JOURNAL OF
ENVIRONMENTAL HYDROLOGY
The Electronic Journal of the International Association for Environmental Hydrology
On the World Wide Web at http://www.hydroweb.com
VOLUME 8 2000

A DYNAMIC SOIL WATER MODEL FOR ENVIRONMENTAL SIMULATION PROBLEMS

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A soil water model of one dimensional flow, using the Runge-Kutta Gill algorithm, is described with the aim of forming a flexible general purpose simulation tool. The problem of 'stiffness' appearing in the traditional finite difference methods approach is discussed, and a numerical algorithm able to overcome it is adopted. The model, based on a flexible numerical approach, is tested with published data. The tests show the model performance to be satisfactory in soil water simulations. The performance of the numerical algorithm is compared with that of a number of alternative numerical methods. The comparison supports the original choice of the algorithm.

INTRODUCTION

Within the wider framework of environmental studies, phenomena of water movement and storage in the soil are of major importance. Reasons for this can be found in the particular significance of these phenomena in relation to the hydrologic cycle, plant growth and crop production, and the movement of chemicals in the environment. A list of processes of the hydrologic cycle that take place within the soil water system would include interception, transpiration, soil evaporation, infiltration, flow of water, storage in the upper soil layers, and drainage. In addition, these processes greatly influence overland flow and groundwater recharge. With respect to environmental problems, subsurface water movement is the key factor, able to adversely affect them through scarcity or excess.

Models of soil water movement are required for simulation of a great number of composite environmental processes. The limitations of such models caused by computational constraints are being reconsidered because of the availability of increasingly powerful hardware. The main problems that need to be considered are, therefore, the difficulties involved with the versatility of the model, its ease of application, and the ease of combination with other environmental models. In this paper the development and implementation of a model using numerical algorithms for one-dimensional soil water flow are discussed. The development places major emphasis on these issues that enhance the versatility of the model and make it readily applicable as a general simulation tool. The mathematical formulation of the model and the standard numerical approaches are first discussed, followed by the limitations of the model using published results. Finally a comparison is carried out between the performance of the adopted solution method and the performances of two other suitable methods.

THEORY

Two properties define the water status of a soil; moisture content and water potential. Water potential is the term used for the potential energy of water in the soil.

The fundamental law that defines the relationship between potential and flow is that of Darcy, which can be expressed as:

$$v_x = K\Delta u / \Delta x \tag{1}$$

Where v_x is the net velocity in the x direction through a soil segment, Δu is the difference in the potential h between the two ends of the segment, Δx is the length of the segment, and K is the hydraulic conductivity of the soil. The minus sign indicates that water flows towards the point of lower potential.

Hydraulic conductivity depends on the pore structure of the soil as well as on its moisture content. As a soil dries, hydraulic conductivity decreases because with the larger soil pores empty, water is transmitted only through the finer ones, which leads to a more restricted and tortuous path.

The fundamental equation for unsaturated flow derives from a combination of the laws of Darcy and continuity. In the case of one-dimensional flow in the x direction through a small volume of soil $dxdydz$, the law of continuity states that:

$$\partial\theta\partial t(dxdydz) = v_x(dydz) - \left[(v_x + \partial v_x / \partial x\ dx)dy\ dz\right] - S \tag{2}$$

where θ is the moisture content of the soil and S is the rate of water abstraction by a sink in the soil

element. Let U be a sink term, defined as the rate of extraction per unit soil volume and expressed as

$$U = S/(dxdydz) \tag{3}$$

Eliminating terms in equation (2) and substituting equation (1) gives

$$\frac{\partial\theta}{\partial t} = \frac{\partial\left[K\frac{\partial u}{\partial x}\right]}{\partial x} - U \tag{4}$$

Using the specific moisture content $C = \partial\theta / \partial\Psi$, this equation can be written as

$$C\frac{\partial y}{\partial t} = \frac{\partial\left[K\frac{\partial u}{\partial z}\right]}{\partial z} - U \tag{5}$$

or

$$C\frac{\partial y}{\partial t} = \frac{\partial\left[K\frac{\partial h}{\partial z}+1\right]}{\partial z} - U \tag{6}$$

where h is the water pressure potential.

