Deterministic finite element solution of unsteady flow and transport through porous media: Model development

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Aguirre, C.G., Madani, A., Mohtar, R. and Haghighi, K. 2005. **Deterministic finite element solution of unsteady flow and transport through porous media: Model development**. Canadian Biosystems Engineering/Le génie des biosystèmes au Canada **47**: 1.29-1.35. A deterministic finite element solution to predict water flow and nutrient movement through porous media was developed and implemented using Visual C++. The model is user-friendly, can be used as a management tool, and is able to predict the NO_3-N losses in subsurface drainage water. The application of either solid or liquid fertilizer can be easily simulated. To reduce computational time, mathematical expressions for the contributions of the flux boundary conditions to the finite element equations were developed analytically and directly introduced into the force vectors. The global system of equations was evaluated using a finite difference approximation in the time domain. The finite element methodology provides a very attractive approach to predict flow and transport of nutrients in soils. **Keywords**: deterministic approach, ground water, water quality, soil, numerical simulations.

Une solution déterministe par éléments finis pour la prédiction de l'écoulement de l'eau et le mouvement des nutriments à travers un médium poreux a été développée et mise en oeuvre en utilisant Visual C++. Le modèle est facile d'utilisation et peut être utilisé comme outil de gestion par la prédiction des pertes de NO_3-N dans les eaux provenant de systèmes de drainage. L'épandage de fertilisants solides ou liquides peut être facilement simulé. De manière à réduire le temps de calcul, des relations mathématiques pour les contributions aux conditions limites de l'écoulement adaptées aux équations des éléments finis ont été développées analytiquement et introduites directement dans les vecteurs forces. Le système global d'équations a été résolu en utilisant une approximation par différences finies dans le temps. La méthodologie des éléments finis est une approche très intéressante pour prédire l'écoulement et le transport des nutriments dans les sols. **Mots clés**: approche déterministe, nappe phréatique, qualité de l'eau, sol, simulations numériques.

INTRODUCTION

The quality of groundwater has become a significant concern throughout the world. Agricultural production has come under greater scrutiny for its potential role in the degradation of water resources (Lovejoy et al. 1997). Surface applied agrochemicals are being detected with increasing frequency in groundwaters worldwide. The detection of these chemicals in drinking water supplies has increased the public concern about the safety of the current agricultural practices and the techniques used to quickly identify and remediate contaminated groundwaters. Prevention of groundwater contamination is absolutely necessary to ensure public safety (Ehteshami et al. 1991).

To protect and preserve groundwater resources, a thorough understanding of the movement of water and transport of contaminants in groundwater aquifers is needed (Cunningham et al. 1999). Groundwater contamination often originates as contamination sources that are frequently located near the soil surface, such as agricultural fields and waste deposits (Jensen and Mantoglou 1992; Mantoglou 1992; Russo et al. 2001). Since the contaminant travels first through the vadose zone, it is very important to obtain accurate predictions of the movement of the water in this domain (Forkel and Celia 1992; Piver and Lindstrom 1991).

To overcome the contamination problem caused by pesticides or other chemicals, detection and prevention approaches are necessary. Continuous monitoring of chemicals in tile and groundwater is difficult, time consuming, and expensive. Finite element modeling may play a role in predicting the movement of water and chemicals through the soil into the groundwater system. The finite element method is a widely accepted and powerful technique for solving systems of differential equations (Aguirre and Haghighi 2002, 2003a, 2003b).

This study presents a general methodology for obtaining the finite element solution of two-dimensional transient unsaturated flow and contaminant transport through porous media. The deterministic formulation is implemented by a finite element code written in Visual C++. The governing differential equation for the unsaturated transient flow is nonlinear and an iterative process is required for the solution of the system of finite element equations.

Transient unsaturated flow and contaminant transport

The movement of water in soils generally results from the combined effect of hydraulic, thermal, and chemical potentials. Darcy (1856) showed that the water flux through a saturated column of packed sand was proportional to the gradient of the elevation and pressure potentials. His experimental results were used by Buckingham (1907) to study steady-state flow in unsaturated soils. Richards (1931) extend Buckingham's formulation to yield a Darcy-scale model for transient water flow in unsaturated soils.

The governing differential equation for two-dimensional transient unsaturated flow through soils is given by Richard's equation (Eq. 1):

$$-\frac{\partial \theta}{\partial t} = C\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial x_i}\left[K(\psi)\frac{\partial(\psi + x_3)}{\partial x_i}\right] \quad i = 1,2,3 \quad (1)$$

where:

ψ = pressure head,
$\theta(\psi)$ = soil moisture content,
C = specific moisture capacity,
$K(\psi)$ = unsaturated hydraulic conductivity, and
x_3 = vertical coordinate, positive downwards.

