

An investigation of a dual-porosity model
for the simulation of unsaturated flow
in a porous medium

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Abstract

A 1-D dual porosity model using Richards' [Richards 1931] coupled non-linear parabolic equations are solved numerically with finite differences. This model is especially appropriate when modelling unsaturated ground water flow in fractured rocks or cracked soils.

Iteration was required to achieve the numerical solution due to the non-linear form of the parabolic equations.

Experiments were made to find the effects of varying parameters on the accuracy, on the convergence of iteration and on the computational effort required to achieve the numerical solution.

Some numerical examples are also included to show the hydraulic plausibility of the numerical results obtained.

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Chapter 1

Dual porosity ground water flow

1.1 Introduction

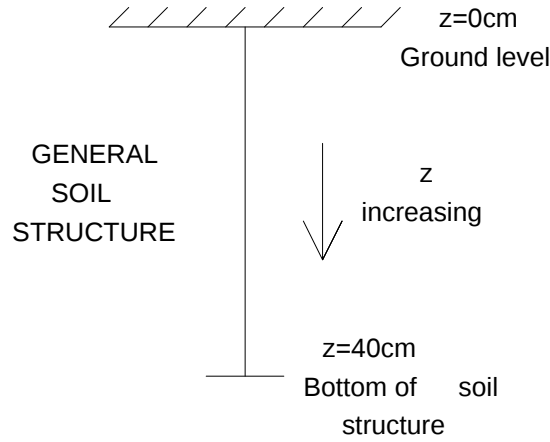


Figure 1.1: The domain of the model.

In this dissertation we will examine the model proposed in the 1993 paper of Gerke and van Genuchten. This model is a one-dimensional dual-porosity model which can be used to study variably saturated water flow in structured soil or fractured rock. The domain of the soil is shown in figure 1.1.

The model consists of superposing two continua at macroscopic level. The two continua are a macropore or fracture pore system and a less permeable matrix pore system. Mobile water exists in both pores. There is an assumption of no horizontal flow taking place since the rock (or soil structure) is assumed to be horizontally homogeneous.

Richard's equation [Richards 1931] describes the variably saturated water flow in both pore systems. The transfer of water between the two pore regions is simulated by means of first-order equations governing the rate.

The model results in two coupled systems of nonlinear partial differential equations which can be solved numerically using Galerkin Finite Element Methods and mass lumping in space (as in [Milly 1985] as 'L1'). The time stepping was achieved by the fully implicit θ method.

The new approach which we are going to introduce here uses the same basic model as used by Gerke and van Genuchten in their 1993 paper, but solves the coupled system of nonlinear partial differential equations by finite difference schemes. In space the integration method [Wood 1993] is used and in time we use the fully implicit θ method. This approach is different to that taken by Gerke and van Genuchten because a different form of mass lumping is implicitly used (as in [Milly 1985] 'L2').

Further, when the numerical solution is available, we will use the program to experiment to try to find the best ways of producing the results. This means trying to find the fastest, most accurate and most reliable way a numerical solution may be obtained given general initial, and boundary conditions of the problem.

Further still, we will also try to investigate the dependence of the numerical solution on different types of initial, and boundary conditions and the ease with which different specifications of numerical solutions may be obtained.

Finally we will conclude this dissertation with some simple numerical examples.

Since we use the same model as Gerke and van Genuchten used (in their 1993 paper), we must explain that model in more detail. This we do in the next section, section 1.2.

1.2 The Model of the Problem

The equations of the dual-porosity model are

$$c_f \frac{\partial h_f}{\partial t} = \frac{\partial}{\partial z} (K_f \frac{\partial h_f}{\partial z} - K_f) - \frac{\gamma_w}{w_f} \quad (1.1)$$

$$c_m \frac{\partial h_m}{\partial t} = \frac{\partial}{\partial z} (K_m \frac{\partial h_m}{\partial z} - K_m) + \frac{\gamma_w}{1 - w_f} \quad (1.2)$$

where c_m and c_f are the specific soil water capacities of the matrix and fracture pores respectively. h_f and h_m are the pressure heads of the fracture and matrix pores respectively. Also K_f and K_m are the hydraulic conductivities of fracture and matrix pores. γ_w is a term representing water transfer from fracture to matrix pores. The term w_f represents the volume of fracture pores as a proportion of total volume. Finally t is time and z is spatial distance (measured downwards with $z=0$ being ground level). 1.1 and 1.2 are forms of Richard's equation [Richards 1931].

The soil retention functions θ_m and θ_f are defined to be the amount of water present in a representative elementary volume of the matrix or fracture pores (respectively), divided by that representative elementary volume.

They are defined here as in [Gerke and van Genuchten 1993] in terms of $\theta_{r(m/f)}$, $\theta_{s(m/f)}$, $\alpha_{(m/f)}$, $h_{(m/f)}$, $n_{(m/f)}$ and $m_{(m/f)}$ as follows

$$\theta_m = \theta_{rm} + (\theta_{sm} - \theta_{rm}) [1 + |\alpha_m h_m|^{n_m}]^{-m_m} \quad (1.3)$$

$$\theta_f = \theta_{rf} + (\theta_{sf} - \theta_{rf})[1 + \alpha_f h_f^{n_f}]^{-m_f} \quad (1.4)$$

where θ_{rf} , θ_{rm} are residual soil water retention constants for fracture or matrix pores. Similarly θ_{sf} , θ_{sm} are the saturated soil retention constants for fracture or matrix pores.

α_m , α_m , α_m or α_f , α_f , α_f are empirical constants for the matrix or fracture pores respectively.

The values of the specific soil water capacities α_m , α_f can be approximated to be the gradient of the soil retention functions θ_m or θ_f with respect to pressure heads h_m or h_f . That is;

$$\alpha_m = -\frac{d\theta_m}{dh_m} \quad (1.5)$$

$$\alpha_f = -\frac{d\theta_f}{dh_f} \quad (1.6)$$

The hydraulic conductivity of the matrix or fracture pores(K_m or K_f) can be thought of as representing the ease(or difficulty)with which water flows through their structures for a given pressure head gradient.This is shown by Darcy's Law [Darcy 1856] .

$$q_m = -K_m \left(\frac{dh_m}{dz} + 1 \right) \quad (1.7)$$

$$q_f = -K_f \left(\frac{dh_f}{dz} + 1 \right) \quad (1.8)$$

where q_m or q_f represent the downward flux of water flow in the matrix or fracture pores.