By defining D as $D=C(h)$ the previous equation becomes

$$D(h,z)\frac{\partial u}{\partial t} = \frac{\partial\left[K(h,z)\frac{\partial u}{\partial z}\right]}{\partial z} - U(z,t) \tag{7}$$

Since $h = u - z$

$$D(u-z,z)\frac{\partial u}{\partial t} = \frac{\partial\left[K(u-z,z)\frac{\partial u}{\partial z}\right]}{\partial z} - U(z,t) \tag{8}$$

Equation (8) forms the basis of the soil water model. Its solution in the time interval dt and space interval requires the specification of initial value of the independent variable $u(z, t)$ and the boundary conditions at z_0 and z_1 throughout the time interval in terms of the head h.

NUMERICAL SOLUTION OF THE MATHEMATICAL MODEL

Equation (8) is a parabolic partial differential equation in two independent (t, z) and one dependent variable. As the coefficients of C and K are functions of h, the equation is nonlinear.

Using the Taylor expansion approximation for the central-difference (three-point) operators for the first and second derivatives of U with respect to x at node I as

$$\left[\frac{\theta h}{\theta x}\right]_i = \frac{h_{i+1} - h_i}{2\Delta x} \tag{9}$$

$$\left[\frac{\vartheta^2 h}{\vartheta x^2}\right]_i = \frac{h_{i+1} - 2h_i + h_{i+1}}{\Delta x^2} \tag{10}$$

in equation (6) leads to a different discretized form

$$C\frac{\theta h}{\theta t} = K\frac{\vartheta^2 h}{\vartheta z^2} + \frac{\vartheta K}{\vartheta z}\left[\frac{\vartheta h}{\vartheta z} + 1\right] - U \tag{11}$$

From equation (9) one can deduce that

$$\frac{h_{i+1} - h_i}{\Delta z} = \left[\frac{\vartheta h}{\vartheta z}\right]_{i+\frac{1}{2}} \tag{12}$$

where $1+\frac{1}{2}$ refers to the midpoint between i and i+1. Equation (6) can therefore be approximated by,

$$C_i\left[\frac{\vartheta h}{\vartheta t}\right]_i = \frac{1}{\Delta z}\left[K_{i+\frac{1}{2}}\left[\frac{h_{i+1} - h_i}{\Delta z} - 1\right] - K_{i-\frac{1}{2}}\left[\frac{h_i - h_{hi-1}}{\Delta z} - 1\right]\right] - U_i \tag{13}$$

Equation (13) is known as the "local balance" model (Vauclin et al., 1979) because it expresses the water balance of a soil element between $i-\frac{1}{2}$ and $i+\frac{1}{2}$. In a number of studies a discretized approximation to equation 13 has been used:

$$C_i\left[\frac{\vartheta h}{\vartheta t}\right]_i = K_i\left[\frac{h_{i+1} - 2h_i + h_{i-1}}{\Delta z^2}\right] + \left[\frac{K_{i+\frac{1}{2}} - K_{i-\frac{1}{2}}}{\Delta z}\right]\left[\frac{h_{i+1} - h_{i-1}}{2\Delta z}\right] - U_i \tag{14}$$

Vauclin et al. 1979 report that schemes based on equation (14), also known as "the decomposed model", performed generally worse than those based on the local balance model.

To approximate the time derivative, central differences can again be used

$$\left[\frac{\vartheta h}{\vartheta t}\right]^{j+\frac{1}{2}} = \frac{h^{j+1} - h^j}{\Delta t} \tag{15}$$

or, alternatively, backward differences, and forward differences

$$\left[\frac{\vartheta h}{\vartheta t}\right]^{j+1} = \frac{h^{j+1} - h^j}{\Delta t} \tag{16}$$

$$\left[\frac{\vartheta h}{\vartheta t}\right]^{j} = \frac{h^{j+1} - h^j}{\Delta t} \tag{17}$$

The use of forward differences leads to an explicit model in which the difference equations for each node at time-step *j* can be readily solved in terms of the values of *h* in step *j*-1. Models of this type are easy to program and each time step is computationally relatively inexpensive. The preservation and of stability and accuracy, however, dictates the use of very small time steps making the scheme relatively inefficient (Haverkamp et al., 1977).