Advection (movement with the water stream) is the main mechanism for the transport of solutes in soils. The first models that tried to describe the advection transport assumed that the flow was uniform and the average velocity of water was a good approximation for the movement of solutes (Rible and Davis 1955). Unfortunately, this approach could not explain the longitudinal spreading of initially sharp solute fronts. A Fickian diffusion approximation was suggested by Aronofsky and Helen (1957) to model the spreading of solutes.

The transport equation that assumes that the dispersive solute flux is a Fickian process has been called the Convection Dispersion Equation (CDE) or the Advection Dispersive Equation (ADE). The CDE is widely used for modeling solute transport in soils (Nielsen et al. 1986; Van Genuchten 1991). The CDE for an ideal nonreactive conservative solute transport in unsaturated flow (assuming constant density and viscosity) is given by:

$$\frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial x_i}\left[E_{ij}\frac{\partial c}{\partial x_i} - cq_i\right] \qquad i, j = 1,2,3 \qquad (2)$$

where:

c = concentration of transported solute,
E_{ij} = local bulk dispersion coefficient (hydrodynamic dispersion and molecular diffusion are included), and
q_i = local specific discharge.

The local dispersion tensor for a two-dimensional problem may be written in the form (Bear 1972):

$$\left[E_{ij}\right] = \begin{bmatrix} \alpha_L q & 0 \\ 0 & \alpha_T q \end{bmatrix} \qquad (3)$$

where: α_L, α_T = local longitudinal and transversal dispersivities, respectively.

A finite element formulation to solve Eqs. 1 and 2 follows.

FINITE ELEMENT FORMULATION

The dependent variable (in this case ψ) has an infinite number of values in any continuum problem. This happens because the dependent variable is a function of each point in the solution domain and the problem has an infinite number of unknowns. The finite element discretization procedure reduces the number of unknowns to a finite number by dividing the solution domain into elements and by expressing the unknown dependent variable in terms of approximating functions within each element. These approximating functions are defined in terms of the values of the dependent variable at specified locations. These locations are called nodes or nodal points. In the case of unsaturated flow, the capillary tension head is approximated by:

$$\psi(x_1, x_2, x_3, t) \approx \overline{\psi}(x_1, x_2, x_3, t) = \sum_{i=1}^{n} N_i(x_1, x_2, x_3)\psi_i(t) \qquad (4)$$

where:

$\psi(x_1, x_2, x_3, t)$ = exact capillary tension head value at any location within an element,
$\overline{\psi}(x_1, x_2, x_3, t)$ = approximated value at the same location,
$N_i(x_1, x_2, x_3)$ = interpolation function at node *i*, and
n = number of nodes per element.

In the case of contaminant transport, the chemical concentration is approximated by:

$$c(x_1, x_2, x_3, t) \approx \bar{c}(x_1, x_2, x_3, t) = \sum_{i=1}^{n} N_i(x_1, x_2, x_3)c_i(t) \quad (5)$$

where:

$c(x_1, x_2, x_3, t)$ = exact chemical concentration value at any location within an element, and
$\bar{c}(x_1, x_2, x_3, t)$ = approximated value at the same location,
c_i = chemical concentration value at node *i*.

The finite element method can be based on several minimization techniques. The most popular, and chosen to be used in this work, is the weighted residual method. In the weighted residuals approach, an approximate solution is substituted into the governing differential equation, and a residual term is generated. This residual is then minimized over the solution domain.

Describing a general differential equation by

$$L(\phi) = 0 \qquad (6)$$

where:

L = a general differential operator, and
ϕ = the dependent variable.

Substituting the approximation solution $\bar{\phi}$ into the governing equation yields:

$$L(\bar{\phi}) = R(x_1, x_2, x_3, t) \neq 0 \qquad (7)$$

where R = the residual term.

This residual is multiplied by a weighting function, integrated over the solution domain, and forced to be zero.

In this finite element formulation, the weighted residual method chosen is the Galerkin approach in which the weighting function is the same function used for the solution approximation. The advantage of this method, relative to other methods such as the variational approach, is that it has no restriction with respect to the governing equation.