Gerke and van Genuchten(in their 1993 paper)use the van Genuchten formulae [van Genuchten 1980] for the hydraulic conductivity of the matrix and fracture pores (K_m or K_f)in terms of their hydraulic conductivity at saturation,as follows

$$K_m(K_{em}) = K_{sm} \left(\frac{K_{em}}{K_{sm}} \right)^{1/m_m} [1 - (1 - (K_{em}/K_{sm})^{1/m_m})^{m_m}]^2 \quad (1.9)$$

$$K_f(K_{ef}) = K_{sf} \left(\frac{K_{ef}}{K_{sf}} \right)^{1/m_f} [1 - (1 - (K_{ef}/K_{sf})^{1/m_f})^{m_f}]^2 \quad (1.10)$$

where K_{sm} or K_{sf} is the hydraulic conductivity at saturation of the matrix or fracture pores.The effective saturation parameters K_{em} and K_{ef} are defined in terms of the water content functions

$$K_{ef} = \frac{K_f}{K_{sf}} \frac{\theta_{rf}}{\theta_{sf}} \quad (1.11)$$

$$K_{em} = \frac{K_m}{K_{sm}} \frac{\theta_{rm}}{\theta_{sm}} \quad (1.12)$$

Boundary and initial conditions are necessary to solve equations 1.1, 1.2 and these will be discussed in Chapter 2.

As noted by Gerke and van Genuchten[1993] the above model needs modification when the water downflow at the surface(caused by rainfall-for example)is larger than the matrix pores can absorb by themselves.If the water downflow is not so large that the entire absorption capacity of the soil is exceeded then a solution is

$$f \quad f \qquad f \quad m$$

$$f \quad \frac{f}{f}$$

$$m \quad \frac{m}{m}$$

$$\begin{array}{cc} f & m \\ f & m \\ & f \quad m \end{array}$$

$$f \quad m \quad f \quad m$$

$$\frac{f \quad m}{\quad}$$

$$f$$

$$f$$

$$\frac{\quad}{\quad}$$

$$\frac{\quad}{\quad} \quad \frac{\quad}{\quad}$$

$$\frac{\quad}{\quad} \quad \frac{\quad}{\quad}$$

$$\frac{\quad}{\quad} \quad \frac{\quad}{\quad}$$

Now using 1.18

$$q = \frac{w_f Q_f}{A_f} + \frac{Q_m}{A} \quad (1.24)$$

Now using 1.19

$$q = \frac{w_f Q_f}{A_f} + \frac{Q_m(1 - w_f)}{A_m} \quad (1.25)$$

ie.from 1.14 and 1.15 we get equation 1.13 .

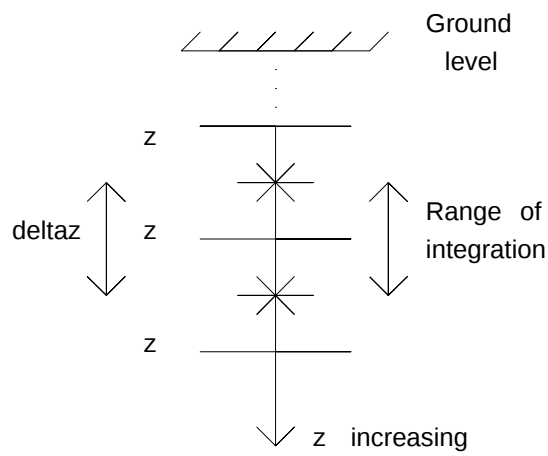


Figure 2.1: How 2.6 may be spatially integrated.

Since f is a constant the left hand side of 2.7 may be integrated to give

$$\int_{z_{j-\frac{1}{2}}}^{z_{j+\frac{1}{2}}} (f - f) dz = f \left(\left[\int_{z_{j+\frac{1}{2}}}^{z_{j+\frac{1}{2}}} (f - f) dz \right] - \left[\int_{z_{j-\frac{1}{2}}}^{z_{j-\frac{1}{2}}} (f - f) dz \right] \right) \quad (2.9)$$

Now from 2.7 by using the approximation of 2.8 and the result of 2.9 we obtain

$$f \left(\left[\int_{z_{j+\frac{1}{2}}}^{z_{j+\frac{1}{2}}} (f - f) dz \right] - \left[\int_{z_{j-\frac{1}{2}}}^{z_{j-\frac{1}{2}}} (f - f) dz \right] \right) = \Delta \left(\left[\int_{z_j}^{z_j} (f - f) dz \right] + \frac{1}{2} \left[\int_{z_j}^{z_j} (f - f) dz \right] + \frac{1}{2} \left[\int_{z_j}^{z_j} (f - f) dz \right] \right) \quad (2.10)$$

In the above equation it is obvious that some function values need to be evaluated mid-point between two spatial nodes. Since we only have values of these functions at the nodes, it is clear that some form of averaging will be required. In

$$f_{j+\frac{1}{2}} = \frac{f_{j+1} + f_j}{2} \quad f_{j-\frac{1}{2}} = \frac{f_j + f_{j-1}}{2} \quad f_j = \frac{f_{j+\frac{1}{2}} + f_{j-\frac{1}{2}}}{2}$$

$$\begin{aligned}
& m([\quad m]_{j+\frac{1}{2}} (\frac{[\quad m]_{j+1}}{\Delta^2} \frac{[\quad m]_j}{2} - \frac{[\quad m]_{j+\frac{1}{2}}}{\Delta}) - m([\quad m]_{j-\frac{1}{2}} (\frac{[\quad m]_j}{\Delta^2} \frac{[\quad m]_{j-1}}{2} - \frac{[\quad m]_{j-\frac{1}{2}}}{\Delta}) \\
& = -m[\quad m]_j + \frac{1}{w} [\quad a \quad m]_j - \frac{1}{w} [\quad a \quad f]_j
\end{aligned} \tag{2.12}$$

Now if we rearrange 2.11 then we obtain

$$\begin{aligned}
& [\quad f]_{j+1} (\frac{f[\quad f]_{j+\frac{1}{2}}}{\Delta^2}) - [\quad f]_j (\frac{f[\quad f]_{j+\frac{1}{2}}}{\Delta^2} + \frac{f[\quad f]_{j-\frac{1}{2}}}{\Delta^2} + \frac{1}{w} [\quad a]_j) + [\quad f]_{j-1} (\frac{f[\quad f]_{j-\frac{1}{2}}}{\Delta^2}) \\
& + [\quad m]_j (\frac{1}{w} [\quad a]_j) = -f[\quad f]_j + \frac{f[\quad f]_{j+\frac{1}{2}}}{\Delta} - \frac{f[\quad f]_{j-\frac{1}{2}}}{\Delta}
\end{aligned} \tag{2.13}$$

