INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS, VOL. 11, 287–301 (1990)

A FORMAL FINITE ELEMENT APPROACH FOR OPEN BOUNDARIES IN TRANSPORT AND DIFFUSION GROUND-WATER PROBLEMS

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SUMMARY

In the application of the finite element method to diffusion and convection–dispersion equations over a ground-water domain, the Galerkin technique was used to incorporate Neumann (or second-type) and Cauchy (or third-type) boundary conditions. While mass movement through open boundaries is *a priori* unknown, these boundaries are usually treated as a zero Neumann condition at some far distance from the domain of interest. Nevertheless, cheaper and better solutions can be obtained if these unknown conditions are adequately incorporated in the weak formulation and in the transient solution schemes (open boundary condition). Theoretical and numerical proofs are given of the equivalences between this approach and a 'well-posed' problem in a semi-infinite domain with a zero Neumann condition at a boundary placed at infinity. Transport and diffusion equations were applied in one dimension to show the numerical performances and limitations of this procedure for some linear and non-linear problems. No *a priori* limitations are foreseen in order to find similar solutions in two or three dimensions. Thus the spatial discretization in the proximity of open boundaries could be drastically reduced to the domain of interest.

KEY WORDS Finite element Transport Diffusion Ground-water Open boundaries Boundary conditions

INTRODUCTION

Of particular concern in this study is the realistic modelling of open boundaries for diffusion and convection–dispersion equations over a ground-water domain. Mass movement through open boundaries depends essentially on the volumetric sources and sinks as well as on the conditions imposed on other boundaries of the domain. Meanwhile, the lack of information associated with open boundaries is usually avoided by a zero Neumann condition at some far distance from the domain of interest.[1]

In the case of a transport equation it is known that inflow boundaries can be well represented by a Cauchy condition.[2] Typical transport phenomena in ground-water problems include the movement of heat and solutes in a porous medium. For this kind of problem, mass movement through typical outflow or open boundaries is *a priori* unknown.

The diffusion equation over a ground-water domain describes the water flow through a saturated or partially saturated porous medium. This equation can be linear or non-linear. Typical inflow boundaries include the infiltration or precipitation rate at the soil surface. A non-zero Neumann condition describes this second-type boundary.[3] However, inflow or outflow boundaries are only known when a Dirichlet condition can be imposed. Otherwise, important errors can arise because of the lack of information about the amounts of water that the system is

0271–2091/90/110287–15$07.50

Received September 1989
Revised December 1989

able to pick up or to release through the boundary. In order to avoid most of these errors, an impervious second-type condition must be imposed somewhere sufficiently far from the domain of interest. A classical example of inflow and outflow open boundaries can be found in the linear ground-water saturated flow under a dam. Both inflow and outflow boundaries are represented by vertical boundaries placed upstream and downstream in a two-dimensional profile. Another example of an open boundary that could be taken into account concerns the non-linear flow through the bottom boundary of an unsaturated soil where a deep water table can be found.

A one-dimensional finite element model is used to simulate the simultaneous transport of water, heat and solutes in saturated or partially saturated porous media. The numerical model MELEF-3v presented in this study was applied to predict the behaviour of frozen soils[4] as well as the effects of temperature on the fate of pesticides in the unsaturated zone.[5] In the present study the behaviour of diffusion and convection–dispersion processes is analysed for open boundaries by the finite element method. Depending on the characteristics of these boundaries and on the type of problem, better solutions can be obtained if a formal approach, also called an open boundary condition, is adequately incorporated in the weak formulation and in the transient solution schemes related to the finite element method.

GOVERNING EQUATIONS

Diffusion

The equation for the transient flow of water in a slightly compressible and partially saturated soil can be written[6–8]

$$\rho m(H)\frac{\partial H}{\partial t}=\frac{\partial}{\partial x_i}\left\{K(H)_{ij}\frac{\rho}{\eta}\frac{\partial H}{\partial x_j}\right\}+Q, \tag{1}$$

where ρ is the water density, H is the water potential ($H=P+\rho gz$), P is the water pressure, $K(H)_{ij}$ is the intrinsic permeability tensor, η is the dynamic viscosity, m is the specific moisture capacity and Q is a positive value when describing a source function. In (1), $i, j=1, 2, 3$ both stand for summation. The above equation is non-linear because of the dependence of m and K on the state variable H.

Transport

The equation for the unsteady transport of heat in a partially saturated porous medium can also be written[9,10]

$$\bar{c}\frac{\partial T}{\partial t}=\frac{\partial}{\partial x_i}\left\{\bar{K}_{ij}\frac{\partial T}{\partial x_j}\right\}-\rho c\vec{w}_i\frac{\partial T}{\partial x_i}+(T_0-T)cQ, \tag{2}$$

where T is the temperature, $\bar{c}$ is the calorific capacity by unit volume of the porous medium, c is the specific calorific capacity of water, $\vec{w}_i$ is the Darcy velocity vector, $\bar{K}_{ij}$ is the thermal conductivity tensor and T_0 is the known temperature of a source water.

Finally, the convection–dispersion of solutes in partially saturated soils can be expressed as[1,8]

$$\theta\frac{\partial C}{\partial t}=\frac{\partial}{\partial x_i}\left\{\theta D_{ij}\frac{\partial C}{\partial x_j}\right\}-\vec{w}_i\frac{\partial C}{\partial x_i}+(C_0-C)\frac{Q}{\rho}, \tag{3}$$

where C is the dissolved solute concentration, C_0 is the dissolved solute concentration in the source water, θ is the water content and D_{ij} is the hydrodynamic dispersion tensor.

BOUNDARY CONDITIONS

Appropriate boundary conditions are required to solve any of the time-dependent partial differential equations given above. The heat and solute transport equations (2) and (3) have a similar mathematical form. In order to avoid repetitions in subsequent explanations, we indicate for equation (3) the conditions that would also apply to the similar transport equation.