The use of backward or central differences results in an implicit scheme involving a system of nonlinear difference equations, which can only be solved iteratively by a Newton-type method. Although they allow the use of longer time-steps than explicit methods, such nonlinear implicit schemes have not been popular for the solution of the flow equation because they are quite involved to program, are expensive computationally at each time-step and, more importantly, there exists an attractive alternative. This consists of linearizing the difference equations by expressing the specific moisture content and the hydraulic conductivity in terms of a known pressure head. This reduces the *C* and *K* functions to parameter values and the nonlinear system of difference equations to a linear time-varying set. With the use of backward differences the local balance model becomes

$$\hat{C}_i \frac{h_i^{j+1} - h_i^j}{\Delta t} = \frac{1}{\Delta z}\left[\hat{K}_{i+\frac{1}{2}}\left[\frac{h_{i+1}^{j+1} - h_i^{j+1}}{\Delta z} - 1 \right] - \hat{K}_{i-\frac{1}{2}}\left[\frac{h_i^{j+1} - h_{i-1}^{j+1}}{\Delta z} - 1 \right] \right] - U_i \tag{18}$$

where $\hat{C}$ and $\hat{K}$ represent the known values of the parameters. This type of scheme based on backward time differences is known as "fully implicit".

The use of the central-difference approximation yields

$$\hat{C}_i \frac{h_i^{j+1} - h_i^j}{\Delta t} = \hat{C}_i \left[\frac{\vartheta h}{\vartheta t} \right]^{j+\frac{1}{2}} \tag{19}$$

The partial derivative at is expressed as a weighed sum of the partial derivatives at *j* and $j + \frac{1}{2}$. When the weights are both equal to 0.5 the resulting scheme is given by

$$\begin{aligned} \hat{C}_i \frac{h^{j+1} - h_i^j}{\Delta t} = {} & \frac{1}{2\Delta z}\left[\hat{K}_{i+\frac{1}{2}}\left[\frac{h_{i+1}^{j+1} - h_i^{j+1}}{\Delta z} - 1 \right] - \hat{K}_{i-\frac{1}{2}}\left[\frac{h_i^{j+1} - h_{i-1}^{j+1}}{\Delta z} - 1 \right] \right] + \\ & + \frac{1}{2\Delta z}\left[K^j{}_{i+\frac{1}{2}}\left[\frac{h_{i+1}^j - h_i^j}{\Delta z} - 1 \right] - K^j{}_{i-\frac{1}{2}}\left[\frac{h_i^j - h_{i-1}^j}{\Delta z} - 1 \right] \right] - U_i \end{aligned} \tag{20}$$

and is known as a Crank-Nicholson type scheme (Smith, 1985, Vauclin, 1979).

For both the totally implicit and the Crank-Nicholson type models estimates for $\hat{C}$ and $\hat{K}$ are required. The estimates for $\hat{C}$ must approximate $C^{j+\frac{1}{2}}$ and for $\hat{K}$, K^{j+1}. The simplest and most commonly used method is to assume that for any particular time mode

$$\left.\begin{aligned}\hat{C} &= C\left(h^{i}\right)\\ \hat{K} &= K\left(h^{j}\right)\end{aligned}\right\} \qquad (21)$$

There is an additional requirement for estimates of $K_{i+\frac{1}{2}}$ and $K_{i-\frac{1}{2}}$. These are estimated either as some type of average of K_{i-1}, K_i and K_{i+1}, or from estimates of h at $i+\frac{1}{2}$ and $i-\frac{1}{2}$, which are themselves evaluated as averages of h_{i-1}, h_i and h_{i+1}.

These methods are widely adopted to the solution of the flow equation for soil water movement. In the following paragraphs the problems with these methods and different approaches to the numerical solution of the soil water model are examined.

LIMITATIONS OF TRADITIONAL SCHEMES - IMPLICIT MODELS

Finite-difference methods solve partial differential equations by discretizing all variables in both space and time. In the case of a nonlinear partial differential equation, the difference equations that result from the discretization are also nonlinear.