We will now represent 2.13 in a clearer form

$$_{-f} + \quad_{-m} = \quad_{-f} + \quad_{-m} \tag{2.14}$$

where $\quad_{-f} = [\quad f_{j-1} \quad f_j \quad f_{j+1}]^T$ and where $\quad_{-m} = [\quad m_{j-1} \quad m_j \quad m_{j+1}]^T$
also where

$$\begin{aligned}
& = \begin{pmatrix} \ddots & & \ddots & & \ddots \\ 0 & \frac{w_f[K_f]_{j-\frac{1}{2}}}{\Delta z^2} & (\frac{w_f[K_f]_{j+\frac{1}{2}}}{\Delta z^2} + \frac{w_f[K_f]_{j-\frac{1}{2}}}{\Delta z^2} + \frac{1}{w} [\quad a]_j) & \frac{w_f[K_f]_{j+\frac{1}{2}}}{\Delta z^2} & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \\
& = \begin{pmatrix} \ddots & & \ddots & & \ddots \\ 0 & \frac{1}{w} [\quad a]_j & 0 & & \\ \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \\
& = \begin{pmatrix} \ddots & & \ddots & & \ddots \\ 0 & f[\quad f]_j & 0 & & \\ \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \\
& \vdots \\
& \quad_{-m} = \begin{pmatrix} \frac{w_f[K_f]_{j+\frac{1}{2}}}{\Delta z} & \frac{w_f[K_f]_{j-\frac{1}{2}}}{\Delta z} \\ \vdots & \vdots \end{pmatrix}
\end{aligned}$$

$$\begin{array}{ccccccc}
k+\frac{1}{2} & k+1 & & k+\frac{1}{2} & k+1 & & k+\frac{1}{2} & k & & k+\frac{1}{2} & k & & k+\frac{1}{2} \\
-f & & & -m & & & -f & & & -f & & & \\
\hline
\end{array}$$

$$\begin{array}{ccccccc}
k+\frac{1}{2} & +1 & & +\frac{1}{2} & +1 & & +\frac{1}{2} & +1 & & +\frac{1}{2} \\
\hline
\end{array}$$

$$\begin{array}{ccccccc}
+1 & & +\frac{1}{2} & & +\frac{1}{2} & & +\frac{1}{2} \\
+1 & \frac{+1}{2} & & +1 & \frac{+1}{2} & & +1 \\
\hline
\end{array}$$

$$\begin{array}{ccccccc}
+1 & & +\frac{1}{2} & & +1 & & +\frac{1}{2} \\
+1 & \frac{+1}{2} & & +1 & \frac{+1}{2} & & +1 \\
\hline
\end{array}$$

where

$$[\]_j^{k+\frac{1}{2}} = \left(\frac{f[\]_{j+\frac{1}{2}}^{k+\frac{1}{2}}}{\Delta^2} + \frac{f[\]_{j-\frac{1}{2}}^{k+\frac{1}{2}}}{\Delta^2} \right) \frac{f[\]_j^{K+\frac{1}{2}}}{w_a j^{k+\frac{1}{2}}}$$

[illegible]

$$\frac{k+1}{-}$$

$$\begin{array}{ccc} & & k+1 \\ \text{---} & \text{---} & \text{---} \\ & k+1, p+1 & \\ \text{---} & & \text{---} \end{array}$$

$$\overline{\quad}^{k+1,p+1} \quad \overline{\quad}^{k+1,p} \quad \overline{\quad}^{k+1,p+1} \quad \overline{\quad}^{k+1,p}$$

$$\begin{array}{ccccc} \text{---} & k+1,0 & & k,p & & \frac{k}{k-1} & & k,p & & k-1,q \\ & & & & & & & & & \text{---} \end{array}$$

k

								-

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Chapter 3

General Results

3.1 General properties of the numerical solution

3.1.1 Oscillation

No oscillation was experienced in the numerical results in time and in space. In addition it was noted that consecutive iterates (of a time-step) did not oscillate. The behaviour of the consecutive iterates not oscillating can probably be explained by the lumping of the mass matrix which has (implicitly) taken place in our solution (according to 'L2' in [Milly 1985]) but which was done differently in the 1993 paper of Gerke and van Greuchten (according to 'L1' in [Milly 1985]).

In [Ouyang and Xiao 1994] there is a result stated regarding a linear parabolic problem which we have transformed to relevant variables, as follows;

$$\frac{\partial h}{\partial t} = \alpha \nabla^2 h(z, t) + f(z, t) \quad (3.1)$$

(where h represents the pressure head in either of the two pores and α is constant) Similar boundary and initial conditions to the ones we used in this problem are assumed.

The solution of equation 3.1 in space is assumed by finite element methods. This procedure is assumed to give the following equation;

$$[M]\dot{\underline{h}}(t) + [K]\underline{h}(t) = \underline{F} \quad (3.2)$$

(where now $\underline{h}$ is assumed to be the form of pressure heads as used in 2.21). Ouyang and Xiao assume the problem has been discretized in time by the θ method and then give the following condition (equation 3.3) as a sufficient condition of the non-oscillation of the numerical solution in *time*. The inequality of equation 3.3 is valid because $K_{ij} < 0$ if $i \neq j$ and $K_{ii} > 0$.

$$\max_{i,j} \left[\frac{M_{ij}}{-\theta K_{ij}} \right] (i \neq j) \leq \Delta t \leq \min_i \left[\frac{M_{ii}}{(1-\theta)K_{ii}} \right] \quad (3.3)$$

Using our method of numerical discretization on equation 3.1 we may assume that the mass matrix M (as shown in 3.2) is in fact lumped and hence $M_{ij} (i \neq j)$

terms are zero. Further since we use the *fully* implicit θ method we may take θ to be equal to 1. Hence we conclude that condition 3.3 shows that our numerical solution on 3.1 will not oscillate in *time* when discretized by the numerical method we have used.

This result on our method of discretization of equation 3.1 applies to oscillation of the numerical solution in time but does not apply to the oscillation in *space* or to the oscillation of the iterates which may occur during the iteration of a time-step. However we conjecture that the result of [Ouyang and Xiao 1994] may suggest an explanation for the non-oscillation of our numerical solution (to equations 1.1 and 1.2) in *time* which we observe in this dissertation. Further investigation is required to confirm this conjecture.

3.1.2 Stability

Stability is not an issue in the numerical solution because a fully implicit difference scheme is used.

3.1.3 Convergence

By convergence we mean the ability of the pressure head values to converge to a new value for the new time-step, as the iterations continue. If the consecutive pressure head values begin to diverge, then convergence is unlikely.