Several types of conditions are possible on the boundaries Γ.[8]

1. First-type or Dirichlet boundary condition

$$\left.\begin{array}{ll} H(x_i, t)=H_1 & \text{for equation (1)} \\ C(x_i, t)=C_1 & \text{for equation (3)} \end{array}\right\} \text{ on } \Gamma_1, \tag{4}$$

where H_1 and C_1 are respectively the prescribed hydraulic heads and dissolved solute concentrations on the boundary Γ_1. This condition can be usually prescribed for equation (1) at inflow or outflow boundaries. In the case of the transport equation (3), the Dirichlet condition is often well known on inflow boundaries.

2. Second-type or Neumann boundary condition

$$\left.\begin{array}{ll} -K(H)_{ij}\dfrac{\rho}{\eta}\dfrac{\partial H}{\partial x_j}n_i=q_{\mathrm{H}} & \text{for equation (1)} \\ -\theta D_{ij}\dfrac{\partial C}{\partial x_j}n_i=\bar{q}_{\mathrm{C}} & \text{for equation (3)} \end{array}\right\} \text{ on } \Gamma_2, \tag{5}$$

where q_{H} and $\bar{q}_{\mathrm{C}}$ are the prescribed water flux and diffusive flux of solute along the boundary (n_i is the unit outward normal vector to the boundary). Usually, q_{H} is only known for inflow boundaries (e.g. precipitation rate) as well as for assumed impermeable boundaries ($q_{\mathrm{H}}=0$). On the other hand, $\bar{q}_{\mathrm{C}}$ is not often known for outflow boundaries. In spite of this, the water flux and the diffusive flux of solute are in general considered as non-existent along these unknown boundaries.

3. Third-type or Cauchy boundary condition

$$\left(-\theta D_{ij}\frac{\partial C}{\partial x_j}+\vec{w}_i C\right)n_i=q_{\mathrm{C}} \quad \text{for equation (3)} \quad \text{on } \Gamma_3, \tag{6}$$

where q_{C} is the prescribed total contaminant flux, i.e. the diffusive flux plus the convective flux of solute:

$$q_{\mathrm{C}}=\bar{q}_{\mathrm{C}}+\vec{w}_i C n_i=\bar{q}_{\mathrm{C}}+\frac{q_{\mathrm{H}}}{\rho}C.$$

Mixed boundary conditions are required along those inflow boundaries of the system where infiltration of water occurs:

$$q_{\mathrm{C}}=\frac{q_{\mathrm{H}}}{\rho}C^*,$$

where C^* are prescribed concentrations of the solute in the influx water. At inflow boundaries either (4) or (6) is prescribed. Along impermeable boundaries we have

$$\vec{w}_i n_i=0,$$

and it is common to assume $\bar{q}_{\mathrm{C}}=0$, so q_{C} is equal to zero as well.[1]

The water flux (q_H) and diffusive flux of solute ($\bar{q}_C$) are not often known at outflow boundaries. The water flux is not always known at inflow boundaries either. However, and even if the conditions at a specific boundary are unknown, inflow or outflow boundaries to diffusion and convection–dispersion equations cannot always be physically defined as open boundaries.

Open boundaries

First let us consider the convection–dispersion problem. All boundary conditions are based on the requirement that for any boundary surface the tracer mass flux (mass per unit area of boundary surface) normal to the boundary must be equal on both sides of a given fixed boundary.[11]

Let us suppose that superscript * denotes the porous medium domain external to the boundary. When the external domain is also a porous medium, e.g. the same porous medium as the one inside the domain, the requirement that the normal mass fluxes be equal on both sides of this boundary is expressed by

$$-\theta D_{ij}\frac{\partial C}{\partial x_j}n_i+\frac{q_H}{\rho}C=-\theta D_{ij}\frac{\partial C^*}{\partial x_j}n_i+\frac{q_H}{\rho}C^*. \tag{7}$$

The left-hand part of this equation indicates the unknown mass flux inside the domain. This flux is dependent on the solution C at this point of the boundary.

For a continuous feed solution (the tracer solution is injected at a prescribed rate), equation (7) becomes a Cauchy boundary:[2]

$$-\theta D_{ij}\frac{\partial C}{\partial x_j}n_i+\frac{q_H}{\rho}C=\frac{q_H}{\rho}C^* \quad \text{on } \Gamma_3. \tag{8}$$

This condition implies in itself a discontinuity of the concentration and its derivatives at the boundary. However, if this boundary is located at infinity, where continuity would prevail ($C^*=C$), the same unsteady solutions as those obtained for a steady Cauchy condition in the finite domain can be obtained over the shared part of the semi-infinite domain if in the latter a zero Neumann condition at infinity is prescribed,

$$-\theta D_{ij}\frac{\partial C}{\partial x_j}n_i=0 \quad \text{on } \Gamma_2 \text{ at infinity,} \tag{9}$$

and if initial conditions in both domains are the same, continuous and in conformity with the latter Cauchy and Neumann conditions (taking for granted that the physical properties are also the same in both cases). Then we could say that an inflow Cauchy condition on a boundary would work similarly to a zero Neumann condition at infinity if certain conditions of continuity are initially respected close to the boundary. We will also prove this assumption numerically.

In order to establish the feasibility of the so-called open boundaries, it can be assumed that wherever the boundary is located there is no discontinuity and therefore $C^*=C$. Then (7) yields

$$-\theta D_{ij}\frac{\partial C}{\partial x_j}n_i=-\theta D_{ij}\frac{\partial C^*}{\partial x_j}n_i=\bar{q}_C\neq 0 \quad \text{on } \Gamma_2, \tag{10}$$

which means that there is also continuity in the derivative. This would give the same solutions, under the same and continuous initial conditions, as

$$-\theta D_{ij}\frac{\partial C}{\partial x_j}n_i=-\theta D_{ij}\frac{\partial C^*}{\partial x_j}n_i=0 \quad \text{on } \Gamma_2 \text{ at infinity,} \tag{11}$$

on a boundary at infinity in a semi-infinite domain. Then, in both cases, the Neumann boundary equations (10) and (11) will give the same transient solutions over both shared domains if the physical properties do not change from near inside to outside the open boundary (from the finite domain to the semi-infinite one). The initial conditions must also be the same, continuous and in conformity with the last zero Neumann condition at infinity. In transport problems, outflow boundaries are continuous and can be defined as typical open boundaries. The open boundary condition (10) needs to be formally incorporated on boundaries Γ_2 as well as into the weak formulation and in the transient solution schemes related to the finite element method, just as the inflow Cauchy condition (8) is usually incorporated on boundaries Γ_3.[1]

