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NUMERICAL MODEL FOR SATURATED-UNSATURATED FLOW IN DEFORMABLE POROUS MEDIA, PART II: THE ALGORITHM

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Numerical Model For Saturated-Unsaturated Flow In Deformable Porous Media, Part II: The Algorithm

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NUMERICAL MODEL FOR SATURATED-UNSATURATED FLOW IN DEFORMABLE POROUS MEDIA, PART II: THE ALGORITHM

by

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ABSTRACT

An integrated finite difference algorithm is presented for numerically solving the governing equation of saturated-unsaturated flow in deformable porous media. Recognizing that stability of the explicit equation is a local phenomenon, a mixed explicit-implicit procedure is used for marching in the time domain. In this scheme, the explicit changes in potential are first computed for all elements in the system, following which, implicit corrections are made only for those elements for which the stable time step is less than the time step being used. Time step sizes are automatically controlled in order to optimize the number of iterations, control maximum change in potential during a time step and to obtain desired outputs. Time derivatives, estimated

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on the basis of system behavior during two previous time steps, are used to start the iteration process and to evaluate non-linear coefficients. Boundary conditions and sources can vary with time or with the dependent variable. Input data are organized into convenient blocks. Accuracy of solutions can be affected by modeling errors, different types of truncation errors and convergence errors. The algorithm constitutes an efficient tool for analyzing linear and non-linear fluid flow problems in multi-dimensional, heterogeneous porous media with complex geometry. An important limitation is that the model cannot conveniently handle arbitrary anisotropy and other general tensorial quantities.

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INTRODUCTION

The mathematical consideration of transient groundwater motion in saturated-unsaturated porous media leads to the solution of initial-boundary value problems. The earliest approach for numerically solving these problems was that of the finite differences, in which the partial differential equation of groundwater motion is directly approximated at each point of interest in the flow region. In recent times it has become evident that by posing the initial-boundary value problem in an integral form rather than in the form of a differential equation, a great deal of power can be gained in numerical analysis, especially in regard to handling complex geometries of the flow region. The remarkable growth and popularity of the finite element method over the past decade attests to the advantages of an integral formulation of the problem. In the present work we will make use of an integral formulation which has been termed an Integrated Finite Difference Method (IFDM). The basic philosophy of this method and its relation to the finite element method (FEM) has been discussed elsewhere (Narasimhan and Witherspoon, 1976a). Combining the IFDM with a mixed explicit-implicit iterative scheme for advancing in time domain, Edwards (1968, 1972) developed a powerful computer code called TRUMP for determining transient and steady state temperature distributions in multidimensional, heterogeneous systems with arbitrary geometry. Since conductive heat transfer is analogous to the flow of fluids in porous media, the basic calculational model of the TRUMP algorithm has been incorporated in the present work into a computer program called TRUST for studying transient groundwater movement in variably saturated deformable porous media.

THE GOVERNING EQUATION

It was shown in Part I of this series of papers (Narasimhan and Witherspoon, 1976b) that the transient movement of groundwater in variably saturated deformable porous media can be described by an integral equation of the form

$$G + \int_{\Gamma} \rho_w \frac{k\rho_w g}{\mu} \vec{\nabla}(z + \psi) \cdot \vec{n} \, d\Gamma = M_c \frac{D\psi}{Dt} \tag{1}$$

in which

$$M_c = V_s \rho_w \left[S e \rho_{wo} \beta g + S \gamma_w \chi' a_v + e \frac{dS}{d\psi} \right] \tag{1a}$$

The quantity ψ occurring in the time derivative on the right hand side of (1) represents an average pressure head over the volume element bounded by the surface Γ and D/Dt denotes a material derivative. Equation (1) is in general non-linear since G, ρ_w, k and M_c can be dependent on ψ or t.

Consider an appropriately small subregion of the flow region (Figure 1) over which the variation of ψ is not rapid and let the average properties of this volume element be associated with a representative nodal point ℓ. Furthermore, let the volume element be so chosen that the lines joining the nodal point ℓ to its neighbors be normal to the interfaces between the respective elements. We will assume that the average properties such as ψ associated with each nodal point are functions only of time while the spatial variation of these average properties between adjacent nodal points can be represented by a simple linear relation which is independent of time. Then applying (1) to the element in Figure 1, we can write

$$G_\ell + \sum_m \rho_w \frac{k\rho_w g}{\mu} \left[\frac{(z_m + \psi_m) - (z_\ell + \psi_\ell)}{d_{\ell,m} + d_{m,\ell}} \Gamma_{\ell,m} \right] = M_{c,\ell} \frac{\Delta\psi_\ell}{\Delta t} \tag{2}$$

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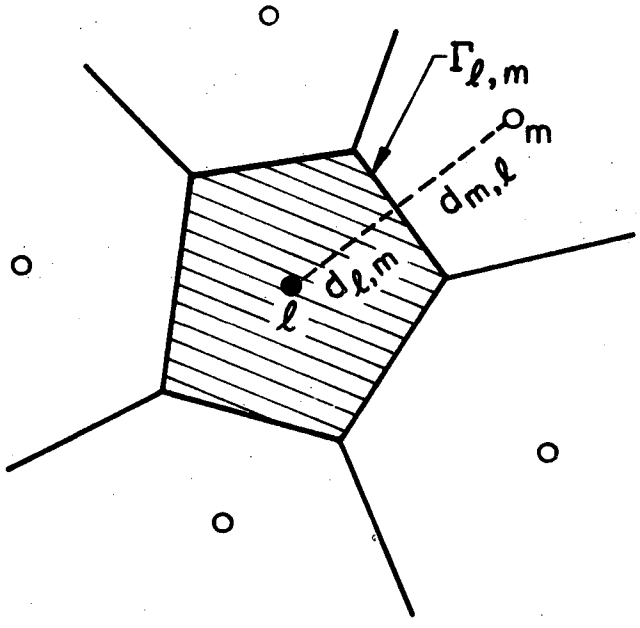

Fig. 1. Volume element associated with nodal point ℓ.