To start with a fixed time and space-step is used, but later it was found to be beneficial to have a varying time-step. But in this section we shall assume the time-step to be fixed.

Often the only criterion for choosing the space and time-step was whether the iterative solution would converge. Decreasing the space-step (for a fixed overall soil depth) was found to have a detrimental effect on the convergence of the solution and decreasing the time-step was found to have a beneficial effect on the convergence (these results are also backed up by some of the results of section 3.6)

In the paper [Neuman 1973] it is suggested that the lumping of the mass matrix is necessary for convergence in an unsaturated flow. Indeed both Gerke and van Grenchten and the author did lump their mass matrices.

However Wood and Calver in their 1990 paper concluded that the distributed mass matrix should be used in saturated-unsaturated subsurface flow because it gives increased accuracy. This conclusion may be inappropriate in our case because we are dealing with unsaturated flow.

3.2 Applying rainfall

3.2.1 Boundary conditions

We briefly discussed boundary conditions in chapter 2. However it is perhaps appropriate for us to comment some more on how the boundary conditions were implemented in this numerical solution.

Usually Neumann boundary conditions were implemented. Therefore fictitious points had to be created in order to achieve these Neumann conditions. Strictly speaking these fictitious points are not within the soil structure and are not recorded in any results we show in future sections.

Upper boundary conditions

Using equations 1.7 and 1.8 these rainfall fluxes can be turned into pressure head gradients. The evaluation of the hydraulic conductivity term in 1.7 and 1.8 is at the point just below the fictitious point.

Once the pressure head gradient has been evaluated then the pressure head at the space point two space-steps below the fictitious point is changed by an amount in accordance with the gradient of the pressure head, until it reaches the value to be assigned at the fictitious point. This is shown in figure 3.1 .

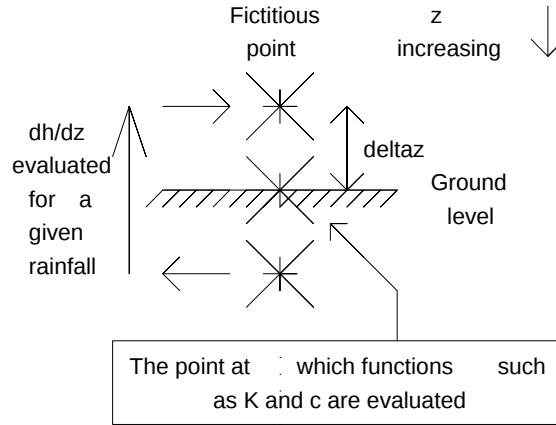


Figure 3.1: How upper boundary conditions are evaluated.

Later in this dissertation we may refer to ‘no flow’ boundary conditions which merely means imposing a zero velocity of rainfall at the upper boundary.

Lower boundary conditions

These are almost always ‘free flow’ boundary conditions. They are said to represent the unimpeded release of water as it exits from the soil structure (into a water table, for example).

These boundary conditions are simply implemented by making the value at the fictitious point (which is one vertical space-step below the lower boundary) equal that at the space node on the lower boundary.

More generally, the velocity of the flux of rainfall formed the upper boundary condition, and the lower boundary condition remained ‘free flow’ (as before).

3.2.2 General properties

Generally the number of iterates required for each time-step (for fixed time-step) varied from problem to problem and varied as the fixed time-step varied for each prob-

-5

-85

problem to that which would result if the boundary flow was introduced immediately. The gradual 'run-in' is really only of use if the steady-state solution of the soil is sought. If the numerical solution must approximate the solution which introduces the flow immediately at *all* times then a much better approach is to initially reduce the time-step and then gradually increase it as the system recovers from the shock of the initially imposed boundary conditions.

3.4 Varying the time-step

As we indicated in the previous section, this seems (in most cases) to be the most superior way of letting the program deal with extreme or abruptly imposed boundary conditions. It is not difficult to modify the program to be able to cope with a varying time-step length. Some method of varying the time-step must be implemented so that the number of iterates achieved remains roughly constant (per time-step) over the running of the numerical solution. Of course the time-step length must only be varied slowly since a large variation may cause the time-stepping procedure to approximate a wildly inaccurate value of the next time-step and hence convergence may be threatened. However in our experimentations we found the program to be fairly robust to time-stepping changes, and easily able to cope with a halving of time-steps over one time-step.

We will now include a specific numerical example. We comment on a program which changes the time-step depending on the number of iterates being required to achieve convergence on the last time-step. The program is given a single number of iterates (or a range of iterate values) and if the program produces a number less than this (per time-step) then it increases the time-step by a factor of 10 per cent. If the program exceeds this number by 1 then the time-step is decreased by a factor of 10 per cent. If the program exceeds this number by a number greater than 1 then the time-step is halved. Hence usually the program achieves a constant number of iterates (per time-step).

Numerical example

In the following example we introduce a specified rainfall into the soil structure with specified initial pressure head. The depth of the soil sample is 40cm and the space-step is also specified below. A tolerance of 10^{-3} cm was used (unless stated otherwise). A transfer term assuming rectangular shaped blocks of size 1cm was used. In all cases a 'free-flow' boundary condition was imposed at the lower end of the soil structure.

We show the results in the form of a table 3.1. In case (a) an initial time-step of 10^{-3} days and space-step of 1cm are used, with initial pressure heads of -100cm in both pores. We imposed 'no-flow' boundary conditions at the top. We measured the total number of iterates to reach 0.1 days. In case (b) we used the same initial conditions as in case (a) but now with an initial time-step of 5×10^{-4} days with initial pressure heads of -50cm in both pores. In this case a flow of 0.5cm/day was also imposed to both the matrix and fracture pores. We measured the total number of iterates required to reach 0.05 days. In case (c) we used the same conditions as in

iterates per time step	total number of iterates for case(a)	total number of iterates for case(b)	total number of iterates for case(c)	total number of iterates for case(d)	total number of iterates for case(e)
2	320	450	107	86	472
3	214	1051	112	97	338
4	206	395	109	101	323
5	202	232	117	109	322
6	207	230	117	114	321
7	224	231	123	118	346
8	213	232	139	130	358
9	230	236	140	130	388

was not this small then the iteration of the solution(at a given time-step)would simply not converge to a solution for the next time-step in a finite number of iterations.However as the numerical solution changes(with time)the program may not need to maintain such a small time-step in order to maintain convergence(because conditions may have become less severe or may have become less saturated)and in some cases the time-step may safely increase by an order of more than 1000.There-

	iter.(a2)	$[\Psi]_{2,2}(a)$	$[\Psi]_{4,2}(a)$	iter.(a3)	$[\Psi]_{4,3}(a)$	iter.(b2)	$[\Psi]_{4,2}(b)$
0.6	24	0.99051	0.999122	11	0.999862	12	0.999903
0.7	22	0.99050	0.998926	10	0.999851	11	0.999879

-3

-5

-4

4,2

3,2

4

3

there is no benefit to be had from introducing it. Other methods of accelerating the iteration process (such as Newton[Conte-and-de-Boar-1980]) are also not applicable due to the effort required to form the various differentials. Newton also requires a very good starting value for convergence to be achieved.

