MATHEMATICAL MODELS FOR PREDICTION OF SOIL MOISTURE PROFILES

by

H. J. Morel-Seytoux

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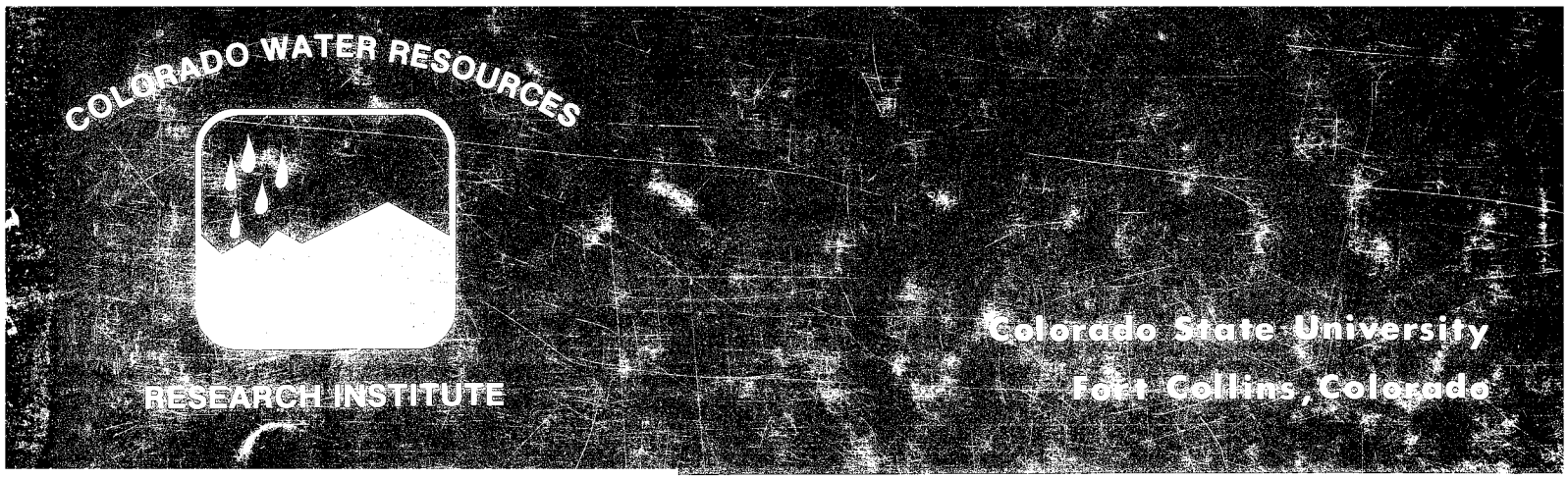

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MATHEMATICAL MODELS OF SOIL MOISTURE PROFILES USING TWO-PHASE FLOW THEORY

by

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ABSTRACT

Three methods of analysis for prediction of infiltration and water content profiles in a soil column are presented.

The first method is the more or less classical finite difference approach except that the governing equations are those deduced from two-phase flow theory. As a result the determination of the water content at the soil surface before ponding is facilitated. Similarly after ponding the calculation of the capacity infiltration rate is more stable than with the usual finite difference approximations to Richards' equation. The second method is purely analytical. It "speaks" as results such as ponding time are obtained explicitly in terms of the various parameters of the problem (hydraulic conductivity, effective capillary drive, initial water content, etc.). Each solution applies for a particular value of the exponent n in the power law form of the relative permeability vs. normalized water content curve. Solutions have been obtained for $n = 1,2,3,4,6$ and 8. Profiles look realistic. Nevertheless, the results are approximate. A third method, a hybrid method, tries to combine the advantages of the numerical and analytical techniques by retaining the versatility of the numerical method and the low cost of the analytical method. The hybrid method is illustrated in depth for the case $n = 1$. The case $n = 2$ has been discussed previously in the literature (Morel-Seytoux, 1982). Results for the case $n= 4$ are given without derivation. The case $n = 4$ has been implemented

operationally in a computer program SOILMOP. Tests (though limited) indicate that accuracy with SOILMOP is comparable with existing difference code for the Richards' equation and is 25 times cheaper. The hybrid technique appears to have a significant potential.

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RESEARCH OBJECTIVES

The overall objective of the research was the development of a surface-subsurface hydrologic model that portrays accurately fluid movement in the unsaturated zone and is so cost-effective that it can be incorporated readily in complex models for prediction of the evolution of water quality both in the unsaturated zone and in the underlying aquifer.

ACHIEVEMENTS OF CONTRACT

It is not desirable to repeat in this completion report all the results obtained over the past three years and the detailed procedures by which they were obtained. These results and procedures can (or will) be found in one thesis (Ross, 1982), one report (Ross and Morel-Seytoux, 1982), and several papers in preparation.

Rather a brief review of the methods of attack and a sample of results will be given. Generally speaking the thrust of the research has been in the direction of development of new and imaginative methods that will greatly reduce the cost of management studies of the quality of water in the vadose zone and in the connected aquifer without significant reduction in accuracy. In this regard the project was successful.

GOVERNING EQUATIONS FOR SOIL MOISTURE EVOLUTION

The nomenclature used in this report follows the accepted practice for the description of moisture evolution from the two-phase (water and air) flow point of view (e.g. Morel-Seytoux, 1979). The basic governing equations are the water volume conservation equation:

$$\frac{\partial \theta}{\partial t} + \frac{\partial v_w}{\partial z} = 0 \tag{1}$$

with the usual notations (Morel-Seytoux, 1979, p. 17) and the v-integral equation:

$$v = \frac{\tilde{K}[h_{au} - h_{ab} + H_c(\theta_u) + \int_b^u f_w dz]}{\int_b^u \mu_r dz} \tag{2}$$

where the subscripts u and b refer to prevailing conditions at the top (upper boundary) and bottom of a soil column. In Eq. (2) $H_c(\theta_u)$ is the effective capillary drive (Morel-Seytoux, 1979, p. 20). The dependence of the effective capillary drive on the value of water content at the bottom (lower boundary) is not shown explicitly in this notation for the sake of brevity. The water velocity v_w is given by the relation:

$$v_w = vF_w = vf_w + G_w - \frac{\partial \theta}{\partial z} \tag{3}$$

with the usual notations (Morel-Seytoux, 1979, p. 24).

Given the expression of v_w in Eq. (3) the conservation equation, Eq. (1), becomes more explicitly:

$$\frac{\partial\theta}{\partial t} + \frac{\partial}{\partial z}\left(vf_w + G_w - E_w \frac{\partial\theta}{\partial z}\right) = 0 \qquad (4)$$

(In later sections the subscript w in f_w, G_w, and E_w will be dropped for simplicity.) Eqs. (2) and (4) provide two equations for the unknowns $\theta(z,t)$ and $v(t)$. The solution of this system of 2 equations can be obtained (approximately) by numerical techniques (e.g. finite difference method) or analytically.

APPROXIMATE NUMERICAL FORMULATION

Discretization and Mean Water Content

An integral form of Eq. (1) is:

$$\frac{\partial}{\partial t}\left[\int_{z_1}^{z_2} \theta dz\right] = v_w^1 - v_w^2 \tag{5}$$

where the indices 1 and 2 refer to two arbitrary levels in the soil column. If Δz represents the distance between these two levels, then Eq. (5) can be rewritten in the form:

$$\frac{\partial \bar{\theta}}{\partial t} = \left(\frac{v_w^1 - v_w^2}{\Delta z}\right) \tag{6}$$

where $\bar{\theta}$ is the *average* water content at a given time over the interval Δz in a *mass balance* sense. In the finite difference technique the flow domain is discretized. Figure 1 illustrates the selected grid system. Application of Eq. (6) to the cell j yields the finite difference *spatial* approximation:

$$\frac{\partial \theta_j}{\partial t} = (v_{w,j-\frac{1}{2}} - v_{w,j+\frac{1}{2}})/\Delta z_j \tag{7}$$

where j is the cell index, θ_j is the mean water content in cell j and $j-\frac{1}{2}$ (and similarly $j + \frac{1}{2}$) is an index that refers to the location (level) of the boundary (interface) between cell j-1 and cell j. The finite difference (simplest) *temporal* approximation of Eq. (7) is:

$$\theta_j^v = \theta_j^o + (v_{w,j-\frac{1}{2}} - v_{w,j+\frac{1}{2}}) \frac{\Delta t}{\Delta z_j} \tag{8}$$

where θ_j^v represents the (new) mean water content in cell j at the end of the time step of duration Δt whereas θ_j^o represents the (old) value at

