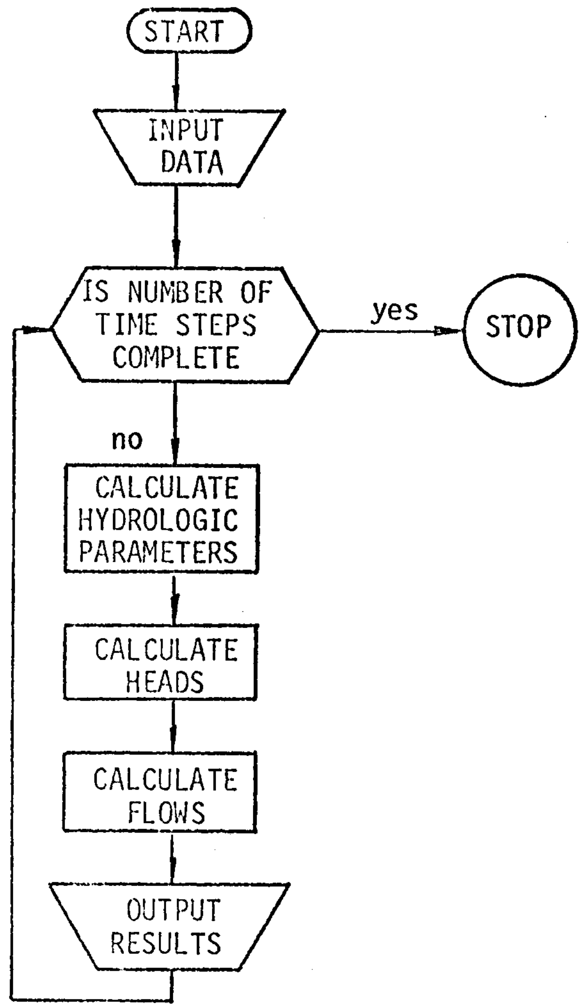

Figure 2. WTSHED2 - WTSHED4 sequence of events.

In practice, the situation is more complex than the one explained. There are many storm events between the successive observations of moisture content. It may not be practical to reduce the time interval between the observations to account for every storm.

A mathematical model is developed to simulate the movement of moisture and thus determine the vertical distribution of moisture content during the time interval between successive observations. The time distribution of flux at the upper boundary of the control volume is determined by Darcy's law. The time distribution of the change in storage of moisture within the control volume is determined from the distribution of moisture calculated by solving the mathematical model. The time distribution of natural groundwater recharge is described by equation 3.1.1.

3.2 Development of Simulation Model.

The development of a mathematical model to simulate the flow of gravitational water is described below.

3.2.1 Basic Assumptions.

The following assumptions are made in the development of the mathematical model.

i) The moisture variation in the soil below the zone of influence of evapotranspiration is in the linear range of the pressure-moisture curve, figure 5(a).

ii) The unsaturated hydraulic conductivity varies in the linear range for these same values of moisture, figure 5(b).

iii) The effects of hysterisis and flow of air are neglected.

vi) Darcy's law is valid.

3.2.2 Modification of Richards' Equation.

The linear relationship between hydraulic conductivity, $K(\Theta)$, and moisutre content, Θ, is expressed as

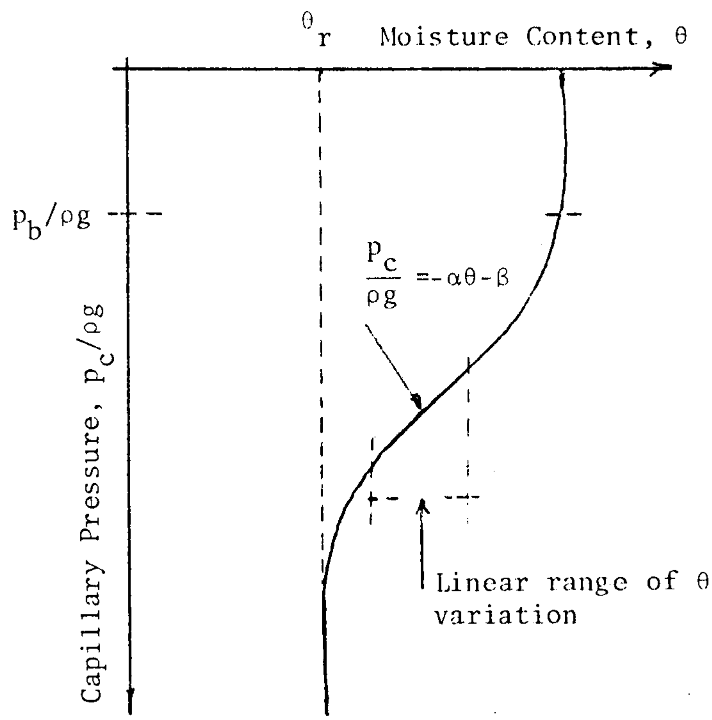

Figure 5(a). Typical curve of capillary pressure $p_c/\rho g$, versus moisture content, θ.

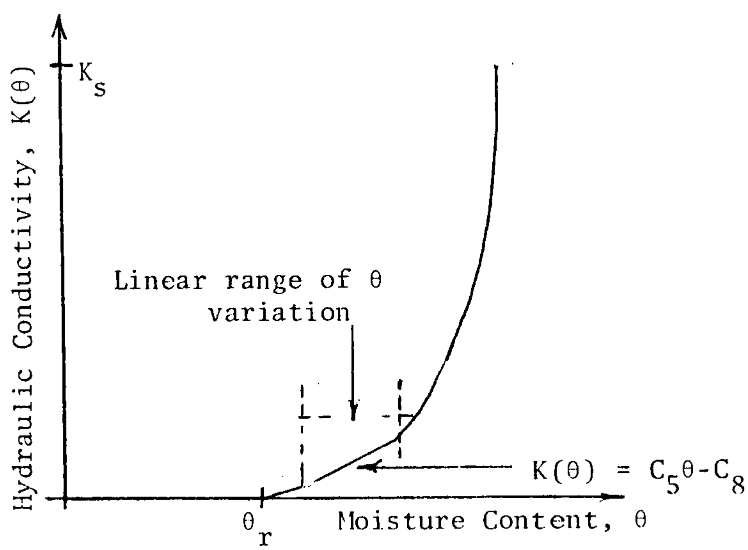

Figure 5(b). Typical curve of hydraulic conductivity, $K(\theta)$ versus moisture content, θ.

$$K(\theta) = C_5\theta - C_8 \tag{3.2.2.1}$$

where C_5 and C_8 are constants.

Similarly, the linear relationship of capillary pressure, p_c, with moisture content, θ , can be expressed as

$$p_c/\rho g = -\alpha\theta - \beta \tag{3.2.2.2}$$

where α and β are constants.

The generalized Darcy's law for one-dimensional vertical flow of water in unsaturated soil is

$$\bar{q} = - K(\theta) \frac{\partial}{\partial z} [- \frac{p_c}{\rho g} + z] \qquad \text{(de Wiest, 1969)} \tag{3.2.2.3}$$

where

$\bar{q}$ is the flux of water considered positive downward,

$K(\theta)$ is the unsaturated hydraulic conductivity,

p_c is the capillary pressure defined as the pressure of free water in equilibrium with the soil at the point in question,

z is the vertical distance from a datum plane measured positively downward from the soil surface.

Assuming that on a macro-scale, the differential form of the continuity equation is valid (the functions describing the flow and their derivatives are continuous and that the soil water is incompressible) the one-dimensional flow equation for the general case, is expressed as

$$\frac{\partial\theta}{\partial t} = - \frac{\partial}{\partial z} [-K(\theta) \frac{\partial}{\partial z} (- \frac{p_c}{\rho g} + z)] \quad . \tag{3.2.2.4}$$

Using the fact that gravitational potential decreases with depth,

$$\frac{\partial\theta}{\partial t} = - \frac{\partial}{\partial z} [K(\theta) \frac{\partial p_c/\rho g}{\partial\theta} \frac{\partial\theta}{\partial z} + K(\theta)] \quad .$$

Substituting equations 3.2.2.1 and 3.2.2.2 into 3.2.2.4 yields

$$\frac{\partial\theta}{\partial t} = - \frac{\partial}{\partial z} [\alpha(C_5\theta - C_8) \frac{\partial\theta}{\partial z} + (C_5\theta - C_8)]$$

$$= \frac{\partial}{\partial z} [(C_1\theta - C_3) \frac{\partial\theta}{\partial z}] - \frac{\partial}{\partial z} (C_5\theta - C_8) \qquad (3.2.2.5)$$

where

$$C_1 = -C_5 \cdot \alpha$$

$$C_3 = -C_8 \cdot \alpha$$

$$C_8 = \frac{C_3 \cdot C_5}{C_1} \quad . \qquad (3.2.2.6)$$

The coefficients C_1 , C_3 , C_5 and C_8 characterize the properties of the soil and they vary in space for a non-homogeneous medium.

Expansion of equation 3.2.2.5 gives,

$$\frac{\partial\theta}{\partial t} = C_1\theta \frac{\partial^2\theta}{\partial z^2} + C_1(\frac{\partial\theta}{\partial z})^2 + \frac{\partial C_1}{\partial z} \theta \frac{\partial\theta}{\partial z} - C_3 \frac{\partial^2\theta}{\partial z^2} - \frac{\partial C_3}{\partial z} \frac{\partial\theta}{\partial z}$$

$$-C_5 \frac{\partial\theta}{\partial z} - \frac{\partial C_5}{\partial z} \theta + \frac{\partial C_8}{\partial z} \quad .$$

Linearizing the spatial variation of the coefficients C_1 , C_3 , C_5 and C_8 i.e., designating $\partial C_1/\partial z = C_2$, $\partial C_3/\partial z = C_4$, $\partial C_5/\partial z = C_6$ and $\partial C_8/\partial z = C_7$, and neglecting the higher detree term, $(\partial\theta/\partial z)^2$ as described by Wang, 1968, we get,

$$\frac{\partial\theta}{\partial t} = C_1\theta \frac{\partial^2\theta}{\partial z^2} + C_2\theta \frac{\partial\theta}{\partial z} - C_3 \frac{\partial^2\theta}{\partial z^2} - (C_4+C_5) \frac{\partial\theta}{\partial z} - C_6\theta + C_7 \quad .$$

Writing $C_4+C_5 = C_{45}$,

$$\frac{\partial\theta}{\partial t} = C_1\theta \frac{\partial^2\theta}{\partial z^2} + C_2\theta \frac{\partial\theta}{\partial z} - C_3 \frac{\partial^2\theta}{\partial z^2} - C_{45} \frac{\partial\theta}{\partial z} - C_6\theta + C_7 \quad .(3.2.2.7)$$

Equation 3.2.2.7 is the mathematical model that describes the flow of moisture in partially saturated soil. The coefficients $C_1, \ldots, C_7$ have to be estimated to use this equation as a simulation model and estimation procedures are developed in the next section.

Soil water diffusivity, $D(\theta)$ (Childs and Collis-George, 1950), is defined as the product of the hydraulic conductivity, $K(\theta)$, given by equation 3.2.2.1 and the slope of the soil water characteristic curve is found by taking the derivative of equation 3.2.2.2 with respect to θ. The expression for soil water diffusivity can be written as

$$D(\theta) = (C_1\theta - C_3) \tag{3.2.2.8}$$

where C_1 and C_3 are given by equation 3.2.2.6.