However in [Gerke and van Genuchten 1993] Picard iteration with Cooley under-relaxation [Cooley 1983] is used which suggests that the iterations (of a time-step) *do* oscillate. This is because if their iterates *do not* oscillate then the under-relaxation scheme used would be of no benefit. It should be noted that although we suspect the iterates did oscillate this is **not** explicitly stated anywhere in [Gerke and van Genuchten 1993].

Since we suspect the iterates(of a time-step)oscillate when ‘L1’ mass lumping is used but the iterates do not oscillate when ‘L2’ mass lumping is used then we conclude that the ‘L1’ form of mass lumping is probably preferable. We conclude this because as long as the iterates(of a time-step)oscillate then their convergence may be accelerated by the Cooley algorithm. If the iterates do not oscillate then their convergence can not be easily accelerated.

The same procedure of varying the parameter value Ω as in equation 2.25 may be applied to the initial iterate of the new time-step. However, since the solution does not oscillate in time either it seems likely that similar results will be obtained. We tried values of $\Omega = 0.5$ and $\Omega = 1.0$ and found the value of $\Omega = 1.0$ to be superior(as one would expect for a non oscillating problem). This value of Ω was then adopted.

3.6 Numerical difficulties

We now aim to quantify the numerical difficulty associated with solving different types of numerical problem.

Numerical example

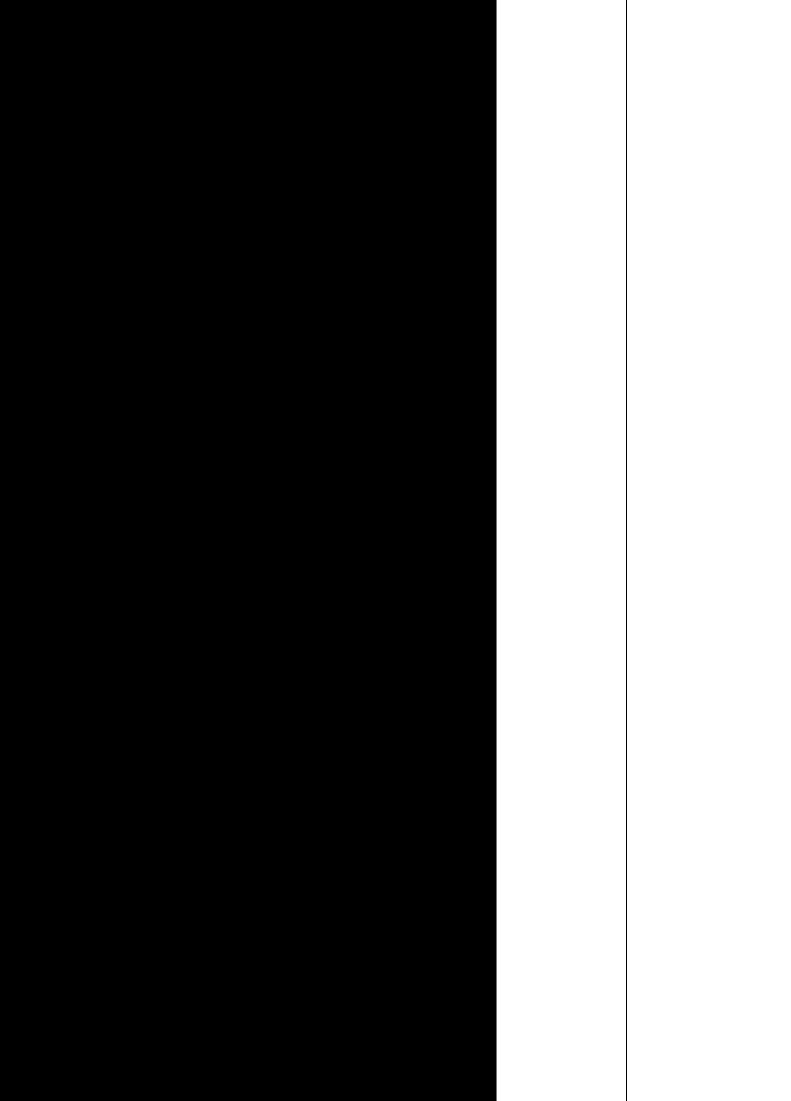
To achieve this aim we set the computer a set of problems(or cases)which only vary by one aspect. To quantify the difficulty that the computer has we will produce a table similar to table 3.1 .However now only 5 iterates(per time-step)were aimed for and no other values were taken(ie.variable time-step was used as described in the previous section).

The larger the total number of iterates required,the harder the computer finds the problem(in general–there are some exceptions). There are different cases to be considered.

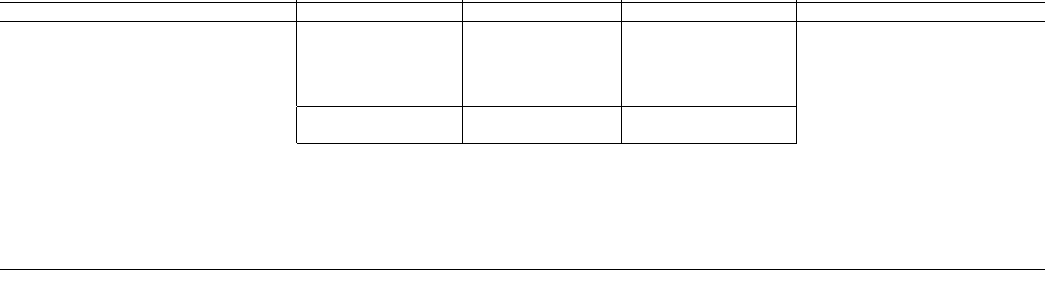
Case(a)is the same as case(a)from the previous section,ie.using a 40cm depth of soil,a tolerance of 10^{-3} cm,initial(variable) time-step of 10^{-3} days with initial pressure heads of -100cm in both matrix and fracture pores. We were assuming a transfer term which assumed that the average rectangular shaped matrix block size was 1cm and also setting the space-step to be 1cm. Finally a‘no flow’condition was assumed on the upper surface and a‘free flow’boundary condition was assumed on the lower surface. We counted the number of iterations required to

reach a time of 0.1 days.