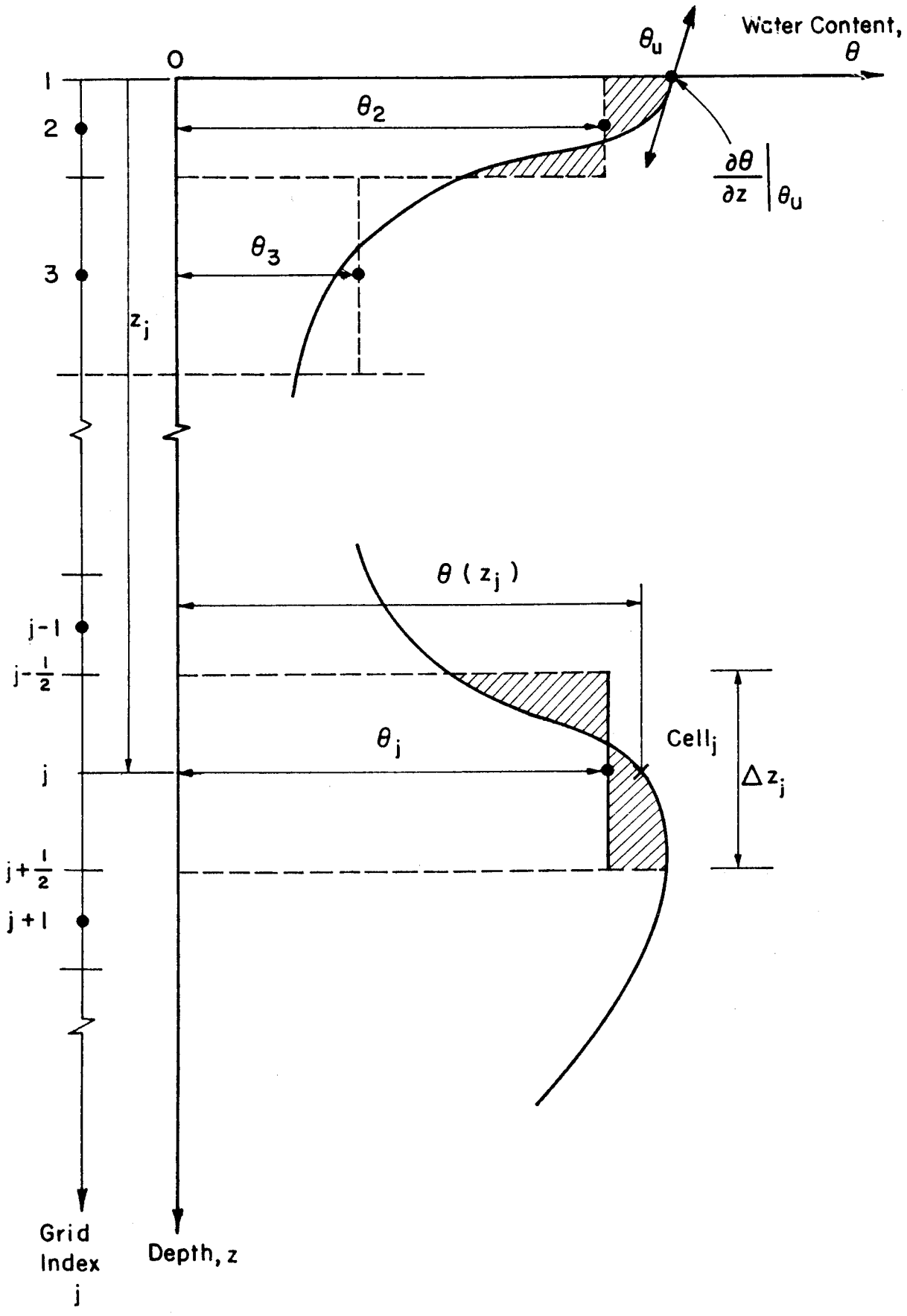

Figure 1. Typical Finite Difference Grid Geometry, Notation and Indexing

the beginning of the time step. It is important to be fully aware that θ_j is not really a numerical approximation for the true value of θ at level z_j but more accurately an approximation for the mean water content in cell j. The fundamental difference in physical meaning between θ_j and $\theta(z_j)$ is illustrated on Figure 1. It is also clear from the figure that θ_2 is not the value of θ at depth z_2. The two values coincide only if the water content profile is truly straight within a given cell.

Estimation of Water Fluxes (Velocities) at Cell (Block) Interfaces (Boundaries)

It is (also) important to realize that Eq. (8) will naturally conserve water in every cell even if the fluxes at the cell boundaries are calculated erroneously. To complete the finite difference approximation it remains to select an expression for the fluxes at the cell boundaries. From the water conservation meaning of Eq. (8) it is clear that the best estimate for $v_{w,j-\frac{1}{2}}$ should be a *time* average over the interval Δt. Its exact estimation however would require the continuous solution for θ in time at such boundaries. In the finite difference scheme values of θ are calculated only as spatial averages for a cell and only at discrete times. The value of $\bar{v}_{w,j-\frac{1}{2}}$ (time average) of $v_{w,j-\frac{1}{2}}$ is estimated as a weighted mean of the values at time t^o and at time t^v. The simplest finite difference form for v_w from Eq. (3) is at any time:

$$v_{w,j-\frac{1}{2}} = vf_{j-\frac{1}{2}} + G_{j-\frac{1}{2}} - E_{j-\frac{1}{2}} 2\left(\frac{\theta_j - \theta_{j-1}}{\Delta z_j + \Delta z_{j-1}}\right) \qquad (9)$$

The functions f, G, and E evaluated at interface of index $j-\frac{1}{2}$ can be evaluated as mean values of the same functions at the grid points j-1

and j. Thus for example an approximation for $f_{j-\frac{1}{2}}$ is $f_{j-\frac{1}{2}} = \frac{1}{2}[f(\theta_j) + f(\theta_{j-1})]$. Alternately one can calculate the mean value of θ at grid points j and j-1 thus $\theta_{j-\frac{1}{2}} = \frac{1}{2}(\theta_j + \theta_{j-1})$ and next evaluate $f(\theta_{j-\frac{1}{2}})$. Actually the weights are not both $\frac{1}{2}$ for variable grid size. For variable grid size, with the first method of spatial averaging, then:

$$f_{j-\frac{1}{2}} = \frac{\Delta z_j \; f(\theta_{j-1}) + \Delta z_{j-1} \; f(\theta_j)}{\Delta z_{j-1} + \Delta z_j} \tag{10}$$

The values of $G_{j-\frac{1}{2}}$ and $E_{j-\frac{1}{2}}$ are calculated similarly for the old values of θ, θ^o. Then $v_{w,j-\frac{1}{2}}$ is calculated for the new values of θ, θ^v. The time average is then calculated as a weighted mean of the values of v_w at the old time and at the new time, with weights λ^o and λ^v, both positive and adding to 1. Denoting by $v^o_{w,j-\frac{1}{2}}$ the value of $v_{w,j-\frac{1}{2}}$ at the old time and similarly by $v^v_{w,j-\frac{1}{2}}$ for the new time, Eq. (8) takes the form:

$$\theta^v_j = \theta^o_j + \left[\lambda^o(v^o_{w,j-\frac{1}{2}} - v^o_{w,j+\frac{1}{2}}) + \lambda^v(v^v_{w,j-\frac{1}{2}} - v^v_{w,j+\frac{1}{2}})\right]\frac{\Delta t}{\Delta z_j} \tag{11}$$

Finite Difference Approximation

Grouping terms involving unknown values, the new values, on the left side of the equation, Eq. (11) takes the form:

$$-\lambda^v \, v^v_{w,j-\frac{1}{2}} \frac{\Delta t}{\Delta z_j} + \theta^v_j + \lambda^v v^v_{w,j+\frac{1}{2}} \frac{\Delta t}{\Delta z_j} = \theta^o_j$$

$$+ \lambda^o \, (v^o_{w,j-\frac{1}{2}} - v^o_{w,j+\frac{1}{2}}) \frac{\Delta t}{\Delta z_j} \tag{12}$$

The terms v^v_w involve several unknown θ^v at grid points j-1, j and j+1. The dependence of $v^v_{w,j-\frac{1}{2}}$ as can be seen explicitly in Eq. (9) and implicitly in Eq. (10) on θ^v_j and θ^v_{j-1} is not linear. To linearize

Eq. (12) in the θ^v the f, G, and E functions are evaluated at a previously estimated value of θ^v, the $m^{\underline{th}}$ iterate estimate of θ^v denoted θ^m. Substitution of the expression for $v_{w,j-\frac{1}{2}}$ (and $v_{w,j+\frac{1}{2}}$) from Eq. (9) into Eq. (12) yields an equation for the unknowns θ^v, namely:

$$-\lambda^v \left\{ v^m f^m_{j-\frac{1}{2}} + G^m_{j-\frac{1}{2}} - 2E^m_{j-\frac{1}{2}} \left(\frac{\theta^v_j - \theta^v_{j-1}}{\Delta z_j + \Delta z_{j-1}} \right) \right\} \frac{\Delta t}{\Delta z_j}$$

$$+ \theta^v_j + \left\{ \lambda^v v^m f^m_{j+\frac{1}{2}} + G^m_{j+\frac{1}{2}} - 2E^m_{j+\frac{1}{2}} \left(\frac{\theta^v_{j+1} - \theta^v_j}{\Delta z_j + \Delta z_{j+1}} \right) \right\} \frac{\Delta t}{\Delta z_j}$$

$$= \theta^o_j + \lambda^o \left(v^o_{w,j-\frac{1}{2}} - v^o_{w,j+\frac{1}{2}} \right) \frac{\Delta t}{\Delta z_j} \qquad (13)$$

Ordering the unknowns in order of increasing index Eq. (13) takes the final explicit form:

$$-\lambda^v \frac{2\Delta t \, E^m_{j-\frac{1}{2}}}{\Delta z_j (\Delta z_j + \Delta z_{j-1})} \theta^v_{j-1} + \left[1 + 2\lambda^v \frac{\Delta t}{\Delta z_j} \left(\frac{E^m_{j-\frac{1}{2}}}{\Delta z_j + \Delta z_{j-1}} + \frac{E^m_{j+\frac{1}{2}}}{\Delta z_j + \Delta z_{j+1}} \right) \right] \theta^v_j$$

$$- \lambda^v \frac{\Delta t \quad 2E^m_{j+\frac{1}{2}}}{\Delta z_j (\Delta z_j + \Delta z_{j+1})} \theta^v_{j+1}$$

$$= \theta^o_j + \lambda^o \left(v^o_{w,j-\frac{1}{2}} - v^o_{w,j+\frac{1}{2}} \right) \frac{\Delta t}{\Delta z_j} + \lambda^v \left[v^m \left(f^m_{j-\frac{1}{2}} - f^m_{j+\frac{1}{2}} \right) \right.$$

$$\left. + \left(G^m_{j-\frac{1}{2}} - G^m_{j+\frac{1}{2}} \right) \right] \frac{\Delta t}{\Delta z_j} \qquad (14)$$

Eq. (14) applies at all the internal nodes of the system i.e. for j = 3, N-2 and in this case each equation involves 3 unknowns. The values of θ at the upper boundary denoted θ_u or θ_1 and at the lower boundary denoted θ_b or θ_N are given as boundary conditions. Eq. (14) applies also for j = 2 but in this case there are only 2 unknowns (θ_2 and θ_3). Similarly for j = N-1 the 2 unknowns are θ_{N-2} and θ_{N-1}.

To simplify notations a little bit let us define some composite variables, namely:

$$b^m_{j,j-1} = \lambda^v \frac{\Delta t \quad 2E^m_{j-\frac{1}{2}}}{\Delta z_j (\Delta z_j + \Delta z_{j-1})} \tag{15}$$

$$vf + G = vF \tag{16}$$

Eq. (14) takes the briefer form:

$$-b^m_{j,j-1}\ \theta^v_{j-1} + \left[1 + \left(b^m_{j,j-1} + b^m_{j,j+1}\right)\right]\theta^v_j - b^m_{j,j+1}\ \theta^v_{j+1}$$

$$= \theta^o_j + \lambda^o\left(v^o_{w,j-\frac{1}{2}} - v^o_{w,j+\frac{1}{2}}\right)\frac{\Delta t}{\Delta z_j} + \lambda^v\left(v^m\ F^m_{j-\frac{1}{2}} - v^m\ F^m_{j+\frac{1}{2}}\right)\frac{\Delta t}{\Delta z_j} \tag{17}$$

With the choice of $\lambda^o = 1$, $\lambda^v = 0$ the system of Eqs. (17) is said to be explicit. In that case there is only one unknown θ^v_j per equation. With the choice $\lambda^o = 0$ and $\lambda^v = 1$ it is fully implicit. For $\lambda^o = \lambda^v = \frac{1}{2}$ it is the Crank-Nicolson scheme. In the latter cases there are 3 unknown θ per equation.