Note that the quantity within the summation sign in (2) represents the flux rate across the interface between elements ℓ and m. The quantities k and ρ_w in (2) are therefore to be evaluated at the interface $\Gamma_{\ell,m}$ between the elements. When there is material heterogeneity and elements ℓ and m are composed of different materials, we will use a harmonic mean permeability (Edwards, 1968; Narasimhan, 1975) in order to preserve continuity of flux at the interface. Thus

$$\bar{k}_{\ell,m} = \frac{k_\ell k_m (d_{\ell,m} + d_{m,\ell})}{k_\ell d_{m,\ell} + k_m d_{\ell,m}} \tag{3a}$$

and

$$\bar{\rho}_{w,\ell,m} = \frac{\rho_{w,\ell}\rho_{w,m}(d_{\ell,m} + d_{m,\ell})}{\rho_{w,\ell}\, d_{m,\ell} + \rho_{w,m}\, d_{\ell,m}} \tag{3b}$$

For convenience we shall define the conductance of the interface between elements ℓ and m by

$$U_{\ell,m} = \bar{\rho}_{w,\ell,m} \frac{\bar{k}_{\ell,m}\bar{\rho}_{w,1,m}g}{\mu} \frac{\Gamma_{\ell,m}}{(d_{\ell,m} + d_{m,\ell})} \tag{4}$$

Physically, $U_{\ell,m}$ denotes the rate of flux across the interface ℓ,m due to a unit difference between $(z_m + \psi_m)$ and $(z_\ell + \psi_\ell)$.

In the light of (4), (2) becomes

$$G_\ell + \sum_m U_{\ell,m} [(z_m + \psi_m) - (z_\ell + \psi_\ell)] = M_{c,\ell} \frac{\Delta\psi_\ell}{\Delta t} \tag{5}$$

Assuming z_m and z_ℓ to be constants during Δt, if we let $\psi_m = \psi_m^\circ$ and $\psi_\ell = \psi_\ell^\circ$ in (5) where the superscript $^\circ$ denotes the known initial values at the beginning of the interval Δt, we obtain

$$G_\ell + \sum_m U_{\ell,m} [(z_m + \psi_m^\circ) - (z_\ell + \psi_\ell^\circ)] = M_{c,\ell} \frac{\Delta\psi_\ell}{\Delta t} \tag{6}$$

In (6) all the quantities are known except $\Delta\psi_\ell$. Equation 6 is hence explicit and $\Delta\psi_\ell$ can be computed by the simple relation

$$\Delta\psi_{\ell,exp} = \frac{\Delta t}{M_{c,\ell}} \left\{ G_\ell + \sum_m U_{\ell,m}[(z_m + \psi_m^\circ) - (z_\ell + \psi_\ell^\circ)] \right\} \tag{7}$$

For an element ℓ whose boundary surface may partly coincide with portions of the boundary of the overall flow region, (7) could be generalized as

$$\Delta\psi_{\ell,exp} = \frac{\Delta t}{M_{c,\ell}} \left\{ G_\ell + \sum_b U_{\ell,b}[(z_b + \bar{\psi}_b) - (z_\ell + \psi_\ell^\circ)] + \sum_m U_{\ell,m}\,[(z_m + \psi_m^\circ) - (z_\ell + \psi_\ell^\circ)] \right\} \tag{8}$$

If we seek to solve the problem explicitly, we need to set up one such simple equation as in (8) for each point ℓ and compute $\Delta\psi_\ell$ directly.

Despite its simplicity, the explicit equation is limited to small time steps, since the solution of (8) can become unstable with time if Δt exceeds a critical value. The phenomenon of stability, however, is local in nature (Richtmeyer and Morton, 1967). Based on physical considerations (Dusinberre, 1961; Narasimhan, 1975) or based on an analysis of error propagation (O'Brien et al, 1951; Evans et al., 1954), it can be shown that the time step which is critical to stability of the solution in the vicinity of element ℓ is given by

$$\Delta t_\ell = \frac{M_{c,\ell}}{\sum_m U_{\ell,m}} \tag{9}$$

In order to be able to progress rapidly in the time domain using conveniently large time steps, we seek to write (5) in an implicit form by the substitution

$$\psi_m = \psi_m^\circ + \lambda\Delta\psi_m \tag{10a}$$

$$\psi_\ell = \psi_\ell^\circ + \lambda\Delta\psi_\ell \ , \quad 0 \leq \lambda \leq 1 \tag{10b}$$

and obtain

$$\Delta\psi_\ell = \frac{\Delta t}{M_{c,\ell}} \left\{ G_\ell + \sum_b U_{\ell,b} \left[(z_b + \bar{\psi}_b) - (z_\ell + \psi_\ell^\circ + \lambda\Delta\psi_\ell) \right] + \sum_m U_{\ell,m} \left[(z_m + \psi_m^\circ + \lambda\Delta\psi_m) - (z_\ell + \psi_\ell^\circ + \lambda\Delta\psi_\ell) \right] \right\} \tag{11}$$

Note that for $\lambda = 0$, (11) reduces to (8). The three cases, $\lambda = 0$, $\lambda = 0.5$ and $\lambda = 1.0$ are respectively known as forward differencing, central differencing and backward differencing procedures.

Collecting similar terms, $\Delta\psi_\ell$ can be split up into an explicit and an implicit component. Thus from (11) and (8)

$$\Delta\psi_\ell = \Delta\psi_{\ell,exp} + \frac{\lambda\Delta t}{M_{c,\ell}} \left\{ -\sum_b U_{\ell,b} \Delta\psi_\ell + \sum_m U_{\ell,m} (\Delta\psi_m - \Delta\psi_\ell) \right\} \tag{12}$$

The local nature of stability and the form of (12) suggest that in order to carry out the solution process over the whole flow domain, one could first compute $\Delta\psi_{\ell,exp}$ for all the nodal points in the flow region and compute the implicit correction only for those elements whose stability limit is exceeded by Δt. As far as is known Edwards (1968) is the first to have taken advantage of the local nature of the stability phenomenon and combined explicit and implicit procedures in the calculations of a single time step. We will call this the mixed explicit-implicit approach.