After comparing a large number of variations on the two principal models of equations (18) and (20), Vauclin et al. (1979) recommended the use of a totally implicit model with estimates $\hat{C}$ and $\hat{K}$ given by equations (21) and (22) and estimates of $K_{i+\frac{1}{2}}$ given by the geometric mean, $\sqrt{K_i K_{i+1}}$.

At each time-step the solution of a vector equation is of the form,

$$\left(\bar{I}-\bar{A}\right)u^{j+1}=\bar{b} \qquad (22)$$

where $\bar{I}$ is the identity matrix. Equation (22) can either be solved iteratively or by a simple efficient algorithm. In a comparative study Vauclin et al. (1979) showed that the Thomas algorithm based solution is computationally more efficient than the iterative one.

When an explicit linearization is combined with a backward difference discretization for the time derivative (equation 18), the following system of equations is derived:

$$u^{j+1}=\Delta t\,\bar{A}^{j}u^{j+1}+\bar{u}+\Delta t\,\bar{s}^{j} \qquad (23)$$

where $\bar{A}$ is the matrix and $s_i=-\frac{U_i}{e_i}$.

This system was solved at each time step using library routines.

A COMPARISON BETWEEN INTEGRATION ALGORITHMS

Selection of the appropriate integrator for the solution of the system is imperative to the success of the method. Problems reported in the integration of systems of ordinary differential equations that

have been arrived at by the spatial discretization of a partial differential equation have mainly to do with the stiffness often associated with problems involving such systems. The dependence of the time discretization method on the space discretization of traditional differential of equations makes it advisable that standard explicit Runge-Kutta algorithms are not used as general purpose routines. Instead, methods exhibiting a more extensive region of stability should be implemented.

In the following, the proposed method is compared with the performance of two other integration routines. The first algorithm is based on one of the widely used Runge-Kutta formulae by Kuo (1981). The second is based on the standard implicit finite difference method with explicit linearization of the discretized equations. The method was recommended by Vauclin et al. (1979) and Haverkamp et al. (1977) on the basis of their comparison tests. As it is their tests that have been used here, the inclusion of the method provides a reference point between the results of these two methods and the present work.

THE RUNGE-KUTTA METHOD

Runge-Kutta formulae are the most popular integrators for systems of ordinary differential equations. However, they are often inefficient when applied, as is the case here, because of the so called "stiffness" that equations describing physical systems exhibit when there are transient components which vary in time at widely different rates

The Runge-Kutta-Fehlberg algorithm used for comparison in this study is the well known method of the fourth order, which means that at each integration step it requires four evaluations of $\overline{\Im}$ (h, t) in $u = \overline{\Im}$ (h, t). It uses evaluations to approximate a fourth order method. At each step, the difference between the results of the second and third order methods is assumed to be indicative of the local error and is used to choose an appropriate length for the next time step. If the maximum difference, max $\left|h_i^j - h_i^{j+1}\right|$, between the second and the third order results are not greater than a prespecified error tolerance Δ, the step is regarded as successful. If not, the calculations are repeated using a new time step. After each evaluation of u^j and u^{j+1}, the time step is updated using

$$\Delta t(new) = \delta\Delta(old) \tag{24}$$

where,

$$\delta = 0.84\left(\frac{\varepsilon}{\max\left|h_i^{j=1} - \hat{h}_i^{j+1}\right|}\right) \tag{25}$$

GILL ALGORITHM

The Gill algorithm is an example of a family known as "semi implicit" proposed by Kuo. It is actually a modification of the explicit Runge-Kutta method that involves the Jacobian matrix of the system of ordinary differential equations. The explicit part involves the linearization of system equation that involves the use of water addition, hydraulic conductivity and specific moisture content values calculated at the start of the time step, through the whole of the time step. The whole system can be written as $\overline{\Im}(h,t) = \overline{A}h + q$, where $\overline{A}$ is the matrix containing the Jacobian matrix of system equations and q is constant. Following this the Gill algorithm as described by Kuo (1981) can be

written as follows:

$$h_m^k = h_m^{k-1} + a^{k+1}\left[f^{\,k-1}\Delta t - q^{k-1}\right] \tag{26}$$

$$q^k = \left(1-3a^k\right)q^{k-1} + 2a^k q^{k-1}\overline{A}\Delta t \tag{27}$$

where

$$q^{(0)} = 0 a^1 = 1/2,\ a^2 = 1-\left(\sqrt{2}/2\right), \text{and}\, a^3 = 1+\left(\sqrt{2}/2\right) \tag{28}$$

k = 1,2,3... the three steps of the method, and Δt is a prespecified time step. The method is implicit in the evaluation of q^1 *and* q^2.