Finite element equations for transient unsaturated flow

The governing differential equation for the transient unsaturated flow is given by Eq. 1. The residual equation for each element is obtained by applying the Galerkin Method to Eq. 1:

$$\left\{R^{(e)}\right\} = -\int_A N^T \left\{\frac{\partial}{\partial x_i}\left[K(\psi)\frac{\partial(\psi + x_1)}{\partial x_i}\right] - C\frac{\partial \psi}{\partial t}\right\} dA \quad (8)$$

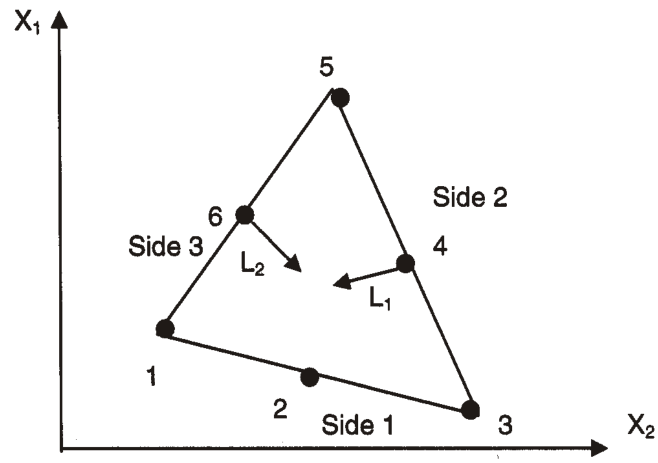

Fig. 1. A typical 6-noded triangular element (with quadratic shape functions) and area coordinates.

where:

N = shape functions of the element, and
A = element area.

Six-noded triangular elements are used in this study (Fig. 1) (Segerlind 1984; Rao 1989; Istok 1990). The quadratic shape functions in area coordinates are given by:

$$N_1 = L_1(2L_1 - 1) \tag{9}$$

$$N_2 = 4L_1L_2 \tag{10}$$

$$N_3 = L_2(2L_2 - 1) \tag{11}$$

$$N_4 = 4L_2(1 - L_1 - L_2) \tag{12}$$

$$N_5 = 1 - 3(L_1 + L_2) + 2(L_1 + L_2)^2 \tag{13}$$

$$N_6 = 4L_1(1 - L_1 - L_2) \tag{14}$$

in which L_1, L_2 = area coordinates of the triangle.

The diffusive terms are evaluated using integration by parts:

$$-\int_A N^T \left\{ \frac{\partial}{\partial x_i} \left[K_{ii} \frac{\partial \psi}{\partial x_i} \right] \right\} dA$$

$$= -\int_A \left\{ K_{ii} \frac{\partial}{\partial x_i} \left(N^T \frac{\partial \psi}{\partial x_i} \right) \right\} dA + \int_A \left\{ K_{ii} \frac{\partial N^T}{\partial x_i} \frac{\partial \psi}{\partial x_i} \right\} dA \tag{15}$$

Applying Green's Theorem to the first integral on the right hand side (RHS) of Eq. 15 results in:

$$-\int_A N^T \left\{ \frac{\partial}{\partial x_i} \left[K_{ii} \frac{\partial \psi}{\partial x_i} \right] \right\} dA$$

$$= -\int_{\Gamma_{bc}} \left\{ \left\{ N^T K_{ii} \frac{\partial \psi}{\partial n} \right\} \right\} d\Gamma_{bc} + \int_A \left\{ K_{ii} \frac{\partial N^T}{\partial x_i} \frac{\partial \psi}{\partial x_i} \right\} dA \tag{16}$$

where:

n = unit outward vector to the boundary, and
Γ_{bc} = element boundary.

Substituting into the residual, Eq. 8, gives:

$$\left\{R^{(e)}\right\} = -\int_{\Gamma_{bc}} \left\{ N^T K_{ii} \frac{\partial \psi}{\partial n} \right\} d\Gamma_{bc} + \int_A \left\{ K_{ii} \frac{\partial N^T}{\partial x_i} \frac{\partial \psi}{\partial x_i} \right\} dA$$

$$-\int_A N^T \frac{\partial K_{11}}{\partial x_1} dA + \int_A N^T C \frac{\partial \psi}{\partial t} dA \tag{17}$$

