Tridimensional and multi-layer modelling of transfers in unsaturated porous medium.

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Modélisation multi-couche et en 3 dimensions des transferts à travers la zone non saturée

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ABSTRACT: Waste disposal sites are usually protected from rainfall by sloping capillary barriers which cannot be modelled by classical unsaturated zone monodimensional models. A 3-dimensional and multilayer finite differences model has been developed. This model - MARTHE - has a system of nested grids with irregular rectangular meshes which guarantees a higher accuracy in given areas. The time discretization follows a special implicit scheme which allows large time steps with perfect flow balance. The flow equations are solved by a preconditioned conjugate gradient solver which is fast and accurate. An example of its application: the simulation of flows through a capillary barrier receiving rainfall is described.

RESUME : Dans les sites de stockage de déchets en surface, l'isolation vis-à-vis des pluies est généralement réalisée par des barrières capillaires inclinées dont le fonctionnement ne peut être simulé par les modèles monodimensionnels classiques en zone non saturée. Un modèle à différences finies, à la fois multicouches et tridimensionnel a donc été réalisé. Ce modèle -le modèle MARTHE - utilise un maillage formé de parallélépipèdes irréguliers avec possibilité de maillages emboîtés (gigognes), pour assurer une précision maximale en certaines zones. La discrétisation du temps se fait selon un schéma particulier, totalement implicite, permettant de grands pas de temps de calculs tout en conservant des bilans parfaitement équilibrés. La résolution des équations est assurée par la méthode des gradients conjugués avec préconditionnement qui est très performante. Un exemple d'application du modèle est présenté: la simulation des écoulements à travers une barrière capillaire soumise à la pluie.

1 INTRODUCTION

Wastes stored in superficial formations must be protected from the infiltration of rainfall which could generate and transport leachate to the underlying aquifers. A capillary barrier made by the superposition of two graded sloping layers of granular material is a very efficient way of preventing rainfall infiltration. As the layers are sloping, the design and management of such a capillary barrier can only be managed in transient state through 2 or 3-dimensional numerical models of transport in unsaturated porous media.

The main difficulty is due to the non-linear character of the flow equation from which the velocities are determined. From the velocities, and the variations of water content, the transport can be calculated using the random walk method with particles (Kinzelbach, 1988) in a scheme adapted to transient state (Thiéry and Iung, 1990, 1991; Thiéry, 1991).

2 FLOW MODELLING

The following assumptions are made:

- isothermal flow;
- non-swelling soils (the porosity is invariant);
- incompressible fluid (water);
- infinite permeability for air.

With these assumptions the general flow equation is:

$$\mathrm{div}[K\ \mathrm{Grad}H] = S_S \frac{\partial H}{\partial t} + q \qquad (1)$$

where:

H: hydraulic head at location x, y, z [L]

q : volumetric density of inflow (injection) or outflow (abstraction) [T^{-1}]

S_S : specific storage [L^{-1}]
K : hydraulic conductivity for water [LT^{-1}].

2.1 Spatial discretization

Discretization is by finite differences with a pure implicit method. Writing the balance equation between the central mesh and its 6 neighbours (North, South, East, West, Up and Down) yields:

$$\sum_{v=1}^{6} K_v \circ A \circ (H_v - H_c) / D_v + Q_i = STO / D_t \quad (2)$$

Where:

A	=	exchange area
D_V	=	distance to neighbouring node in direction v
k_V	=	internal hydraulic conductivity in direction v
Q_i	=	internal injection (source term)
STO	=	storage in the mesh
D_t	=	duration of time step
c	=	index of central mesh
v	=	index of neighbouring mesh in direction v
VOL	=	geometric volume of the mesh
θ	=	volumetric water content
θ_r	=	residual water content
θ_S	=	saturated water content
S_S	=	specific storage
Z	=	elevation (positive upwards)
Dg	=	variation of variable g
h	=	pressure head = H – Z
ES	=	equivalent specific storage coefficient
N	=	number of meshes
K_S	=	saturated hydraulic conductivity

The hydraulic conductivity is a function of pressure head h:

$$K = f(h) = f(H - Z)$$

2.2 Storage

The storage term is divided into two components:

- a term proportional to the variation of water content Dθ
- a compressibility term, according to the relative saturation $\theta/\theta s$

$$STO = VOL \, . \, [D\theta + (\theta/\theta_S) \, . \, S_S \, . \, DH] \, / \, Dt \quad (3)$$