The soil water flux, by Darcy's law is expressed as

$$\begin{aligned} \bar{q} &= -D(\theta)\frac{\partial\theta}{\partial z} + K(\theta) \\ &= -(C_1\theta - C_3)\frac{\partial\theta}{\partial z} + (C_5\theta - C_8) \quad . \end{aligned} \tag{3.2.2.9}$$

3.3 Statistical Model to Estimate the Simulation Model Coefficients.

As indicated above the mathematical model developed to simulate the flow of gravitational water is described by equation 3.2.2.7. This equation has six coefficients and they have to be estimated for each depth level from the observed soil moisture data.

For accurate determination of spatial derivatives of moisture content, θ, a polynomial is fit to the values of θ as a function of z and estimates of values of θ at each depth are calculated. These estimated values of θ, for a particular location, are used to determine the quantities $\partial\theta/\partial z$, $\partial^2\theta/\partial z^2$, $\theta\,\partial^2\theta/\partial z^2$ and $\theta\,\partial\theta/\partial z$. Techniques are available (Greville, 1969; Nilson, 1970) to fit spline functions and perform numerical differentiations to a given set of equally spaced or unequally spaced data points.

The mathematical model developed can be viewed under the theory of General Linear Hypothesis Model I of Full Rank (Graybill, 1961) as an analog or prediction model, where $\partial\theta/\partial t$ is a random variable depending on known quantities of θ , $\partial\theta/\partial z$, $\partial^2\theta/\partial z^2$, $\theta\ \partial\theta/\partial z$ and $\theta\ \partial^2\theta/\partial z^2$.

It is assumed that the quantity $\partial\theta/\partial t$ cannot be measured accurately and involves a measurement error. This error is considered to be purely random and unbiased. For example, if n observations

$$\{(\frac{\partial\theta}{\partial t})_i,\ \theta_i,\ (\frac{\partial\theta}{\partial z})_i,\ (\frac{\partial^2\theta}{\partial z^2})_i,\ (\theta\frac{\partial\theta}{\partial z})_i,\ (\theta\frac{\partial^2\theta}{\partial z^2})_i,\ i=1,\ldots,n\}$$

are made either randomly or by design at a point in the porous medium, then

$$(\frac{\partial\theta}{\partial t})_i = (\frac{\partial\Theta}{\partial T})_i + e_i \qquad , \qquad i=1,\ldots,n$$

where

$(\frac{\partial\theta}{\partial t})_i$ = observed value of change in moisture content θ , with time t , at a point z .

$(\frac{\partial\Theta}{\partial T})_i$ = true value of change in moisture content θ , with time at the same point.

e_i = measurement error at point z .

and n = number of observations.

For Case B of model I (Graybill, 1961), it will be considered that the expected value of each e_i is zero, the e_i are uncorrelated, and the e_i have a common unknown variance $\sigma^2_{\partial\Theta/\partial T}$ (Shchigolev, 1965); that is,

$$E(\bar{e}) = \bar{0} \quad , \quad E(\bar{e}\bar{e}^T) = \sigma^2_{\partial\Theta/\partial T}\bar{I}$$

and

$$\mathrm{Cov}(e_i, e_j) = 0 \quad , \quad i=1,\ldots,n \quad , \; j=1,\ldots,n \quad , \quad i \neq j$$

Designating $\partial\theta/\partial t = y$, $\theta\, \partial^2\theta/\partial z^2 = x_1$, $\theta\, \partial\theta/\partial z = x_2$, $\partial^2\theta/\partial z^2 = x_3$, $\partial\theta/\partial z = x_4$, $\theta = x_5$ and $C_7 = x_6$, equation 3.2.2.7 for a particular value of z can be expressed as

$$y_i = C_1(x_1)_i + C_2(x_2)_i - C_3(x_3)_i - C_{45}(x_4)_i + C_6(x_5)_i + (x_6)_i + e_i \quad , \quad i=1,\ldots,n$$

and in the matrix form

$$\bar{Y} = \bar{m}\bar{X} + \bar{e} \quad . \tag{3.3.1}$$

It will be considered that each variable $(x_i, i=1,\ldots,N)$ is known exactly in equation 3.3.1, the parameters $\bar{m}$ are unknown and the probability distribution of e_i is unspecified. Applying the method of least-squares, that is, estimating $\bar{m}$ that minimizes $\bar{e}\bar{e}^T$, we get

$$\frac{\partial}{\partial \bar{m}}(\bar{e}\bar{e}^T) = 2\bar{X}^T\bar{Y} - 2\bar{X}^T\bar{X}\bar{m} = 0 \quad .$$

The least-squares estimate of $\bar{m}$ is therefore

$$\hat{\bar{m}} = (\bar{X}^T\bar{X})^{-1}\bar{X}^T\bar{Y} \quad . \tag{3.3.2}$$

The unbiased estimate of σ^2_y based on the least-squares estimate of $\bar{m}$ is given by

$$\hat{\sigma}^2_y = \frac{\bar{Y}^T\bar{Y} - \hat{\bar{m}}\bar{X}^T\bar{Y}}{(n-N)} \tag{3.3.3}$$

The values of the coefficients change in magnitude and sign from point to point depending on the nature of the non-homogeneity. The set of equations given by 3.2.2.7 with the appropriate coefficients constitute the mathematical simulation model to describe the flow of gravitational water in partially saturated non-homogeneous porous media.

The coefficients $C_1,\ldots,C_N$, in simple terminology, are the regression coefficients. The variables are either first or second space derivatives or their functions and relate to fixed z. The algebraic sign of these coefficients are therefore governed by the algebraic signs of the variables. These variables change in sign depending on the actual moisture profile and the kind of non-homogeneity.

Figure 6(a) shows a plot of θ in natural soil in the field as a function of z at one point in time for a case in which downward flow was maintained through the profile in which a stratum of coarse sand existed between strata of finer material. It is assumed that the contact between coarse and finer materials was not abrupt. This assumption enables one to define the derivative of θ with respect to z. If the stratification was abrupt, the derivative would not exist because θ as a function of z is discontinuous at the contact, even though pressure is continuous. The signs of $\partial\theta/\partial z$ at the upper and lower merger points are opposite in nature. The sign of $\partial^2\theta/\partial z^2$ is negative at the inflection points in the sand.

Figure 6(b) shows a plot of θ as a function of z for the case in which the same stratum of sand was placed between strata of gravel. The signs of $\partial\theta/\partial z$ are different at the two merger points of these materials. But, they are opposite in nature compared to the case in figure 6(a). Similarly the sign of $\partial^2\theta/\partial z^2$ is positive in this case. It is therefore possible that the same type of material may be characterized by the same coefficients with opposite signs depending on its juxtaposition with other types of materials in the strata.

Equation 3.3.2 gives the estimate for the six parameters C_1, C_2, C_3, C_{45}, C_6, C_7 of the mathematical model. These parameters characterize the property of the porous medium at a particular value of z. These parameters at other elevations are calculated to simulate the

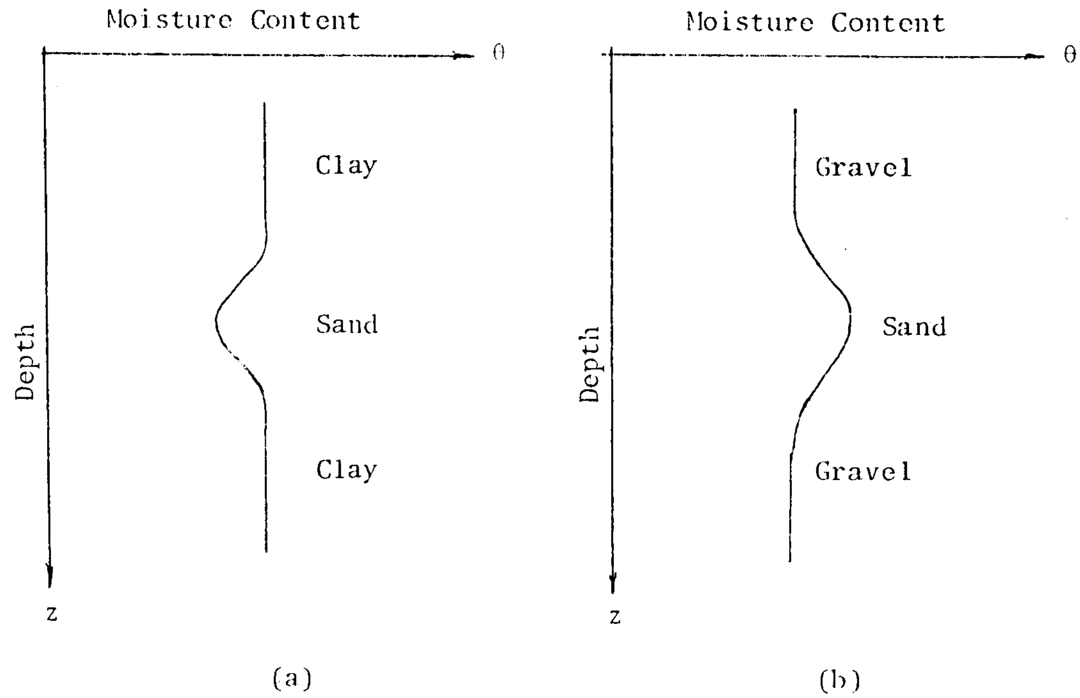

Figure 6. Distribution of moisture content (θ)at one point in time, during downward flow through partially saturated nonhomogeneous soil.

flow through the porous medium. The spatial variation of the parameter C_3 i.e., $\partial C_3/\partial z = C_4$ is calculated by fitting a spline function to the values of C_3. This enables one to find the value of C_5 which is equal to C_{45}-C_4 (section 3.2.2). The value of the parameter C_8 is given by equation 3.2.2.6, and is $C_8 = (C_3 \cdot C_5)/C_1$. The coefficients C_5 and C_8 are not required in the simulation model, however, they are required in determining the unsaturated hydraulic conductivity defined by equation 3.2.2.1.

3.4 Finite-Difference Solution.

Equation 3.2.2.7 has no exact solution; therefore, a Finite-Difference approximation is utilized to allow a numerical solution with a digital computer. Application of the Finite-Difference approach requires subdivision of the gravitational water zone into a system of finite grids.

Approximating equation 3.2.2.7 by the Crank-Nicholson (1947) difference scheme leads to the following expression.

$$\frac{(\theta_j^{t+1}-\theta_j^t)}{\Delta t} = C_{1j}\{\frac{(\theta_j^{t+1}+\theta_j^t)}{2}[(\frac{\theta_{j+1}^t-2\theta_j^t+\theta_{j-1}^t}{2\Delta z^2}) + (\frac{\theta_{j+1}^{t+1}-2\theta_j^{t+1}+\theta_{j-1}^{t+1}}{2\Delta z^2})]\}$$

$$+ C_{2j}(\frac{\theta_j^{t+1}+\theta_j^t}{2})[(\frac{\theta_{j+1}^t-\theta_{j-1}^t}{2\Delta z}) + (\frac{\theta_{j+1}^{t+1}-\theta_{j-1}^{t+1}}{2\Delta z})]$$

$$- C_{3j}[(\frac{\theta_{j+1}^t-2\theta_j^t+\theta_{j-1}^t}{2\Delta z^2}) + (\frac{\theta_{j+1}^{t+1}-2\theta_j^{t+1}+\theta_{j-1}^{t+1}}{2\Delta z^2})]$$

$$- C_{45j}[(\frac{\theta_{j+1}^t-\theta_{j-1}^t}{2\Delta z}) + (\frac{\theta_{j+1}^{t+1}-\theta_{j-1}^{t+1}}{2\Delta z})]$$

$$- C_{6j}(\frac{\theta_j^{t+1}+\theta_j^t}{2}) + C_{7j} \quad . \qquad (3.4.1)$$

The j notation refers to the grid point for which a particular equation is written and the superscript t represents the time level of computation. The Crank-Nicholson differencing scheme averages θ both in time and space. Figure 7 illustrates the physical significance of $\partial\theta/\partial t$.