THE IMPLICIT METHOD

When an explicit linearization is combined with a backward difference discretization for the time derivative, equation (23) describes the relevant system.The system was solved at each time step using library routines.

AN OVERVIEW OF THE COMPUTER PROGRAM

The soil water program has been programmed in Pascal. The design of the program has been influenced by two aims. Firstly, to achieve flexibility with regard to the application of the model to different simulation problems. This has meant a high degree of modularity, with each subroutine carrying out a specific task. Secondly, to structure the problem so as to allow the addition of other dynamic models coupled to that of soil water model. The program consisted of three main components. The input component capable of adjusting its inputs to changing environmental conditions (Manoliadis, 1994), the integration of ordinary equations, and output. The program is designed to allow for the inclusion of additional models, each one of the three sections has as input key variables that can easily communicate with other programs (i.e. soil moisture of each step). The subroutines that may need modification are those related to the soil types.

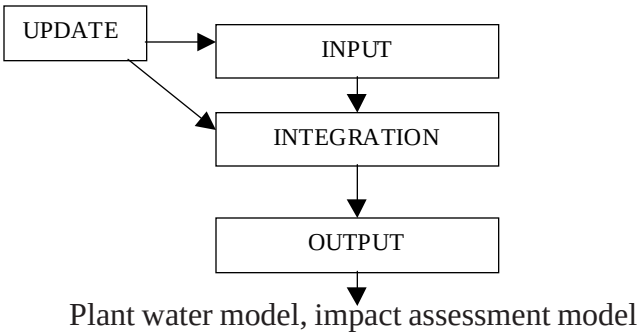

Figure 1. Structure of the computer program.

VALIDATION OF THE SOIL WATER MODEL SIMULATION

Validation of the soil water model has been carried out using two sets of published results reporting the infiltration of water in homogeneous sand and clay columns under restricted initial and boundary conditions. These initial conditions of the simulation were provided by the pressure head profile observed just prior to the commencement of water application. During infiltration the surface boundary conditions were given by the sequence of application rates (Figures 2a and 2b).

The simulations carried out were of the infiltration into fine sand tests presented in Haverkamp et al. (1977). In both tests, the three methods described used an identical grid spacing of 2 cm. The grid depths were 90 cm (Figure 3a) and 60 cm (Figure 3b) for the constant pressure and constant flux experiments.