MIXED EXPLICIT-IMPLICIT ITERATIVE SCHEME

The iterative scheme used in the present work is an adaptation and a generalization of one discussed by Evans et al. (1954). The scheme is unconditionally stable provided the coefficients in the equation are not very

strongly dependent on ψ. Convergence is generally rapid but the number of iterations necessarily depends on the relative number and time constants of interconnected implicit elements in the system and the relative values of conductances between such elements.

The equation for the iterative scheme is obtained from (12) by making the following substitutions (Edwards, 1968):

$$\Delta\psi_\ell, \text{ left hand side} = \Delta\psi_\ell^{p+1} \tag{13a}$$

$$\Delta\psi_\ell, \text{ right hand side} = (1 + s)\,\Delta\psi_\ell^{p+1} - s\Delta\psi_\ell^{p} \tag{13b}$$

$$\Delta\psi_m, \text{ right hand side} = \Delta\psi_m^{p} \tag{13c}$$

The acceleration factor s should be greater than zero for convergence. A value of s = 0.2 was empirically chosen by Edwards (1968) by minimizing the total required machine time for a large group of test problems. However, s is always set to zero on the first time step and for any time step in which no implicit elements are interconnected.

Making the above substitutions and solving for $\Delta\psi_\ell^{p+1}$ we obtain

$$\Delta\psi_\ell^{p+1} = \Delta\psi_{\ell,\exp} + \frac{\lambda\Delta t}{M_{c,\ell}} \sum_m^{\exp} U_{\ell,m}\,\Delta\psi_{m,\exp} + \sum_m U_{\ell,m}\,\Delta\psi_m^{p} + \frac{sZ_\ell\Delta\psi_\ell^{p}}{\left[1 + \frac{\lambda\Delta t}{M_{c,\ell}}\,(1 + s)\,Z_\ell\right]} \tag{14}$$

in which

$$Z_\ell = \sum_b U_{\ell,b} + \sum_m U_{\ell,m} \tag{15}$$

For the first iteration (p = 0), the following values are used:

$$\Delta\psi_\ell^{\circ} = \Delta t\,\dot{\psi}_\ell \tag{16a}$$

$$\Delta\psi_m^{\circ} = \Delta t\ \dot{\psi}_m \tag{16b}$$

where $\dot{\psi}_\ell$ and $\dot{\psi}_m$ are judiciously estimated values of time derivative. The difference between successive values of $\Delta\psi_\ell$ in the iteration is given by

$$E_\ell^{p+1} = \Delta\psi_\ell^{p+1} - \Delta\psi_\ell^{p} \tag{17}$$

In the light of (14), (17) can be immediately written as

$$E_\ell^{p+1} = \frac{\frac{\lambda\Delta t}{M_{c,\ell}}\left[\sum_m U_{\ell,m}(\Delta\psi_m^{p} - \Delta\psi_m^{p-1}) + sZ_\ell\ (\Delta\psi_\ell^{p} - \Delta\psi_\ell^{p-1})\right]}{\left[1 + \frac{\lambda\Delta t}{M_{c,\ell}}\ (1 + s)\ Z_\ell\right]} \tag{18}$$

or

$$E_\ell^{p+1} = \frac{\frac{\lambda\Delta t}{M_{c,\ell}}\left[\sum_m U_{\ell,m}\ E_m^{p} + sZ_\ell\ E_\ell^{p}\right]}{\left[1 + \frac{\lambda\Delta t}{M_{c,\ell}}\ (1 + s)\ Z_\ell\right]} \tag{19}$$

In equation (19) note that E_ℓ at iteration p+1 is expressed in terms of the known values of E_ℓ, E_m at p+1 iteration. This procedure eliminates unnecessary recalculation of the fixed quantities in (14).

To implement the iterative scheme, the values of $\Delta\psi_\ell^1$ are first computed using (14), (16a) and (16b) and the values of E_ℓ^1 are calculated by

$$E_\ell^1 = \Delta\psi_\ell^1 - \Delta t\ \dot{\psi}_\ell \tag{20}$$

Then, E_ℓ^2 is calculated using (19) and $\Delta\psi_\ell^2$ is obtained by the relation

$$\Delta\psi_\ell^2 = \Delta\psi_\ell^1 + E_\ell^2 \tag{21}$$

This scheme is continued until convergence criteria are satisfied. If the convergence criteria are not satisfied within a limit of 80 iterations, then the results of the time step are discarded and a new Δt, half as large, is

used and the calculations carried out. If the new time step has already reached a minimum prescribed value, then the problem is ended and convergence failure is assumed.

The convergence criterion is intimately related to the quantity ψ_{vary}, which is one half of the maximum change in ψ allowed at any nodal point in the system during a given time step. The net correction to the fluid mass content and the fluid mass capacity of all the implicit elements in the system for the p^{th} iteration are given by

$$\Delta H^p_{net} = \sum_{\ell}^{implicit} M_{c,\ell} E^p_{\ell} \tag{22a}$$

$$M_{c,net} = \sum_{\ell}^{implicit} M_{c,\ell} \tag{22b}$$

The iteration procedure is stopped when the following criteria are satisfied for all elements excluding those for which $M_{c,\ell}$ is zero (the zero volume elements).

$$\Delta H^p_{net} < 10^{-5} (M_{c,net}) (\psi_{var}) \tag{23a}$$

$$E^p_{\ell,max} < 10^{-4}(\psi_{var}) \tag{23b}$$

After the final changes in ψ have been found for all the implicit elements, final corrections must be made to $\Delta\psi$ in all the explicit elements connected to implicit elements in order to obtain the correct mass balance. The complete equation for explicit elements connected to implicit elements is as follows

$$\Delta\psi_{\ell,exp.,\ corrected} = \Delta\psi_{\ell,exp} + \frac{\lambda\ \Delta t}{M_{c,\ell}} \left[\sum_{m}^{m=implicit} U_{\ell,m}(\Delta\psi_m - \Delta\psi_{\ell,exp}) \right] \tag{24}$$

Corrections must also be made to the fluxes calculated for all those internal connections involving implicit elements.