In case(b)we used the same conditions as in case(a) except our initial(variable) time-step was 10^{-4} days,the space-step was 0.5cm.In case(o)a space-step of 2cm



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total number of iterates for case(j)	total number of iterates for case(k)	total number of iterates for case(l)
354	294	317

Table 3.10: Table showing the effects of varying matrix block sizes for *differing* pressure heads in fracture and matrix pores

Our results also show that there is a very large increase in the amount of numerical work required to find a solution with a halved space-step. In fact this increase in work is even larger than is suggested by the table (see table 3.4) because the amount of numerical work done(per iterate) was larger in case(b) than case(a) because there were a greater number of spatial nodes present.

As we have suggested earlier on in the dissertation, it seems (from the results of table 3.6) that the program computes less saturated conditions more easily than more saturated conditions.

The results also show us that changing the average matrix block size seems to have a relatively small effect on the increase in the amount of numerical work required when the pressure heads in the two media are similar (see Table 3.7). However the effects seem to be more marked when the pressure head differences are larger (see Table 3.10).

It also seems that doubling or halving the soil depth does not change the total number of iterates required (see Table 3.8). However, as with Table 3.4, the amount of numerical work required is still substantially increased.

When some rainfall is applied (0.2cm/day) there is a significant increase in the amount of numerical work needed to obtain a numerical solution (see Table 3.9). This is probably as a result of the ‘shock’ of immediately introducing the boundary conditions and not so much as a result of the numerical solution becoming more saturated (as it does not have time to become significantly saturated). In fact applying a slightly lesser amount of rainfall (eg. 0.1cm/day as case(m) shows) can actually need less numerical work than case(a) required, which had no rainfall applied. We think the reason for this is because ‘no-flow’ boundary conditions at the top of the soil structure actually cause more of a ‘shock’ to the program than just letting a small amount of water flow into the surface to replace the water ‘free-flowing’ out of the soil at the lower end.

3.7 Evaluating the functions at mid-points

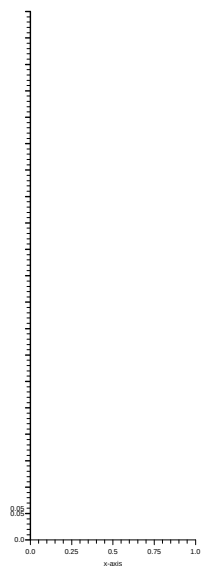
As is mentioned earlier in this dissertation (in Chapter 2), the way in which the value of the functions (ie the hydraulic conductivity of the specific soil water capacity) are taken at the mid-point of two nodes is to evaluate the functions at the pressure head values of the two adjacent nodes and then take the arithmetic average.

However another way of attacking the problem is to average the pressure head val-

ues at the two adjacent nodes the function's value is calculated (ie. evaluate the functions' value at the averaged pressure head). In so doing one will find that there is a significant reduction of the number of function calls required. Since the function evaluations are somewhat complicated and therefore time consuming, there is a significant advantage to be had in averaging the pressure head values before calling the function.

We set a tolerance of 10^{-3} days, initial pressure heads of -100cm in both pores, initial (variable) time-step of 10^{-3} days, space-step to be 1cm, depth of soil to be 40cm, average rectangular matrix block size to be 1cm, the number of iterates aimed for (with variable time-step) was 5, and finally we take the results at time = 0.2 days.

Using the averaging the function calls the computer took 34.9 seconds (in time) and used 359 iterates. In using the averaging the function calls the computer took 19.7 second and 358 iterates. (Please note that we are convinced that the differences in time that we observed are not as the result



For the purpose of simplicity we will assume that the pressure head values may take either Fig.3.2 case two or Fig.3.2 case three(with the y-axis being the value of the pressure-head and the x-axis being the depth of the soil structure).This is a large assumption which is motivated by the form of the boundary conditions at the lower surface of the soil(these two types of pressure head distributions can be seen in the numerical results of figures 4.6 , 4.7 , 4.9 and 4.10).This assumption will be especially wrong when oscillatory boundary conditions are to be applied to the soil.

We will now explore the accuracy of the two methods of evaluation of the value of the K function at a mid-node in *space*.Firstly we will assume that the pressure head distribution has the form of Fig.3.2 case two.

Here the average value of the pressure heads at the two nodes(d and e in case 2 of figure 3.2)will be 0.5.By observing the assumed distribution for K(case one) it is clear that $h=0.5$ returns a value of about 0.05.For $h=1$ (the value of the pressure head at node d)we find that K returns a value of 1.0 and for $h=0$ (the value of the pressure head at node e)we find that K returns a value of 0.0.Therefore by averaging *after* we obtain a value of 0.5 for the value of the function K at the midpoint of the two nodes.

In fact the value of the pressure head(case two) at $\text{depth}=0.5$ (ie.the midpoint of the two nodes,d and e,in space)is 0.05,which returns a value of K(case one) being approximately equal to 0.0.So in *this* (ie.case two) averaging *before* is the more accurate of the two methods and it will also require less computational time to evaluate the solution.

However a similar argument concludes that if the pressure head distribution has the distribution as given in case three then the averaging *after* scheme is the more accurate(or the closer to the correct value).

Therefore we conclude that,for these two simple examples,neither of the two methods is superior on a general pressure head distribution.This implies that it is better to use the averaging *before* method since it does not lose out on accuracy and produces a result in about half the time.

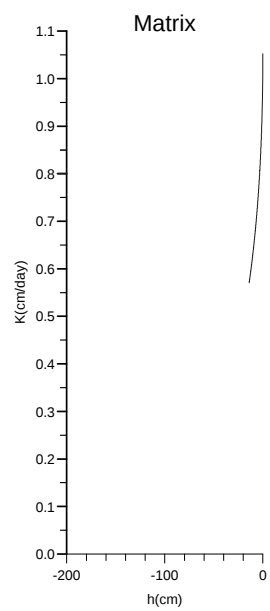
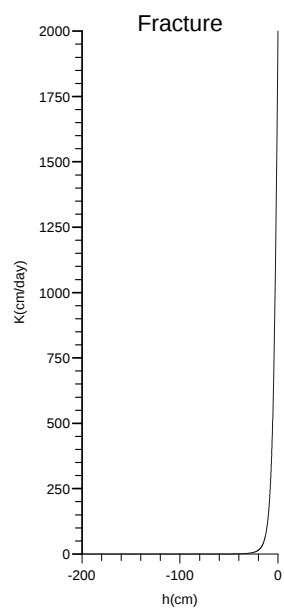
As stated earlier,we have used a large number of simplifying assumptions.We will comment on the inadequacies of our previous argument as follows.