There are unknown outflow or inflow boundary conditions for water diffusion problems that imply a continuity of the hydraulic head or its derivatives close to the boundary. If this boundary corresponds to a typical open boundary, its conditions need to be treated in the same way as condition (10) would be:

$$-K(H)_{ij}\frac{\rho}{\eta}\frac{\partial H}{\partial x_j}n_i=q_{\mathrm{H}}\neq 0 \quad \text{on } \Gamma_2, \tag{12}$$

where q_{H} is not known on a boundary located at a finite distance. This means that this kind of boundary can be eventually substituted by a zero Neumann condition at infinity in a semi-infinite domain:

$$-K(H)_{ij}\frac{\rho}{\eta}\frac{\partial H}{\partial x_j}n_i=0 \quad \text{on } \Gamma_2 \text{ at infinity.} \tag{13}$$

Classical examples of inflow and outflow open boundaries for water diffusion problems can be found in the linear ground-water saturated flow under a dam. Another example of an open boundary could be the non-linear flow through the bottom boundary of an unsaturated soil where there is a deeper water table. We will see later whether the non-linearities involved allow us to define such a boundary in this way.

If a formal numerical approach for open boundaries on a finite domain is reliable, it could be interpreted as an open condition of the second kind. However, we have seen that open boundaries need to be clearly defined within a physical context.

FINITE ELEMENT FORMULATION

The Galerkin technique is used to determine approximate solutions to equations (1)–(3) under the appropriate initial and boundary conditions. Full details of the solution procedures involved will not be given here; however, an outline of our numerical scheme is presented below to provide some idea of how the different types of boundary conditions were dealt with (for more details, see References 1 and 8).

Transport

An estimate of the solution C can be represented as the product of an appropriate shape function N_l and the value of the state variable at required model points C_l:

$$C=\langle N_l\rangle\{C_l\}. \tag{14}$$

Integrating by parts only the dispersion component of the solute transport equation (3), the resulting weak formulation gives the following set of finite element equations in matrix form:

$$[M]\left\{\frac{\partial C}{\partial t}\right\}+[K]\{C\}=\{F\}, \tag{15}$$

where $[M]$ and $[K]$ are $n \times n$ matrices and $\{F\}$ is a vector of length n (the nodal points of the discretized system: $l=1, 2, \ldots, n$). These are expressed by

$$M_{kl}=\sum_e \int_{\Omega^e} [\theta N_k]\,\mathrm{d}\Omega \quad \text{for } k=l, \qquad M_{kl}=0 \quad \text{for } k\neq l$$

(this is a diagonalized form where the nodal time derivatives are weighted averages over the entire flow region[8]),

$$K_{kl}=\sum_e \left[\int_{\Omega^e} \left(\theta D_{ij} \left[\frac{\partial N_k}{\partial x_i} \frac{\partial N_l}{\partial x_j} \right] + \vec{w}_i \left[N_k \frac{\partial N_l}{\partial x_i} \right] \right) \mathrm{d}\Omega + \int_{\Omega^e} \frac{Q}{\rho} [N_k N_l]\,\mathrm{d}\Omega \right],$$

$$F_k=\sum_e \left\{ \int_{\Omega^e} \frac{Q}{\rho} C_0 \{N_k\}\,\mathrm{d}\Omega + \oint_{\Gamma^e} \{N_k\} \theta D_{ij} \frac{\partial C}{\partial x_j} n_i\,\mathrm{d}\Gamma \right\},$$

where e indicates summation over the elements joining at node k ($k=1, 2, \ldots, n$), Ω is the domain of the flow regime and $N_{k,l}$ are spatial shape functions. The vector $\{F\}$ depends on the conditions at the boundaries Γ.

With the representation given by (14), the Dirichlet or first-type boundary conditions are satisfied at the prescribed concentration nodes on Γ_1 directly by the shape functions. Thus for these nodes (15) is not actually written. Therefore in this equation the boundary integral is to be extended to Γ_2 and Γ_3 only.

If formulation (15) is followed we set

$$\oint_{\Gamma_3} \{N_k\} \theta D_{ij} \frac{\partial C}{\partial x_j} n_i\,\mathrm{d}\Gamma = \oint_{\Gamma_3} \frac{q_{\mathrm{H}}}{\rho} [N_k N_l] \{C_l\}\,\mathrm{d}\Gamma - \oint_{\Gamma_3} \frac{q_{\mathrm{H}}}{\rho} C^* \{N_k\}\,\mathrm{d}\Gamma \tag{16}$$

along inflow, mixed or Cauchy boundaries with q_{H} and C^* prescribed;

$$\oint_{\Gamma_2} \{N_k\} \theta D_{ij} \frac{\partial C}{\partial x_j} n_i\,\mathrm{d}\Gamma = 0 \tag{17}$$

along impermeable boundaries;

$$\oint_{\Gamma_2} \{N_k\} \theta D_{ij} \frac{\partial C}{\partial x_j} n_i\,\mathrm{d}\Gamma = \oint_{\Gamma_2} \theta D_{ij} n_i \left[N_k \frac{\partial N_l}{\partial x_j} \right] \{C_l\}\,\mathrm{d}\Gamma \tag{18}$$

along typical outflow or open boundaries.

Note that by this treatment, this latter condition can be interpreted as a self-imposed condition leading to an ill-posed problem. Even though this condition could be seen actually as self-imposed, it must be used only on boundaries that have been defined as open, i.e. that would work as a zero Neumann condition at infinity over a hypothetical semi-infinite domain.