PREPARATIONS FOR NEXT TIMESTEP

The following preparations are essential before carrying out the calculations for each time step.

Reclassification of Elements

The computer program provides options for solving a given problem using explicit forward differencing, implicit central or backward differencing or mixed explicit-implicit procedures. When the mixed explicit-implicit procedure is followed, reclassification of explicit elements to implicit elements can take place if the time step is less than a prescribed maximum and if any explicit elements remain. Under those conditions, whenever the time step reaches the limit of 2/3 of the smallest time constant for any explicit element in the system, the corresponding explicit element and all other explicit elements with time constants no more than 20 percent larger are reclassified as implicit elements. No further reclassification is thus needed until the time step increases by at least 20 percent. Thus, the conditions for reclassifying explicit elements are as follows:

i) mixed explicit-implicit procedure is used;

ii) current time step $\Delta t = \Delta t_{max}$, where $\Delta t_{max} = \min [2/3\ \Delta t_{stab}, \Delta t_{large}]$, in which Δt_{stab} is the smallest time constant for any explicit element in the system and Δt_{large} is the upper limit chosen for Δt;

iii) ℓ is explicit and $\Delta t_{\ell} \leq 1.8\ \Delta t_{max}$.

Control of Time Step

The algorithm is designed to automatically control the size of the time step in a gradual manner so that the total number of iterations needed for convergence as well as the maximum change in ψ during a time step are optimized. The upper and the lower limits for Δt are controlled by the input parameters Δt_{large} and Δt_{small} which may be prescribed through input or automatically controlled within the program. Within these limits, Δt is controlled by the ratio

$$R = \frac{\psi_{vary}}{(\Delta\psi_{max}, \nu)_{max}} \tag{25}$$

The parameter ν denotes product of ψ_{vary} and 1/40 of the number of iterations needed for convergence or the maximum percentage change that took place in any tabulated property, whichever is larger. If $R < 0.5$ and $\Delta t > \Delta t_{small}$, the last time step calculations are rejected, Δt halved and the calculations repeated. For $R \geq 0.5$, a new ratio R' is defined as

$$R' = \begin{cases} R^2, & R' \geq 0.5, \quad 0.5 \leq R \leq 1.0 \\ 0.5\ (1 + R), & R' \leq 2.0, \quad R > 1.0 \end{cases} \tag{26}$$

Then, the new Δt is calculated as the product of R' and the Δt of the last time step. In addition, the size of Δt is also adjusted appropriately to obtain printouts at any specified time intervals.

Estimation of Time Derivatives

Time derivatives of ψ are used to estimate the average pressure heads during the time step, to evaluate ψ-dependent tabulated properties and to obtain the first estimate of $\Delta\psi$ for implicit elements to begin the iterative mass balance calculations.

At the end of each time step the calculated values of $\Delta\psi$ are used to estimate the time derivatives for the next time step. The estimate makes use of

the ratio of the maximum rates of change during the two preceding time steps to obtain approximately second order accuracy. If the maximum rate of change is decreasing with time, it is assumed that the potentials throughout the flow region are exponentially approaching equilibrium with the same exponent. On the other hand, if the maximum rate of change is increasing, the assumption is made that the potential changing most rapidly is following a quadratic curve and that the ratio between successive slopes is the same for all elements.

Consider first the case of exponential decay. Looking at Figure 2, let ψ be expressed by

$$\psi = \psi_o \, e^{-\alpha t} \tag{27}$$

Then, $\dot{\psi} = -\alpha\psi_o \, e^{-\alpha t}$ and $\dot{\psi}_o = \dot{\psi}\Big|_{t=0} = -\alpha\psi_o$. Hence

$$\frac{\dot{\psi}}{\dot{\psi}_o} = e^{-\alpha t} \tag{28a}$$

or

$$\left(\frac{\dot{\psi}}{\dot{\psi}_o}\right)^{1/t} = e^{-\alpha} \tag{28b}$$

In the light of (28b) we can write

$$\left(\frac{\dot{\psi}_2}{\dot{\psi}_1}\right)^{\frac{1}{(\Delta t_1+\Delta t_2)/2}} = \left(\frac{\dot{\psi}_3}{\dot{\psi}_2}\right)^{\frac{1}{(\Delta t_2+\Delta t_3)/2}} \tag{29a}$$

or

$$F_c = \frac{\dot{\psi}_3}{\dot{\psi}_2} = \left(\frac{\dot{\psi}_1}{\dot{\psi}_2}\right)^{-\frac{\Delta t_2+\Delta t_3}{\Delta t_1+\Delta t_2}} \tag{29b}$$