2.3 Linearization

The balance equation in each mesh is non-linear; there are several methods to solve it, as described by Cooley (1983) or more recently by Thiéry (1988, 1990a), Celia *et al.* (1990), Ross (1990) and Kirkland *et al.* (1992). The method that we chose is described by Thiéry (1988). This is an iterative method (with under-relaxation) which always yields perfect balance and, in contrast to the approach of Cooley (1983), is independent of soil functional relations between pressure, water content and hydraulic conductivities. The values of K and STO are the most recent estimations in the iterative process corresponding to the end of the time step. At iteration k+1:

$$D\theta^{k+1} = (H_c - H_b) \cdot [(\theta^k - \theta_b)/(H^k - H_b)] \quad (4)$$

where:

k = iteration number
$H_b = H(t - Dt)$
$\theta_b = \theta(t - Dt)$

Dθ may be written as Dθ = C . DH where C has the dimension of a specific storage or a specific moisture capacity:

$$C = (\theta^k - \theta_b)/(H^k - H_b)$$

Equation (3) then writes as:

$$STO = VOL \cdot [C \cdot DH + (\theta/\theta_S) \, . \, S_S \cdot DH] \, / \, Dt = EM \cdot (H_c - H_b) \quad (5)$$

where:

$$EM = VOL \cdot [(\theta^k - \theta_b)/(H^k - H_b) + (\theta^k/\theta_S) \cdot S_S]/Dt \quad (6)$$

Equation (2) then writes:

$$\sum_v T_v \circ (H_v - H_c) + Q_i = EM \circ (H_c - H_b) \quad (7)$$

which turns into the following algebraic equation for mesh c:

$$\sum_v T_v \circ H_v - \left(\sum_v T_v + EM\right) \circ H_c = -Q_i - EM \circ H_b \quad (8)$$

2.4 Resolution

In a grid of N meshes it is necessary, at each iteration, to solve a linear system of N equations identical to equation (8). This linear system is symmetrical and generates a symmetrical square matrix of dimension N x N. This matrix is very sparse and has non-zero terms only along 7 diagonals; the centre and the 6 neighbours in the 6 directions. This system is solved very efficiently by a preconditioned conjugate gradient - as described by Hill (1990 a and b) - specially adapted to this type of matrix, which is very fast and needs very little memory. As the system is highly non-linear, an under-relaxation coefficient is used to avoid oscillations during the iterative process.

Discretization of time

Time steps are automatically determined to ensure optimal convergence and are indexed on the variations of saturation in the meshes.

2.5 Boundary conditions

Four types of boundary condition are possible:
a) prescribed potential (hydraulic head), pressure or water content
b) no-flow boundary
c) seepage face
d) unit gradient of hydraulic head (natural drainage).

Boundary conditions a) and b) are classical; the implementation of the third boundary condition (seepage face) is as a "tentative prescribed hydraulic head". If the computed hydraulic head at a given iteration becomes greater then the elevation of the node, the head is prescribed to the value of the elevation and there will be seepage. Then, for future iterations, if the calculated flow is negative (seepage), the hydraulic head stays prescribed, otherwise if it is positive (inflow), it is liberated and the hydraulic head will be lower than the elevation (no seepage). This scheme is efficient, as it is shown below. The fourth boundary condition (unit gradient) is implemented by simulating, in the meshes concerned, a density of outflow equivalent to the hydraulic conductivity corresponding to the local hydraulic head.

2.6 Internode weighting

The exchange coefficient between adjacent meshes may be Harmonic mean, Geometric mean (as advised by Vauclin *et al.*, 1979) or Upstream.

3 VERIFICATION OF MODEL

The method described in the previous section has been implemented in the 3-dimensional, Finite Difference Model MARTHE described by Thiéry (1990b). The model has been verified in the unsaturated zone by several severe tests published in the literature, among which are Cooley (1983), Celia (1990) and many others.

3.1 Flow through a square embankment

This is test No 1 as described by Cooley (1983) - flow through a square bank of porous medium of size 10. Hydraulic head is prescribed at 10 (units) over the left boundary and 2 over the right boundary. The right boundary is a seepage face. The functional relations of the soil are:

$h/h_t = [(\theta_s - \theta) / (\theta - \theta_r)]^{bt}$

$K/K_s = [(\theta - \theta_r)/(\theta_s - \theta_r)]^{bk}$

$K/K_s = [1 + (h/h_t)^{1/bt}]^{-bk}$

where:

$h_t = 1.778$; $b_t = 0.25$; $b_k = 4$; $K_s = 10^{-2}$

Figure 1 displays the calculated hydraulic head and the free surface; there is a seepage face at the left boundary from elevation 2 to elevation 4.8. The results are similar to those obtained by Cooley (1983).