Diffusion

Similar to the expression for representing the solute concentrations, an estimate of the solution H can be represented as the product of an appropriate shape function N_l and the value of the state variable at required model points H_l:

$$H=\langle N_l \rangle \{H_l\}. \tag{19}$$

Applying Green's lemma to the water flow equation (1), the resulting weak formulation gives the following set of non-linear equations in matrix form:

$$[M(H)] \left\{ \frac{\partial H}{\partial t} \right\} + [K(H)]\{H\} = \{F(H)\}. \tag{20}$$

These matrices are expressed by

$$M(H)_{kl}=\sum_e \int_{\Omega^e} [\rho m(H) N_k] \, d\Omega \quad \text{for } k=l, \qquad M(H)_{kl}=0 \quad \text{for } k \neq l$$

(which have the diagonalized form[8]),

$$K(H)_{kl}=\sum_e \int_{\Omega^e} \frac{\rho}{\eta} K(H)_{ij} \left[\frac{\partial N_k}{\partial x_i} \frac{\partial N_l}{\partial x_j} \right] d\Omega,$$

$$F(H)_k=\sum_e \left\{ \int_{\Omega^e} Q\{N_k\} \, d\Omega + \oint_{\Gamma^e} \{N_k\} \frac{\rho}{\eta} K(H)_{ij} \frac{\partial H}{\partial x_j} n_i \, d\Gamma \right\}.$$

The vector $\{F\}$ depends on the conditions at the boundaries Γ. In equation (20) the boundary integral is to be extended to Γ_2 and Γ_3 only. If this formulation is followed we set

$$\oint_{\Gamma_2} \{N_k\} \frac{\rho}{\eta} K(H)_{ij} \frac{\partial H}{\partial x_j} n_i \, d\Gamma = 0 \tag{21}$$

along impermeable boundaries;

$$\oint_{\Gamma_2} \{N_k\} \frac{\rho}{\eta} K(H)_{ij} \frac{\partial H}{\partial x_j} n_i \, d\Gamma = -\oint_{\Gamma_2} q_{\mathrm{H}} \{N_k\} \, d\Gamma \tag{22}$$

along known inflow or outflow Neumann boundaries;

$$\oint_{\Gamma_2} \{N_k\} \frac{\rho}{\eta} K(H)_{ij} \frac{\partial H}{\partial x_j} n_i \, d\Gamma = \oint_{\Gamma_2} \frac{\rho}{\eta} K(H)_{ij} n_i \left[N_k \frac{\partial N_l}{\partial x_j} \right] \{H_l\} \, d\Gamma \tag{23}$$

along unknown open boundaries. This condition can be interpreted as a release or sink of water outside the domain in order to avoid its storage at the boundary. Note that this kind of boundary actually requires to have a physical meaning according to the definition of an open boundary. However, non-linear temporal schemes would be needed to solve the transient flow of water in a partially saturated porous medium.

LINEAR SOLUTION METHOD

Transport

The implicit difference scheme has been found to provide good results for the time-dependent nature of equations (15) and (20).[12] In this case, linear convection–dispersion systems can be expressed as

$$[\Delta t \alpha [K] + [M]] \{C_{t+\Delta t} - C_t\} = \{\Delta t (\alpha \{F_{t+\Delta t}\} + (1-\alpha)\{F_t\} - [K]\{C_t\})\}. \tag{24}$$

When $\alpha = 1$ it is called a fully implicit backward scheme, and when $\alpha = 0{\cdot}5$ it is the Crank–Nicholson scheme. If $\{F\}$ depends on the solution, it can be expressed as the sum of two parts:

$$\{F_t\} = [F']\{C_t\} + \{F''\}, \qquad \{F_{t+\Delta t}\} = [F']\{C_{t+\Delta t}\} + \{F''\};$$

that is,

$$\{F_{t+\Delta t}\} = [F']\{\Delta C_t\} + [F']\{C_t\} + \{F''\} = [F']\{\Delta C_t\} + \{F_t\}. \tag{25}$$

In the case of the solute transport the vector $\{F'')$ would consider only the fluxes that would not be dependent on the solution, i.e. the steady volumetric and surface fluxes expressed in vector $\{F\}$ of equation (15). Employing this definition in equation (24) yields

$$[\Delta t\alpha([K]-[F'])+[M]]\{C_{t+\Delta t}-C_t\}=\{\Delta t(\{F_t\}-[K]\{C_t\})\}, \tag{26}$$

where $[F']$ is a $n\times n$ matrix evaluated on the boundaries.

Following this set of finite element equations, the matrix $[F']$ can be written

$$F'_{kl}=\sum_e \oint_{\Gamma_3}\left(\frac{q_{\mathrm{H}}}{\rho}\right)[N_k N_l]\,\mathrm{d}\Gamma \tag{27}$$

along an inflow or Cauchy boundary of the type expressed by equation (16);

$$F'_{kl}=0 \tag{28}$$

along impermeable boundaries (17);

$$F'_{kl}=\sum_e \oint_{\Gamma_2}\theta D_{ij}n_i\left[N_k\frac{\partial N_l}{\partial x_j}\right]\mathrm{d}\Gamma \tag{29}$$

along open boundaries of the type expressed by equation (18).

Diffusion

A linear form of equation (1) would describe the flow of water in a saturated porous medium. Applying the implicit difference scheme and the definitions given above to the linear form of the set of finite element equations (20) yields

$$[\Delta t\alpha([K]-[F'])+[M]]\{H_{t+\Delta t}-H_t\}=\{\Delta t(\{F_t\}-[K]\{H_t\})\}. \tag{30}$$

Expressed in matrix form,

$$F'_{kl}=0 \tag{31}$$

along impermeable (21) and known Neumann boundaries (22);

$$F'_{kl}=\sum_e \oint_{\Gamma_2}\frac{\rho}{\eta}K_{ij}n_i\left[N_k\frac{\partial N_l}{\partial x_j}\right]\mathrm{d}\Gamma \tag{32}$$

along unknown open boundaries of the type expressed by (23).