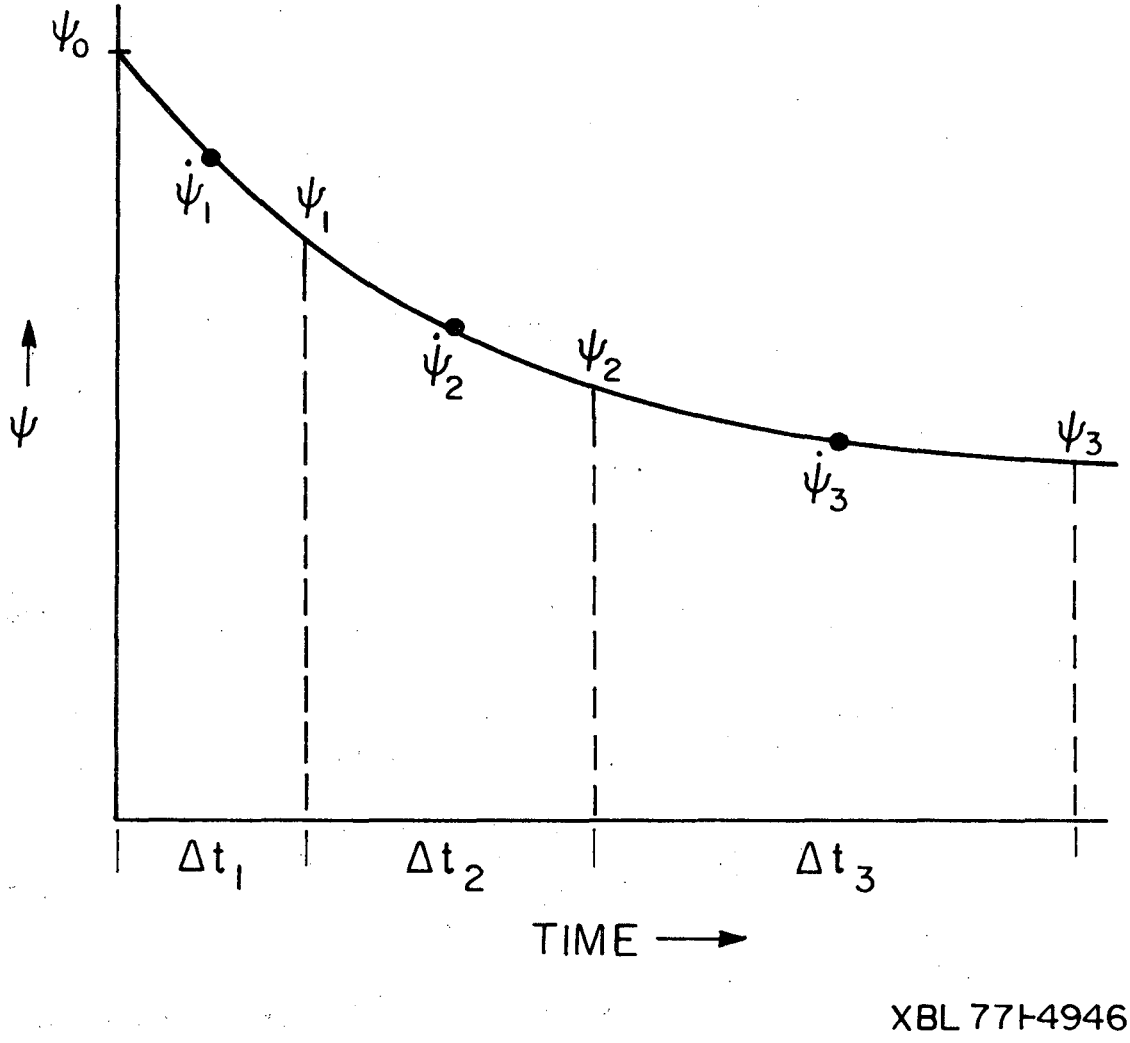

Fig. 2. Estimation of $\dot{\psi}$ for exponential decay.

Consider now the second case in which the maximum rate of change of ψ is increasing with time (Fig. 3). Let ψ be expressed by the quadratic relation

$$\psi = \psi_o + at + bt^2 \tag{30}$$

Then, $\dot{\psi} = a + 2bt$ and $\dot{\psi}_o = \dot{\psi}\Big|_{t=0} = a$. Hence $\dot{\psi} = \dot{\psi}_o + 2bt$. Therefore

$$\frac{\dot{\psi}}{\dot{\psi}_o} - 1 = \frac{2bt}{\dot{\psi}_o} \tag{31}$$

In the light of (31),

$$\frac{\dot{\psi}_2}{\dot{\psi}_1} - 1 = \frac{2b(\Delta t_1 + \Delta t_2)/2}{\dot{\psi}_1} \tag{32a}$$

and

$$\frac{\dot{\psi}_3}{\dot{\psi}_2} - 1 = \frac{2b(\Delta t_2 + \Delta t_3)/2}{\dot{\psi}_2} \tag{32b}$$

Dividing (32a) by (32b) and rearranging terms we obtain

$$F_c = \frac{\dot{\psi}_3}{\dot{\psi}_2} = 1 + (1 - \frac{\dot{\psi}_1}{\dot{\psi}_2})(\frac{\Delta t_2 + \Delta t_3}{\Delta t_1 + \Delta t_2}) \tag{33}$$

Once F_c is calculated using (29b) or (33), the estimate of the time derivative for an element ψ is obtained by

$$\dot{\psi}_{\ell,est} = F_c(\Delta\psi_\ell / \Delta t) \tag{34}$$

in which the quantity $(\Delta\psi_\ell / \Delta t)$ is the rate of change calculated for the last time step.