3.4.1 <u>Computational Technique</u>.

Finite-Difference equations similar to equation 3.4.1 can be written for all the grids, $j=0,1,\ldots,H$. In order to solve the system of non-linear algebraic equations, initial values of θ at time level t for all grids 0 to H and boundary values of θ for all t for the grids 0 and H should be known. The solution of the system of non-linear equations gives the value of θ at time level $t+1$ for all the grids.

A Newton-like method developed by Brown (1969) is adopted to solve the system of non-linear algebraic equations. This method is essentially

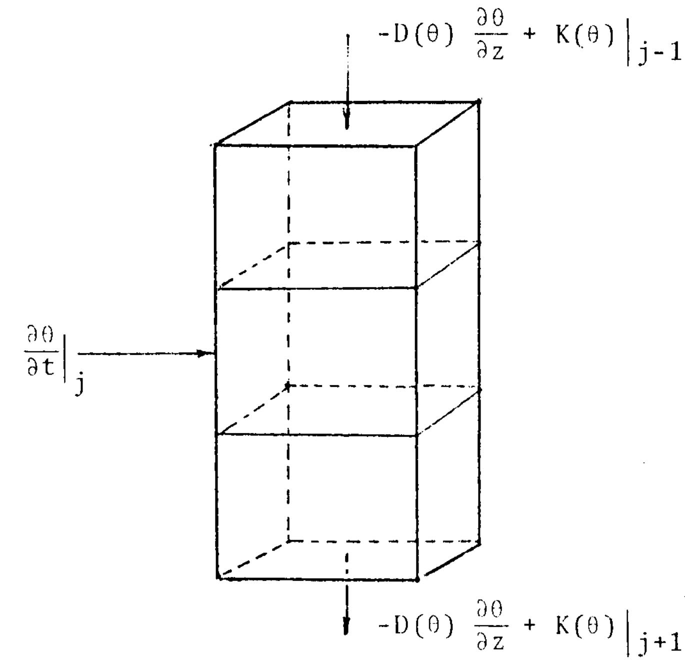

Figure 7. Physical significance of $\partial\theta/\partial t$ in one-dimensional flow equation 3.2.2.7 applied to grid j.

a modified Newton's method based on Gaussian elimination. The iterative procedure developed by him converges and is quadratic in nature. The method is described by Krishnamurthi (1975).

3.4.2 Criteria for Non-Oscillation of Implicit Solution of Partial Differential Equations.

The implicit difference schemes including the Crank-Nicholson scheme under certain conditions become unsatisfactory if the coefficients of the higher order space derivatives are small compared to the coefficients of the lower order ones.

The differential equation developed in this study describing the flow of water in unsaturated soil is given by equation 3.2.2.7. In this equation if the coefficients C_1 , C_2 and C_3 are smaller in value compared to C_{45} and C_6 , the terms $C_{45}\ \partial\theta/\partial z$ and $C_6\theta$ are the controlling factors on the right side of the equation. As a result, the first space derivative over two increments in space, as in the case of Crank-Nicholson scheme, is set equal to the first time derivative over one increment in time. The value of θ_j^t has little influence over spatial derivatives in determining the value of θ_j^{t+1}. Consequently, the value of θ at a given time level oscillates around the true value, though the solutions are considered stable. This can arise even with infinitely small time increments, if the spatial mesh is sufficiently coarse. The extent of this oscillation depends on the relative values of the coefficients $C_1,\ldots,C_7$, Δt and Δz. Price, Varga and Warren (1966) confirm this phenomenon and have developed a method to determine the criteria for the prevention of oscillation of the diffusion-convection equation. The novelty of their results lies in the application of the theory of Oscillatory Matrices of Gantmakher and Krein (1950).

The application of this theory is extended to the mathematical model developed in this study and criteria for non-oscillation of solution have been developed (Appendix C). The criteria are

i) $$\left\{\frac{C_{1j}\theta_j^t - C_{3j}}{\Delta z^2} + C_{6j}\right\} > 0 \qquad (3.4.2.1)$$

and

ii) $$\frac{(C_{1j}\theta_j^t - C_{3j})/\Delta z}{(C_{45j} - C_{2j}\theta_j^t)} > \frac{(C_{45j} - C_{2j}\theta_j^t)}{(C_{1j}\theta_j^t - C_{3j})/\Delta z} > 0 \qquad (3.4.2.2)$$

for $j=0,1,\ldots,H$ and for all t.

3.4.3 Significance of the Criteria for Non-Oscillation of Solutions.

The size of spatial grid Δz indirectly governs the size of time step Δt. The values of the elements of the oscillation matrix A depend on Δz and Δt and should be less than two times the reciprocal of the maximum eigen values of the oscillation matrix for non-oscillatory solution (Appendix C).

It is interesting to note that the criteria for non-oscillation of solutions have a physical meaning. For homogeneous soil, the coefficients C_2 , C_4 and C_6 are zero and the coefficient C_{45} reduces to C_5 . It may be seen that the term $(C_1\theta - C_3)$ represents soil water diffusivity which by definition should be positive for positive values of hydraulic conductivity. The value of C_5 which represents the slope of the linear portion of the curve of the hydraulic conductivity-moisture content relationship, should be positive as hydraulic conductivity increases with increase of moisture content. In other words, the criteria for non-oscillation of Finite-Difference solutions stipulate that the values of hydraulic conductivity, $K(\theta)$ and soil water diffusivity, $D(\theta)$ computed by the simulated value of moisture content, θ should be positive.

For the non-homogeneous soil, the criteria given by equations 3.4.2.1 and 3.4.2.2 ensure that the matrix A (Appendix C) is diagonally dominant.

The magnitude of oscillation depends on the accuracy with which the coefficients of the model are estimated. These coefficients can be determined to a great degree of accuracy, if the hydraulic properties of soil are determined in a laboratory. This procedure involves time and expenditure. Such an approach would be worth the effort if simulation is attempted for a future period of time.

CHAPTER IV

VERIFICATION AND RESULTS OF APPLICATION

4.0 Data Needed for Verification of the Model.

Prior to the application of any model, it must be made certain that it accurately simulates the prototype system. The model is verified when the simulated values of moisture content, hydraulic conductivity and soil water flux compare satisfactorily with similar parameters of the prototype measured either in the field or in the laboratory. The simulated values can also be compared with the exact analytic solution of the model if such a solution is available.

The analytical solutions provided by Philip (1969), Brutsaert (1968) and Parlange (1971) are applicable to homogeneous soils with a uniform initial moisture content and having excess water ponded at the surface. The Parlange solution, though approximate, lends itself easily for verification of a model based on the simplified relationships of moisture content, θ, with capillary pressure head, h, and hydraulic conductivity, K.

4.1 Comparison with Parlange's Solution.

The mathematical model given by equation 3.2.2.7 to simulate flow in non-homogeneous soil has no general analytical solution. The model being versatile, can be verified with an analytical solution for a particular simple solution for flow in homogeneous soil. This will help ensure the validity of the computational techniques and computer program.

Appendix B describes the Parlange solution and the procedure to verify the model for homogeneous soil with simplified linear relationships of θ with $K(\theta)$ and $D(\theta)$. The assumed relationships of θ where $0 \leq \theta \leq 1$ with $K(\theta)$ and $D(\theta)$ are:

$$K(\theta) = C_5 \cdot \theta \tag{4.1.1}$$

and

$$D(\theta) = C_1 \cdot \theta \tag{4.1.2}$$

where C_5 and C_1 are hydraulic conductivity and soil water diffusivity respectively at saturation.

Values of 5cm/day and 250cm^2/day were assumed respectively for C_5 and C_1 for the purpose of verification. The positions of infiltration fronts were calculated for 120 time levels from the solutions of the equations B-7 and B-8 in Appendix B for selected infiltration rates, $C(t)$. The transient soil moisture data which is required as a function of position and time for use in the simulation model were then obtained from the plot of Parlange's solution.

The flow was simulated in this hypothetical homogeneous medium at a given depth for 27 time levels. The values of coefficients C_5 and C_1, simulated values of moisture contents, and the time distribution of flux (recharge) at a particular depth level were obtained from the numerical model of equation 3.2.2.7. The average values for C_5 and C_1 obtained by simulation were respectively 5.1cm/day and 236.4cm^2/day. This compares well with selected values of C_5 = 5.0cm/day and C_1 = 250cm^2/day. The corresponding standard deviations were 1.3cm/day and 82.7cm^2/day.

Figure 8 presents a comparison between the theoretical values of flux obtained for Parlange's solution and computer model values. As can be seen, the percentage deviation between the theoretical values and simulated values are very small and attests to the adequacy of the numerical model. The percentage difference between the theoretical

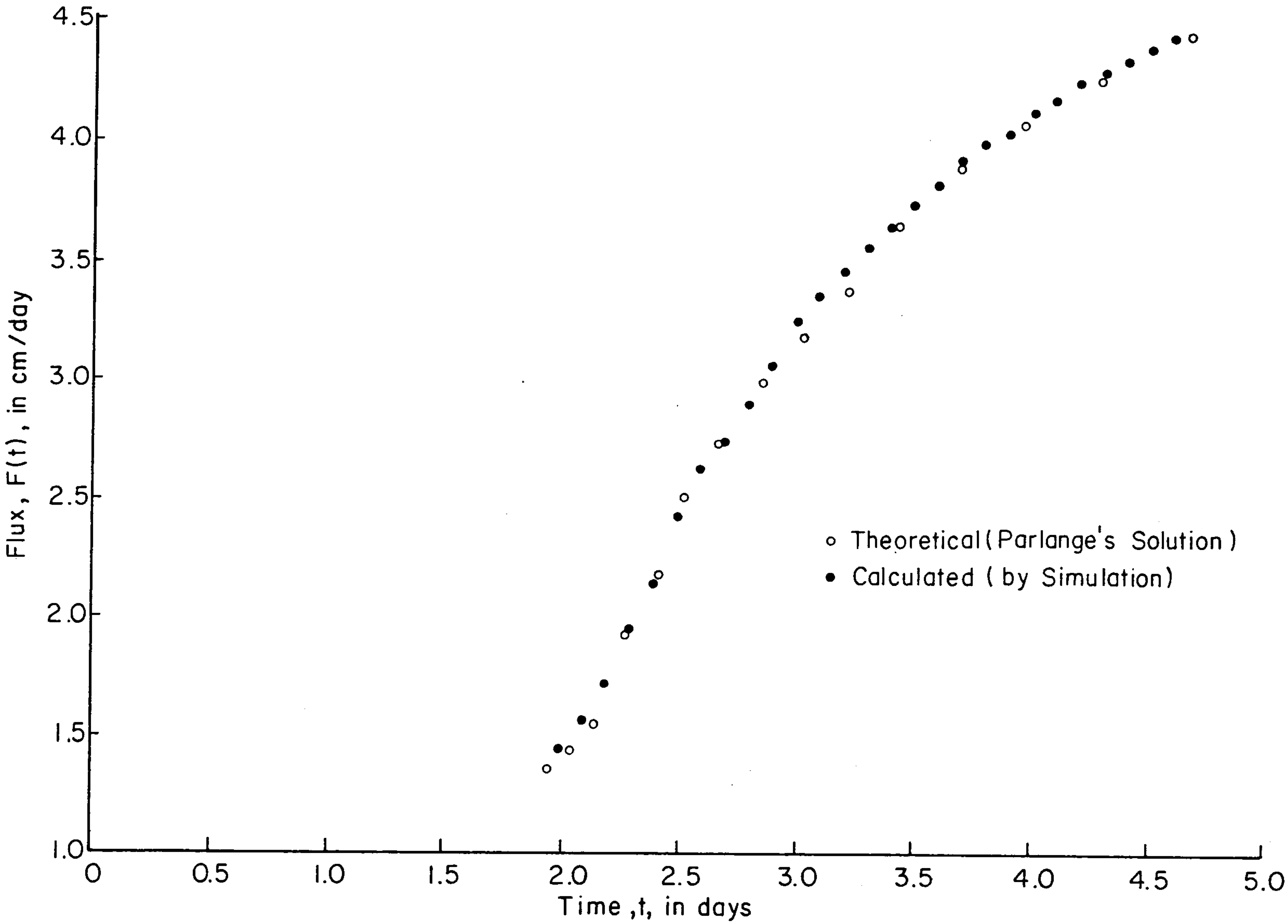

Figure 8. Comparison of flux at one depth level - theoretical (Parlange's solution) versus calculated (by simulation).

values and simulated values of moisture content θ was found to be less than one percent.