UPPER BOUNDARY CONDITIONS

The natural hydrologic conditions at the upper boundary are: a given rainfall rate (it rains), a condition of ponding (it has rained so long that infiltration capacity has been exceeded and water accumulates (ponds) over the soil surface), a condition of ponding (including zero depth) but it no longer rains and evaporation takes place from a very wet soil and finally a condition of limited evaporation when the soil has dried up (evaporation continues but no longer at the potential rate). More concisely these various boundary conditions (b.c.) will be called: rainfall condition, ponded rainfall condition, and evaporation condition.

The mathematical statements of these boundary conditions are applicable for the numerical or the analytical approximations. To discuss these boundary conditions it is best to visualize a typical hydrologic sequence of events, starting with rain over a soil of arbitrary but given initial moisture state. After a while if the rainfall rate is high enough, capacity will be exceeded. The time at which infiltration capacity occurs is called the ponding time. It is not known a priori. It must be calculated. Following ponding and as long as ponding continues (rain or no rain) the boundary condition is no longer that of a given (prescribed) flux but that of a given depth of ponding and a given water content (natural saturation) at least until air starts to escape and bubble out through the ponded depth of water. The so called given ponded depth actually depends on the overland flow process and on the prevailing evaporation rate from a free water surface. With no more rain and no more ponding the boundary condition

turns into one of a given evaporation rate, the evaporation potential. As the soil dries up at the surface the soil reaches its evaporation capacity. After that the soil evaporates at capacity. The time at which the soil reaches its evaporation capacity has not received a particular name. One could call it the "evaporation capacity time". The ponding time is indeed the "infiltration capacity time".

The approach followed to impose any type of boundary condition is to convert it to one of a given water content θ_u at the soil surface. The natural (hydrologic) boundary condition is rarely one of a given water content. Nevertheless the numerical and analytical schemes are developed for a boundary condition which is always one of a prescribed water content at the soil surface $\theta_u(t)$. The trick is to reduce every possible b.c. to one of a given θ_u.

(Given) Rainfall Boundary Condition

With r denoting the rainfall rate (expressed as a velocity) the boundary condition is simply that the water velocity at the soil surface equals the rainfall rate (until ponding time is reached), explicitly:

$$vf(\theta_u) + G(\theta_u) - E(\theta_u) \left.\frac{\partial\theta}{\partial z}\right|_{\theta_u} = r \qquad (18)$$

If Eq. (18) can be solved for θ_u the rainfall boundary condition is converted to one of a given θ_u. In the numerical scheme one expresses v explicitly as a function of θ_u as shown in Eq. (2) and one approximates $\left.\frac{\partial\theta}{\partial z}\right|_{\theta_u}$ in a finite difference form. In Eq. (2) for v at the $m^{\underline{th}}$ iterate level one maintains the dependence of H_c on θ_u but one evaluates

the other terms using the $m^{\underline{th}}$ iterate estimate of the water content profiles. For simplicity let us define:

$$\int_b^u f_w^m \, dz = L_G^m \tag{19}$$

and

$$\int_b^u \mu_r dz = L_R^m \tag{20}$$

The letter L is used mnemonically because the integrals have dimensions of length. The subscripts G and R refer respectively to *gravity* and viscous *resistance* to flow. The superscript indicates the iterative level of the water content profile used to evaluate the integrals. With these notations the expression for v at the $m^{\underline{th}}$ iterate level is:

$$v^m = \frac{\tilde{K}\left[h_{au} - h_{ab} + H_c(\Theta_u) + L_G^m\right]}{L_R^m} \tag{21}$$

Prior to ponding at the soil surface the air is in free contact with the atmosphere and $h_{au} = h_A$ where h_A is atmospheric pressure. The value of h_{ab} will depend on the lower boundary condition. Eq. (18) takes the form:

$$\frac{\tilde{K}}{L_R^m} f(\Theta_u)\left[h_A - h_{ab} + H_c(\Theta_u) + L_G^m\right] + G(\Theta_u) - E(\Theta_u) \left.\frac{\partial\Theta}{\partial z}\right|_{\Theta_u} = r \tag{22}$$

It remains to express $\left.\frac{\partial\Theta}{\partial z}\right|_{\Theta_u}$ in finite difference form. It is clear from Figure 1 that the simple approximation $\frac{\Theta_2 - \Theta_u}{z_2}$ will not be very good specially if z_2 is not very small. To account for the significant curvature of the profile a higher order approximation which makes use of 3 points in the profile rather than the usual 2 points is used, namely:

$$\left.\frac{\partial\theta}{\partial z}\right|_{\theta_u} \cong \frac{\dfrac{\theta_2 - \theta_u}{z_2} - \dfrac{z_2}{z_3}\dfrac{(\theta_3 - \theta_u)}{z_3}}{1 - \dfrac{z_2}{z_3}} \tag{23}$$

Note that for z_3 very large compared to z_2 the expression reduces as expected to the simple approximation $(\theta_2 - \theta_u)/z_2$. This suggests that a good ratio for z_2/z_3 should be of the order of 1/3.

Substitution of Eq. (23) into Eq. (22) yields the equation:

$$\frac{\tilde{K}}{L_R^m}\left[\left(h_A - h_{ab}\right) + H_c(\theta_u) + L_G^m\right] f(\theta_u) + G(\theta_u)$$

$$+ \frac{E(\theta_u)}{z_3 - z_2}\left\{\left(\frac{z_3}{z_2} - \frac{z_2}{z_3}\right)\theta_u - \left(\frac{z_2}{z_3}\theta_3^m - \frac{z_3}{z_2}\theta_2^m\right)\right\} = r \tag{24}$$

Defining the residue function $\rho(\theta_u) = r - v_w$ then explicitly the expression for the residue function is:

$$\rho(\theta_u) = r - \frac{\tilde{K}}{L_R^m}\left[\left(h_A - h_{ab}\right) + H_c(\theta_u) + L_G^m\right] f(\theta_u) - G(\theta_u)$$

$$- \frac{E(\theta_u)}{z_3 - z_2}\left\{\left(\frac{z_3}{z_2} - \frac{z_2}{z_3}\right)\theta_u - \left(\frac{z_2}{z_3}\theta_3^m - \frac{z_3}{z_2}\theta_2^m\right)\right\} \tag{25}$$

The value of θ_u that makes $\rho(\theta_u) = 0$ is the solution. Since all the functions of θ_u involved (such as f, G, E, and H_c) are known what is required is the solution of an explicit nonlinear algebraic equation. The solution is obtained by standard procedures (i.e. systematic trial and error procedure based on successive values of the residue). There is a little problem to start that solution, however. If one were to use

as $0^{\underline{th}}$ iterate values of the profile, the profile values at the beginning of the time step, i.e. at time t^o, the solution for θ_u would be θ_u^o, as it should. Thus an estimate for the new profile at time t^v must be secured before calculation of θ_u can start. One trick is to incorporate the boundary condition $v_w\Big|_{\theta_u} = r$ in the first finite difference equation for the system. Since in Eq. (8) for j = 2, $v_{w,j-\frac{1}{2}}$ is known and equal to r only the finite difference form for $v_{w,j+\frac{1}{2}}$ is needed. As a result in the case j = 2 one can replace the general Eq. (14) by the simpler form:

$$\left[1 + \lambda^v \frac{\Delta t}{\Delta z_2} \frac{2E^m_{2.5}}{\Delta z_2 + \Delta z_3}\right] \theta_2^v - \lambda^v \frac{\Delta t}{\Delta z_2} \frac{2E^m_{2.5}}{\Delta z_2 + \Delta z_3} \theta_3^v$$

$$= \theta_2^o + r \frac{\Delta t}{\Delta z_2} - \lambda^o v^o_{w,2.5} \frac{\Delta t}{\Delta z_2} - \lambda^v v^m F^m_{2.5} \frac{\Delta t}{\Delta z_2} \qquad (26)$$

To start then one uses as $0^{\underline{th}}$ estimate of the θ the old profile values. In that case all terms with superscript m have the same values as they had at the end of the previous time step. By solving Eq. (26) and Eqs. (14) for j = 3, N-1 one obtains the $1^{\underline{st}}$ iterate estimate of the new profile. One can then solve for the $1^{\underline{st}}$ estimate of θ_u by finding the root of $\rho(\theta_u)$. Typically as under a rainfall condition θ_u increases with time $\rho(\theta_u^o)$ for the current profile ($1^{\underline{st}}$ iterate level) will be positive. One then increases θ_u progressively until $\rho(\theta_u)$ changes sign. The first iterate value of θ_u, θ_u^1 has been obtained. One then proceeds to solve again the system of Eqs. (14) for j = 3, ... N-2 and Eq. (26), to obtain the $2^{\underline{nd}}$ iterate level estimate of the profile. Once this is done a new estimate for θ_u, θ_u^2 can be calculated. The procedure is repeated until there is no significant difference between θ_u^m and θ_u^{m-1}.

It is important to note that in this approach the θ_j^m for j = 2,3 ... N-1 are first calculated and then only afterward is θ_u^m calculated. One might refer to this procedure as the θ_u-*last* iterative procedure. This procedure is advantageous for the case of a given (known exactly) flux at the upper boundary. An alternative which treats *really* θ_u as a given (but unknown) boundary condition is to start with a value of θ_u^m, calculate v^m by the equation:

$$v^m = \tilde{K}\left[\frac{h_A - h_{ab} + H_c(\theta_u^m) + L_G^{m-1}}{L_R^{m-1}}\right] \tag{27}$$

solve the system of Eqs. (14) for j = 2,3 ...N-1 (or alternately but less generally Eq. (26) and Eqs. (14) for j = 3, ... N-1) to obtain the θ_j^m and then proceed to obtain θ_u^{m+1} by making the residue $\rho(\theta_u)$ given by Eq. (25) equal to zero. The procedure is then repeated until θ_u^m and θ_u^{m-1} are (practically) the same. As a first estimate of θ_u^1 to start the procedure one can use θ_u^o if $\underline{r}$ has changed. If r has not changed one uses a slightly larger value than θ_u^o. One may refer to this procedure as the θ_u-*first* iterative procedure.

(Ponded) Rainfall Condition

As long as Eq. (24) has a solution, that is as long as there is a θ_u such that $\rho(\theta_u) = 0$ with $\theta_u < \tilde{\theta}$, ponding (surface saturation) does not occur. The indication that ponding does occur during a time step is that $\rho(\theta_u) = 0$ does not have a solution. In this case, and if during the previous time interval there was no ponding, the solution for θ_u^v is (usually) $\tilde{\theta}$. The ponding time is somewhere between t_o and t^v. As the time steps are (usually) reduced as ponding is approached, it is convenient to define $t_p = \frac{t^o + t^v}{2}$ during that interval for which saturation

first occurs. The time interval is broken down into 2 equal time intervals (t_o, t_p) and (t_p, t^v). During the first (half) interval the infiltration rate is still r. One obtains the profile at time t_p using the general procedure except that the $0^{\underline{th}}$ iterate and all $m^{\underline{th}}$ iterates of θ_u are set at the value of $\tilde{\theta}$ (unless there is a situation of air counterflow prevailing). For the second (half) interval it is also known that $\theta_u^v = \tilde{\theta}$. The profile is obtained at time t^v with the boundary condition that $\theta_u^v = \tilde{\theta}$. The profile is calculated with the general procedure except again that all iterate estimates of θ_u are set equal to $\tilde{\theta}$. At the end of the iterative process v^v is obtained. The mean infiltration rate during the time interval (t_p, t^v) is $\frac{r + v^v}{2}$.