In addition to determining F_c as detailed above, appropriate restrictions

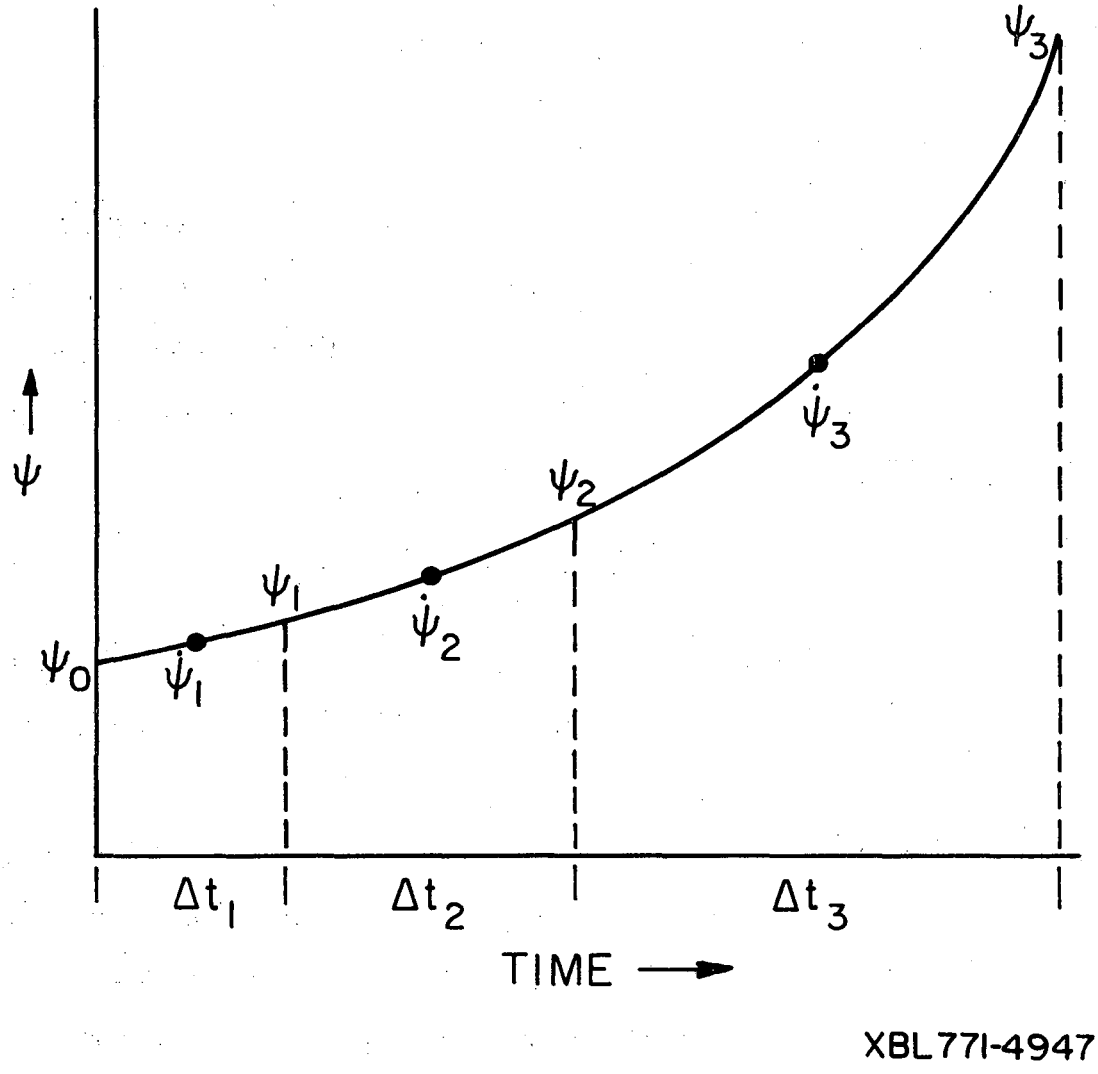

Fig. 3. Estimation of $\dot{\psi}$ for quadratic increase.

are placed on F_c to safeguard against possible sources of instability. For details regarding these, see Edwards (1968). More accurate derivatives could be calculated by saving several successive values of ψ for each case, and using higher order extrapolates. However, since the algorithm only uses first order approximation in space, there is little to be gained in attempting higher order approximation in time without reducing spatial errors.

Estimation of Interpolation Factor, λ

The factor λ is used to estimate the average values of ψ during the time step, (a) for use in evaluating the ψ-dependent properties and (b) for interpolating between initial and final values of ψ for implicit calculations. In the mixed explicit-implicit procedure λ is allowed to vary between 0.57 and 1 depending on F_c. Thus

$$\lambda = [0.57, (1.0, F_c)_{max} /(1.0 + F_c)]_{max} \tag{35}$$

As seen from (35) the minimum value of λ is 0.57 instead of 0.5. This is in order to make sure that the small oscillations which may arise if $\lambda = 0.5$ are damped out.

The form of (35) was chosen by Edwards (1968) to give λ a value close to the interpolation factor required to obtain correct average ψ when the potentials are approaching equilibrium values exponentially, that is, near 0.5 when slopes do not change appreciably over a time step and near 1.0 when large time steps are used near equilibrium.

Evaluation of ψ-Dependent Coefficients

In a variably saturated deformable porous medium the fluid mass capacity as well as permeability are functions of ψ and hence of time. Before carrying out the calculations for a time step both M_c and k are evaluated at an estimated

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average value of ψ for that time step. This estimate is obtained by

$$\bar{\psi}_\ell = \psi^\circ_\ell + \lambda \Delta t \dot{\psi}_\ell \tag{36}$$

In order to compute M_c (equation (1a)) it is necessary that several quantities such as ρ_w, e, s, etc., are to be evaluated at $\bar{\psi}$. It is relatively simple to compute ρ_w with the equation of state: $\rho_w = \rho_{wo} \exp[\rho_{wo} \beta g \bar{\psi}]$. For evaluating the deformation parameters, e and a_v, it is essential to transform $\bar{\psi}$ into an equivalent effective stress. For this purpose, the total stress σ and the volume of solids V_s for each element are calculated at the beginning of the problem and stored in memory. Then, σ' is given by $\sigma' = \sigma - \gamma_w \bar{\psi}$ and e can be calculated either by $e = e_o - (\sigma - \sigma'_o) a_v$ or, for normal consolidation, by $e = e_o - C_c[\log_{10}(\sigma - \sigma'_o)]$.

The functions χ', S and $dS/d\psi$ are tabulated as functions of ψ and hence are to be evaluated by interpolation at $\bar{\psi}$. In particular, the ψ - S relation may be characterized by hysteresis. In the present work, hysteresis is handled in a simple manner with the help of scanning curves.

It was pointed out in Part I of this series papers that k is a function of void ratio (or effective stress) in the saturated zone and of ψ in the unsaturated zone. Just as in the case of the ψ versus S relation, k is tabulated as a function of ψ for $\psi \leq 0$ and is evaluated by interpolation at $\bar{\psi}$. For the saturated zone, k can either be tabulated as a function of σ' or, more easily, k can be evaluated using the index C_k

$$k = k_o \, [2.303 \, (e - e_o)/C_k] \tag{37}$$

BOUNDARY CONDITIONS AND SOURCES

In the present model boundary conditions can be conveniently handled with the help of surface and boundary elements and the surface conductance between them. A surface element is usually a thin element which shares a segment of the external boundary of the flow region.