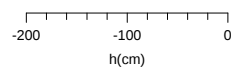
Firstly we have not discussed at all how the pressure head values may vary with time.This is significant because a large amount of timelike averaging between nodes is also necessary.However we hope the distribution may be similar to that of case two or case three,but have no results to prove this.

Secondly the ‘c’ (ie.the specific soil water capacity) functions are also averaged between time nodes and again we have no results(as yet)to give us any indication as to the distribution of this function(in time).However (for non-oscillatory solutions) perhaps we should hope that the distribution is quite close to case two or case three.

Finally(as we have mentioned before)in certain circumstances the spatial distri-

bution of the pressure head values may not be similar to either case two or case





In this numerical example we will show how the model reacts to an initially wet soil(see figure 4 5).This soil will slowly dry because we have a ‘no flow’ boundary condition at the top of the soil structure and a ‘free flow’ boundary condition at the bottom of the soil structure.The initial conditions were of a pressure head of -10cm in both fracture and matrix pores.The length of the soil medium was 40cm, space-steps of 1cm were used and the average rectangular matrix block size was set to be 1.0cm.

By observation of figure 4 3 it is clear that just because the pressure heads are identical(initially)in the matrix and fracture pores does not necessarily mean that their water contents are the same.Nevertheless it is still clear that both media would initially be said to be ‘wet’ as defined by any sensible definition(in fact a more precise definition of ‘wetness’ may be given by equations 1 11 and 1 12).Further,since both the water content functions in the matrix and fracture are monotonic,it is a safe to assume that as the pressure head decreases in one medium then the water content of that medium also decreases.

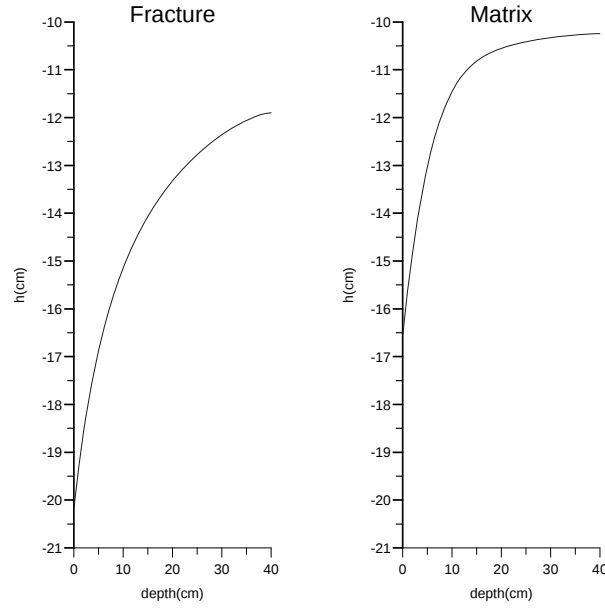
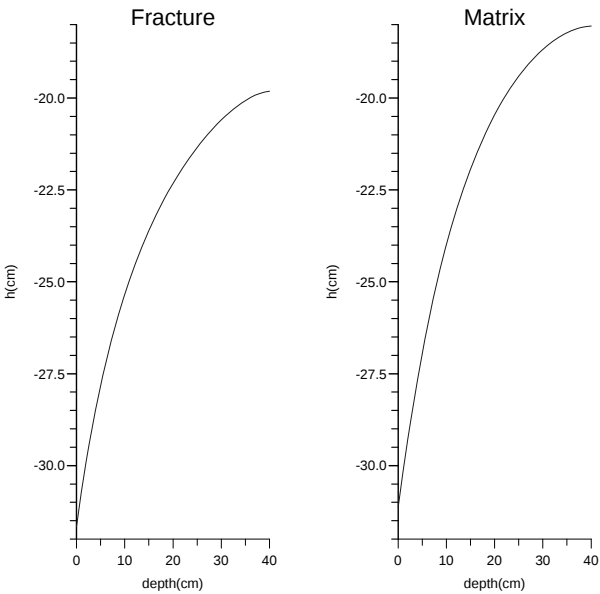
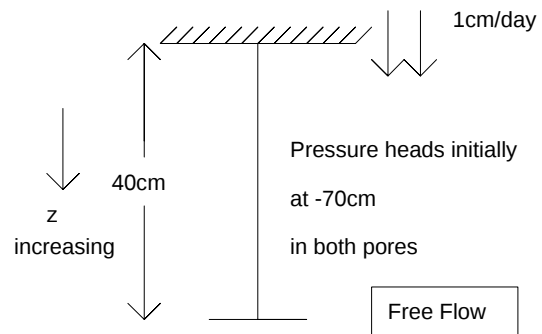


Figure 4.6: Pressure Heads at time=0.01 days

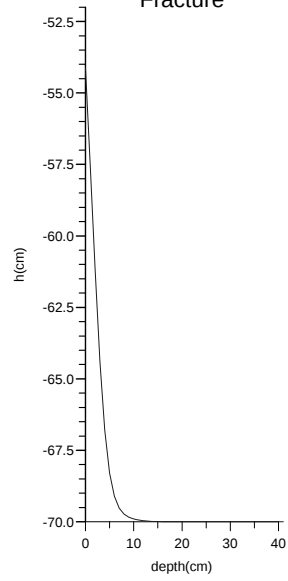
set initially. This may be accounted for by the explanation that since the water is flowing (relatively) slowly in the matrix pores, it has not had time to make the lower end of the soil structure significantly dryer at this short time (0.01 days) after the initial conditions were imposed.