The prior discussion applied to the first interval during which ponding occurred. In general going into a new time step given that during the previous time interval a ponding condition prevailed, one does not know whether a ponded condition will continue to prevail. In other words for each interval it is necessary to seek a solution for θ_u that minimizes $\left|\rho(\theta_u)\right|$. It is important to note that a ponded condition can exist without $\theta_u = \tilde{\theta}$. The minimum of $\left|\rho(\theta_u)\right|$ is not necessarily attained for $\theta_u = \tilde{\theta}$.

For a ponded rainfall condition the value of h_{au} is $h_A + H^o + h_{cu}$ where H^o is the ponded depth of water over the soil surface at time t^o. Eq. (2) applies.

During the given interval the mean infiltration rate is:

$$\bar{I} = \frac{v_w^o\Big|_{z=0} + v_w^v\Big|_{z=0}}{2} \tag{28}$$

($v_w\big|_{z=0}$; $v_{w,1}$; $v_w\big|_{\theta_u}$; I are alternate notations for the infiltration rate). Note that $v_w\big|_{z=0} = v$ only if $\theta_u = \tilde{\theta}$. The ponded depth at time t^v is:

$$H^v = H^o + (r - \bar{I})\Delta t - q\Delta t \tag{29}$$

where q is the overland flow velocity (a likely function of H).

Evaporation Condition

As soon as rain stops whether occurring with some ponded depth or not, evaporation starts. However, if there is a sufficient ponded depth there may be infiltration into the soil as well as evaporation from the free surface. Thus if there is a depth H^o at time t^o in excess of $e_p\Delta t$ where e_p is the potential evaporation rate (velocity), the boundary condition is one of ponded rainfall with a supply rate:

$$r_s = \frac{H^o}{\Delta t} - e_p \tag{30}$$

If H^o is less than $e_p\Delta t$, the value of r_s is set to zero and the time step is reduced to $\Delta t = \frac{H^o}{e_p}$. Naturally at the end of this time interval $H^v = 0$.

If at time t^o there is no rain (or snowmelt) and no depth of ponding ($H^o = 0$) then the evaporation has to come from the soil. The value of θ_u is the solution of Eq. (24) with r replaced by $-e_p$, or in other words the solution of $\rho(\theta_u) = 0$ with $r = -e_p$. As in the case of rainfall (potential infiltration rate) the soil may not be able to evaporate the potential evaporation rate. As infiltration capacity may be reached, so can evaporation capacity be reached. If $\rho(\theta_u)$ cannot be made zero evaporation capacity is reached. The value of θ_u is the

one that minimizes $|\rho(\theta_u)|$. The solution to that minimization problem will provide the maximum possible evaporation rate from the soil:

$$e = -v_w\Big|_{z=0} = -v_w(\theta_u) \tag{31}$$

compatible with the water content profile in the soil.

Iterative Scheme(s) for Determination of Profile

Two such schemes were presented on previous pages. One scheme capitalizes on the fact that the flux at the boundary is (sometimes) exactly known to avoid man balance error over the entire profile. The other scheme is more general. Note that the first scheme can be generalized to account for the fact that under some conditions the flux is not known. In Eq. (26) it suffices to replace r by the mean infiltration rate $\bar{I}$, or rather since $\bar{I}$ is not known to replace r by the m^{th} iterate estimate of $\bar{I}$, $\bar{I}^m$. (In the case of evaporation $\bar{I}$ is negative equal to $-\bar{e}$.) One can choose for the first estimate of $\bar{I}$ its old value $\bar{I}^o$.

CAPACITY INFILTRATION RATE

It is interesting to note that prior to ponding at any time Eq. (2) provides the current (actual) value of v. If at that time the water content θ_u is raised instantaneously to the value $\tilde{\theta}$, the water content profile remaining the same, then Eq. (2) provides the capacity infiltration rate of the soil at that time given the previous history of the soil. Explicitly the capacity infiltration rate at any time is:

$$I_c = \tilde{K} \frac{\left[h_A - h_{ab} + H_c + L_G\right]}{L_R} \tag{32}$$

(There is an exception to that expression when v = 0 steadily, as when the bottom boundary is impervious). At the beginning of a new time step, at time t^o then:

$$I_c^o = \tilde{K} \frac{\left[h_A - h_{ab}^o + H_c + L_G^o\right]}{L_R^o} \tag{33}$$

This information is very valuable because a comparison of I_c^o with the current r provides some information regarding the imminence of ponding. Let t^{-1} be the time at the beginning of the previous time interval, t^o the time at the beginning of current time interval. A linear estimate of the approximate ponding time is:

$$\hat{t}_p = t^o + \frac{\Delta t^o \, (I_c^o - r)}{I_c^{-1} - I_c^o} \tag{34}$$

where I_c^{-1} is I_c at time t^{-1}, and Δt^o is the previous time interval. Thus based on current infiltration capacity and past infiltration capacity one can select a new time interval so that ponding time occurs close to the end of the time interval or close to its middle. In this latter

case the assumption discussed previously that if ponding does occur during interval (t^o, t^v) t_p is conveniently selected as $\frac{t_o + t^v}{2}$, will be a very good (convenient) assumption. The implication is that at the end of one time step after rainfall has started one could closely approximate the forthcoming ponding time. Of course this is not the case because I_c is not a linear function of time. However as ponding time is approached Eq. (34) becomes very informative.

TIME STEP AND GRID SIZE SELECTIONS

Generally speaking as a boundary condition changes and the more radical the change, the smaller the time step should be for the sake of accuracy. Generally as rain starts over a soil θ_u will change much readily. The first time step should always be fairly small. If the rainfall rate is less than $\tilde{K}$ a practical value of the time step would be 1 or a few minutes. In the remaining discussion a value of 1 minute will be selected. It will be referred to as the period for greater generality. The boundary conditions are specified for intervals of one period or a multiple integer of periods. As long as the rainfall rate remains below $\tilde{K}$ even if the rate changes the time step can be kept constant equal to the period. As soon as the rainfall rate rises above $\tilde{K}$ there should be a sequence of 2 time steps of duration 1/10 of a period. The next time step will be 8/10 of a period and thereafter as long as the rainfall rate exceeds $\tilde{K}$ the time step is one period. If rainfall rate changes from an old value $> \tilde{K}$ to a new value $< \tilde{K}$ (including zero if rain stops) the two time steps of 1/10 period followed by a time step of 8/10 of a period are recommended.

As rain proceeds and $r > \tilde{K}$ Eq. (34) will sooner or later suggest that ponding will occur during the next period. The next time step is then selected as $2(\hat{t}_p - t^o)$. It will be the used time step provided that the given rainfall rate continues during this calculated time step. The next time step ends at the next period end. If rain stops before the time $t^o + 2(\hat{t}_p - t^o)$ the time step ends when the current rainfall rate ends.

If ponding occurs during a given interval, as discussed previously the interval is broken down into two time steps. As usual during infiltration taking place at capacity, capacity infiltration rate is calculated at the end of each time step, symbolically $v^o_{w,1}$ for the next time step. If r exceeds $v^o_{w,1}$ the next time step can be taken as a period. Otherwise there is a chance that desaturation will occur and it is wise to reduce the time step in half.

There are other considerations to reduce time step besides those of accuracy. The numerical approximations introduce errors. For example it may happen that during infiltration (before or after ponding) the calculated value of θ^v_2 may exceed θ^v_u even though rain did not decrease. This will happen if due to numerical errors the flux out of cell 2 is underestimated. In the worst case the low estimate of $v^v_{w,2.5}$ is $v^o_{w,2.5}$. If the time step is selected by the formula:

$$\Delta t = \frac{\Delta z_2 \ (\theta^o_u - \theta^o_2)}{r - v^o_{w,2.5}} \tag{35}$$

then under the worst condition of numerical errors θ^v_2 will be equal to θ^o_u and a fortiori less than θ^v_u. This time step estimated from Eq. (35) should be rounded to the nearest 1/10 fraction of a period. As ponding is approached (usually slowly if the rain is steady) θ^o_u and θ^v_u are close and θ^v_2 is close to θ^v_u particularly for a small z_2. The time step may settle for a steady value of 1/10 of a period. In other words the procedure guarantees that $\theta^v_2 < \theta^v_u$ but at the price of a large number of time steps up to ponding time. Following ponding Eq. (35) can be used in the modified form:

$$\Delta t = \frac{\Delta z_2 \ (\theta^o_u - \theta^o_2)}{I^o_c - v^o_{w,2.5}} \tag{36}$$

Under the worst conditions ($I_c^v = I_c^o$, $v_{w,2.5}^v = v_{w,2.5}^o$) Eq. (36) guarantees that θ_2^v will be less than θ_u^o. As infiltration proceeds at capacity θ_2 tends to θ_u and Eq. (36) may lead to smaller and smaller time steps. For cost efficiency it is desirable to use a large value of z_2 (and consequently Δz_2 since $\Delta z_2 = 2z_2$). After ponding and when I_c approaches $\tilde{K}$ it is desirable to use a coarser grid size to describe the moisture profile.

Rule of Thumb for Grid Size and Period Selection

A simple rule to estimate cumulative infiltration depth up to ponding, W_p (Morel-Seytoux, 1982) is to estimate the ponding time, t_p, by the formula:

$$\hat{t}_p = t_{k-1} + \frac{1}{r_k}\left[\frac{(\tilde{\theta} - \bar{\theta}_i)}{r_k^* - 1} - \sum_{\lambda=1}^{k-1} r_\lambda (t_\lambda - t_{\lambda-1})\right] \tag{37}$$

where $\bar{\theta}_i$ is a mean initial water content over a soil depth susceptible to be affected by infiltration at ponding time and r_k is the prevailing rainfall rate in the time interval (t_{k-1}, t_k). The estimate of W_p is:

$$\hat{W}_p = \sum_{\lambda=1}^{k-1} r_\lambda (t_\lambda - t_{\lambda-1}) + r_k(\hat{t}_p - t_{k-1}) \tag{38}$$

An estimate for z_2 is:

$$\hat{z}_2 = \frac{1}{4}\frac{H_c}{\frac{W_p}{\tilde{K}\hat{t}_p} - 1} \tag{39}$$

This will guarantee that at ponding time an assumed piston-like wetting front would have cleared cell 2 already and cell 3 if $\Delta z_3 = \Delta z_2$. In this case the higher order approximation for $\left.\frac{\partial\theta}{\partial z}\right|_{\theta_u}$ will still work as

ponding is approached. For a value of H_c = 10 cm (a reasonable value for several soils), the estimate for $\hat{z}_2$ with a high ratio $\frac{\hat{W}_p}{\tilde{K}t_p}$ = 6 is 5 mm or Δz_2 = 1 cm. It is recommended to use $\Delta z_3 = \Delta z_2$ or $z_3 = 3z_2$. Certainly a minimum value for z_2 is 1 mm (except for studies of soil seals and soil crusts). All depths should be rounded off to the nearest mm (or cm) depending on the magnitude of $\hat{z}_2$.