The model built on differential structure is highly sensitive to the accuracy of the derivatives, especially second derivatives. Consequently, moisture content should be determined as accurately as possible in order to assume reasonable values of the first and second derivatives of θ with respect to depth.

4.2 Field Data Used for Additional Verification.

Conducting field or laboratory experiments to verify the model would be very expensive. The review of literature showed that Nielsen et al. (1973) conducted field experiments to determine the spatial variability of soil water properties. Infiltration was initiated by ponding water on the experimental plots (20 feet x 20 feet) and steady flow was established. The surface of the plots was covered with sheets of plastic to prevent evaporation when infiltration was terminated. The transient soil moisture data were then collected for the drainage cycle.

Transient soil moisture data for plots 7, 9 and 13 were chosen for use in the verification. The soil water characteristic curves for these plots were found to be approximately linear in most cases for the moisture content values from the 5th day to the 50th day of the drainage cycle. Thirty data points, starting at the 5th day and ending at the 50th day of the drainage cycle, were selected for use in the verification of the model.

4.2.1 Results of Verification.

The mathematical simulation technique was applied to the three plots 7, 9 and 13. Moisture content, hydraulic conductivity and soil water flux were calculated by simulation. Figures 9, 10 and 11 show the com-

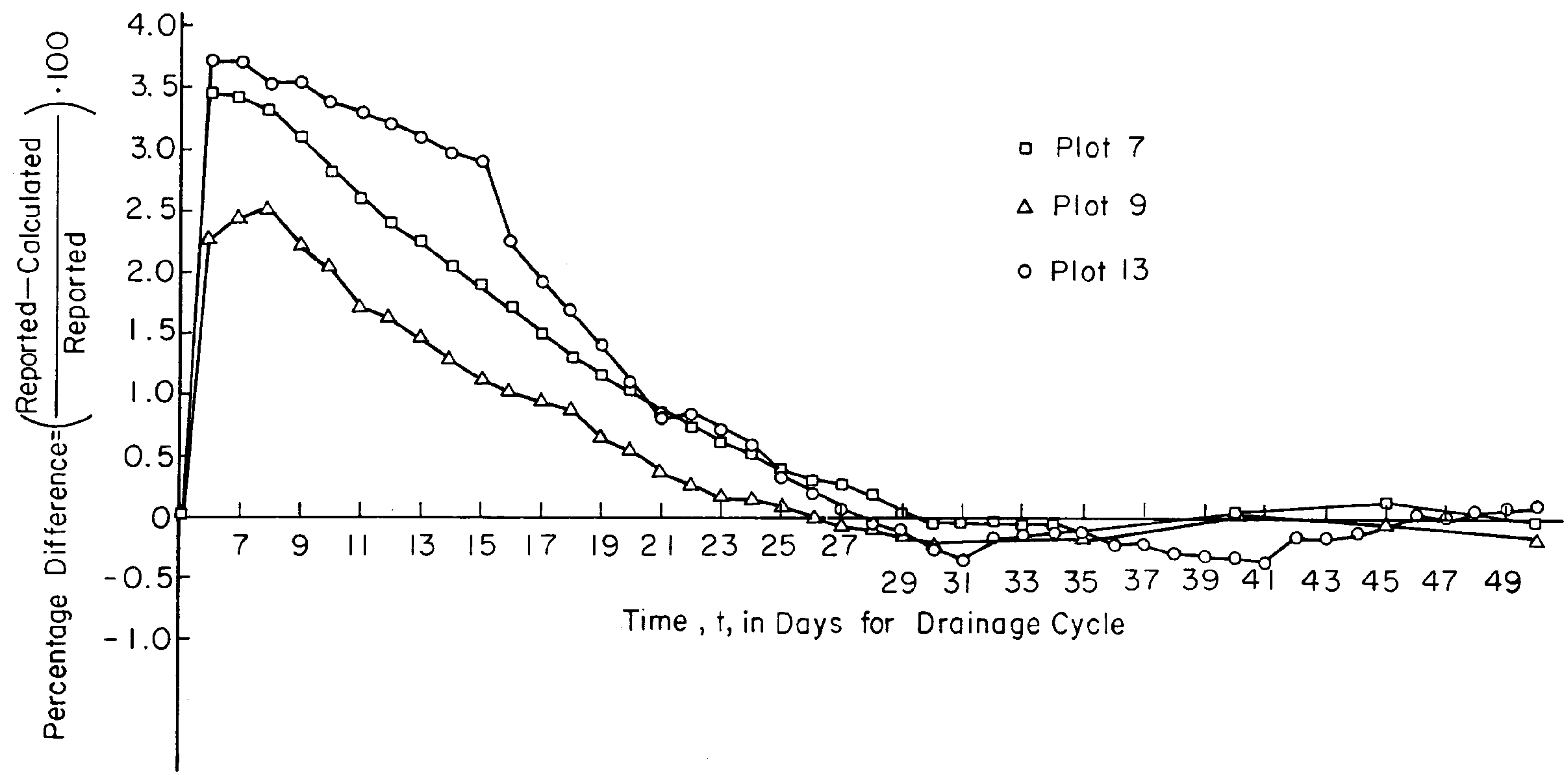

Figure 9. Comparison of moisture content - Reported (Nielsen et al., 1973) versus calculated.

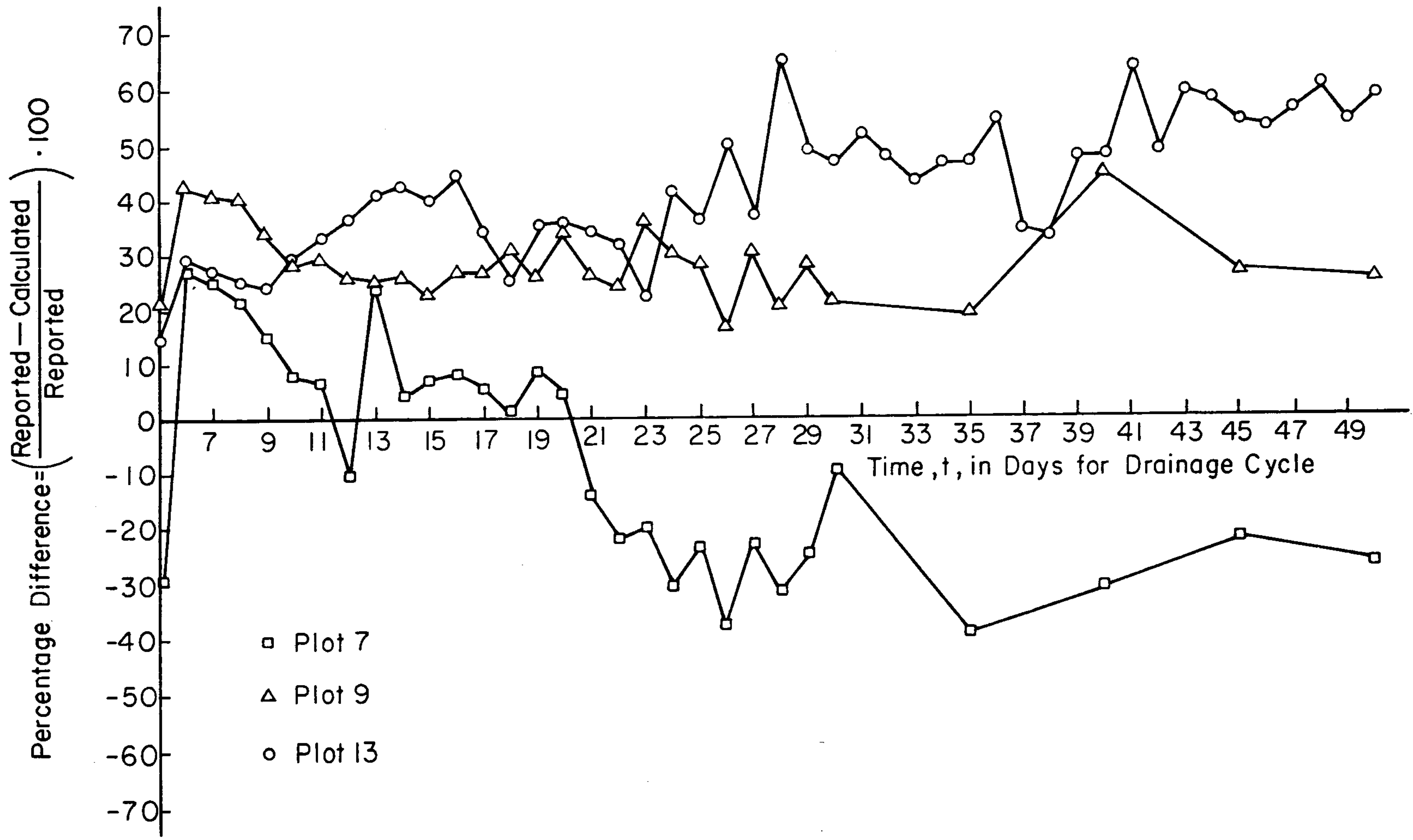

Figure 10. Comparison of hydraulic conductivity - Reported (Neilsen et al., 1973) versus calculated.

