Soil Water Modeling I: A Generalized Simulator of Steady, Two-Dimensional Flow

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A COMPUTATIONAL scheme was developed for solving the steady-state, two-dimensional form of Richards' equation using finite differencing. The successive overrelaxation (SOR) method was used. The computer model developed for implementing the computational scheme was generalized using a technique called subsectioning, which allows application of the model, without internal modification, to a wide range of geometric shapes, hydraulic boundary conditions, and soil distributions. Unsaturated or saturated flow regions or those containing phreatic surfaces may be modeled. The nonlinear nature of Richards' equation was reflected in the overrelaxation coefficient which had a maximum rather than an optimum value. Values higher than maximum caused instability.

INTRODUCTION

Aside from its crucial role in the maintenance of organic life, soil water is an important and active part of the hydrologic cycle. Most groundwater bodies in humid areas are recharged primarily by soil water (Linsley et al. 1958); therefore, movement of the latter is one of the controlling factors for dry weather streamflow, springflow, and the maintenance of groundwater supplies. Soil water content and hydraulic gradients also affect infiltration rates and, therefore, the generation of surface runoff during storm and snowmelt periods.

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Flowing soil water has been found to remove fine particles from soil profiles and has been studied as one of the agents contributing to soil and landscape genesis (Vasilyev 1948; Bunting 1961; Smirnov 1963). Flowing soil water also carries many soluble substances (Buckman and Brady 1969).

To improve our understanding of such processes as surface and subsurface hydrology, soil genesis, landscape morphology development, and the distribution of chemical substances through the landscape, we must study soil water and its movement. For some processes we cannot be satisfied simply to investigate inputs and outputs but must endeavor to define actual flow paths and velocities.

In most situations involving large-scale and large-volume soil water movement, hydraulic head gradients provide the major forces and, along with soil hydraulic conductivity, determine flow paths and velocities (Childs 1969). Numerous mathematical models have been devised to help understand soil water movement under various conditions (Reisenauer et al. 1963, Freeze and Witherspoon 1966, Rubin 1968, Taylor and Luthin 1969, Amerman 1969, Raats 1970, and 1972, Freeze 1971, Pinder and Frind 1971, and Pinder 1973). Reisenauer et al. (1963) have devised a model that has been generalized in that geometry and boundary conditions can be specified as input data.

In developing the model discussed herein, my aim was twofold: (a) to provide a steady-state model of the hydraulic-head distribution of porous-media flow applicable to a wide variety of boundary geometries and flow regions simply by changing input data and (b) to provide sufficiently detailed documentation that others, with only brief acquaintance with digital computer programming or with the field of mathematics involved, could use the model. The model, named STDY2, is fully documented in another publication (Amerman 1976). The purposes of this paper are to briefly describe the model and to discuss a programming concept that could be used to generalize other models. In later papers I will discuss sensitivity of finite difference models to various factors.

MODEL DESCRIPTION

The model is a digital computer program, written in USASI Fortran, which should run on most computers with a minimum of modification. Statements likely to vary from one computer to another are flagged. The model uses the successive overrelaxation (SOR) method of finite differencing applied to the steady-state, two-dimensional form of Richards' equation.

Model capabilities and limitations are as follows:

1 The model simulates two-dimensional soil water flow situations.

2 Flow in the prototype must be at least quasi-steady state.

3 Flow-system geometries approximated with straight-line segments may be complex, including point sinks, point sources, cavities, and impermeable zones within the section.

4 The major axes of the model may be rotated to conform with the slope of the prototype.

5 Hydraulic boundary conditions may be specified for all boundaries in terms of either pressure head or zero, normal, hydraulic-head gradient (impermeable condition). A flux (evaporation or infiltration) can be specified on the upper surface. A hydrostatic distribution of pressure head can be specified along vertical boundaries.

6 The modeled section may contain several soil units with different hydraulic characteristics. The boundaries of these units may be geometrically complex and are approximated as straight-line segments.

7 Hydraulic conductivity (K) as a function of soil water pressure head (h) may be used in tabular form. Alternatively, a user may insert an

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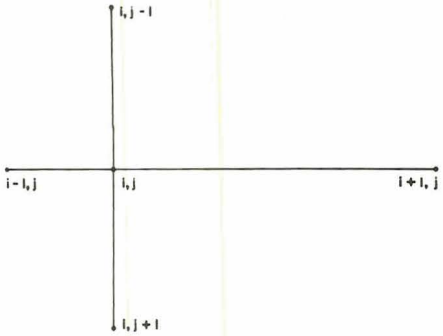

FIG. 1 Stencil for finite difference grid.

equation relating K and h, but this requires some programming ability on his part.