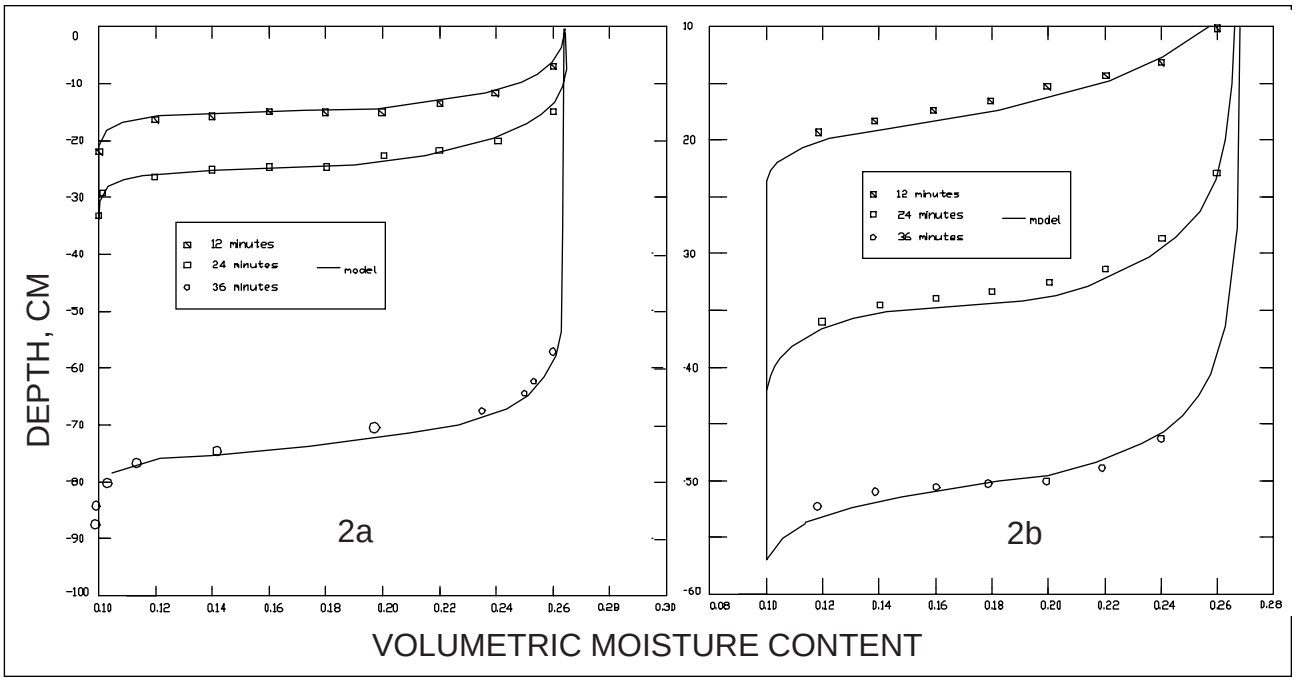

Figure 2a. Infiltration in sand with constant pressure condition at surface. Model simulation and Philip's solution (Haverkamp et al., 1977).

Figure 2b. Infiltration in sand with constant flux condition at surface. Model simulation and experimental measurements from Haverkamp et al., (1977).

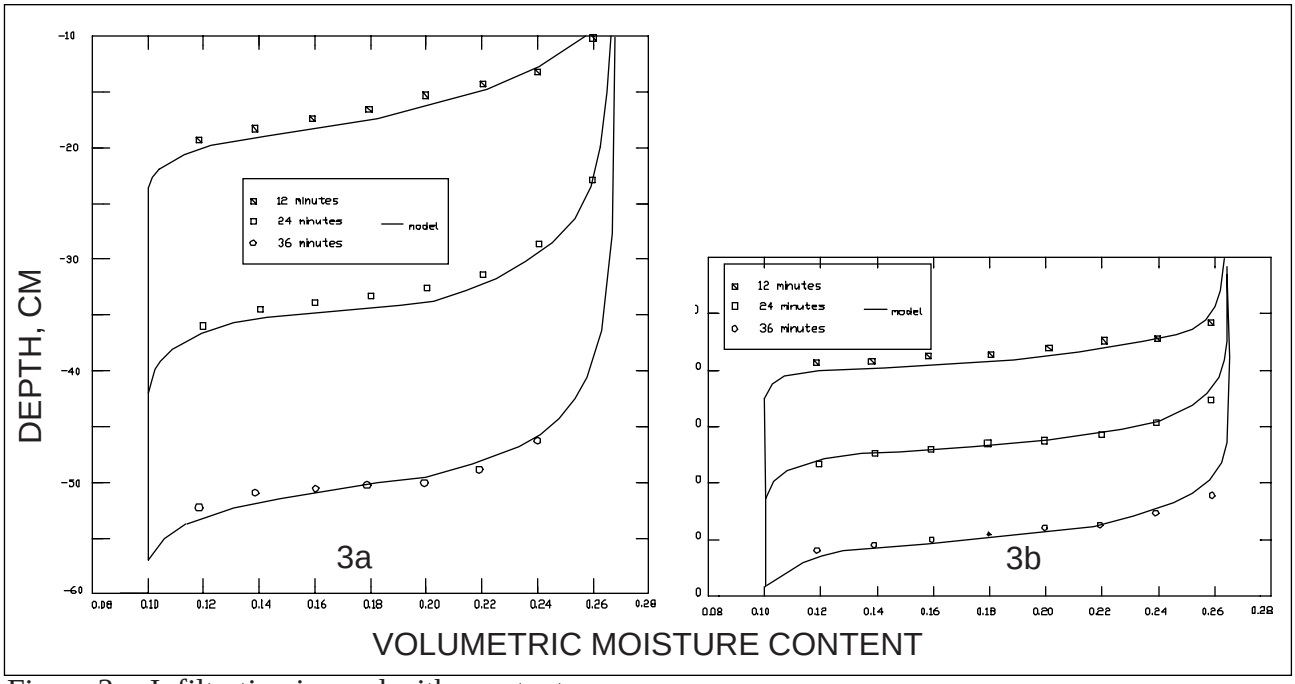

Figure 3a. Infiltration in sand with constant pressure condition at surface. Simulation using Gill's algorithm and Philip's solution (Haverkamp et al., 1977).