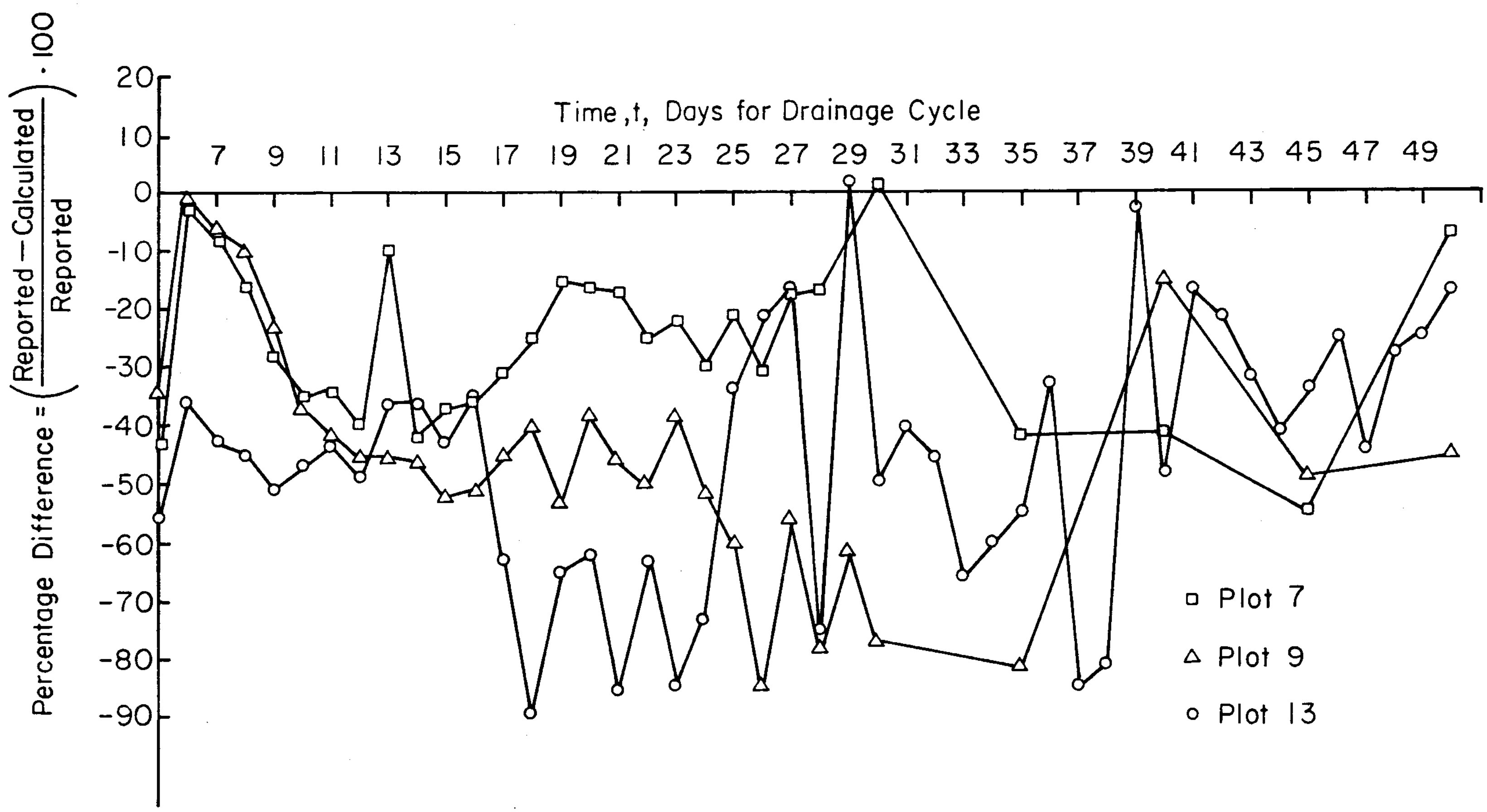

Figure 11. Comparison of soil water flux - Reported (Nielsen et al., 1973) versus calculated.

parison of calculated and reported (computed by Nielsen et al. 1973) values of moisture content, hydraulic conductivity and soil water flux at a 4 foot depth in the experimental plots 7, 9 and 13. Variations between calculated and reported values are found in all cases.

One of the possible reasons for such a variation between calculated and reported values is that the simulation model calculates the flux by Darcy's law (eq3.2.2.9) and assumes that the moisture content within the grid is uniform and the variation of moisture content between the grids is linear. However, Nielsen et al. fitted a spline function to the moisture content data in vertical space for calculating flux and hydraulic conductivity.

The contribution of the diffusivity term to flux was studied in detail for the four foot depth in all the selected plots. In plot 7 the reported values of flux at four foot depth are consistantly lower than the values of hydraulic conductivity. This shows that the diffusivity term does not contribute to downward flux. This becomes obvious from the vertical moisture content profile as the moisture content increases with depth ($\partial\theta/\partial z$ is positive at 4 feet). The calculated values of soil water flux are lower than the calculated values of hydraulic conductivity and this pattern is in agreement with the reported values.

In plots 9 and 13 the calculated values of flux are consistantly higher than the calculated values of hydraulic conductivity. The moisture content profiles for these plots show that $\partial\theta/\partial z$ at four foot depth is negative in these plots. This shows that the diffusivity term contributes to downward flux. Surprisingly, the reported values of flux at four foot depth in plots 9 and 13 are consistently lower than the values of hydraulic conductivity. This explains the big percentage difference between the reported values of hydraulic conductivity and soil water flux to their calculated values using Darcy's law especially for plots 9 and 13. The percentage differences for plot 7 are comparatively smaller.

Judging the results of verification in the light of the foregoing observation, it can be said that the model was verified satisfactorily for non-homogeneous soil, since the magnitudes of errors in the reported values and calculated values were explainable.

4.3 Time Distribution of Natural Groundwater Recharge.

The simulation model developed in this study was applied to three locations within the experimental site of the Central Great Plains Field Station of the USDA-ARS. They were i) near an ephemeral stream course, ii) in a leveled pan, and iii) in fallow land. The computed monthly and yearly values of natural groundwater recharge at these three locations are given in Table 4.1. An average recharge of 4 inches per year is found to exist in this area.

Fig. 12 plots the computed monthly recharge values against time at the three sites. The recharge at the site near the stream course shows large fluctuations of values compared to the recharge through the other two locations. The overall magnitudes of recharge are higher near the stream bed and lower in the fallow land. The fluctuations of recharge from fallow land and the leveled pan are small. The average annual recharge in fallow land was computed to be 2.4 inches. The average annual recharge in the leveled pan was computed to be 4.2 inches. The higher annual recharge in the leveled pan resulted from the diversion of excess surface runoff into the pan and about 5 inches per year in addition to the precipitation falling on the area.

The distribution of recharge for the site near the stream course shows peak values in the months of December, 1969, January, 1970 and

Table 4.1. Computed Distribution of Natural Ground Water Recharge at Three Locations Within the Central Great Plains Field Station Area Near Akron, Colorado.

	Recharge in inches of water					
	Stream course USDA well no. 5		Leveled pan USDA well no. 8		Fallow land USDA well no. 9	
Time (1)	Monthly recharge (2)	Yearly recharge (3)	Monthly recharge (4)	Yearly recharge (5)	Monthly recharge (6)	Yearly recharge (7)
Nov '69	1.263		0.354		0.164	
Dec '69	0.854		0.394		0.153	
Jan '70	0.498		0.437		0.144	
Feb '70	0.343		0.486		0.138	
Mar '70	0.340		0.516		0.140	
Apr '70	0.391		0.452		0.151	
May '70	0.386		0.304		0.162	
Jun '70	0.232		0.222		0.164	
Jul '70	0.104		0.267		0.155	
Aug '70	0.076		0.336		0.137	
Sep '70	0.085		0.352		0.127	
Oct '70	0.214		0.336		0.133	
Nov '70	0.394		0.301		0.145	
Dec '70	0.508		0.277		0.154	
1970		3.571		4.286		1.750
Jan '71	0.526		0.266		0.157	
Feb '71	0.500		0.266		0.154	
Mar '71	0.496		0.274		0.144	
Apr '71	0.568		0.282		0.137	
May '71	0.645		0.277		0.161	
Jun '71	0.647		0.268		0.218	
Jul '71	0.558		0.294		0.248	
Aug '71	0.416		0.346		0.237	
Sep '71	0.328		0.373		0.235	
Oct '71	0.327		0.376		0.252	
Nov '71	0.374		0.358		0.285	
Dec '71	0.421		0.343		0.319	
1971		5.806		3.723		2.547
Jan '72	0.445		0.335		0.346	
Feb '72	0.435		0.334		0.364	
Mar '72	0.414		0.337		0.372	
Apr '72	0.407		0.344		0.370	
May '72	0.433		0.354		0.361	
Jun '72	0.486		0.366		0.346	
Jul '72	0.516		0.377		0.329	
Aug '72	0.467		0.387		0.312	
Sep '72	0.310		0.392		0.296	
Oct '72	0.030		0.388		0.282	
Nov '72	0.022		0.376		0.270	
Dec '72	0.455		0.357		0.262	
1972		4.420		4.347		3.910
Jan '73	0.959		0.334		0.259	
Feb '73	1.323		0.309		0.261	
Mar '73	1.417		0.284		0.270	
Apr '73	1.192		0.269		0.283	
May '73	0.723		0.297		0.294	
Jun '73	0.273		0.341		0.300	
Jul '73	0.121		0.370		0.303	
Aug '73	0.133		0.386		0.303	
Sep '73	0.065		0.394		0.304	
Oct '73	0.019		0.395		0.307	
Nov '73	0.035		0.393		0.309	
Dec '73	0.047		0.389		0.312	
1973		6.307		4.161		3.505
Jan '74	0.069		0.383		0.314	
Feb '74	0.128		0.375		0.315	
Mar '74	0.205		0.366		0.312	
Apr '74	0.259		0.355		0.304	
May '74	0.250		0.344		0.288	
Jun '74	0.201		0.338		0.268	
Jul '74	0.142		0.337		0.246	
Aug '74	0.019		0.303		0.195	

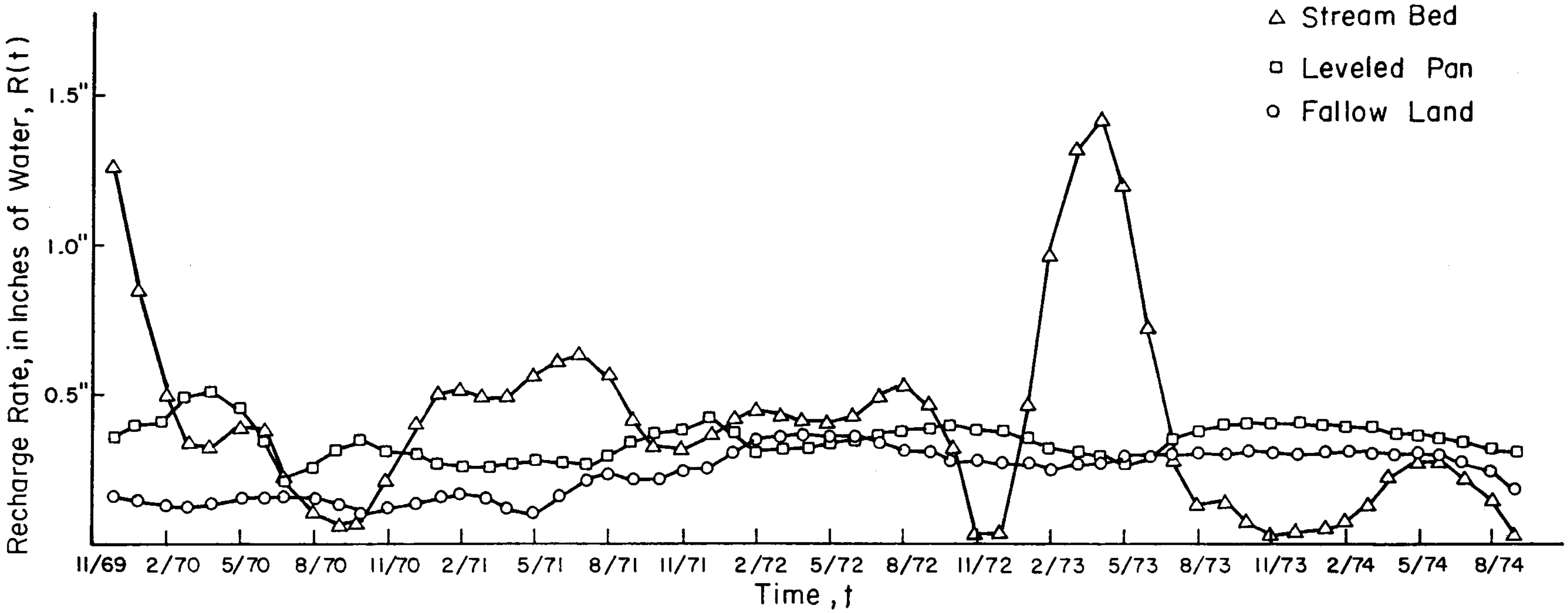

Figure 12. Monthly distribution of natural ground water recharge.

during the months February-June 1973. In the years 1969 and 1973 there was heavier precipitation in spring and summer compared to other years of the study. The precipitation in spring 1973 was intense and combined with the effects of snowmelt, the ephemeral stream was flowing a few times during this period. The recharge of about 1-1½ inches per month during February-June 1973 strongly suggests that this was due to stream flow during this period. The peak recharge in December 1969 might relate to the heavy precipitation events in the summer of that year. Flow was not reported in the stream during this period and it could be possible that the precipitation infiltrated into the soil in May of 1969 and showed up as recharge in December, 1969 and January 1970.