8 A given soil unit is considered isotropic.

9 Hysteresis in the K-h relationship is ignored.

10 Darcy-type flow in the prototype system is assumed.

11 A surface-of-seepage problem is handled by trial and error and requires the user to interact with the model.

12 Convergence checking requires the user to interact with the model. An auxiliary program is provided as an aid for this.

13 The finite-difference grid is specified by means of input data cards. The grid may be square, rectangular, or irregular with grid-size varying over the section.

14 An auxiliary program is provided to change mesh spacings of an existing grid for which a solution already exists.

Input to the model consists of model specifications and, except as provided in No. 7 above, a table of K as a function of h. The user may select one of two model-generated starting arrays of h, or he may submit an array as input data in either punchcard or magnetic tape form.

Output of the model may be divided into four groups:

1 Printed model identification and model specifications.

2 Printed intermediate data for use in checking convergence.

3 Printed array of soil-water hydraulic heads.

4 Array of soil-water pressure heads in printed form and in either punchcard or magnetic tape form.

METHODS

Combining the equations of state and continuity with Darcy's law yields Richards' equation (Richards 1931) for transient, unsaturated flow. It may be written for the steady state and for two dimensions as

$$\frac{\partial}{\partial x}\left(K\frac{\partial H}{\partial x}\right)+\frac{\partial}{\partial y}\left(K\frac{\partial H}{\partial y}\right)=0 \quad \ldots\ldots \quad [1]$$

where

H = hydraulic head = h + z (L)
h = soil-water pressure head (L)
z = position head, vertical distance above a datum (L)
K = K(h), hydraulic conductivity (LT^{-1})
x = distance parallel to the x-axis of the Cartesian coordinate system, positive to the right (L)
y = distance parallel to the y-axis, positive upward (L).

The Cartesian coordinate system may be rotated through an angle α to make the x-axis conform with the predominant slope of the prototype system, i.e., the slope of a soil surface or bedrock. Because K is a function of h, substituting h + z for H is convenient. Making this substitution and introducing α in equation [1] yields

$$\frac{\partial}{\partial x}\left(K\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K\frac{\partial h}{\partial y}\right)+\sin\alpha\frac{\partial K}{\partial x}+\cos\alpha\frac{\partial K}{\partial y}=0$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad [2]$$

Equation [2] is a nonlinear, elliptic-type, partial differential equation. Description of a given problem is complete when boundary geometrics and boundary hydraulic conditions have been specified. There is no general analytical solution for all boundary geometrics, sequences of boundary conditions and K-h distributions. Numerical methods must usually be applied.

The numerical method used by STDY2 is finite differencing with terms developed using the central differencing technique. The resulting system of equations is solved by the iterative scheme known as successive overrelaxation (Forsythe and Wasow 1960, Smith 1965, Greenspan 1968). The finite-difference grid stencil is given in Fig. 1.

STDY2 solves the following SOR finite difference approximation to equation [2]

$$h_{i,j}^{m}=(1-\omega)\,h_{i,j}^{m-1}$$

$$+\omega\left[\frac{2}{\Delta x_-+\Delta x_+}\left(\frac{K_{i-\frac{1}{2},j}^{m-1}}{\Delta x_-}h_{i-1,j}^{m}+\frac{K_{i+\frac{1}{2},j}^{m-1}}{\Delta x_+}h_{i+1,j}^{m-1}\right)\right.$$

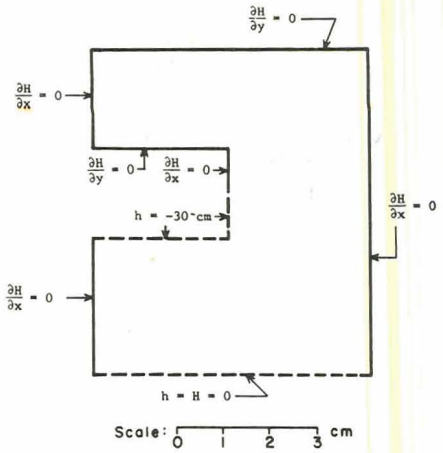

FIG. 2 Example of complex cross section.