NON-LINEAR SOLUTION METHOD

Diffusion

Non-linear algorithms may be employed for non-linear problems with transient parameters. In a ground-water domain the flow of water through partially saturated soils is a typical non-linear phenomenon. Applying the substitution method[12] to (30) gives the following set of equations in matrix form:

$$\begin{aligned}&[\Delta t\alpha([K^{m-1}_{t+\Delta t}]-[F'^{m-1}_{t+\Delta t}])+[M^{m-1}_{t+\Delta t}]]\{H^{m}_{t+\Delta t}-H^{m-1}_{t+\Delta t}\}\\&\quad=[M^{m-1}_{t+\Delta t}]\{H_t-H^{m-1}_{t+\Delta t}\}-\Delta t\alpha[K^{m-1}_{t+\Delta t}]\{H^{m-1}_{t+\Delta t}\}-\Delta t(1-\alpha)[K_t]\{H_t\}\\&\qquad+\{\Delta t((1-\alpha)[F'_t]\{H_t\}+\alpha[F'^{m-1}_{t+\Delta t}]\{H^{m-1}_{t+\Delta t}\}+\{F''\})\}.\end{aligned} \tag{33}$$

In the case of a fully implicit backward scheme ($\alpha = 1$) we can reduce (33) to

$$[\Delta t([K^{m-1}_{t+\Delta t}] - [F'^{m-1}_{t+\Delta t}]) + [M^{m-1}_{t+\Delta t}]]\{H^{m}_{t+\Delta t} - H^{m-1}_{t+\Delta t}\}$$
$$= [M^{m-1}_{t+\Delta t}]\{H_t - H^{m-1}_{t+\Delta t}\} + \{\Delta t(\{F^{m-1}_{t+\Delta t}\} - [K^{m-1}_{t+\Delta t}]\{H^{m-1}_{t+\Delta t}\})\}, \tag{34}$$

where m indicates the number of iterations of the non-linear algorithm.

MODEL VERIFICATION

In a one-dimensional finite element domain, hydraulic heads, temperatures and solute concentrations were represented by spatial quadratic functions (Figure 1). The time step chosen to solve each equation at a particular point in time needs to be smaller or equal to the time taken by the input data or to evaluate transient parameters if this is the case. The time step is then computed by keeping the diffusion parameter within a certain range as well as the Courant and Peclet numbers

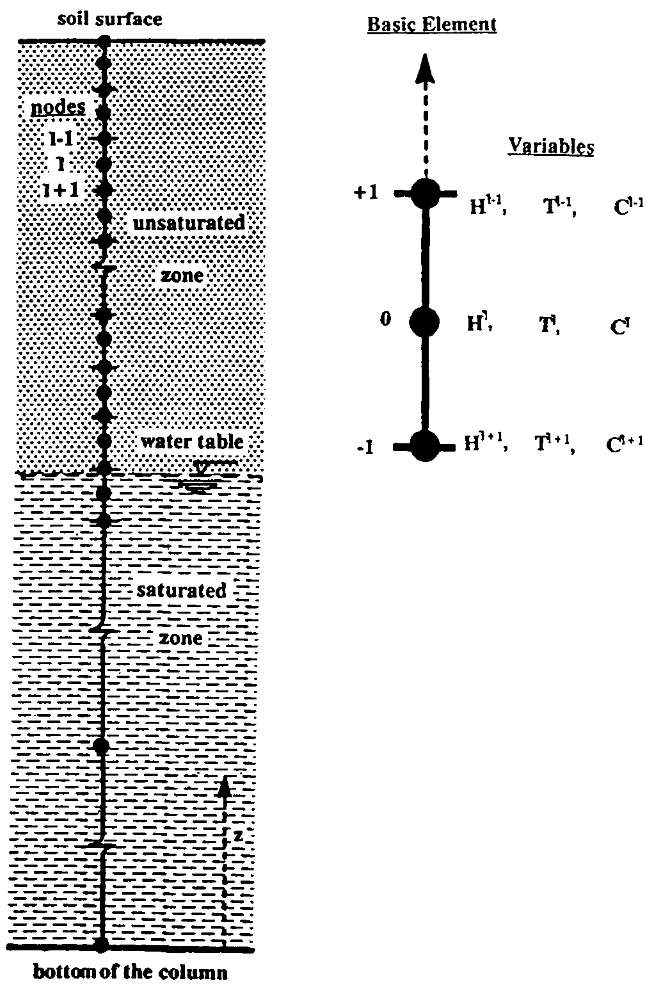

Figure 1. Finite element vertical discretization of the unsaturated–saturated zone of the soil

of the corresponding transport phenomena. The choice of the frequency for evaluating transient parameters depends on the kind of problem, the stability criteria, the precision desired and the CPU time.

The heat and solute transport portions of the model were tested by comparison with the analytical solution proposed by Ogata and Banks.[13] This solution is given in one dimension for linear convection–dispersion using a step input (C_0 or T_0) at $z=0$ and a zero gradient ($\partial C/\partial z$ or $\partial T/\partial z$) at $z=-\infty$. In the case of an outflow boundary it has already been seen that this last condition could be well represented, in a finite element numerical model, by an open boundary condition. If the bottom of the column is an inflow boundary, the above Neumann condition at infinity can be well represented by a third-type or Cauchy condition if continuity is initially respected in the proximity of the boundary (Figure 2). However, a zero Neumann condition is needed only for impermeable boundaries. Otherwise, outflow boundaries at infinity can also be accurately reproduced in a continuous finite domain by an open boundary condition (Figure 3). Therefore, in general transport phenomena, if the bottom of the column is considered to have the characteristics of an outflow open boundary, it does not need an *a priori* known condition and all the results of the discretized domain are able to closely represent the analytical solutions (Figure 4). These latter comparisons are shown for a Darcy velocity, soil porosity, longitudinal dispersivity and thermal conductivity of the solids of $0.24\,\mathrm{m\,day^{-1}}$, 0.4, 0.2 m and $14\,446\,\mathrm{J\,m^{-1}\,day^{-1}\,K^{-1}}$ respectively.