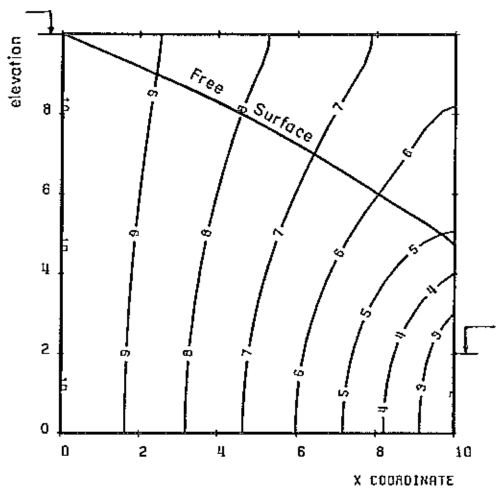


Fig. 1 Flow through a square embankment.

3.2 Test 2. Transient seepage from a stream

This is test No 6 as described by Cooley (1983) - the evolution of an infiltration profile and the response of a water table to infiltration. The soil parameters are identical to those from test No 1 with the additional values: $\theta_r = 5\%$; $\theta_s = 25\%$; $S_s = 10^{-4}$. The aquifer is initially at elevation 2 and the river is suddenly filled with water to elevation 18. Figure 2 displays the free surface (h = 0) at dates 35, 90, 194, 226, 302 and infinite (thick line). The water table has risen at time 194 and a short time later (t= 226) the whole region under the river is saturated. The results were obtained with a relaxation coefficient equal to 0.7 and only weighting by geometric mean was efficient. The results are exactly similar to those described by Cooley (1983). The calculation in steady state necessitated a relaxation coefficient not greater than 0.2.

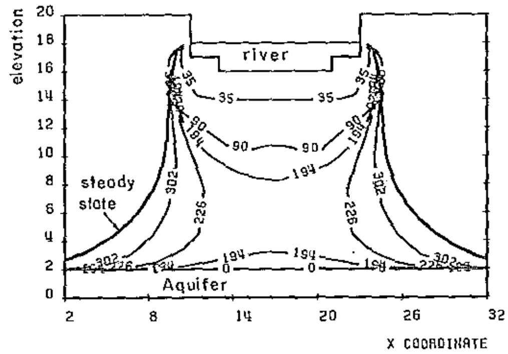


Fig. 2 Transient seepage from a stream.

3.3 *Test 3. Drainage involving multiple seepage faces*

This is test No 4 as described by Cooley (1983) - drainage from an initially saturated canyon wall. The porous medium is composed of 2 aquifers separated by a confining bed 100 times less pervious. The hydraulic head is prescribed at 26 over the left boundary situated at x = 200. The functional laws are the same as for test No 1 but with the following parameters:

aquifers : $h_t = 2.115$; $b_t = 0.25$; $b_k = 4$; $K_s = 100$

confining bed : $h_t = 4.472$; $b_t = 0.50$; $b_k = 4$; $K_s = 0.1$

Figure 3 displays the calculated hydraulic head in steady state and the free surface. There is a small seepage face at the bottom of the lower aquifer (over a height of less than one meter). Within the confining bed there is an "inverted" free surface because of the drainage into the lower aquifer. These results are similar to those of Cooley. A relaxation coefficient not greater than 0.5 was necessary to obtain a smooth convergence.

4 MODELLING OF A CAPILLARY BARRIER

The model MARTHE has been used to simulate a capillary barrier formed by a sandwich of 2 sandy layers separated by a semi-pervious layer of clay. The dimensions of the barrier are 50 x 6.6 m and the slope is 7.5%. The hydraulic conductivity is described by the relation :

$$K/K_s = 1/[1 + (h/h_k)^{bk}]$$

and the retention curve by:

$$h/h_t = [1/S_e - 1]^{bt} \quad \text{for sand}$$

$$h/h_t = [(1/S_e)^{1/(1-bt)} - 1]^{bt} \quad \text{for clay,}$$

where: $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$

The parameters are:

sand: $h_t = 0.15$ m; $b_t = 0.4$; ; $h_k = 0.20$ m; $b_k = 3$; $K_s = 10^{-6}$ m/s; $\theta_r = 2\%$; $\theta_s = 25\%$

clay : $h_t = 20$ m; $b_t = 0.5$; ; $h_k = 0.1$ m; $b_k = 1$; $K_s = 10^{-10}$ m/s; $\theta_r = 10\%$; $\theta_s = 32\%$

(clay parameters were adapted from Brun, 1989) The barrier receives a rainfall equal to 150 mm/year.