Consider now Eq. (35) for this Δz_2 = 1 cm. Consider a rainfall rate of 12 cm/hour or 1 cm/5 minutes. Let us use 5 minutes as the period. Even taking $v^o_{w,2.5} = 0$ the value of Δt, numerically Δt (periods) = $\frac{1}{1}(\theta^o_u - \theta^o_2) = \theta^o_u - \theta^o_2$ will fall below one tenth of a minute only if $\theta^o_u - \theta^o_2$ is less than 0.02.

The problem is more severe after ponding. As infiltration proceeds for a long time at capacity gravity becomes the dominant drive. The velocity of propagation of a given water content into a zone of mean initial water content $\bar{\theta}_i$ is in this case roughly:

$$\left(\frac{dz}{dt}\right)_\theta = \tilde{K}\,\frac{(1 - k_{ri})}{\tilde{\theta} - \bar{\theta}_i}$$

To guarantee that the water content $\theta^o_2 < \tilde{\theta}$ does not move out of cell 2 within a given time step or just barely reach the interface with cell 3 one must be sure that:

$$\Delta t = \frac{(\tilde{\theta} - \theta^o_2)\Delta z_2}{2\tilde{K}[1 - k_{rw}(\theta^o_2)]}$$

or in the limit as θ^o_2 tends to $\tilde{\theta}$:

$$\Delta t = \frac{(\tilde{\theta} - \theta_r)\Delta z_2}{2\tilde{K}\,n} \qquad (40)$$

where n is the exponent in the power law of k_{rw} vs. θ^*. For $\tilde{K}$ = 2 cm/hour = $\frac{1}{6}$ cm/5 minutes, $\tilde{\theta} - \theta_r = 0.2$, $\Delta z_2 = 1$ cm, a sand i.e. n = 5 and from Eq. (40) the numerical value of Δt is:

$$\Delta t = \frac{(0.2)(1)}{2\ (\frac{1}{6})\ 5} = 0.12 \text{ (period)} = 0.6 \text{ minute}$$

Clearly for permeable media as I_c tends to $\tilde{K}$ or less a small grid size is no longer tenable. As soon as the rule for time step given by Eq. (36) becomes too small (e.g. fall below say $\frac{1}{5}$ of a period of 5 minutes) then a new and coarser grid size in the region near the soil surface and deeper needs to be developed. The old profile needs to be redefined in terms of the new grid points. Let z_j and Δz_j refer to the new grid definition, z_i^o and Δz_i^o referring to the old grid system. Let $\hat{\theta}$ refer to the values of θ in the old grid system at time t^o (i.e. initial profile) and θ_j refer to the initial profile but in the new grid system.

Proceeding recursively, then:

$$\Delta z_2\ \theta_2 = \sum_{i=2}^{I(2)} \hat{\theta}_i \Delta z_i^o + \hat{\theta}_{I(2)+1}\left[(z_2 + \frac{\Delta z_2}{2}) - (z^o_{I(2)} + \Delta z^o_{I(2)})\right] \qquad (41)$$

where I(2) refers to the deeper old cell i whose lower boundary is still above the lower boundary of the new cell 2. In the case of Figure 2, I(2) = 4. More generally:

$$(\Delta z_j)\theta_j = \left[z^o_{I(j-1)+1} + \frac{1}{2}\Delta z^o_{I(j-1)+1} - (z_{j-1} + \frac{\Delta z_{j-1}}{2})\right]\hat{\theta}_{I(j-1)+1}$$

$$+ \sum_{i=I(j-1)+2}^{I(j)} \hat{\theta}_i \Delta z_i^o + \hat{\theta}_{I(j)+1}\left[\left(z_j + \frac{\Delta z_j}{2}\right) - \left(z^o_{I(j)} + \frac{\Delta z^o_{I(j)}}{2}\right)\right] \qquad (42)$$

where I(j) is the index of the deepest old cell i whose lower boundary still lies over the lower boundary of new cell j. Eq. (42) is perfectly

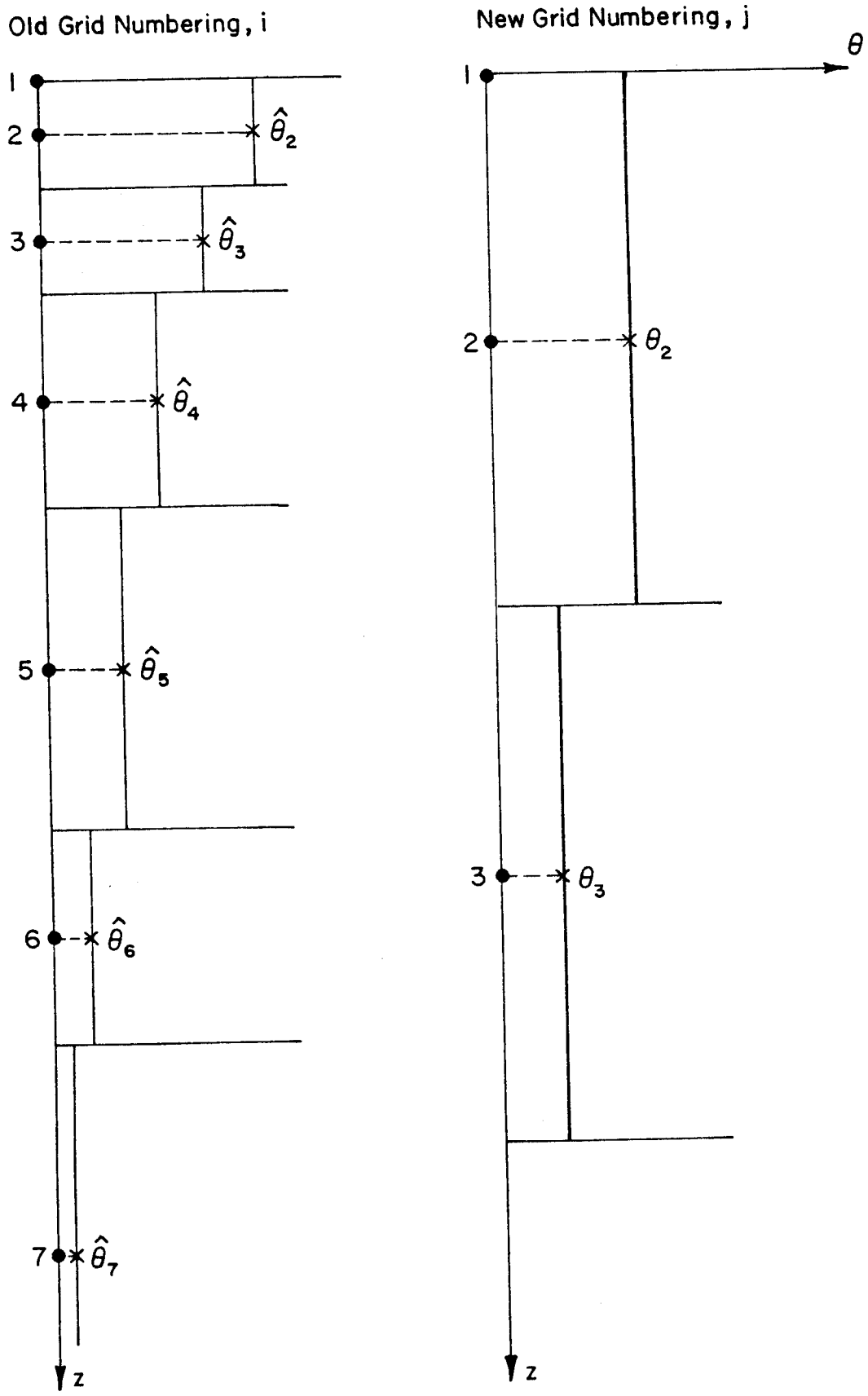

Figure 2. Change in grid size.

general and applies for all j = 3,4 ... N-1 where N refers to the index of the lower boundary in the new grid system. Eq. (42) reduces to Eq. (41) for j = 2 because I(1) = 0, $z_1^o = 0$, $\Delta z_1^o = 0$, $z_1 = 0$ and $\Delta z_i = 0$.

For the case of Figure 2 for j = 3, I(3) = 6, I(2) = 4 and Eq. (42) takes the form:

$$(\Delta z_3)\theta_3 = \left[(z_5^o + \frac{\Delta z_5^o}{2}) - (z_2 + \frac{\Delta z_2}{2})\right]\hat{\theta}_5 + \hat{\theta}_6\,\Delta z_6^o$$

$$+ \hat{\theta}_7\left[(z_3 + \frac{\Delta z_3}{2}) - (z_6^o + \frac{\Delta z_6^o}{2})\right]$$

Given the old grid system characterized by the z_i^o and Δz_i^o, and a new system characterized by the z_j and Δz_j, Eqs. (38) allow the calculation of a new initial profile for the new grid system. The calculations now proceed as before. Eqs. (42) apply whether the new grid is coarser or finer than the old one, or coarser in parts and finer in other parts.

The array I(j) is obtained by comparing the cumulative sum of the Δz_i^o to the cumulative sum of the Δz_j recursively. If $z_i^o + \frac{\Delta z_i^o}{2} < z_j + \frac{\Delta z_j}{2} < z_{i+1}^o + \frac{\Delta z_{i+1}^o}{2}$ then i is the value of I(j). Starting with j = 2 one calculates the difference $z_j + \frac{\Delta z_j}{2} - (z_i^o + \frac{\Delta z_i^o}{2})$ starting with i = 2, then 3 etc. until the difference becomes negative for the first time. Then I(j) = i-1. More generally having just determined I(j-1) one calculates the same difference incrementing i but starting with i = I(j-1) until the difference becomes negative for the first time. I(j) is the last i index value minus one.

APPROXIMATE ANALYTICAL FORMULATION

It should be apparent from the section on time step and grid size selection that for the numerical schemes to predict infiltration accurately small time steps and grid sizes are required. The main value of such computer programs is to serve as benchmark (when used with small time steps and grid sizes) for comparison with simpler and much cheaper schemes. Such schemes have been described in the literature (Morel-Seytoux, 1982) and will not be repeated as a whole. In the literature only the case $n = 2$ was discussed thoroughly. In this section only the case $n = 1$ will be discussed thoroughly to introduce the theory in the simplest mathematical manner. Then results for the (more realistic) case $n = 4$ will be provided without derivation in following sections.