For simulating a prescribed potential at the boundary (Dirichlet problem) a surface element may be connected through a large surface conductance to a boundary element with a prescribed potential. Alternatively, the boundary element could be replaced by a very large element with very large M_c. A prescribed flux boundary (Neumann problem) can be simulated by connecting the surface element through a very small surface conductance to the boundary element with a very large boundary potential, and so choosing the boundary potential that the product of surface conductance and the boundary potential yields the prescribed flux. Prescribed flux can also be handled through a thin surface element generating fluid at a rate equal to the prescribed flux.

The seepage face is an important boundary condition arising in the consideration of saturated-unsaturated flow. On a seepage face two conditions hold: (a) $\psi = 0$ and (b) across a seepage face fluid can only leave but not enter the flow region. To handle the seepage face, a check is carried out the end of each time step if the flux is directed inward or outwards from the flow region across each segment of the seepage face. If directed inward, that segment of the seepage is made an impermeable boundary and the time step calculations are repeated.

Sources or sinks can be conveniently handled by prescribing the fluid generation rates from one or more elements. In the present algorithm, generation rates, prescribed potentials and prescribed fluxes can be tabulated either as functions of ψ or as functions of time.

CALCULATIONAL SCHEME AND ORGANIZATION

At the beginning of a problem, the parameters are initialized and the total stress, volume of solids and the preconsolidation pressure are calculated for each element. Following this, various system parameters are evaluated and summarized.

Before carrying out the time step calculations it is necessary to choose Δt, reclassify elements as needed, estimate time derivates and λ and evaluate the appropriate mean values of k and M_c. The first time step is always set to 10^{-12} so as to start the calculations smoothly and to establish time derivatives. For each time step, $\Delta\psi_{exp}$ and the fluxes due to the explicit changes in potential are first calculated for all elements in the system. Following this, the iterative scheme is employed to make the necessary corrections to $\Delta\psi$ for all the implicit elements in the system. Upon obtaining proper convergence, final corrections are made to all the fluxes involving implicit elements and to the potentials at all explicit elements connected to implicit elements.

If convergence does not occur in 80 iterations or if $\Delta\psi_{max}$ exceeds twice ψ_{var} or if any tabulated quantities change by more than 2 percent, the time step calculations are discarded, Δt halved and the calculations repeated. If the reduced Δt is less than Δt_{small} and more than 40 iterations are required, failure of convergence is assumed and the problem is terminated.

The code TRUST is organized into a main program and the principal subroutines THERM, HYST, FINK, GEN, SURE, SPECK and TALLY. Other subroutines are used for cross referencing, encode-decode, interpolation and other subordinate operations. The main program is used for initializing parameters and for calling the various calculational subroutines. THERM is used for input of material and element properties and for evaluating ψ-dependent coefficients for $\psi > 0$. HYST is used for evaluating material properties when $\psi \leq 0$. The fluxes and the

associated changes in ψ due to the explicit part are calculated in FINK for the internal connections and in SURE for the surface connections. Explicit calculations related to sources or sink are performed in GEN. The implicit iterative calculations as well as the associated corrections to fluid fluxes and the corrections to explicit elements connected to implicit elements are carried out in SPECK. Summarizing the material balance, making all preparations for the next time step and controlling the frequency of output are functions of the subroutine TALLY.

In the present algorithm, input is organized into convenient blocks. All control parameters such as output interval, time limit, choice of differencing scheme, scale factor, symmetry factor, Δt_{small}, Δt_{large}, ψ_{var} and uniform initial conditions are provided through Block 1. Block 2 is used for specifying material properties and Block 3 for properties of the fluid. Geometric properties of elements are specified in Block 4 while Blocks 5 and 6 are used to specify internal and external fluid flow connections. Boundary potentials are specified in Block 7 and Block 8 is used for specifying variable generation rates. Finally Block 9 is used for specifying non-uniform initial conditions.

CONTROL OF ACCURACY

The numerical algorithm described above is subject to different sources of error and an appreciation of these sources is essential for a proper use of the mathematical model. The errors that affect accuracy can be divided into six groups (Edwards, 1968), namely, modeling errors, spatial truncation errors, time truncation errors, ψ-truncation errors, convergence errors and arithmetic truncation errors.

Modeling errors arise from inaccurate material properties, inaccurate

initial and boundary conditions and interpolation errors in evaluating tabulated properties. Such errors can usually be estimated by comparing results using different models of the same system.

Spatial truncation errors occur due to the discretization of the system into finite volume elements for which average values of spatially dependent variables must be evaluated. In the present algorithms, spatial truncation errors can be controlled by dividing the system just finely enough so that nonlinear variations in ψ are fitted within required accuracy by linear interpolation. Just how fine this should be in different parts of the system may be difficult to estimate in advance. Often, a simplified version of the problem may be first solved to help estimate the degree of subdivision required in different parts of the system.

Time truncation errors are caused due to the use of discrete time steps for which average values of time-dependent variables must be estimated. These errors can be controlled by limiting the maximum variation of ψ during a time step. Further, in the present algorithm, time truncation errors are also minimized by the use of a variable weighting factor λ (equation (35)) for increased accuracy in estimating the mean value of ψ during a given time step.

The discrete changes in ψ that occur in each volume element during each time step lead to ψ-truncation errors when ψ-dependent properties are to be evaluated for each volume element. In the present algorithm, such properties are evaluated using the quasi-linear approximation and errors in this regard can be reduced by limiting the variation of ψ during a time step such that material properties vary only slightly from one time step to another.

Convergence errors arise due to the use of an iterative scheme for implicit calculations and the employment of arbitrary convergence criteria, and can be controlled through a proper choice of the error tolerance factors. In heterogeneous systems, convergence may also be affected when thin, highly per-

meable volume elements adjoin elements with low permeability. One method of avoiding this problem is to lump several thin elements into a single large element.

The last important source of errors is that arising from the accumulation of round-off inaccuracies. Such errors are in general unimportant in comparison with the other five sources mentioned above. Truncation errors arising from algebraic addition of terms which are nearly equal but are opposite in sign or which have widely different orders of magnitude can be quite serious. This is one reason why it is necessary to avoid very high conductances between intercommunicating volume elements, by lumping their elements together.