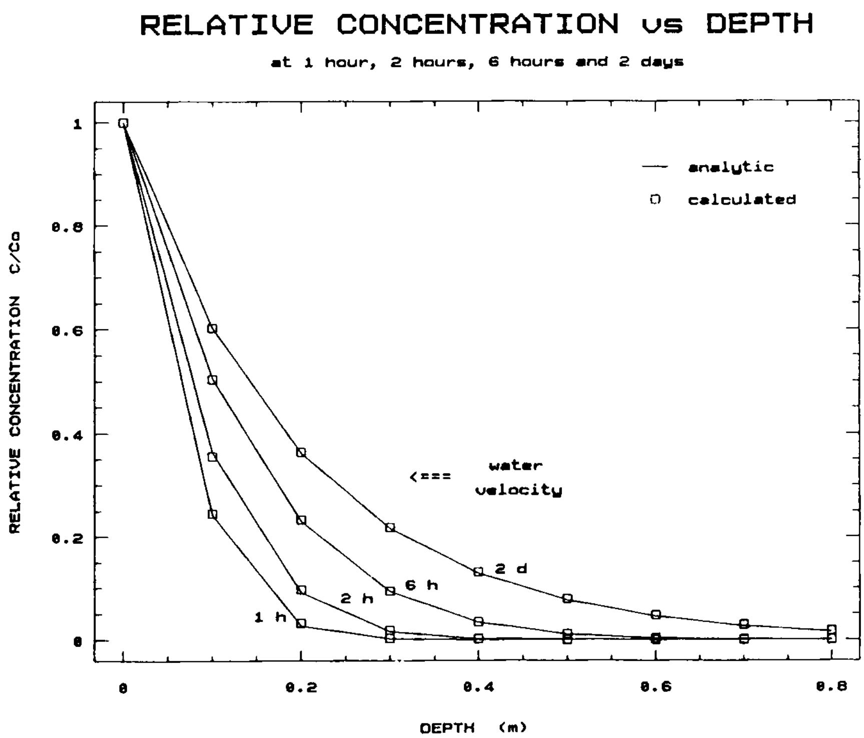

Figure 2. Comparison of numerical model and analytical solution results for the convection–dispersion of a solute when the water velocity is oriented upwards. Cauchy boundary conditions are imposed at the bottom of the column

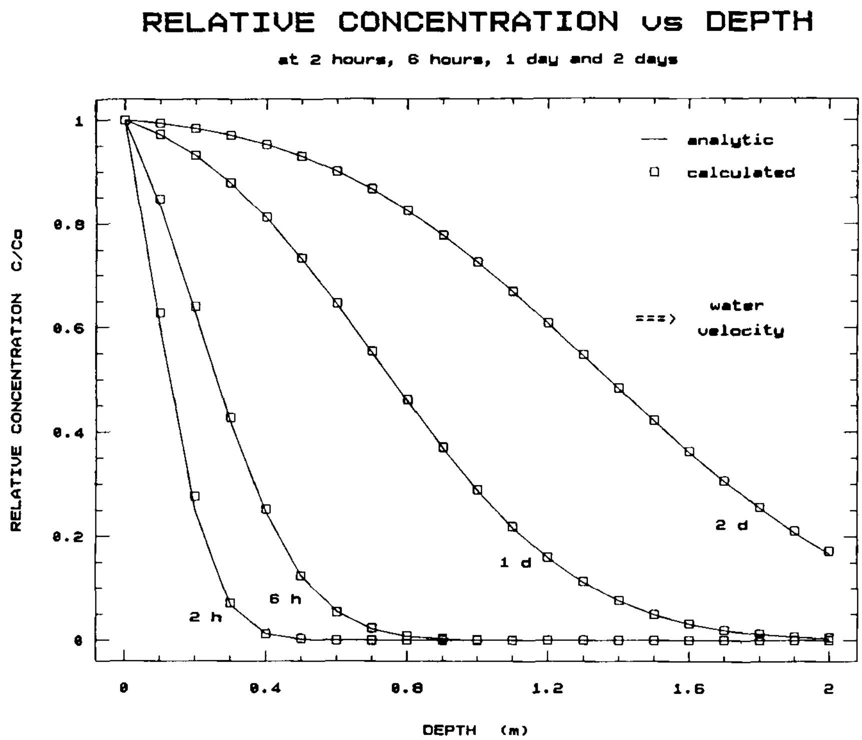

Figure 3. Comparison of numerical model and analytical solution results for convection–dispersion of a solute when the water velocity is oriented downwards. Open boundary conditions are imposed at the bottom of the column

Testing the accuracy of numerical schemes used to solve the one-dimensional transient non-linear water flow equation is limited by the scarcity of suitable analytical solutions. In order to avoid this difficulty, equation (1) can be expressed in the Richards form

$$\frac{\partial \theta}{\partial t}=\frac{\partial}{\partial z}\left\{\frac{K_0}{\eta}K_r\frac{\partial P}{\partial \theta}\frac{\partial \theta}{\partial z}\right\}+\rho g\frac{K_0}{\eta}\frac{\partial K_r}{\partial z}, \tag{35}$$

where K_0 and K_r are the saturated intrinsic and relative permeabilities of water respectively ($K=K_0K_r$). Putting $K_r=S$ and $P=a\ln S$ yields

$$\frac{n\eta}{K_0}\frac{\partial S}{\partial t}=a\frac{\partial^2 S}{\partial z^2}+\rho g\frac{\partial S}{\partial z}, \tag{36}$$

where S is the water saturation, n is the porosity and a is a constant defined for each type of soil. Equation (36) has the form of a transport equation and therefore it can also be compared to the analytical solution of Ogata and Banks.[13] The physical properties used hereafter for the simulations concerning the transient flow of water correspond quite well to a fine sand, lightly silty soil. The hypothetical impervious boundary condition at $z=-\infty$ could be represented in the unsaturated water flow equation (1) by making $\partial H/\partial z=\rho g$ at the top of the discretized column sufficiently far from the water table (Figure 5). The results show nearly steady conditions after 6 h of water intake from a water table towards the unsaturated zone of an initially almost dry soil.