Over each element, the following variables are approximated by polynomial shape functions relating them to their nodal values:

$$\psi^{(e)} = [N]\{\psi\} \tag{18}$$

$$\frac{\partial \psi^{(e)}}{\partial t} = [N]\{\dot{\psi}\} \tag{19}$$

$$K_{ii}^{(e)} = [N]\{K_{ii}\} \tag{20}$$

$$C^{(e)} = [N]\{C\} \tag{21}$$

Substituting the interpolation expressions (Eqs. 18-21) into Eq. 17 and rearranging into matrix form yields:

$$\left\{R^{(e)}\right\} = \left[p^{(e)}\right]\{\dot{\psi}\} + \left[s^{(e)}\right]\{\psi\} - \left\{f^{(e)}\right\} \tag{22}$$

The capacitance matrix [$p^{(e)}$] is evaluated using the lumped formulation to give:

$$\left[p^{(e)}\right] = \int_A [N]^T ([N]\{C\})[N] dA \tag{23}$$

The stiffness matrix [$s^{(e)}$] is given by:

$$\left[s^{(e)}\right] = \int_A \left\{ [N]\{\hat{K}_{ii}\} \frac{\partial [N^T]}{\partial x_i} \frac{\partial [N]}{\partial x_i} \right\} dA \tag{24}$$

The force vector {$f^{(e)}$} is:

$$\left\{f^{(e)}\right\} = \int_A [N]^T \frac{\partial [N]}{\partial x_1} \{K_{11}\} dA \tag{25}$$

Combining the element matrices and summing over all the elements using the direct stiffness procedure, yields:

$$[P]\{\dot{\psi}\} + [S]\{\psi\} - \{F\} = 0 \tag{26}$$

where:

[P]=global capacitance matrix,
[S]=global stiffness matrix,
{F}=global force vector,
{ψ}=mean capillary tension head value, and
{$\dot{\psi}$}=$d\{\psi\}/dt$.

The global system of equations is evaluated using a finite difference approximation in the time domain (Segerlind 1984):

$$([P] + \beta \Delta t [S])\{\psi\}_{t+\Delta t}$$

$$= ([P]) - (1-\beta)\Delta t [S]\{\psi\}_t + \Delta t\left((1-\beta)\{F\}_t + \beta\{F\}_{t+\Delta t}\right) \tag{27}$$

The Crank-Nicholson method (β = 1/2) was chosen in order to avoid numerical oscillations.

Prescribed values along the boundaries are directly introduced in the final system of equations (Eq. 27) as:

$$\psi(x_i,t)_\Gamma = \psi_\Gamma \tag{28}$$

The other type of boundary condition is a prescribed flux along the boundaries:

$$q(x_i)_\Gamma = q_n \tag{29}$$

The contribution of prescribed flux over the boundary to the final system of equations is given by the expression:

$$-\int_{\Gamma_{bc}} \left\{ N^T K_{ii} \frac{\partial \psi}{\partial n} \sin\Theta \right\} d\Gamma_{bc}$$

$$= q_n \int_{\Gamma_{bc}} [N]^T d\Gamma_{bc} + \int_{\Gamma_{bc}} [N]^T [N]\{K_{11}\} d\Gamma_{bc} \tag{30}$$

where Θ = angle to the outward normal.

It should be noted that the last integral of Eq. 30 is only evaluated when the component of the prescribed flux in the direction is not zero.

The integrals in Eq. 30 are evaluated for each element where the flux is prescribed. To decrease computational time, these integrals are evaluated analytically. The shape functions of the quadratic triangular element (Eqs. 9-14) are substituted into Eq. 30. The area coordinates, L_1 and L_2, reduce to one-dimensional shape functions over each side, and the integral over the edge of a triangular element can be replaced by a line integral written in terms of local coordinates. The results of the integrals on the RHS of Eq. 30 are included in the force vector of the elements since they are independent of the unknown variables.

The set of finite element equations for transient unsaturated flow given by Eq. 26 is solved by an iterative procedure in which a simple convergence sequence and an underrelaxation method of variable updating are used (Taylor and Hughes 1981). A summary of the procedure is as follows:

(a) Assume initial values of the unknowns ψ_t.

(b) Solve for the updated values $\psi_{t+\Delta t}$.

(c) Evaluate $(\psi_{t+\Delta} - \psi_t)/\psi_{t+\Delta}$ at all nodes. If these values are smaller than a pre-specified tolerance, then the calculation is complete. The tolerance value for pressure head is assumed to be 0.1 .

(d) If the differences in (c) are not all smaller than the specified tolerance, then the nodal values are updated as:

$$\psi_{t+\Delta t,n+1} = \psi_{t+\Delta t,n} + \Lambda(\psi_{t+\Delta t,n} - \psi_{t,n})$$

where: Λ = underrelaxation coefficient,
n = subscript for current iteration, and
$n+1$ = subscript for new iteration.