Figure 4 displays the calculated hydraulic head and the free surface in steady state. With these parameters, most of the rainfall is drained in the upper sandy layer, the rest (4.3 mm, i.e., 2.9%) flows quasi-vertically through the clay, which is saturated except for the lower half meter, and reaches the lower sandy layer

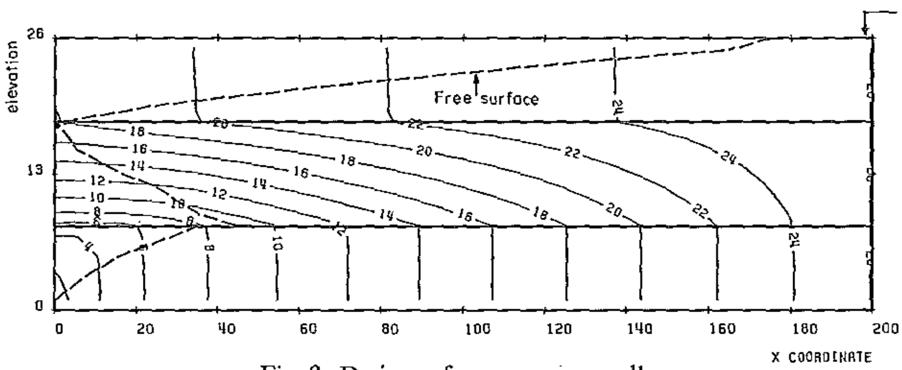


Fig. 3 Drainage from a canyon wall.

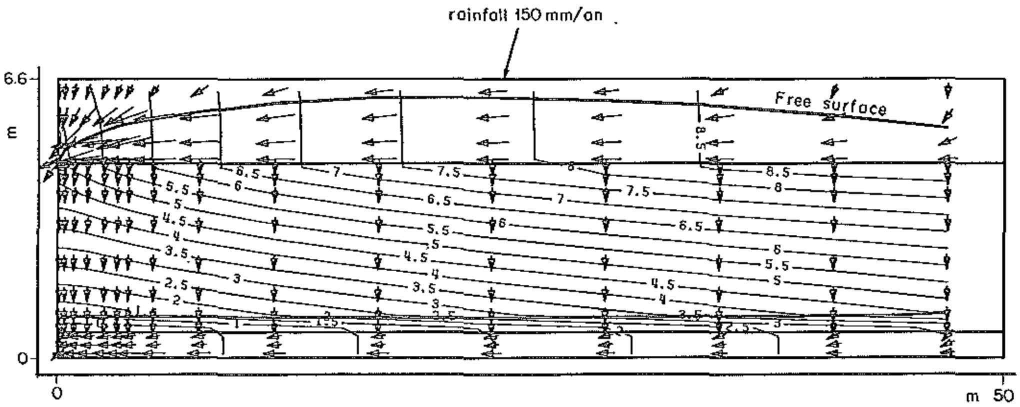
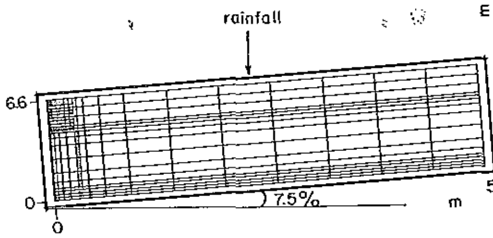
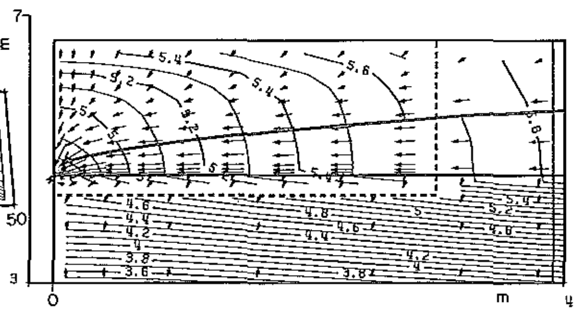


Fig. 4 Flow through a sloping capillary barrier: velocity and head gradient.



a) Total grid.



b) Upper left part of flow.

Fig. 5 Nested grid for the capillary barrier.

(mostly saturated) where it is drained. The same calculation has been done with a nested grid (Figure 5a). Figure 5b displays the upper left part of the grid and shows the free surface with great accuracy. A calculation in transient state has shown that the steady state is reached after more than 10 years.

5 CONCLUSIONS

A new scheme has been derived for the modelling in steady state and in 3 dimensions of flow in a porous medium in the unsaturated zone. This scheme, though very simple, is very efficient and accurate and may be used with any functional relations of the soil. Complex boundary conditions such as seepage faces are taken into account easily and the system of nested grid used in MARTHE is very flexible and enables a fine discretization in zones of interest. The model may be applied to design a capillary barrier in order to select the optimal geometry and to study its reaction in transient state under various sequences of rainfall.

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