4.3.1 Comparison with the Results of Reddell (1967).

Reddell used a Finite-Difference steady-state method to determine the areal distribution of yearly natural recharge over the entire High Plains of Colorado. The Central Great Plains Field Station lies in the area where an average yearly recharge of 1-2 inches was computed by Reddell. His model assumed that the state of dynamic equilibrium existed in the Ogallala formation which is the main aquifer of the area. This meant that the average recharge was balanced by an equal amount of natural discharge. His model could be interpreted to compute the values of natural recharge and its areal distribution to maintain the state of dynamic equilibrium within the aquifer.

Before the year 1957, the aquifer was not fully developed and the assumption that the aquifer was in dynamic equilibrium might be valid. The state of dynamic equilibrium no longer exists after the large scale development of the aquifer. There are changes in water table elevations (Hofstra, 1971) in all parts of the High Plains. In the Central Great

Plains area near Akron, an increase of water table elevation from 0-4 feet was reported during the period 1964-71. This was confirmed by the observation of water table elevations at wells 5, 8 and 9 respectively near the ephemeral stream course, in the leveled pan and in the fallow land. Figure 13 plots water table elevations in these wells against time. An increase in water table elevation up to 3 feet was noticed in these wells during the period 1969-74. The rise of water table was not uniform during the 5 year period of the study. A rise of 2 feet occurred during the last year. During the first four years, the water table rose by 1 foot. This pattern seemed to agree generally with distribution of recharge through the location near the ephemeral stream. The water table level responded similarly in all the three wells irrespective of the rates of recharge through the respective locations. This was obvious because of nearness of these three locations and groundwater flow in the north-easterly direction forming a common phreatic surface. This strongly suggests that the area gets recharge through the two ephemeral streams running east-west, one each on the southern and northern parts of the area.

An annual recharge of 1-2 inches is required in this area to maintain the water table at the existing level. This is in accordance with Reddell's (1967) model developed on the basis of dynamic equilibrium. The continuous rise of the water table in this area justifies the higher recharge computed by the technique developed in this study.

4.4 Use of Mathematical Model for Predicting Future Recharge and Development of Areal Structure.

The mathematical model developed in this study expressed in equation 3.2.2.7 is a second order, non-linear, parabolic partial differential

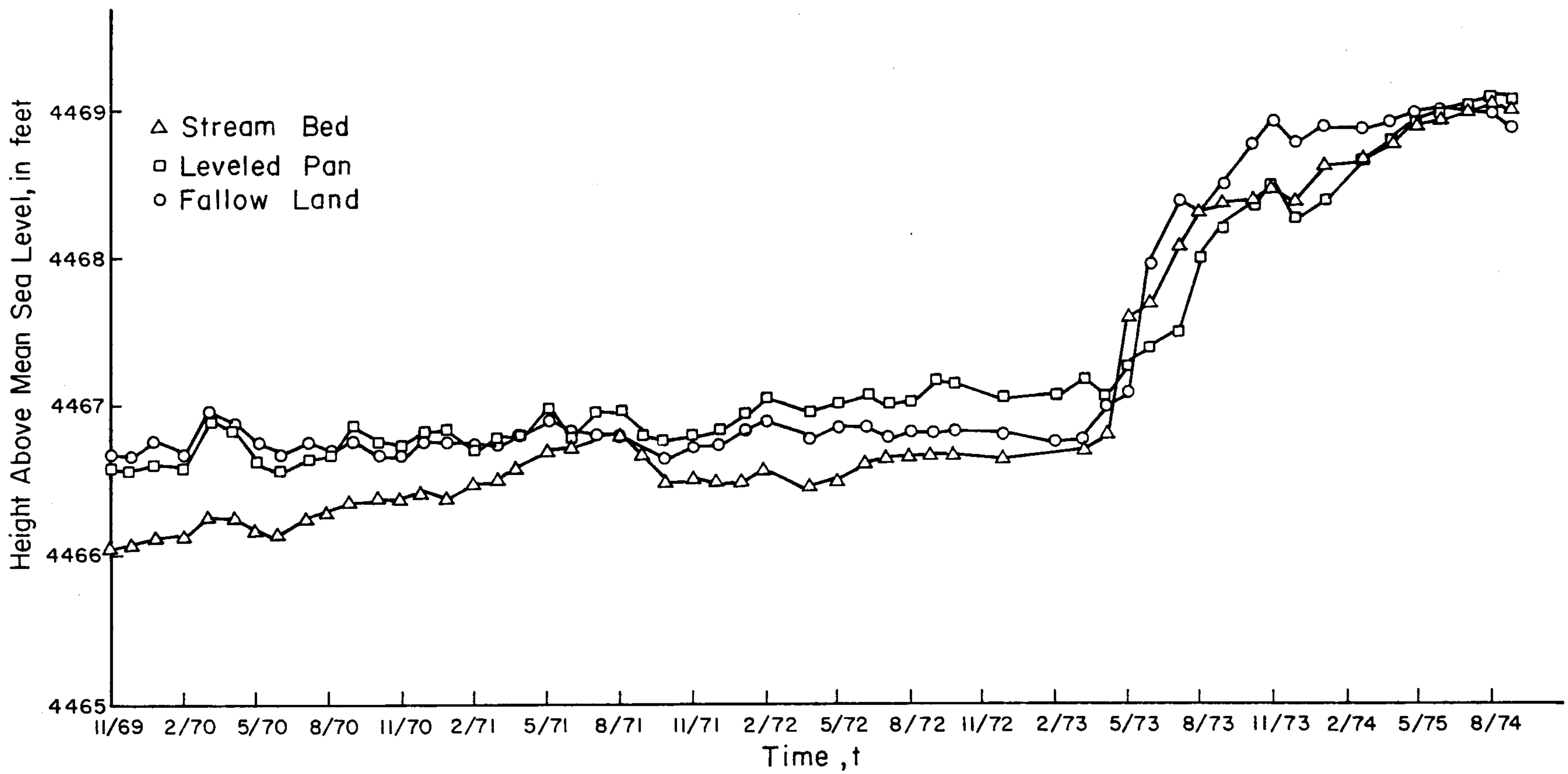

Figure 13. Water level changes in the experimental wells (USDA-ARS, Annual Reports).

equation and requires two boundary conditions besides initial condition for solution. For use of the model for future periods of time, the two boundary conditions must be specified. It is possible to use the water table as the lower boundary. The determination of moisture content at the upper boundary is difficult. Chien (1972) developed a stochastic model for movement of moisture within vadose media. The shortcoming of his approach was that he used a linear stochastic model to describe flow in partially saturated soil described by Richards' equation which is a highly non-linear partial differential equation. A linear stochastic model is applicable if the Richards' equation is linearized by suitable transformation of the variable, θ . It would then become possible to use existing precipitation models to determine the moisture content at the upper boundary. This constitutes a separate study by itself and such a study is strongly recommended.

For use of the mathematical model at other locations, the characteristic curves for the soil at these locations must be known besides initial and boundary conditions. Once time distributions of recharge at different locations are determined, techniques (Rayner, 1967; Karplus, 1972) are available to develop an areal structure.

The difference in the values of precipitation series and recharge series is a measure of water available for artificial recharge. The identification of the system is possible once the input (precipitation series) and output (recharge series) are known. The identification can be characterized by natural parameters like soil type, topography and plant cover. Complete topographic maps and soil survey maps are not available for the High Plains of Colorado. And, therefore, objective number 3 of the proposal could not be evaluated.

4.5 Computer Program.

A Fortran IV computer program was developed to determine the time distribution of natural groundwater recharge at one station. The program required moisutre content data measured as a function of vertical position and time at one station. The main program RECHAR utilized twenty-one subroutine subprograms and one function subprogram. Flow charts and a computer program listing were included in the dissertation by Krishnamurthi (1975). He also presented data on the computer time required for solving the various phases of the problem.

V. CONCLUSIONS AND RECOMMENDATIONS

The first objective of the research proposal was to develop a technique to determine the time distribution of natural groundwater recharge from a suitable descriptor of the process. This objective was totally fulfilled by the development of a mathematical model using transient soil moisture data as the descriptor of recharge. The technique was verified both by analytical solution and experimental data. The second objective was successfully accomplished by application of the technique to an experimental site of the USDA-ARS on the High Plains of Colorado. The time distribution of natural recharge computed using the technique compared favorably with the results of Reddell (1967). With regard to the third objective, complete topographic and soil data for the High Plains of Colorado were not available. Accordingly, an accurate evaluation of the use of soils maps for selecting artificial recharge sites could not be undertaken.

To apply the technique to other locations and for future periods of time, characteristic curves of the soil in these locations, initial and boundary conditions to solve the mathematical model must be known. Techniques are available to develop an areal structure from point time series data. Identification of parameters from precipitation series (input) and recharge series (output) is possible adopting existing techniques of system analysis.

5.1 Conclusions.

i) A mathematical model was developed to simulate the flow of gravitational water in non-homogeneous soil using transient soil moisture data. The simulation model assumed that the moisture content of unsaturated soil below the zone of influence of evapotranspiration varied in the linear range of the soil water characteristic curve. The coefficients of the model characterize the hydraulic propoerties of soil and their spatial variability.

ii) The model was verified for homogeneous soil using the analytical solution of Parlange (1971). The agreement was very good.

iii) The model was verified for non-homogeneous soil using field results of Nielsen et al. (1973). The magnitude of errors in the values calculated by simulation and in the values reported was similar and the possible reasons for the differences were expressed.

iv) The technique was applied to determine the time distribution of natural ground water recharge at three locations within the experimental site of the Central Great Plains Field Station of USDA-ARS, near Akron, Colorado. An average annual recharge of four inches was found to exist in that area. This was higher than the values of Reddell (1967). A water table rise of 3 feet in this area during the study period coincided with the higher values of recharge obtained by the developed model.

v) Use of this technique for other locations and for prediction of future recharge is possible if the hydraulic properties of soil and initial and boundary conditions are specified.

5.2 Recommendations

i) Research efforts for development of a procedure to predict the recharge using the simulation approach is urged.

ii) Laboratory experiments to verify the model for non-homogeneous soil are recommended.

iii) The model built on differential structure is highly sensitive to derivatives, especially to second derivatives. Accurate determination of spatial derivatives is possible if moisture detection by continuous logging equipment is made.

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APPENDIX A

A STOCHASTIC MODEL FOR RECHARGE USING WATER TABLE AS DESCRIPTOR

Precipitation occurs as a random variable and the resulting natural groundwater recharge should also be a random variable. Therefore, natural ground water recharge is a stochastic process. It is assumed that the deterministic component of a water table time series can be removed by standard procedures and the random component describes the recharge process. Identification of water table fluctuations and their removal from time series data due to external pumping, deep seepage from irrigation and barometric pressure variations are difficult in the absence of accurate data. However, an approximate estimation of total recharge by a stochastic model is possible if water table time series data exist for a long period of time for a virgin aquifer.