At this point we should perhaps mention the transfer term. This regulates the

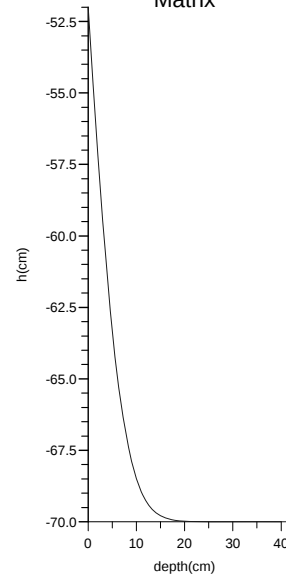




Fracture



Matrix



f

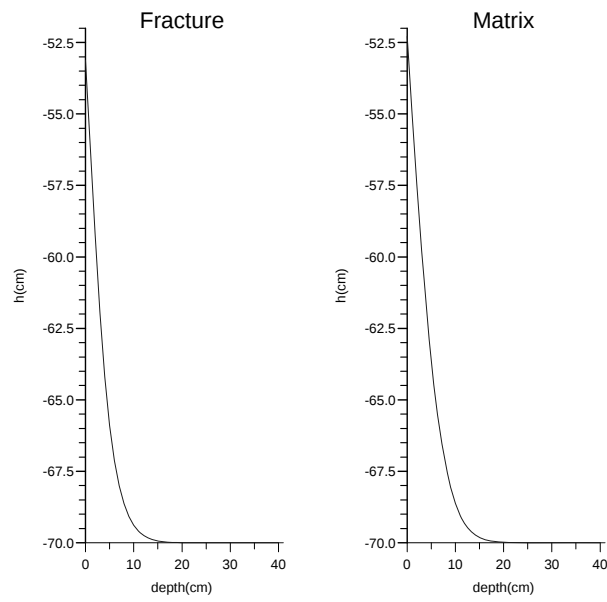


Figure 4.10: Pressure Heads at time=0.04 days with average matrix size=1.0cm

difficulty in modeling the interaction between the two pore systems which is resulting here and which (of course) will be dependent on the average matrix block size as figures 4 9 and 4 10 show.

No oscillation was observed in time,space or in the consecutive iterates of a time-step.

The gradual introduction of rainfall was found to have a beneficial effect on the convergence of the numerical solution(as opposed to its immediate introduction)

A variable time-step was found to be a necessity for producing our numerical solution in an efficient number of time-steps.

We also conclude that it is probably better to calculate nonlinear terms by averaging the values of the pressure heads to adjacent nodes(in time or space)*before* calculating the corresponding hydraulic conductivity or specific soil water capacity.

Finally(as the graphical examples show)we conclude that the dual-porosity model produces plausible results for certain initial and boundary conditions.

Bibliography

- [Beven and Germann 1982] Keith Beven and Peter Germann. *Macropores and Water Flow in Soils*. Water Resources Research, Vol.18, No.5, Pages 1311-1325, (October 1982).
- [Conte-and-de-Boor-1980] Conte, S.D. and de Boor, C. *Elementary numerical analysis*. McGraw-Hill, (1980).
- [Cooley 1983] Cooley, R.L. *Some new procedure for numerical solution of variably saturated flow problems*. Water Resources Research, 19, 1271-1285, (1983).
- [Darcy 1856] Darcy, H. *Les fontaines publiques de la ville de Dijon*. Dalmont, Paris, (1856).
- [Gerke and van Genuchten 1993] Gerke, H.H. and Van Genuchten, M.T. *A Dual-Porosity Model for simulating the Preferential Movement of Water and Solutes in Structured Porous Media*. Water Resources Research, 29, 305-319, (1993).
- [Milly 1985] Milly, P.C.D. *A mass-conservative procedure for time-stepping in models of unsaturated flow*. Adv. Water Resources, Volume 8, 32-36, (March 1985).
- [Neuman 1973] Neuman, S.P. *Saturated-unsaturated seepage by finite elements*. J. Hydraul. Div. Am. Soc. Civ. Eng., 99, 2233-2250, (1973).
- [Ouyang and Xiao 1994] Huajiang Ouyang and Ding Xiao. *Criteria for elimination oscillation in analysis of heat-conduction equation by finite-element method*. Communications in numerical methods in engineering, Vol.10 453-460, (1994).
- [Richards 1931] Richards, L.A. *Capillary conduction of liquids through porous mediums*. Physics, 1, 318-33, (1931).

- [van Genuchten 1980] van Genuchten ,M.T.*A closed-form equation for predicting the hydraulic conductivity of unsaturated soils*.Soil Sci.Soc.Am.J.,44,892-898,(1980).
- [Wood 1993] Wood ,W.L.*Introduction to numerical methods for water resources*.Clarendon Press,Oxford,(1993).
- [Wood and Calver 1990] Wood ,W.L.and Calver ,A.*Lumped Versus Distributed Mass Matrices in the Finite Element Solution of Subsurface Flow*.Water Resources Research,26,819-825,(May 1990).

Symbol.	Description.
$a(L)$	average distance from centre of matrix block to its bounday.
$c_m(L^{-1})$	specific soil water capacity of matrix pores.
$c_f(L^{-1})$	specific soil water capacity of fracture pores.
$\underline{h}(L)$	average pressure head of matrix and fracture pores.
$h_f(L)$	pressure head of fracture pores.
$h_m(L)$	pressure head of matrix pores.
$K_a(L/T)$	hydraulic conductivity of fracture/matrix interface.
$K_f(L/T)$	hydraulic conductivity of fracture pores.
$K_m(L/T)$	hydraulic conductivity of matrix pores.
$K_{sf}(L/T)$	hydraulic conductivity at saturation of fracture pores.
$K_{sm}(L/T)$	hydraulic conductivity at saturation of matrix pores.
m_m	$m_m = 1 - \frac{1}{n_m}$
m_n	$m_n = 1 - \frac{1}{n_n}$
n_m	experimental constant for matrix pores.
n_f	experimental constant for fracture pores.
l	experimental constant
$q_f(L/T)$	flux of water in fracture pores
$q_m(L/T)$	flux of water in matrix pores.
s_{ef}	effective saturation of fracture pores
s_{em}	effective saturation of matrix pores
$t(T)$	temporal variable(starting with $t=0$ initially)
w_f	volume of fractual pores as a proportion of total volume
w_m	volume of matrix pores as a proportion of total volume
$z(L)$	spatial variable(measured downwards with $z=0$ being ground-level).
$\alpha(L^2/T)$	constant.
$\alpha_w^*(L^{-2})$	experimental constant depending on size and structure of matrix pores.
β	empirical constant depending on the structure of the soil.
γ	empirical constant.
$\gamma_w(T^{-1})$	term representing water transfer from fracture to matrix pores
$\Delta t(T)$	time-step.
$\Delta t_k(T)$	time stepped by the kth time step.
$\Delta z(L)$	spatial-step.
θ	parameter in the θ method of time stepping.
θ_f	soil water retention function for fracture pores.
θ_m	soil water retention function for matrix pores.
θ_{rf}	residual soil water retention constant for fracture pores.
θ_{rm}	residual soil water retention constant for matrix pores.
θ_{sf}	saturated soil water retention constant for fracture pores.
θ_{sm}	saturated soil water retention constant for matrix pores.
Λ	maximum absolute difference in pressure heads of consecutative iterates.
Ψ	specified ratio of Λ terms as given in equation 3.4.
ω	relaxation parameter in the iteration of a time step.
Ω	relaxation parameter in the time stepping approximation.