For each time step, the process (a) through (d) is repeated until the tolerance criteria are met at all nodal points within the domain and on all boundary points subject to a flux boundary condition.

FINITE ELEMENT EQUATIONS FOR TRANSIENT CONTAMINANT TRANSPORT

The transient contaminant transport governing differential equation is given by Eq. 2. The residual equation for each element is obtained by applying the Galerkin Method to Eq. 2:

$$\{R^{(e)}\} = -\int_A N^T \left\{ -\left(c\frac{\partial q_i}{\partial x_i} \right) - \left(q_i \frac{\partial c}{\partial x_i} \right) \right.$$

$$\left. + \frac{\partial}{\partial x_i}\left(E_{ij}\frac{\partial c}{\partial x_j} \right) - \theta\frac{\partial c}{\partial t} - c\frac{\partial \theta}{\partial t} \right\} dA \tag{31}$$

The diffusive terms are evaluated using integration by parts:

$$-\int_A N^T \left\{ \frac{\partial}{\partial x_i}\left[E_{ij}\frac{\partial c}{\partial x_j} \right] \right\} dA$$

$$= -\int_A \left\{ \frac{\partial}{\partial x_1}\left[N^T E_{ij}\frac{\partial c}{\partial x_1} \right] - E_{ij}\frac{\partial N^T}{\partial x_i}\left[\frac{\partial c}{\partial x_i} \right] \right\} dA \tag{32}$$

Applying Green's Theorem to the first term of the integral on the right hand side (RHS) of Eq. 32gives:

$$-\int_A \left\{ \frac{\partial}{\partial x_1}\left[N^T E_{ij}\frac{\partial c}{\partial x_1} \right] \right\} dA = -\int_{\Gamma_{bc}} N^T E_{ij}\frac{\partial c}{\partial x_n} d\Gamma_{bc} \tag{33}$$

Substituting into the residual, Eq. 31, results in:

$$\{R^{(e)}\} = -\int_A N^T \left\{ -\left(c\frac{\partial q_i}{\partial x_i} \right) - \left(q_i \frac{\partial c}{\partial x_i} \right) \right.$$

$$\left. + E_{ij}\frac{\partial N^T}{\partial x_i}\left(\frac{\partial c}{\partial x_j} \right) - \theta\frac{\partial c}{\partial t} - c\frac{\partial c}{\partial t} \right\} dA - \int_{\Gamma_{bc}} N^T E_{ij}\frac{\partial c}{\partial x_n} d\Gamma_{bc} \tag{34}$$

Over each element, the following variables are approximated by polynomial shape functions relating them to their nodal values:

$$c^{(e)} = [N]\{c\} \tag{35}$$

$$q_i^{[e]} = [N]\{q_i\} \tag{36}$$

$$q^{(e)} = [N]\{q\} \tag{37}$$

$$\theta^{(e)} = [N]\{\theta\} \tag{38}$$

$$\alpha_L^{(e)} = [N]\{\alpha_L\} \tag{39}$$

$$\alpha_T^{(e)} = [N]\{\alpha_T\} \tag{40}$$

Substituting the interpolation expressions (Eqs. 35-40) into Eq. 34 and rearranging in matrix form yields:

$$\{R^{(e)}\} = [p^{(e)}]\{\dot{c}\} + [s^{(e)}]\{c\} - \{f^{(e)}\} \tag{41}$$

The capacitance matrix $[p^{(e)}]$ is evaluated using the lumped formulation and is given by:

$$\left[p^{(e)}\right] = -\int_A [N]^T [N]\{\theta\}[N]dA \tag{42}$$

The stiffness matrix $[s^{(e)}]$ is:

$$\left[s^{(e)}\right] = \int_A \left\{ \left(N^T[N]\frac{\partial[N]}{\partial x_i}\{q_i\} \right) + \left(N^T[N]\{q_i\}\frac{\partial[N]}{\partial x_i} \right) + \Theta N^T[N] - E_{ij}\frac{\partial N^T}{\partial x_i}\frac{\partial[N]}{\partial x_i} \right\} dA \tag{43}$$

where $\Theta^{(e)}$ is given by :

$$\Theta^{(e)} = \frac{\bar{\theta}^{(e)}_{t+\Delta t} - \bar{\theta}^{(e)}_{t}}{\bar{\theta}^{(e)}_{t+\Delta t}} \tag{44}$$

The subscript $t + \Delta t$ is related to the results obtained in the current time interval and the subscript t is related to the results obtained in the last time interval. The mean values for moisture content ($\bar{\theta}$) are obtained as the arithmetic mean among the nodes over each element.