The phenomenon of fluid motion in one dimension in an unconfined aquifer is described by the following partial differential equation.

$$\frac{\partial}{\partial x} \left(Kh \frac{\partial H}{\partial x}\right) = S_y \frac{\partial H}{\partial t} - R \qquad \text{A.1}$$

where

K = hydraulic conductivity

h = Aquifer's saturated thickness

H = Water table elevation above datum

S_y = Specific yield

R = Recharge Rate

t = Time

x = Spatial coordinate .

Assuming that the aquifer is homogeneous and the water table fluctuations are small compared to aquifer thickness, h, it is possible to remove h from within the partial derivative which essentially linearizes equation A.1 to

$$Kh \frac{\partial^2 H}{\partial x^2} = S_y \frac{\partial H}{\partial t} - R \qquad \text{A.2}$$

Finite differencing the equation A.2 using an explicit difference scheme results in

$$\frac{Kh}{\Delta x^2} (H^t_{x+\Delta x} - 2H^t_x + H^t_{x-\Delta x}) = \frac{S_y}{\Delta t} (H^{t+1}_x - H^t_x) - (\frac{R^{t+1} + R^t}{2}) \qquad \text{A.3}$$

Designating

$$\frac{2\Delta t \ Kh}{\Delta x^2} = \alpha \qquad \text{A.4}$$

$$2S_y = \delta \qquad \text{A.5}$$

and

$$\Delta t \ (R^{t+1} + R^t) = r^{t+1} + r^t \qquad \text{A.6}$$

and substituting equations A.4, A.5 and A.6 in equation A.3, we have

$$\alpha(H^t_{x+\Delta x} - 2H^t_x + H^t_{x-\Delta x}) = \delta(H^{t+1}_x - H^t_x) - r^{t+1} - r^t \qquad \text{A.7}$$

Assuming

$$H_x = \overline{H}_x + \lambda_x$$

$$H_{x+\Delta x} = \overline{H}_{x+\Delta x} + \mu_{x+\Delta x}$$

$$H_{x-\Delta x} = \overline{H}_{x-\Delta x} + \psi_{x-\Delta x}$$

$r = \overline{r} + \Omega_x$ and substituting these in

equation A.7 we have

$$\delta(\overline{H}_x + \lambda_x^{t+1}) = (\delta - 2\alpha)\ (\overline{H}_x + \lambda_x^t) + \alpha\ (\overline{H}_{x+x\Delta x} + \overline{H}_{x-\Delta x} + \mu^t_{x+\Delta x} + \psi^t_{x-\Delta x})$$

$$+ 2\overline{r} + \Omega_x^{t+1} + \Omega_x^t \qquad \text{A.7}$$

or,

$$\lambda_x^{t+1} = (\frac{\delta-2\alpha}{\delta})\ \lambda_x^t + \frac{1}{\delta}\ \{-2\alpha\overline{H}_x + 2\overline{r} + \alpha\ (\overline{H}_{x+\Delta x} + \overline{H}_{x-\Delta x})$$

$$+\alpha\ (\mu^t_{x+\ x} + \psi^t_{x-\Delta x} + \Omega_x^{t+1} + \Omega^t_x)\ \} \qquad \text{A.8}$$

Equation A.8 is analogous to a first order auto regressive model where λ_x is the stochastic variable and $(\frac{\delta-2\alpha}{\delta})$ is the autoregressive coefficient. The other terms in equation A.8 constitute "noise" and it is assumed that it is "white".

The expected value of the "white noise" terms should be zero and

$$\varepsilon\{\frac{1}{\delta}[-2\alpha\overline{H}_x + 2\overline{r} + \alpha(\overline{H}_{x+\Delta x} + \overline{H}_{x-\Delta x}) + \alpha(\mu^t_{x+\Delta x} + \psi^t_{x-\Delta x})$$

$$+ \Omega^{t+1}_x + \Omega^t_x]\} = 0$$

or,

$$\frac{1}{\delta}\{-2\alpha\overline{H}_x + 2\overline{r} + \alpha(\overline{H}_{x+\Delta x} + \overline{H}_{x-\Delta x})\} + \varepsilon\{\alpha(\mu^t_{x+\Delta x} + \psi^t_{x-\Delta x})$$

$$+ \Omega^{t+1}_x + \Omega^t_x\} = 0 \qquad \text{A.9}$$

From equation A.9, it is evident that

$$-2\alpha\overline{H}_x + 2\overline{r} + \alpha(\overline{H}_{x+\Delta x} + \overline{H}_{x-\Delta x}) = 0$$

$$\overline{r} = \frac{\alpha}{2}(2\overline{H}_x - \overline{H}_{x+\Delta x} - \overline{H}_{x-\Delta x}) \qquad \text{A.10}$$

Time series analysis of water table data yields the coefficient $(\frac{\delta-2\alpha}{\delta})$. For known values of δ, α can be calculated.

Equation A.10 gives the recharge during the discrete time Δx, where $\overline{H}_{x-\Delta x}$, $\overline{H}_x$ and $\overline{H}_{x+\Delta x}$ are the average water table elevations adjusted for the effects of external pumping, deep seepage and other causes at three locations Δx apart in the direction of flow.

Equation similar to A.10 can be developed for two dimensional flow equation.

The model is ideally suited for virgin aquifers and to aquifers where accurate data on pumping, seepage and pressumer variations are available.

APPENDIX B

SOLUTION TO THE ONE-DIMENSIONAL INFILTRATION EQUATION

The infiltration process due to forces of gravity and gradient of water pressure is described by (Philip, 1969)

$$\frac{\partial z}{\partial t} + \frac{\partial}{\partial \theta}\left[\frac{D(\theta)}{(\partial z/\partial \theta)}\right] = \frac{dK(\theta)}{d\theta} \qquad \text{B-1}$$

where $D(\theta)$ is the soil water diffusivity and $K(\theta)$ the hydraulic conductivity; $z(\theta,t)$ is the position or depth of a point in a homogeneous one-dimensional field where the moisture content is θ at time, t . Parlange (1971) derived an analytical solution to equation B-1 using the following conditions:

$$\begin{aligned} &t=0\ , \quad z>0\ , \quad \theta=0 \\ &t\geq 0\ , \quad z=0\ , \quad \theta=1 \end{aligned} \qquad \text{B-2}$$

This approximate solution, valid for all times, is expressed in the following two equations;

$$t = \int_0^1 \frac{\theta D(\theta)}{K^2(\theta)} \left\{ \ln \frac{K(\theta)+C(t)}{C(t)} - \frac{K(\theta)}{K(\theta)+C(t)} \right\} d\theta \qquad \text{B-3}$$

and

$$z = -\int_\theta^1 \frac{D(\theta)d\theta}{K(\theta)+C(t) \int_0^\theta \left\{ \int_\theta^1 \frac{D(\theta)d\theta}{[K(\theta)+C(t)]^2} \right\} d\theta \Big/ \int_0^1 \left\{ \int_\theta^1 \frac{D(\theta)d\theta}{[K(\theta)+C(t)]^2} \right\} d\theta} \qquad \text{B-4}$$

where $C(t)$ is the infiltration rate and is a function of time. The advantage of this solution is that values of z and t for selected θ can be easily obtained for known function of $K(\theta)$ and $D(\theta)$.

The mathematical model expressed in equation 3.2.2.7 was based upon the assumption that the moisture content, θ varies linearly with both capillary pressure, $p_c/\rho g$ and hydraulic conductivity, $K(\theta)$. These linear relations are given in equations 3.2.2.2 and 3.2.2.1 respectively. For the purpose of checking the computer program, simplified relationships of θ with $D(\theta)$ and $K(\theta)$ are assumed in the Parlange solution to be

$$D(\theta) = C_1 \cdot \theta \tag{B-5}$$

and

$$K(\theta) = C_5 \cdot \theta \tag{B-6}$$

where C_1 and C_5 are specified coefficients.

Equations B-5 and B-6 are substituted in equations B-3 and B-4 and upon integration equation B-3 reduces to

$$t = \frac{C_1}{C_5^{\,3}} \{C_5 + 2C(t)\} \cdot \ell n\{ \frac{C_5 + C(t)}{C(t)} \} - \frac{2C_1}{C_5^{\,2}} \tag{B-7}$$

and equation B-4 becomes

$$z = -\int_{\theta}^{1} \frac{C_1 \theta d\theta}{C_5\theta + \{C(t)\theta[1 + \frac{C(t)}{C(t)+C_5} + \ell n \frac{C(t)+C_5}{C(t)+C_5\theta}] - \frac{2C^2(t)}{C_5}[\ell n \frac{C(t)+C_5\theta}{C(t)}]\} \Big/ 1 + \frac{C(t)}{C(t)+C_5} + \frac{2C(t)}{C_5} \ell n[\frac{C(t)}{C(t)+C_5}]} \tag{B-8}$$

For an assumed value of $C(t)$ $(C(t) \leq -C_5)$, equation B-7 gives the value of time, t. To determine the position, z at the computed time, t for different values of θ, equation B-8 has to be integrated numerically with appropriate lower limits for θ. The computation is repeated for other values of $C(t)$ to obtain a plot of infiltration front at different time levels.

Moisture content data, θ, as a function of position, z, and time, t, are required for the purpose of using the simulation model developed in the study. The solutions of equations B-7 and B-8 give the position, z as a function of θ and t. The analytical data $\theta(z,t)$, can be obtained from the solutions for $z(\theta,t)$ by developing a graph of the position of the wetting front with time.

The analytical data obtained in the fashion described above is used in the computer program and the coefficients C_1 and C_5 calculated by the model is compared with those originally specified in Parlange's equation and a comparison between the model and Parlange's solution can be obtained.

APPENDIX C

CRITERIA FOR NON-OSCILLATION OF IMPLICIT SOLUTION

The spatial finite difference approximation of equation 3.2.2.7 for grids $j=0,1,\ldots,H$, where H is the number of grids, is

$$\left(\frac{\partial\theta}{\partial t}\right)_j^{t+1} = C_{1j}\{\left(\frac{\theta_j^{t+1}+\theta_j^t}{2}\right)[\left(\frac{\theta_{j+1}^t-2\theta_j^t+\theta_{j-1}^t}{2\Delta z^2}\right) + \left(\frac{\theta_{j+1}^{t+1}-2\theta_j^{t+1}+\theta_{j-1}^{t+1}}{2\Delta z^2}\right)]\}$$

$$+ C_{2j}\left(\frac{\theta_j^{t+1}+\theta_j^t}{2}\right)[\left(\frac{\theta_{j+1}^t-\theta_{j-1}^t}{2\Delta z}\right) + \left(\frac{\theta_{j+1}^{t+1}-\theta_{j-1}^{t+1}}{2\Delta z}\right)]$$

$$- C_{3j}[\left(\frac{\theta_{j+1}^t-2\theta_{j-1}^t+\theta_{j-1}^t}{2\Delta z^2}\right) + \left(\frac{\theta_{j+1}^{t+1}-2\theta_j^{t+1}+\theta_{j-1}^{t+1}}{2\Delta z^2}\right)]$$

$$- C_{45j}\left(\frac{\theta_{j+1}^t-\theta_{j-1}^t}{2\Delta z}\right) + \left(\frac{\theta_{j+1}^{t+1}-\theta_{j-1}^t}{2\Delta z}\right) - C_{6j}\left(\frac{\theta_j^{t+1}+\theta_j^t}{2}\right) + C_{7j} \quad .$$