CONCLUDING REMARKS

Like any other approximate method, the algorithm presented in this paper has its advantages and limitations. Perhaps the strongest point of the present model is that it attempts to pose and solve a problem physically. Intrinsically, the chief limitation of the model is that the finite difference gradient approximation is inadequate to handle general tensorial properties such as anisotropy and stress. To handle these properties in a most general way, it is essential to evaluate tangential gradients along surfaces. To some extent, the anisotropy problem can be overcome in the present model by orienting the elements parallel to the principal axes of anisotropy. Since the permeability tensor does not usually rotate with time, this method of handling anisotropy must be adequate for handling many practical problems of interest. However, a similar logic cannot be extended for handling the stress tensor, which generally rotates with time. Therefore, the present approach is at a disadvantage in respect of handling multidimensional stress fields. Numerically, the power of the present model lies in the face that it is inherently multidimensional and the iterative

0 0 0 0 4 7 0 6 1 3 3

scheme employed avoids the large requirements of computer storage associated with direct solution algorithms.

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NOMENCLATURE

a_v	Coefficient of compressibility	$[LT^2/M]$
C_c	Compression index	[1]
C_s	Swelling index	[1]
C_k	Index relating e and log k	[1]
$d_{\ell,m}$	Perpendicular distance from nodal point ℓ to the interface between elements ℓ and m	[L]
e	Void ratio	[1]
e_o	Reference value of e at σ'_o	[1]
E_ℓ	Difference in $\Delta\psi_\ell$ of an implicit element over two successive iterations	[L]
E_ℓ^p	Value of E_ℓ at p^{th} iteration	[1]
F_c	Factor used in estimating time derivatives	[1]
g	Gravity	$[L/T^2]$
G	General symbol for source or sink, associated with a finite subdomain	[M/T]
G_ℓ	Source or sink at element ℓ	[M/T]
H	Fluid mass content	[M]
ΔH_{net}^p	Net change in fluid mass content of all implicit elements, between iterations p and (p - 1)	[M]
k	Intrinsic permeability	$[L^2]$
k_ℓ	Intrinsic permeability of element ℓ	$[L^2]$
$\bar{k}_{\ell,m}$	Mean permeability evaluated at the interface between elements ℓ and m	$[L^2]$
k_o	Permeability at reference void ratio e_o	$[L^2]$
M_c	Fluid mass capacity	[M/L]
$M_{c,\ell}$	Fluid mass capacity of element ℓ	[M/ℓ]
$M_{c,net}$	Net fluid mass capacity of all the implicit elements in the system	[M/ℓ]

0 0 0 0 4 7 0 6 1 3 4

n	Porosity	[1]
$\vec{n}$	An outward unit normal	[1]
p	Iteration number	[1]
R	Ratio used in control of time step	[1]
R'	Ratio used in control of time step	[1]
s	An acceleration factor	[1]
S	Saturation	
t	Time	[T]
Δt	Time interval	[T]
Δt_{ℓ}	Stability limit of time constant of element ℓ	[T]
Δt_{small}	Smallest time step allowable	[T]
Δt_{large}	Largest time step allowable	[T]
Δt_{max}	Maximum time step size at which certain explicit elements would would require classification as implicit elements	[T]
Δt_{stab}	Largest stable time step for explicit zones	[T]
$U_{\ell,b}$	Surface conductance between element ℓ and the external surroundings	[M/LT]
$U_{\ell,m}$	Conductance of the interface between ℓ and m	[M/LT]
V	Volume	$[L^3]$
V_s	Volume of solids	$[L^3]$
z	General symbol for elevation	[L]
z_{ℓ}	Elevation of the nodal point ℓ	[L]
Z_{ℓ}	Sum of the conductances of all the surface segments bounding element ℓ	$[L^2/T]$
α	An exponent	[1]
β	Compressibility of water	$[LT^2/M]$
Γ	Boundary surface of an element	$[L^2]$

$\Gamma_{\ell,m}$	Interface between elements ℓ and m	$[L^2]$
γ_w	Specific weight of water	$[M/LT^2]$
λ	Interpolation factor	[1]
μ	Viscosity of water	[M/LT]
ν	Product of ψ_{vary} and 1/40 of the number of iterations required for convergence or the largest percentage variation in a tabulated property, whichever is greater	[1]
ρ_w	Density of water	$[M/L^3]$
$\rho_{w,o}$	Reference density of water at atmospheric pressure	$[M/L^3]$
$\rho_{w,\ell}$	Average density of water in element ℓ	$[M/L^3]$
$\bar{\rho}_{w,\ell,m}$	Mean density of water evaluated at the interface between elements ℓ and m	$[M/L^3]$
σ	Total stress	$[M/LT^2]$
σ'	Effective stress	$[M/LT^2]$
σ'_o	Reference effective stress at which $e = e_o$	$[M/LT^2]$
χ'	Parameter correlating change in effective stress and change in pore pressure	[1]
ψ	Pressure head	[L]
ψ_b	Pressure head of boundary element	[L]
$\bar{\psi}_b$	Mean boundary pressure head	[L]
ψ_ℓ	Pressure head of element	[L]
ψ_{vary}	One half of the maximum variation of ψ allowed during any time step	[L]
$\bar{\psi}$	Estimated mean pressure head during Δt	[L]
$\dot{\psi}_\ell$	Estimated time derivative for element ℓ	[L/T]
ψ^o_ℓ	Pressure head of element ℓ at the beginning of a time step	[L]

0 0 0 0 4 7 0 6 1 3 5

$\Delta\psi_{exp}$	Explicit change in ψ	[L]
$\Delta\psi_{imp}$	Implicit change in ψ	[L]
$\Delta\psi_{max}$	Maximum change in ψ during a time step	[L]
$\Delta\psi_{\ell}^{p}$	Change in $\Delta\psi_{\ell}$ during p^{th} iteration	[L]

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