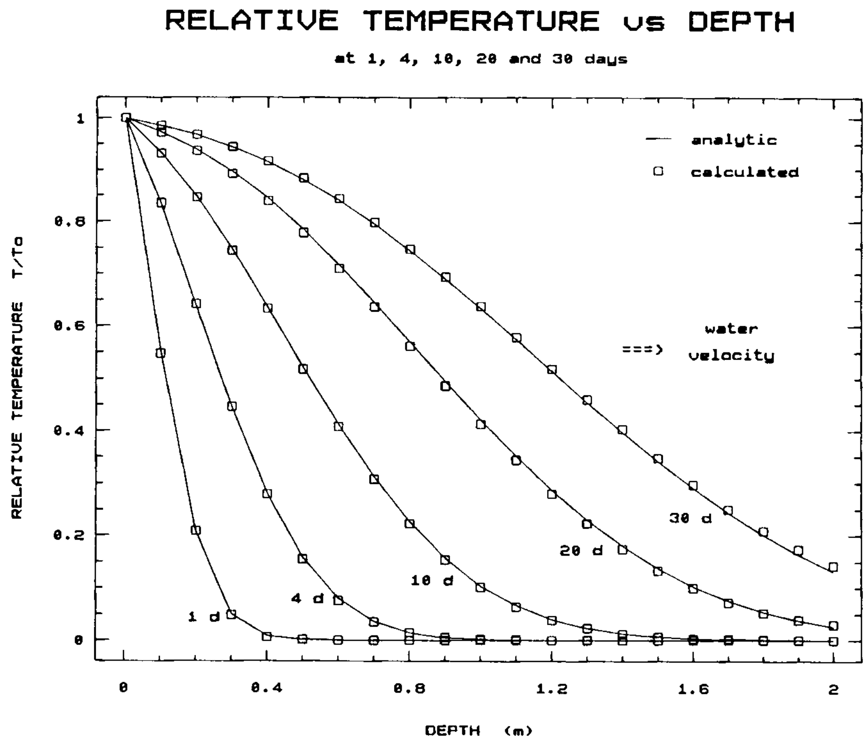

Figure 4. Comparison of numerical model and analytical solution results for convection–dispersion of heat when the water velocity is oriented downwards. Open boundary conditions are imposed at the bottom of the column

In one-dimensional ground-water phenomena the non-linear flow through the bottom boundary of an unsaturated soil could be interpreted as a nearly open boundary. This assumption would become more and more true if a deeper water table were connected by capillarity to the unsaturated domain of interest. However, existent non-linearities imply transient and therefore different physical properties between this boundary and the lower unsaturated soil. Furthermore, nearly zero but non-zero Neumann conditions can be found at a deep and steady water table. Figure 6 shows one-dimensional solutions for three different boundary conditions at the bottom of an initially steady unsaturated column with a 10 m deep water table: (a) Dirichlet condition at the 10 m deep steady water table; (b) open condition at a depth of 2 m; (c) zero Neumann condition at a depth of 2 m. At the top of the one-dimensional soil column, water infiltrates at the rate of 1 cm day^{-1}. As could be expected, the solutions for boundary conditions (a) and (b) compare quite well. Figure 7 shows solutions for a similar soil column where an infiltration of 2 cm day^{-1} occurs at the surface. A steady unsaturated soil with a 5 m deep water table can be defined initially, and three similar boundary conditions at a suitable bottom of the column can also be prescribed: (a) Dirichlet condition for the steady 5 m deep water table; (b) open condition at a depth of 2 m; (c) zero Neumann condition at a depth of 2 m. In this case the hydraulic heads for boundary conditions (a) and (b) compare worse than for the case of Figure 6. Our conclusion is that open boundaries cannot be defined for non-linear phenomena over a finite domain. The reason is that, first, the same physical properties cannot always be respected on the correspondent semi-infinite domain. Then, the examples concerning the hypothetical open boundary conditions

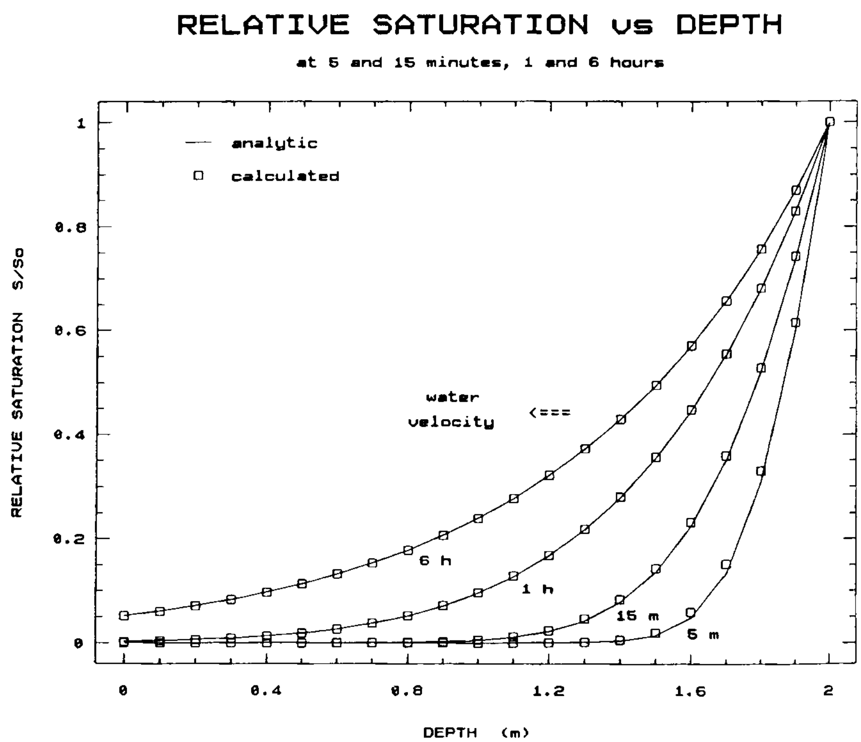

Figure 5. Comparison of numerical model and analytical solution results for water intake from a 2 m deep water table towards the unsaturated zone of an initially dry soil

of Figures 6 and 7 cannot be considered to have actual open boundaries. Secondly, the assumed zero Neumann condition at infinity is not respected at a boundary where a Dirichlet condition would control the position of a steady water table. Nevertheless, for the type of non-linearity we are working with, numerical simulations taking into account initially steady and open boundary conditions have proved to give better results for deeper water tables and lighter infiltration rates. This means that, near the surface of the soil, non-linear unsaturated problems could be quite accurately treated by a suitable open boundary condition if this boundary is near enough to the domain of interest but far enough from the water table position. However, the reliability of this formal approach for two and three dimensions remains its greatest interest.

In all of the above cases the Crank–Nicholson time-dependent scheme shows the most precise results.