Figure 3b. Infiltration in sand with constant flux conditions at surface. Simulation using Gill's algorithm and measurements from Haverkamp et al., 1977.

RESULTS AND DISCUSSION

For the Runge-Kutta methods, the lower boundary condition was one of constant pressure. With the Gill and implicit methods, a no-flow boundary condition was used. Output for the validation of the model proposed are shown in Figures 2a and 2b. Simulation results are shown in Figure 3a for the constant pressure, and Figure 3b for the constant flux tests. In the constant pressure test, the three methods performed very similarly. The differences occurred near the lower end of the grid due to the different lower boundary conditions employed. In the constant flux test, the difference between the three methods becomes more apparent, with the explicit Runge-Kutta method performing worse, but only by a small fraction, than the implicit and Gill difference methods.

The performance of three methods with respect to the accuracy of simulation of the infiltration front is very similar. Any small differences cannot be regarded as conclusive because there exists the additional complicating factor of the different error control used by each method. The accuracy of the Runge-Kutta method is controlled through the specification of a local error tolerance. With the implicit and Gill algorithm methods, the control is less direct, through the choice of time step. Table 1 shows the tolerance values, computer central processing unit times and percentage error in water balance for the three integration methods in the constant flux test.

Table 1. Algorithm Performance Parameters

Method	Error Tolerance	Time-step (min)	Balance Error (%)	CPU Time(s)
Runge-Kutta	.01	-	+14.45	6.7
Gill algorithm	-	0.10	+0.93	1.6
Implicit	-	0.10	+0.40	0.4

The relationship between computer time and error in water balance is probably the most objective criterion for assessing the relative efficiency of the algorithms. This relationship, based on three simulations of the constant flux test by each method, is shown in Table 1. There are wide differences in performance between the four methods, with the Gill and implicit methods being the most, and the Runge-Kutta the least efficient.

The results of these tests agree with the conclusions of Haverkamp et al. (1977) that, in general, all numerical time integration schemes are able to successfully simulate infiltration events, but that totally explicit schemes are far less efficient than the others. The results also confirm that the Gill algorithm may be used as a general purpose soil water flow model. Although its performance here has been very similar to the implicit finite difference model, over longer runs with changing environmental conditions its ability to change the length of the time step would be expected to make it the more efficient of the other two models.

SUMMARY AND CONCLUSIONS

Models of subsurface water movement are required in the simulation of a great number of composite environmental processes. Besides their obvious importance as descriptions of an integral part of such processes, they are also important from a practical modeling aspect because they tend to form the computationally most expensive and, therefore, limiting part of composite models. The mechanics of water movement in the soil are quite well understood in comparison to other

environmental processes. The application of this understanding to practical problems, however, has been hampered by the fact that soil water modeling usually creates models specific to particular problems with a resulting absence of models of more general applicability. The limitations caused by the computational requirements of real life problems are being steadily raised by the spreading availability of increasingly powerful hardware. The main problems that need to be considered are, therefore, the difficulties involved in obtaining representative parameter values for use with the models and the non-availability of models that, once implemented, can be used in a variety of applications with little modification.

In this paper the development and implementation of a model for one dimensional soil water flow is discussed. The development places major emphasis on features that enhance the versatility of the model and make it more readily applicable as a general simulation tool.

The development of the model has been carried out to meet the following objectives:

* Ease of combination with models of other environmental processes,

* Ability to simulate flow under combined saturated-unsaturated conditions,

* Independence of numerical parameter specification (e.g. time step) from type of application, and

* Modular structure allowing the isolated alteration and validation of individual model components.

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