The force vector $\{f^{(e)}\}$ is equal to zero for the large-scale transient transport equation, thus:

$$\left\{f^{(e)}\right\} = 0 \tag{45}$$

Combining the element matrices and summing over all the elements, using the direct stiffness procedure, yields:

$$[P]\{\dot{c}\} + [S]\{c\} = \{0\} \tag{46}$$

The global system of equations is evaluated using a finite difference approximation in the time domain (Segerlind 1984):

$$\left([P] + \beta\Delta t[S]\right)\{c\}_{t+\Delta t} = \left([P] - (1-\beta)\Delta t[S]\right)\{c\}_t \tag{47}$$

Prescribed values along the boundaries are directly introduced in the final system of equations (Eq. 47):

$$c(x_1, x_2)_\Gamma = c_\Gamma \tag{48}$$

The integrals in the capacitance matrices (Eqs. 23, 42), stiffness matrices (Eqs. 24, 43), and force vectors (Eq. 25, 45) are evaluated numerically using Gauss-Legendre quadrature in order to obtain higher accuracy. Before being solved, the integrals are rewritten in terms of area coordinates. For example, the integral in the expression for the capacitance matrix for contaminant transport (Eq. 42) is rewritten in area coordinates as:

$$\left[p^{(e)}\right] = \int_A [N]^T([N]\{C\})[N]dA$$
$$= \int_0^1 \int_0^{1-L_2} N^T([N]\{C\})[N]\det[J]dL_1 dL_2 \tag{49}$$

where the jacobian matrix is defined as:

$$[J] = \begin{bmatrix} \dfrac{\partial x_2}{\partial L_1} & \dfrac{\partial x_1}{\partial L_1} \\ \dfrac{\partial x_2}{\partial L_2} & \dfrac{\partial x_1}{\partial L_2} \end{bmatrix} \tag{50}$$

Nine sampling points and weighting functions are used to evaluate numerically the integrals in Eqs. 23 - 25 and 42 -45. The values for the shape functions and their derivatives are computed at each sampling point.

SOLUTION METHODOLOGY

The solution methodology used to solve transient unsaturated flow and contaminant transport problems are summarized as follows:

(a) At $t = 0$, the tension head, initial chemical distribution, and soil properties are given and boundary conditions are specified.

(b) The finite element equations for the transient unsaturated flow (Eq. 27) are solved numerically by Gauss elimination.

(c) Tension head values are obtained at each node.

(d) The volumetric moisture content profile is evaluated using the tension head values.

(e) Steps (b) through (e) are repeated until the desired convergence criteria are met.

(f) The velocity field is computed using the tension head values.

(g) The finite element equations for the transient contaminant transport (Eq. 47) are solved numerically by Gauss elimination.

(h) Chemical concentration values are obtained at each node.

(i) Time is increased.

(j) The above steps are repeated until $t = t_f$.

A finite element code (written in Visual C++ programming language) was developed for the solution of Eqs. 27 and 47. The program has the option to solve just for flow, just for contaminant transport, or for both. A flow chart summarizing the code modules is displayed in Fig. 2.

The first step consists of providing data on material properties, numerical parameters, and geometry. The nonlinear flow equation is solved iteratively. The stiffness (Eq. 24) and capacitance (Eq. 23) matrices and force vector (Eq. 25) are computed for each element and are assembled using the direct stiffness procedure to create the global capacitance and stiffness matrices and force vector. The boundary conditions are applied. The global system of equations is evaluated using a finite difference approximation in the time domain. Results for ψ are computed at each node. The convergence of pressure head is checked for each node. The convergence criterion of pressure head values is based on the percent difference between two successive iterations at each point of the discretization domain. Convergence is attained when the percent difference is smaller than 0.1 for all nodes. The velocity field is evaluated using the calculated head pressure values. The stiffness (Eq. 42) and capacitance (Eq. 43) matrices and force vector (Eq. 45) are computed for each element and are assembled using the direct stiffness procedure to create the global capacitance and stiffness matrices and force vector. The boundary conditions are applied. The global system of equations is evaluated using a finite difference approximation in the time domain. Results for c are computed at each node. Time is increased and if it is smaller