Constant Rainfall Rate Case

It has been shown (Morel-Seytoux, 1982) that the normalized water content of the soil surface, θ_u^*, is the solution of the (approximate) differential equation:

$$\frac{d\theta_u^*}{dt} = \frac{r}{\tilde{\theta} - \theta_r} \frac{(\theta_\ell^* - \theta_i^*)}{H_{b\ell}} \left[\frac{r^* - k_{rw}(\theta_u)}{\theta_u^* - \theta_i^*} \right] \tag{43}$$

where H_b is defined similarly to H_c except that f_w is replaced by k_{rw} and the subscript ℓ refers to the limiting value of water content at the soil surface. If $r^* < 1$ the value of θ_ℓ^* is:

$$\theta_\ell^* = (r^*)^{\frac{1}{n}} \tag{44}$$

and otherwise it is 1. Eq. (43) in the case $n = 1$ can be integrated without difficulty to yield:

$$(r^* - \theta_i^*)\ \ell n\left(\frac{r^* - \theta_{j-1}^*}{r^* - \theta_u^*}\right) - \left(\theta_u^* - \theta_{j-1}^*\right) = \frac{r}{\tilde{\theta} - \theta_r} \frac{\theta_\ell^* - \theta_i^*}{H_{b\ell}} (t - t_{j-1}) \qquad (45)$$

where θ_{j-1}^* is the value of θ_u^* at time t_{j-1}. For a constant rainfall rate case starting with a uniform initial water content of value $\theta_i = \theta_r$, Eq. (45) simplifies to:

$$r^*\left(\ell n\ \frac{r^*}{r^* - \theta_u^*}\right) - \theta_u^* = \frac{rt}{\tilde{\theta} - \theta_r} \frac{\theta_\ell^*}{H_{b\ell}} \qquad (46)$$

The time of occurrence of a water content θ at the soil surface is:

$$T(\theta) = \frac{(\tilde{\theta} - \theta_r)}{r} H_{b\ell} \left\{\frac{r^*}{\theta_\ell^*}\ \ell n\left(\frac{r^*}{r^* - \theta^*}\right) - \frac{\theta^*}{\theta_\ell^*}\right\} \qquad (47)$$

In particular the ponding time is:

$$t_p = \frac{(\tilde{\theta} - \theta_r)}{r} H_b \left\{r^*\ \ell n\left(\frac{r^*}{r^* - 1}\right) - 1\right\} \qquad (48)$$

For large r^* Eq. (48) has the asymptotic form:

$$t_p = \frac{(\tilde{\theta} - \theta_r)H_b}{r} \frac{r^*}{2(r^* - 1)^2} \qquad (49)$$

indicating a shorter ponding time than predicted by the Mein and Larson formula.

The profile is obtained by integration of:

$$\frac{\partial \theta^*}{\partial z} = - \frac{(\theta_\ell^* - \theta_i^*)}{H_{b\ell}} [r^* - k_{rw}(\theta)^*] \qquad (50)$$

which in the case of $\theta_i = \theta_r$ and $n = 1$ yields:

$$z = \frac{H_{b\ell}}{\theta_\ell^*}\ \ell n\left(\frac{r^* - \theta^*}{r^* - \theta_u^*}\right) \qquad (51)$$

Eq. (51) applies for a ponding or no ponding situation. The ponding situation is of greater interest. Prior to ponding the total velocity is given by the general Eq. (2) giving in this case:

$$v = \frac{\tilde{K}\left[H_c(\theta_u,\theta_b) + H_b \int_o^{\theta_u^*} f_w \frac{d\theta^*}{r^* - \theta^*}\right]}{H_b \int_o^{\theta_u^*} \mu_r \frac{d\theta^*}{r^* - \theta^*}} \qquad (52)$$

In particular the infiltration capacity is given by Eq. (52) replacing $H_c(\theta_u,\theta_b)$ by its maximum value, H_c. Eq. (52) requires numerical integration. After ponding the infiltration rate is given by Eq. (52) with $\theta_u = \tilde{\theta}$ and $\theta_u^* = 1$.

After ponding Eqs. (50) and (51) no longer apply. The profile after ponding is given by the expressions:

$$z_\theta = z_p(\theta) + r(t-t_p)\, vF'(\theta) \qquad \text{for } \theta_f \leq \theta \leq \tilde{\theta} \qquad (53)$$

$$\text{and} \quad z_\theta = z_p(\theta) + r(t-t_p)\left[\frac{vF(\theta_f) - vF(\theta_i)}{\theta_f - \theta_i}\right] \qquad \text{for } \theta_i \leq \theta \leq \theta_f \qquad (54)$$

where $z_p(\theta)$ is the location of θ at ponding time and θ_f is the water content value at point of tangency of line drawn from point of coordinates (θ_i, vF_i) to the vF curve.

Alternative Scheme

Prior to ponding all rainfall infiltrates. The area under the profile must at all times be equal to rt. This requirement takes the mathematical form:

$$rt = \int_{\theta_u^*}^{\theta_i^*} (\theta - \theta_i)\, dz \qquad (55)$$

In the case $\theta_i^* = 0$ and $n = 1$, this equation simplifies to:

$$rt = \int_0^{\theta_u^*} \theta^* \, (\tilde{\theta} - \theta_r) \, \frac{H_{b\ell}}{\theta_\ell^*} \, \frac{d\theta^*}{r^* - \theta^*} = (\tilde{\theta} - \theta_r) \, \frac{H_{b\ell}}{\theta_\ell^*} \left[r^* \ell n \left(\frac{r^*}{r^* - \theta_u^*} \right) - \theta_u^* \right] \tag{56}$$

Eq. (56) can be used to eliminate $H_{b\ell}/\theta_\ell^*$ from Eq. (51) to yield a more explicit form of the profile before ponding at time t:

$$z = \left(\frac{rt}{\tilde{\theta} - \theta_r} \right) \frac{\ell n \left(\frac{r^* - \theta^*}{r^* - \theta_u^*} \right)}{r^* \ell n \left(\frac{r^*}{r^* - \theta_u^*} \right) - \theta_u^*} \tag{57}$$

The slope of the profile at time t prior to ponding is given by Eq. (50) more explicitly after elimination of $H_{b\ell}$ in the form:

$$\frac{\partial \theta^*}{\partial z} = - \frac{(\tilde{\theta} - \theta_r) \, (r^* - \theta^*)}{rt} \left[r^* \, \ell n \left(\frac{r^*}{r^* - \theta_u^*} \right) - \theta_u^* \right] \tag{58}$$

In particular at the soil surface the slope has the value:

$$\left. \frac{\partial \theta^*}{\partial z} \right|_{z=0} = - \frac{(\tilde{\theta} - \theta_r)}{rt} \, (r^* - \theta_u^*) \left[r^* \, \ell n \left(\frac{r^*}{r^* - \theta_u^*} \right) - \theta_u^* \right] \tag{59}$$

This result is a very important one for later sections because it provides the slope solely in terms of θ_u.

Practical Prediction of Infiltration

It is clear that for prediction of infiltration such an analytical scheme is far cheaper than with the finite difference scheme. Indeed it suffices to calculate t_p from Eq. (48), a very simple calculation. Prior to t_p, I = r. If desired a profile of water contents can be calculated at various times from Eq. (57). Exploitation of Eq. (57) requires the prior determination of θ_u^*. Due to the form of Eq. (46) it

is easier to select a value of θ_u^* (in the range θ_i^* to θ_ℓ^*) and calculate t from Eq. (46). (A refinement of the method is to replace the ratio $\theta_\ell^*/H_{b\ell}$ by θ_u^*/H_{bu}). Once θ_u^* and t have been determined the profile can be obtained from Eq. (57).

Following ponding Eqs. (53) and (54) provide the profiles if wanted. The infiltration rate can be given by the generalized forms of the Green and Ampt equations provided by Morel-Seytoux (1982, p. 229, Eqs. 84 and 85).

Variable Rainfall Rate Case

In this case Eq. (43) applies for t in the interval (t_{j-1}, t_j) during which the rainfall rate remains constant at the value r_j. However the term $(\theta_\ell^* - \theta_i^*)/H_{b\ell}$ must be reinterpreted. Its original meaning is that of an average value of $k_{rw} \frac{dh_c}{d\theta^*}$ in the range of integration (t_{j-1}, t_j) in which θ_u^* starts at value θ_{j-1}^* and ends at $\theta_{\ell j}^*$. For $r_j^* < 1$ the limiting value of $\theta_{\ell j}^*$ is $(r_j^*)^{1/n}$. For $r_j^* > 1$ it is 1. For variable rainfall rate Eq. (43) must be replaced by the expression:

$$\frac{d\theta_u^*}{dt} = \frac{r_j}{\tilde{\theta} - \theta_r} \frac{(\theta_{\ell j}^* - \theta_{j-1}^*)}{H_{bj}} \left[\frac{r_j^* - k_{rw}(\theta_u^*)}{\theta_u^* - \theta_i^*} \right] \tag{60}$$

where H_{bj} is defined as:

$$H_{bj} = \int_{h_c(\theta_{\ell j}^*)}^{h_c(\theta_{j-1}^*)} k_{rw}\, dh_c \tag{61}$$

The integration of Eq. (60) yields for θ_u^* an implicit relation of the form:

$$(r_j^* - \theta_i^*)\, \ell n \left(\frac{r_j^* - \theta_{j-1}^*}{r_j^* - \theta_u^*} \right) - (\theta_u^* - \theta_{j-1}^*) = \frac{r_j}{\tilde{\theta} - \theta_r} \frac{\theta_{\ell j}^* - \theta_{j-1}^*}{H_{bj}} (t - t_{j-1}) \tag{62}$$

Time of Appearance of a Water Content

It is given by the expression:

$$T(\theta) = t_{j-1} + \frac{(\tilde{\theta} - \theta_r)H_{bj}}{(\theta^*_{\ell j} - \theta_{j-1})r_j}\left\{(r^*_j - \theta^*_i)\ \ell n\left(\frac{r^*_j - \theta^*_{j-1}}{r^*_j - \theta^*}\right) - (\theta^* - \theta^*_{j-1})\right\} \quad (63)$$

Eq. (63) only applies for the θ for which $T(\theta)$ falls in the interval (t_{j-1}, t_j). It is important to fully realize the nature (meaning) of the symbols. In Eqs. (60), (62) and (63) θ_i is the *minimum* value of water content in the initial profile (*not necessarily uniform*). The initial value of θ_u say θ_{ui} is not the same as θ_i if the initial profile is not uniform. If however $\theta_i(0)$, initial water content at $z = 0$, is $< \theta_r$, then the initial value of θ_u is θ_r. For the first time interval Eq. (62) has the form:

$$(r^*_1 - \theta^*_i)\ \ell n\left(\frac{r^*_1 - \theta^*_{ui}}{r^*_1 - \theta^*_u}\right) - (\theta^*_u - \theta^*_{ui}) = \frac{r_1}{\tilde{\theta} - \theta_r}\left(\frac{\theta^*_{\ell 1} - \theta^*_{ui}}{H_{b1}}\right)t \quad (64)$$

with $H_{b1} = \int_{h_c(\theta^*_{\ell 1})}^{h_c(\theta^*_{ui})} k_{rw}\, dh_c$. Another notation for θ^*_{ui} is θ^*_o. For the second time interval Eq. (62) has the form:

$$(r^*_2 - \theta^*_i)\ \ell n\left(\frac{r^*_2 - \theta^*_1}{r^*_2 - \theta^*_u}\right) - (\theta^*_u - \theta^*_1) = \frac{r_2}{\tilde{\theta} - \theta_r}\ \frac{(\theta^*_{\ell 2} - \theta^*_1)}{H_{b2}}\ (t - t_1) \quad (65)$$

with $H_{b2} = \int_{h_c(\theta^*_{\ell 2})}^{h_c(\theta^*_1)} k_{rw}\, dh_c$, etc...