CONCLUSIONS

A one-dimensional finite element model taking into account a formal approach for open boundaries in typical ground-water problems has been developed. The Galerkin technique, in conjunction with several types of boundaries and initial conditions, was used to solve water diffusion, heat and solute transport in saturated–unsaturated soils.

Open conditions have been developed to take into account open boundaries for linear and non-linear ground-water systems. The equivalences between outflow–inflow boundary conditions at a

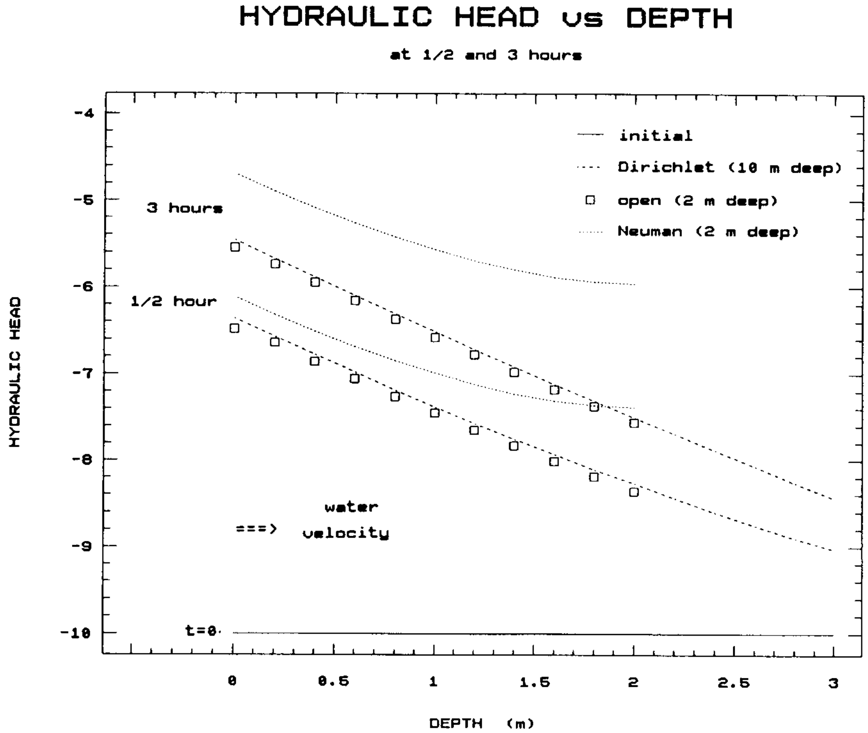

Figure 6. Comparison of numerical results for water infiltration (1 cm day^{-1}) in a 10 m thick unsaturated column where three different conditions were imposed on hypothetical boundaries at a depth of 2 and 10 m

finite distance and at infinity have been established. In the case of linear transport phenomena, Cauchy and open conditions for inflow and outflow boundaries respectively placed at a finite distance have been found to reproduce accurately the corresponding zero Neumann conditions at infinity. Applications also take into account the described open boundary conditions for one-dimensional water flow in non-linear unsaturated soils. No physical meaning or actual conditions have been found in one dimension to justify the existence of an open boundary within the unsaturated zone. This would imply the existence of an impervious Neumann condition in a semi-infinite domain which would keep the same physical properties as the finite domain. Nevertheless, for this kind of non-linearity, more precise solutions in the unsaturated zone can be obtained for deeper water tables and lighter infiltration rates. In the same way we do not see *a priori* limitations to applying this technique to other numerical problems, in two or three dimensions, as long as zero Neumann conditions at infinity have a real physical meaning for the kind of problem to be solved. Even though this is not actually the case, certain lightly non-linear open boundaries could be solved by this formal approach without a significant loss of accuracy.

The heat and solute transport, as well as the flow portions of the numerical model, were precisely compared with analytical solutions. In general, the open boundary condition consumes less computer time and allows more accurate simulations of linear and non-linear diffusion and transport problems.

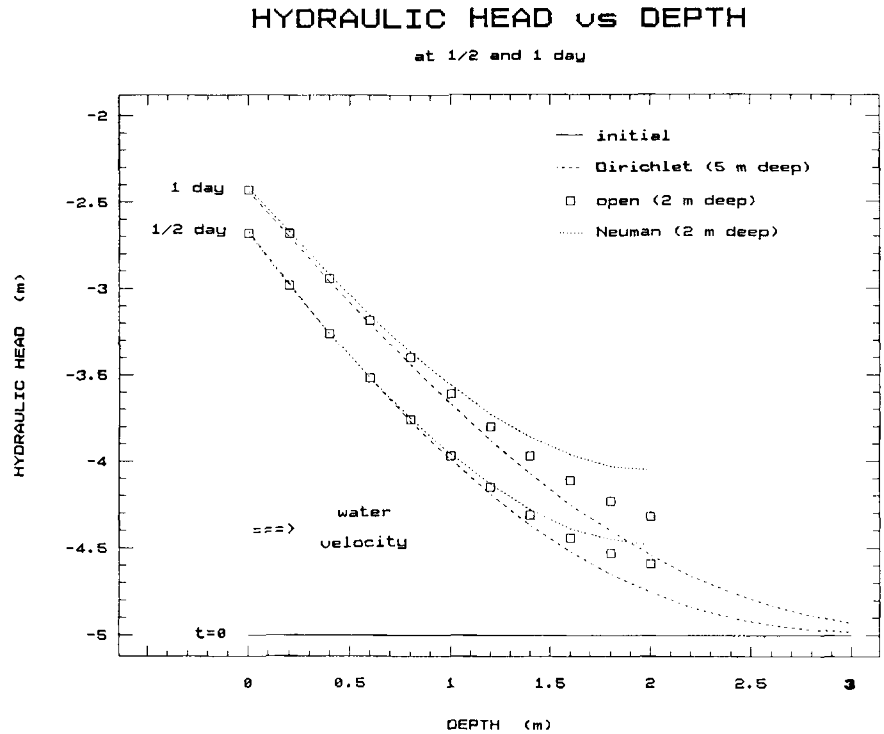

Figure 7. Comparison of numerical results for water infiltration (2 cm day^{-1}) in a 5 m thick unsaturated column where three different conditions were imposed on hypothetical boundaries at a depth of 2 and 5 m

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