Assuming that the coefficients $C_{1j}\{(\theta_{j+1}^{t+1}+\theta_j^t)/2\}$ and $C_{2j}\{(\theta_j^{t+1}+\theta_j^t)/2\}$ are held constant for each time increment at the values they have at the beginning of the increment, which essentially linearizes the equation within the time increment and rearranging the terms, we get

$$\left(\frac{\partial\theta}{\partial t}\right)_j^{t+1} = \theta_{j-1}^{t+1}\{\frac{C_{1j}\theta_j^t}{2\Delta z^2} - \frac{C_{2j}\theta_j^t}{2\Delta z} - \frac{C_{3j}}{2\Delta z^2} + \frac{C_{45j}}{2\Delta z}\}$$

$$- \theta_j^{t+1}\{\frac{C_{1j}\theta_j^t}{\Delta z^2} - \frac{C_{3j}}{\Delta z^2} + \frac{C_{6j}}{2}\} + \theta_{j+1}^{t+1}\{\frac{C_{1j}\theta_j^t}{2\Delta z^2} + \frac{C_{2j}\theta_j^t}{2\Delta z} - \frac{C_{3j}}{2\Delta z^2} - \frac{C_{45j}}{2\Delta z}\}$$

$$+ \theta_{j-1}^t\{\frac{C_{1j}\theta_j^t}{\Delta z^2} - \frac{C_{2j}\theta_j^t}{2\Delta z} - \frac{C_{3j}}{2\Delta z^2} + \frac{C_{45j}}{2\Delta z}\}$$

$$- \theta_j^t\{\frac{C_{1j}\theta_j^t}{\Delta z^2} - \frac{C_{3j}}{\Delta z^2} + \frac{C_{6j}}{2}\} + \theta_{j+1}^t\{\frac{C_{1j}\theta_j^t}{2\Delta z^2} + \frac{C_{2j}\theta_j^t}{2\Delta z} - \frac{C_{3j}}{2\Delta z^2} - \frac{C_{45j}}{2\Delta z}\}$$

$$- \frac{C_{6j}\theta_j^t}{2} + C_{7j} \quad .$$

In the above equation, the terms with superscipt t are known at the beginning of the time increment and held constant during the time interval. Lumping these known values with C_{7j} and designating the sum as S_j and setting

i) $\dfrac{C_{1j}\theta_j^t - C_{3j}}{2\Delta z^2} = \delta_{1j}$ and

ii) $\dfrac{C_{45j} - C_{2j}\theta_j^t}{2\Delta z} = \delta_{2j}$

and rewriting the equation

$$\left(\frac{\partial\theta}{\partial t}\right)_j^{t+1} = \theta_{j-1}^{t+1}\{\delta_{1j}+\delta_{2j}\} - \theta_j^{t+1}\{\delta_{1j}+\frac{C_{6j}}{2}\} + \theta_{j+1}^{t+1}\{\delta_{1j}-\delta_{2j}\} + S_j \quad .$$

This set of difference equations for $j=0,1,\ldots,H$ can be written in matrix form as

$\left(\frac{\partial\bar{\Theta}}{\partial T}\right)^{t+1} = -\bar{A}\bar{\Theta}^{t+1} + \bar{B}$, for $t>0$ where $\bar{A}$ is a real matrix of size $H+1,H+1$ and $\bar{\Theta}^{t+1}$ and $\bar{B}$ are column vectors with $H+1$ components given by

$$\bar{A} = \left|\begin{array}{cccccc} \{\delta_{1j}+\frac{C_{6j}}{2}\}, & -\{\delta_{1j}-\delta_{2j}\}, & \cdots & & & \\ -\{\delta_{1j}+\delta_{2j}\} & , \{\delta_{1j}+\frac{C_{6j}}{2}\} & , -\{\delta_{1j}-\delta_{2j}\} & , \cdots & & \\ & \cdots & \cdots & \cdots & \cdots & \\ & & \cdots & \cdots & \cdots & \\ & & & \cdots & \cdots & \\ & & & -\{\delta_{1j}+\delta_{2j}\} & , \{\delta_{1j}+\frac{C_{6j}}{2}\} & , -\{\delta_{1j}-\delta_{2j}\} \\ & & & & , -\{\delta_{1j}+\delta_{2j}\} & , \{\delta_{1j}+\frac{C_{6j}}{2}\} \end{array}\right|$$

$$\bar{\Theta}^{t+1} = \begin{vmatrix} \theta_0^{t+1} \\ \theta_1^{t+1} \\ \cdot \\ \cdot \\ \cdot \\ \theta_H^{t+1} \end{vmatrix} \quad \text{and} \quad \bar{B} = \begin{vmatrix} S_0 \\ S_1 \\ \cdot \\ \cdot \\ \cdot \\ S_H \end{vmatrix}$$

Our objective in this analysis is to show that the matrix $\bar{A}$ has positive real and distinct eigen values for certain values of δ_{1j}, δ_{2j} and C_{6j} which makes the solution non-oscillatory.

Let $\bar{D}$ = diag $(d_0, d_1, \ldots, d_H)$ be an $H+1, H+1$ diagonal matrix having non-zero diagonal entries which alternate in sign, i.e., $d_i(-1)^{i+1}|d_i|$, $0 \leq i \leq H$. Then the resultant matrix $\bar{D}^{-1}\bar{A}\bar{D}$ may be seen to reduce to,

$$\begin{vmatrix} -1/d_0 & & & & & & \\ & 1/d_1 & & & & & \\ & & \cdot & & & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ & & & & & & 1/d_H \end{vmatrix} \begin{vmatrix} \{\delta_{1j}+\frac{C_{6j}}{2}\}, & -\{\delta_{1j}-\delta_{2j}\}, & \ldots & & \\ -\{\delta_{1j}+\delta_{2j}\}, & \{\delta_{1j}+\frac{C_{6j}}{2}\}, & -\{\delta_{1j}-\delta_{2j}\}, & \ldots & \\ \ldots & \ldots & \ldots & \ldots & \\ & \ldots & \ldots & \ldots & \\ & & \ldots & \ldots & \ldots \\ & \ldots, & -\{\delta_{1j}+\delta_{2j}\}, & \{\delta_{1j}+\frac{C_{6j}}{2}\}, & -\{\delta_{1j}-\delta_{2j}\} \\ & & \ldots, & -\{\delta_{1j}+\delta_{2j}\}, & \{\delta_{1j}+\frac{C_{6j}}{2}\} \end{vmatrix} \begin{vmatrix} -d_0 & & & & & & \\ & d_1 & & & & & \\ & & \cdot & & & & \\ & & & \cdot & & & \\ & & & & \cdot & & \\ & & & & & \cdot & \\ & & & & & & d_H \end{vmatrix}$$

$$\left|\begin{array}{l}\{\delta_{1j}+\frac{C_{6j}}{2}\},\ \{\delta_{1j}-\delta_{2j}\}\frac{d_1}{d_0}\ ,\ \dots\dots\dots\dots\dots \\ \{\delta_{1j}+\delta_{2j}\}\frac{d_0}{d_1}\ ,\ \{\delta_{1j}+\frac{C_{6j}}{2}\},\ \{\delta_{1j}-\delta_{2j}\}\frac{d_2}{d_1}\ ,\ \dots\dots \\ \qquad \dots\dots\dots\dots\dots \\ \qquad\qquad \dots\dots\dots\dots \\ \qquad\qquad\qquad ,\ \{\delta_{1j}+\delta_{2j}\}\frac{d_{H-1}}{d_H}\ ,\ \{\delta_{1j}+\frac{C_{6j}}{2}\}\end{array}\right|$$

We can select the $|d_i|$ as a function of δ_{1j} and δ_{2j} for positive values of $\{\delta_{1j}+C_{6j}/2\}$ and for $\delta_{1j}/\delta_{2j} > \delta_{2j}/\delta_{1j} > 0$ so that the matrix $\bar{D}^{-1}\bar{A}\bar{D}=\bar{E}$ reduces to

$$\bar{E} = \left|\begin{array}{l}\{\delta_{1j}+\frac{C_{6j}}{2}\},\ \{\frac{\delta^2_{1j}-\delta^2_{2j}}{\delta_{1j}\delta_{2j}}\},\ \dots\dots\dots\dots\dots \\ \{\frac{\delta^2_{1j}-\delta^2_{2j}}{\delta_{1j}\delta_{2j}}\},\ \{\delta_{1j}+\frac{C_{6j}}{2}\},\ \{\frac{\delta^2_{1j}-\delta^2_{2j}}{\delta_{1j}\delta_{2j}}\},\ \dots\dots \\ \qquad \dots\dots\dots\dots\dots \\ \qquad\qquad \dots\dots\dots\dots \\ \qquad\qquad\qquad ,\ \{\frac{\delta^2_{1j}-\delta^2_{2j}}{\delta_{1j}\delta_{2j}}\},\ \{\delta_{1j}+\frac{C_{6j}}{2}\}\end{array}\right|$$

Several facts about the matrix $\bar{D}^{-1}\bar{A}\bar{D}=\bar{E}$ can now be stated. First, $\bar{E}$ is a real matrix with all positive elements. Next, $\bar{A}$ is an irreducibly diagonally dominant matrix with positive diagonal entries for $\delta_{1j}/\delta_{2j} > \delta_{2j}/\delta_{1j} > 0$ and for $\{\delta_{1j}+C_{6j}/2)\} > 0$. Therefore, $\bar{E}$ is a positive definite matrix. Further, this diagonal dominance implies, that the successive principal minors of $\bar{E}$ are positive. Since the super-diagonal and sub-diagonal of $\bar{E}$ have positive entries for $\delta_{1j}/\delta_{2j} > \delta_{2j}/\delta_{1j} > 0$ and for $\{\delta_{1j}+C_{6j}/2\} > 0$, it follows from the definition (Gantmakher, 1959) that $\bar{E}$ is an oscillation matrix, i.e., all minors of $\bar{E}$, whether principal or not, are non-negative, and positive powers of $\bar{E}$ have all its minors positive. As an oscillation matrix has real distinct eigen values (Gantmakher, 1959), we deduce that the matrix $\bar{A}$ has real distinct eigen values for the following criteria

i) $\{\delta_{1j} + C_{6j}/2\} > 0$, and

ii) $\delta_{1j}/\delta_{2j} > \delta_{2j}/\delta_{1j} > 0$ for all j , $j=0,1,\ldots,H$.

When these criteria are violated, the eigen values μ_i of $\bar{A}$ are of the form (Price et al., 1966)

$$\mu_i = \{\delta_{1j} + \frac{C_{6j}}{2}\} + i\gamma_j \quad ; \quad 0<j<H \quad \text{where } \gamma_j \text{ is real}$$

and

$$\max(\gamma_j) > 2\{\frac{\delta_{1j}^2 - \delta_{2j}^2}{\delta_{1j}\delta_{2j}}\} \cos\frac{\pi}{H+2} \qquad \text{(Smith, 1965)}$$

which shows that there always exists eigen values of $\bar{A}$ with non-zero imaginary part.

When these criteria are satisfied, the real and distinct eigen values μ_i of $\bar{A}$ and with associated eigen vectors, $\bar{V}_i$, the solution of the equation

$$\left(\frac{\partial\bar{\Theta}}{\partial T}\right)^{t+1} = -\bar{A}\bar{\Theta}^{t+1} + \bar{B}$$

can be expressed as

$$\bar{\Theta}^{t+1} = \sum_{i=0}^{H} d_i\{1-\exp(-t\mu_i)\}\bar{V}_i \quad , \quad t \geq 0$$

where

$$\bar{A}^{-1}\bar{B} = \sum_{i=0}^{H} d_i\bar{V}_i \quad .$$

Price et al. (1966) have found that there could be oscillation even with infinitely small time increments, i.e., with finite difference approximations, if the spatial mesh is sufficiently coarse. They have proved that for Crank-Nicholson approximation, oscillations are eliminated if:

$$0 < \Delta t \leq \frac{2}{\max\mu_i}$$

where μ_i is a positive real eigen value of the $\bar{A}$ matrix.