Ponding Time

One first tries for ponding in the first time interval, solving Eq. (62) for t_p with $\theta_u^* = 1$, explicitly:

$$t_p = \frac{(\tilde{\theta} - \theta_r)H_{b1}}{r_1(1 - \theta_o^*)} \left\{ (r_1^* - \theta_i^*) \ell n \left(\frac{r_1^* - \theta_o^*}{r_1^* - 1} \right) - (1 - \theta_o^*) \right\} \tag{66}$$

If t_p is less than t_1, ponding does occur in first time interval and it has been found. If t_p is greater than t_1, ponding does not occur during the first interval. One then performs the calculations for the next interval and the next, etc. If it has been found that t_p does not occur in interval $(0, t_{j-1})$ one then recalculates it from the relation:

$$t_p = t_{j-1} + \frac{(\tilde{\theta} - \theta_r)\, H_{bj}}{r_j(1 - \theta_{j-1}^*)} \left\{ (r_j^* - \theta_i^*) \ell n \left(\frac{r_j^* - \theta_{j-1}^*}{r_j^* - 1} \right) - (1 - \theta_{j-1}^*) \right\} \tag{67}$$

Note that if in any interval r_j is $< \tilde{K}$ there is no need to calculate a ponding time. Note also that to exploit Eq. (67) θ_{j-1}^* must be known. For example to proceed with second interval calculation one must know θ_1^*. That will require the implicit solution of nonlinear algebraic Eq. (64) for unknown $\theta_u^* = \theta_1^*$ at time $t = t_1$.

Water Content Profile

The general form of the equation for the slope of the water content profile is:

$$\frac{\partial \theta^*}{\partial z} = - \frac{\left(\theta_{\ell j}^* - \theta_{j-1}^* \right)}{H_{bj}} \left[r^* - k_{rw}(\theta^*) \right] \tag{68}$$

Integration of Eq. (68) yields the profile at a given time t in the interval (t_{j-1}, t_j) for the case $n = 1$ for new water contents (i.e. for $\theta_{j-1}^* \leq \theta^* \leq \theta_u^*$ if θ_u increases or $\theta_u^* \leq \theta^* \leq \theta_{j-1}^*$ if θ_u decreases during the time interval) in the form:

$$z = \frac{H_{bj}}{\theta^*_{\ell j} - \theta^*_{j-1}} \ell n\left(\frac{r^*_j - \theta^*}{r^*_j - \theta^*_u}\right) \tag{69}$$

The position of the water contents already present in the soil prior to time t_{j-1}, defines a new profile at time t given by the equation:

$$z = z_{j-1}(\theta) + z(\theta^*_{j-1}) \tag{70}$$

where $z_{j-1}(\theta)$ is the location of (old) water content θ at time t_{j-1} and $z(\theta^*_{j-1})$ is the position at time t of old water content at soil surface obtained from Eq. (69). Exploitation of Eqs. (69) and (70) requires that $\theta^*_u(t)$ be calculated from Eq. (62). In practice one would calculate the profiles at the discrete times $t_1, t_2, \ldots t_{j-1}, t_j, \ldots$ etc.

It should be noted that the profiles may display peaks and troughs. The same value of a given water content may appear at several different depths. The label "new" for a water content refers to the fact that this value has appeared (maybe again) at the soil surface during the current time interval. It is not necessarily new to the profile.

Alternate Form of Water Content Profile

Prior to ponding all rainfall infiltrates. The incremental change in area during time interval $t - t_{j-1}$ is $r_j(t - t_{j-1})$. Expressing mathematically this material balance requirement yields the relation:

$$\begin{aligned} r_j\,(t - t_{j-1}) &= (\tilde{\theta} - \theta_r) \int_0^{z(\theta^*_{j-1})} (\theta^* - \theta^*_i)dz \\ &= (\tilde{\theta} - \theta_r) \int_{\theta^*_u}^{\theta^*_{j-1}} (\theta^* - \theta^*_i) \frac{dz}{d\theta^*} d\theta^* \end{aligned} \tag{71}$$

or using Eq. (68) more explicitly:

$$r_j\,(t - t_{j-1}) = (\tilde{\theta} - \theta_r)\,\frac{H_{bj}}{\theta^*_{\ell j} - \theta^*_{j-1}} \int_{\theta^*_u}^{\theta^*_i} \frac{(\theta^* - \theta^*_i)\,d\theta^*}{r^* - \theta^*} \tag{72}$$

which after integration yields precisely Eq. (62). Thus mass balance is satisfied.

One can use Eq. (62) to eliminate the ratio $H_{bj}/(\theta^*_{\ell j} - \theta^*_{j-1})$ from Eq. (69) with the result for the "new" water contents:

$$z = \frac{r_j(t - t_{j-1})}{\tilde{\theta} - \theta_r}\;\frac{\ell n\left(\dfrac{r^*_j - \theta^*}{r^*_j - \theta^*_u}\right)}{(r^*_j - \theta^*_i)\,\ell n\left(\dfrac{r^*_j - \theta^*_{j-1}}{r^*_j - \theta^*_u}\right) - (\theta^*_u - \theta^*_{j-1})} \tag{73}$$

The interesting aspect of Eq. (73) is that it will preserve water balance *regardless* of the *actual* relationship between θ_u and t. This remark will be thoroughly utilized in later sections.

The slope of the profile at time t prior to ponding is given by Eq. (68) and more explicitly after elimination of $H_{bj}/(\theta^*_{\ell j} - \theta^*_{j-1})$ in the form:

$$\frac{\partial\theta^*}{\partial z} = -\frac{(\tilde{\theta} - \theta_r)}{r_j(t-t_{j-1})}\left\{(r^*_j - \theta^*_i)\,\ell n\left(\frac{r^*_j - \theta^*_{j-1}}{r^*_j - \theta^*_u}\right) - \theta^*_u - \theta^*_{j-1}\right\}(r^* - \theta^*) \tag{74}$$

and in particular at the soil surface:

$$\left.\frac{\partial\theta^*}{\partial z}\right|_{z=0} = -\frac{(\tilde{\theta} - \theta_r)}{r_j(t-t_{j-1})}\left\{(r^*_j - \theta^*_i)\,\ell n\left(\frac{r^*_j - \theta^*_{j-1}}{r^*_j - \theta^*_u}\right) - \left(\theta^*_u - \theta^*_{j-1}\right)\right\}(r^* - \theta^*_u) \tag{75}$$

Again this result is important for later sections because it provides the slope solely in terms of θ_u.

Practical Prediction of Infiltration

Typically one would check for ponding time in first time interval $(0,t_1)$ using Eq. (67) for j = 1. If $t_p > t_1$ one calculates the pre-ponding water content profile at time t_1 by first calculating θ_1^* from Eq. (62) for j = 1 then the profile from Eqs. (73) and (70) for j = 1. Then one checks for ponding in second interval, using Eq. (67) for j = 2. If the calculated value exceeds t_2 one calculates the profile at time t_2 by calculating θ_2^* from Eq. (62) for j = 2 then the profile from Eqs. (73) and (70) for j = 2. Then one checks for ponding in next interval, etc. Sooner or later t_p will fall in an interval (t_{j-1}, t_j). When this happens one calculates the profile at ponding time from Eqs. (73) and (70) with $t = t_p$ and $\theta_u^* = 1$. Naturally until ponding time I = r.

Following ponding the procedures to determine profiles and capacity infiltration rate are the same as for the case of constant rainfall rate. The new profiles are:

$$z_\theta = z_{j-1}(\theta) + r_j(t - t_{j-1})\, vF'(\theta) \qquad \text{for } \theta_f \leq \theta \leq \tilde{\theta} \qquad (76)$$

$$z_\theta = z_{j-1}(\theta) + r_j(t - t_{j-1})\left[\frac{vF(\theta_f) - vF(\theta_i)}{\theta_f - \theta_i}\right] \qquad \text{for } \theta_i \leq \theta \leq \theta_f \qquad (77)$$

where $z_{j-1}(\theta)$ represents the position of water content θ at time t_{j-1}. The index (j-1) may also refer to ponding (p).

HYBRID FORMULATION

Based on the remark that the profiles obtained analytically in the previous section prior to ponding automatically satisfy mass balance regardless of the actual relation between θ_u and t, a new approach was conceived. After all Eqs. (43) and (60) are only approximate. The approximations were made to obtain explicit analytical solutions. The satisfaction of the boundary condition of a given rainfall rate at the soil surface previously given as Eq. (18) requires the knowledge not only of θ_u but also of $\frac{\partial\theta}{\partial z}$ at soil surface. By numerical techniques in order to find θ_u one must find the entire profile through the soil. Why not replace in the boundary condition the slope by an analytical approximate solution such as given by Eq. (75) and solve algebraically for the only remaining unknown θ_u while using the correct soil functions $f(\theta)$, $G(\theta)$ and $E(\theta)$ which only appear approximately in the analytical solutions as average values over a range of water contents?