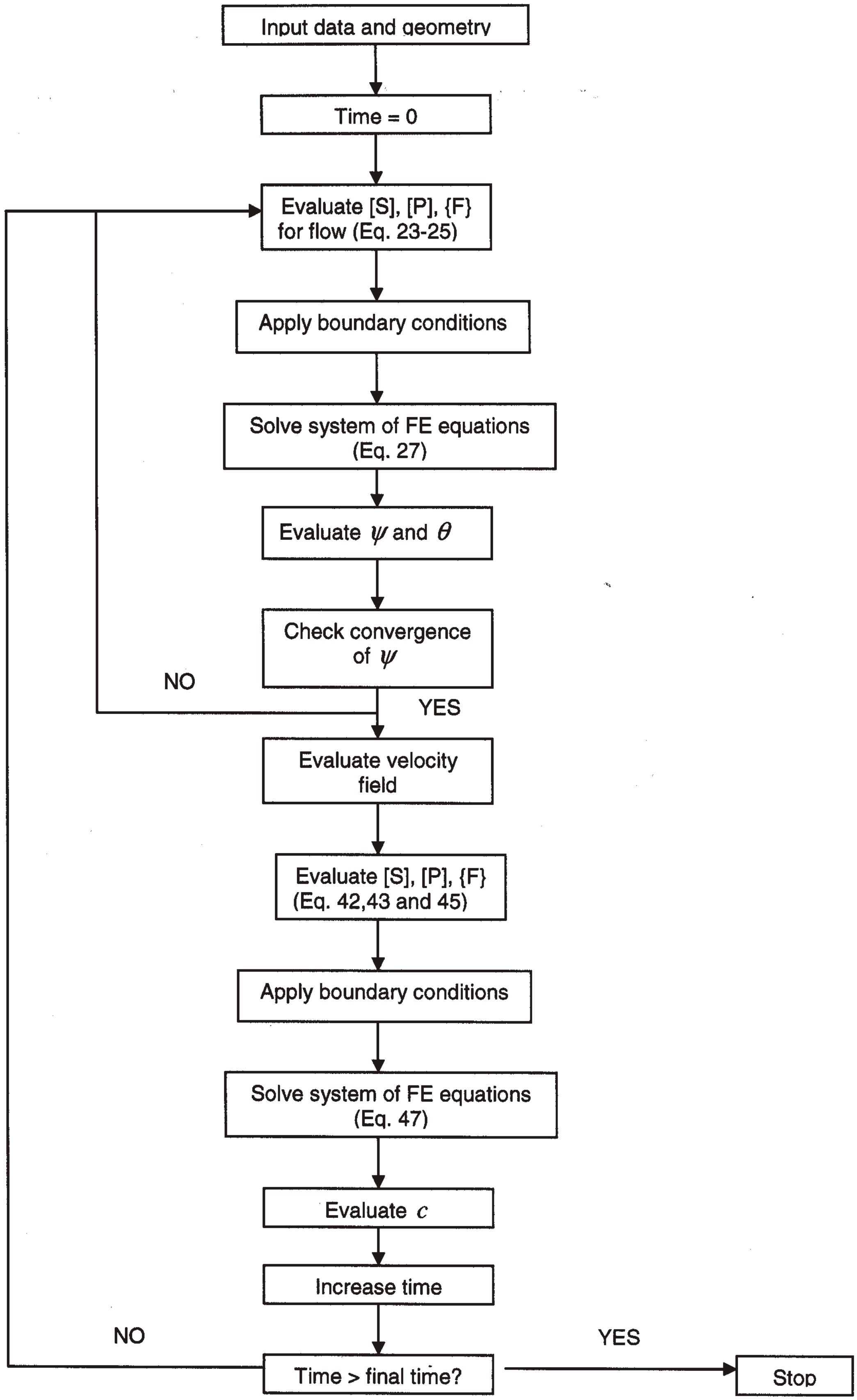

Fig. 2. Schematic presentation of the finite element solution process and code.

than the final time of simulation, the finite element flow and transport equations are solved again.

The input data required to run the finite element code consists of:

(a) finite element mesh information: node coordinates, connectivity matrix, specification of boundary conditions, and initial conditions.

(b) control parameters: underrelaxation factor, total time of simulation, time step, tolerance limit, and maximum number of iterations.

(c) material properties: expressions for K_{ii} and θ, α_L and α_T.

The time step was selected such that it consisted of the largest time step that would not produce numerical oscillation of the finite element results.