Case n = 1

In this case the boundary condition for θ_u takes the form:

$$r = vf(\theta_u) + G(\theta_u) + E(\theta_u)\,\frac{(\tilde{\theta} - \theta_r)}{r(t^v - t^o)}\,(r^* - \theta_u^*)\left\{(r^* - \theta_i^*)\,\ell n\left(\frac{r^* - \theta_u^{*o}}{r^* - \theta_u^*}\right)\right\} - (\theta_u^* - \theta_u^{*o}) \tag{78}$$

where θ_u^o is known water content at soil surface at old time t^o, θ_u is unknown value of water content at soil surface at new time t^v and r is the current prevailing rainfall rate. Strictly speaking v is given by Eq. (2) or for a semi-infinite case and using a Green-Ampt type approximation to estimate the gravity and resistance terms by the expression:

$$v = \tilde{K} \frac{\left[H_c(\theta_u) + \frac{W}{\tilde{\theta} - \theta_i}\right]}{\frac{W}{\tilde{\theta} - \theta_i}} \tag{79}$$

Substitution of Eq. (79) in Eq. (78) yields:

$$\tilde{K} \frac{\left[(\tilde{\theta} - \theta_i)\, H_c(\theta_u) + W^v\right]}{W^v} f(\theta_u) + G(\theta_u) \tag{80}$$

$$+ \frac{E(\theta_u)(\tilde{\theta} - \theta_r)}{r(t^v - t^o)} \left\{ (r^* - \theta_u^*)\,(r^* - \theta_i^*)\, \ell n \left(\frac{r^* - \theta_u^{*o}}{r^* - \theta_u^*} \right) - (\theta_u^* - \theta_u^{*o}) \right\} = r$$

It is interesting to compare Eqs. (80) and (24). In Eq. (24) old (iterate) values of the profile are used whereas in Eq. (80) only the unknown value of θ_u at time t^v appears. Thus solution of Eq. (80) is more efficient since it does not require iteration. Otherwise the equations have a very similar structure. As Eq. (23) provided a higher approximation for the estimation of the slope at the soil surface than the usual $\frac{\theta_2 - \theta_u}{z_2}$ (to which it reduces for large $\frac{z_3}{z_2}$ ratio), Eq. (75) provides an even higher approximation. It is also interesting to note that Eq. (80) shows the influence of the time step $(t^v - t^o)$ explicitly on the solution; Eq. (24) does not. The influence of the time step is felt in Eq. (24) through the numerical calculations of L_G^m, L_R^m, θ_2^m and θ_3^m.

Whereas in Eq. (75) the assumption n = 1 for the exponent in the power law for relative permeability was made, nevertheless in Eq. (80) the true curves for f, G, and E can be used, curves based on the true k_{rw} for which n is not 1. The numerical solution for θ_u^* (t) provides a better solution than use of Eq. (62). Once Eq. (80) has been solved

for θ_u^v profiles can be obtained from Eq. (73) at time t^v for the new water contents and by Eq. (70) for the old water contents.

Actually Eq. (79) forces ponding time on the solution because at $\theta_u = \tilde{\theta}$, f = 1, G and E are zero and one obtains:

$$\tilde{K} \frac{\left[(\tilde{\theta} - \theta_i)H_c + W^v\right]}{W^v} = r \tag{81}$$

A more accurate procedure is to use for v the more coherent approximation, namely:

$$v = \frac{\left[\tilde{K} H_c \theta_u + L_G(\theta_u)\right]}{L_R(\theta_u)} \tag{82}$$

where $L_G(\theta_u)$ is calculated as:

$$L_G(\theta_u) = L_G(\theta_u^o) + \frac{r(t^v - t^o) \int_{\theta_u^{*o}}^{\theta_u^*} f_w \frac{d\theta^*}{r^* - \theta^*}}{(\tilde{\theta} - \theta_r)\left[(r^* - \theta_i^*)\, \ell n\left(\frac{r^* - \theta_u^{*o}}{r^* - \theta_u^*}\right) - (\theta_u^* - \theta_u^{*o})\right]} \tag{83}$$

The integral in the numerator of Eq. (83) can be approximated as:

$$\int_{\theta_u^{*o}}^{\theta_u^*} f_w \frac{d\theta^*}{r^* - \theta^*} = \frac{1}{2}\left[f_w(\theta_u^{*o}) + f_w(\theta_u^*)\right] \ell n\left(\frac{r^* - \theta_u^{*o}}{r^* - \theta^*}\right) \tag{84}$$

The integral in the denominator can be approximated similarly.

Successive substitutions finally lead to a better form of Eq. (80), namely:

$$\tilde{K}\left[\frac{H_c(\theta_u) + L_G(\theta_u^o) + \dfrac{r(t^v - t^o)\left[f_w(\theta_u^{*o}) + f_w(\theta_u^*)\right]\ell n\left(\dfrac{r^* - \theta_u^{*o}}{r^* - \theta_u^*}\right)}{2(\tilde{\theta} - \theta_r)\left[(r^* - \theta_i^*)\,\ell n\left(\dfrac{r^* - \theta_u^{*o}}{r^* - \theta_u^*}\right) - (\theta_u^* - \theta_u^{*o})\right]}}{L_R(\theta_u^o) + \dfrac{r(t^v - t^o)\left[\mu_r(\theta_u^{*o}) + \mu_r(\theta_u^*)\right]\ell n\left(\dfrac{r^* - \theta_u^{*o}}{r^* - \theta_u^*}\right)}{2(\tilde{\theta} - \theta_r)\left[(r^* - \theta_i^*)\,\ell n\left(\dfrac{r^* - \theta_u^{*o}}{r^* - \theta^*}\right) - (\theta_u^* - \theta_u^{*o})\right]}}\right] f_w(\theta_u)$$

$$+ G(\theta_u) + \frac{E(\theta_u)(\tilde{\theta} - \theta_r)(r^* - \theta_u^*)}{r(t^v - t^o)}\left\{(r^* - \theta_i^*)\ell n\left(\frac{r^* - \theta_u^{*o}}{r^* - \theta_u^*}\right) - (\theta_u^* - \theta_u^{*o})\right\} = r \tag{85}$$

Case n = 4

The case n = 1 is not realistic. However for sands a value of n = 4 is very realistic. For this reason similar equations were derived in this case. The results can be found in two publications (Ross, 1982; Ross and Morel-Seytoux, 1982). Figure 3 shows typical predicted profiles of water content using soil characteristic data measured in the laboratory. In the laboratory experiments were performed to observe ponding time under various rainfall conditions. The ponding times were also calculated by the computer program SOILMOP (Ross and Morel-Seytoux, 1982) and the values were compared in Table 1. The agreement is quite reasonable.

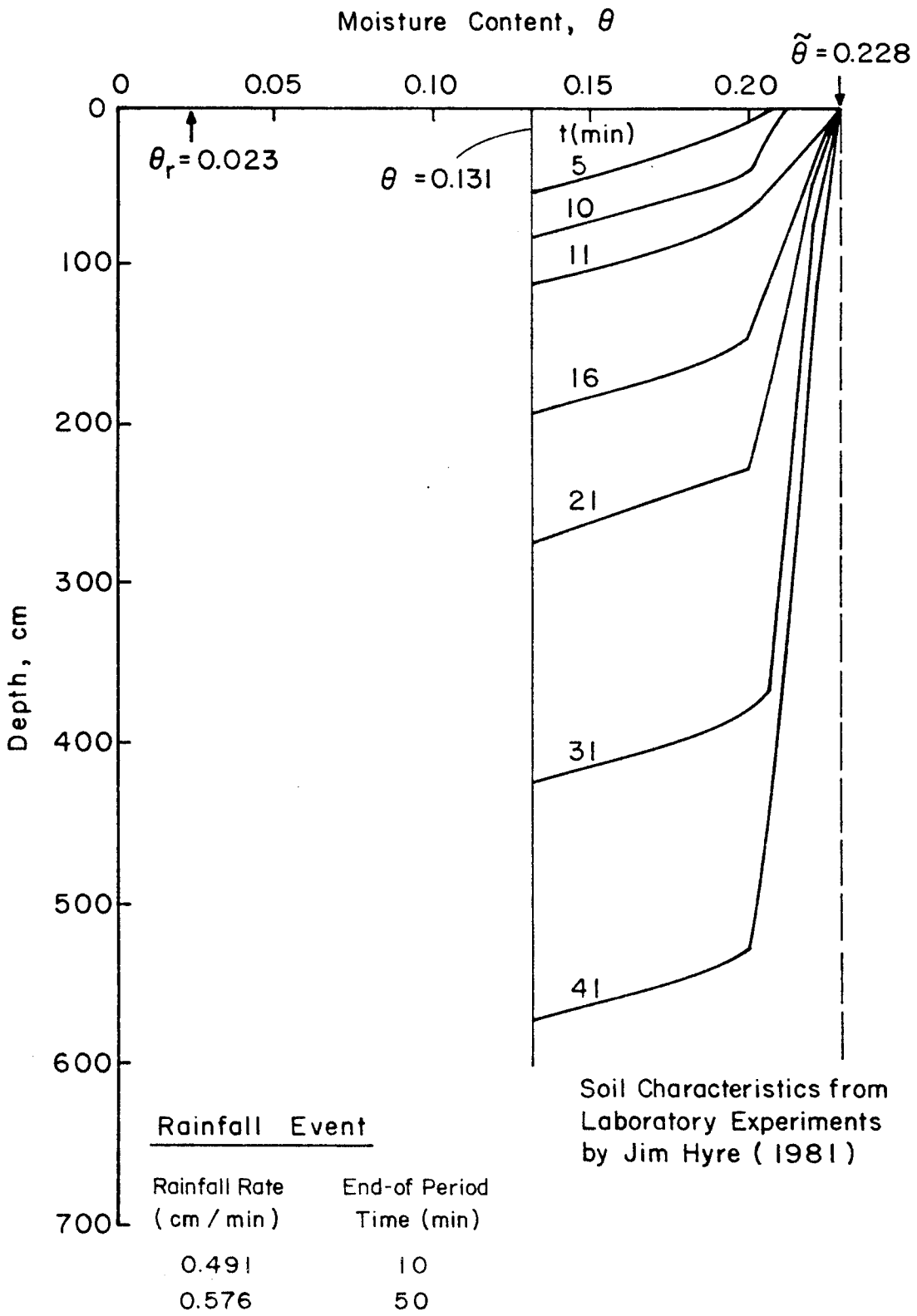

Figure 3. Water content profiles at selected times.

Table 1. Comparison of Calculated Ponding Times and Observed Values in Experiments (Hyre, 1981)

Rainfall Event		Initial Water Content	Observed Ponding Time (min)	Calculated Ponding Time* (min)
rate (cm/min)	end-of-period time (min)			
0.677	constant	0.126	5.2	4
1.160	constant	0.123	0.93	1
0.491 0.576	10 20	0.131	13	11
0.508 0.550	10 22	0.127	18	14
0.542	constant	0.123	21.5	16

*Reported ponding times were rounded to the nearest minute greater than or equal to the calculated ponding time.

CONCLUSIONS

New techniques of solution for prediction of infiltration and water content profiles were developed. Comparison of results of the hybrid analytical-numerical techniques with laboratory measurements indicates that the technique is sufficiently accurate. Comparison of the new technique with an existing finite-difference program was difficult because the finite difference program was not well documented and it did not accept readily different analytical expressions for the soil characteristics. In addition the finite difference model was expensive to run. SOILMOP (Ross and Morel-Seytoux, 1982) was about 25 times cheaper to run than the finite difference model. In order to pursue the comparisons further it was decided to develop a finite difference program that could solve both the Richards equation and the governing equations derived from the two-phase formulation. The finite difference equations are presented in this report. The programs however are not yet fully operational and documented, but are expected to be in late 1983.

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