CONCLUSION

A deterministic finite element solution to predict water flow and contaminant movement through porous media was developed and implemented. The computer model was written in Visual C++ and can be used to better simulate the movement of contaminants in the vadose zone. Since the contaminant travels first through the vadose zone, it is crucial to obtain more realistic predictions of the movement of the water in this region. To reduce computational time, mathematical expressions for the contributions of the flux boundary conditions to the force vector were developed analytically. The governing differential equation for the unsaturated transient flow is nonlinear and an iterative process was required for the solution of the system of finite element equations. The solution methodology as well as the input data required to run the model were presented.

REFERENCES

Aguirre, C.G. and K. Haghighi. 2002. Finite element analysis of transient contaminant transport: A stochastic approach. *Transactions of the ASAE* 45(6): 2049–2059.

Aguirre, C.G. and K. Haghighi. 2003a. Stochastic finite element analysis of transient unsaturated flow in porous media. *Transactions of the ASAE* 46(1): 163–173.

Aguirre, C.G. and K. Haghighi. 2003b. Stochastic modeling of transient contaminant transport. *Journal of Hydrology* 276(1-4):224-239.

Aronofsky, J.S. and J.P. Heller. 1957. A diffusion model to explain mixing of flowing miscible fluids in porous media. *AIME Petroleum Transactions* 210:345-349.

Bear, J. 1992. *Dynamics of Fluids in Porous Media*. New York, NY: American Elsevier Publishing Co.

Buckingham, E. 1907. Studies on the movement of soil moisture. Bulletin No. 38. Washington, DC: USDA Bureau of Soils.

Cunningham J.A., M.N. Goltz and P.V. Roberts. 1999. *Journal of Hydrologic Engineering* 4(4):377-380.

Darcy, H. 1856. Les Fontaines Publiques de la Ville de Dijon. Cited in Hubert, M.K.,1969, *The Theory of Groundwater Motion and Related Papers*. New York, NY: Hafner Publishing Co.

Ehteshami M., R.C. Peratala, H. Eisele, H. Deer and T. Tindall. 1991. Assessing pesticide contamination to groundwater: A rapid approach. *Ground Water* 29(6):862-868.

Forkel, C. and M.A. Celia. 1992. Numerical simulation of unsaturated flow and contaminant transport with density and viscosity dependence. Computational methods in water resources IX. Mathematical Modeling in Water Resources, Computational Mechanics Publications, MA 2: 351–359.

Istok, J. 1990. *Groundwater Modeling by the Finite Element Method*. Water Resources Monograph No. 13. Washington, DC: American Geophysical Union.

Jensen, K.H., and A. Mantoglou. 1992. Application of stochastic unsaturated flow theory, numerical simulations and comparisons to field observations. *Water Resources Research* 28:(1), 269-284.

Lovejoy, S.B., J.G. Lee, T.O. Randhir and B.A. Engel. 1997. Research needs for water quality management in the 21st century: A spatial decision support system. *Journal of Soil and Water Conservation* 52:18-22.

Mantoglou, A. 1992. A theoretical approach for modeling unsaturated flow in spatially variable soils: Effective flow models in finite domains and nonstationarity. *Water Resources Research* 28: 251-267.

Nielsen, D.R., M. Th. Van Genuchten and J.W. Biggar. 1986. Water flow and solute transport processes in the unsaturated zone. *Water Resources Research* 22(9):89S-108S.

Piver, W.T. and F.T. Lindstrom. 1991. Numerical methods for describing chemical transport in the unsaturated zone of the subsurface. *Journal of Contaminant Hydrology* 8:243-262.

Rao, S.S. 1989. *The Finite Element Method in Engineering*. Boston, MA: Butterworth-Heinemann.

Rible, J.M. and L.E. Davis. 1955. Ion exchange in soil columns. *Soil Sci*ence 79:41-47.

Richards, L.A. 1931. Capillary conduction of liquids through porous mediums. *Physics* 1:318-333.

Russo D., J. Zaidel and A. Laufer. 2001. Numerical analysis of flow and transport in a combined heterogeneous vadose zone-groundwater system. *Advances in Water Resources* 24:49-62.

Segerlind, L.J. 1984. *Applied Finite Element Analysis*, 2nd edition. New York, NY: John Wiley and Sons.

Taylor, C. and T.G. Hughes.1981. *Finite Element Programming of the Navier-Stokes Equations*. Swansea, UK: Pineridge Press Ltd.

Van Genuchten, M.Th. 1991. Recent progress in modeling water flowand chemical transport in the unsaturated zone. In *Hydrological Interactions Between Atmosphere, Soil and Vegetation - Proceedings of the Vienna Symposium,* 169-183. Publication No. 204, IAHS.