$$+\frac{2}{\Delta y_-+\Delta y_+}\left(\frac{K_{i,j-\frac{1}{2}}^{m-1}}{\Delta y_-}h_{i,j-1}^{m}+\frac{K_{i,j+\frac{1}{2}}^{m-1}}{\Delta y_+}h_{i,j+1}^{m-1}\right)$$

$$+\sin\alpha\frac{K_{i-1,j}^{m-1}-K_{i+1,j}^{m-1}}{\Delta x_-+\Delta x_+}+\cos\alpha\frac{K_{i,j-1}^{m-1}-K_{i,j+1}^{m-1}}{\Delta y_-+\Delta y_+}\Bigg]$$

$$\div\left[\frac{2}{\Delta x_-+\Delta x_+}\left(\frac{\Delta x_+\cdot K_{i-\frac{1}{2},j}^{m-1}+\Delta x_-\cdot K_{i+\frac{1}{2},j}^{m-1}}{\Delta x_-\cdot\Delta x_+}\right)\right.$$

$$\left.+\frac{2}{\Delta y_-+\Delta y_+}\left(\frac{\Delta y_+\cdot K_{i,j-\frac{1}{2}}^{m-1}+\Delta y_-\cdot K_{i,j+\frac{1}{2}}^{m-1}}{\Delta y_-\cdot\Delta y_+}\right)\right]$$

$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad [3]$$

where

m = values obtained during the current iteration,
m-1 = values obtained during the preceding iteration,
ω = overrelaxation factor.

$$K_{i-\frac{1}{2},j}=\frac{K_{i-1,j}+K_{i,j}}{2},$$

$$K_{i+\frac{1}{2},j}=\frac{K_{i,j}+K_{i+1,j}}{2}$$

$$K_{i,j-\frac{1}{2}}=\frac{K_{i,j-1}+K_{i,j}}{2},$$

$$K_{i,j+\frac{1}{2}}=\frac{K_{i,j}+K_{i,j+1}}{2},$$

Δx_- = mesh increment to left of node, i,j,
Δx_+ = mesh increment to right of node, i,j,
Δy_- = mesh increment above node, i,j,

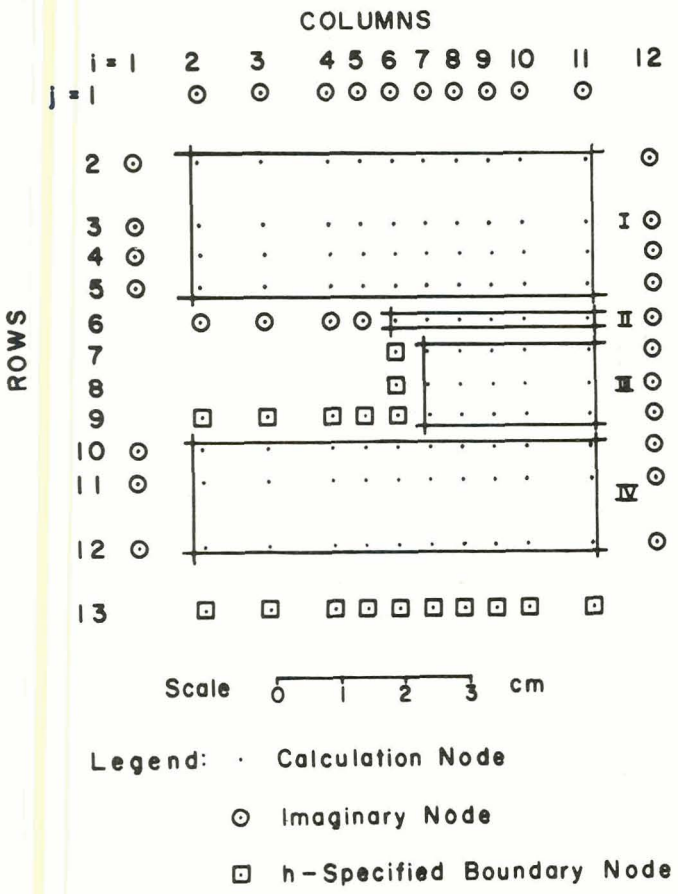

FIG. 3 Row subsections for Fig. 2.

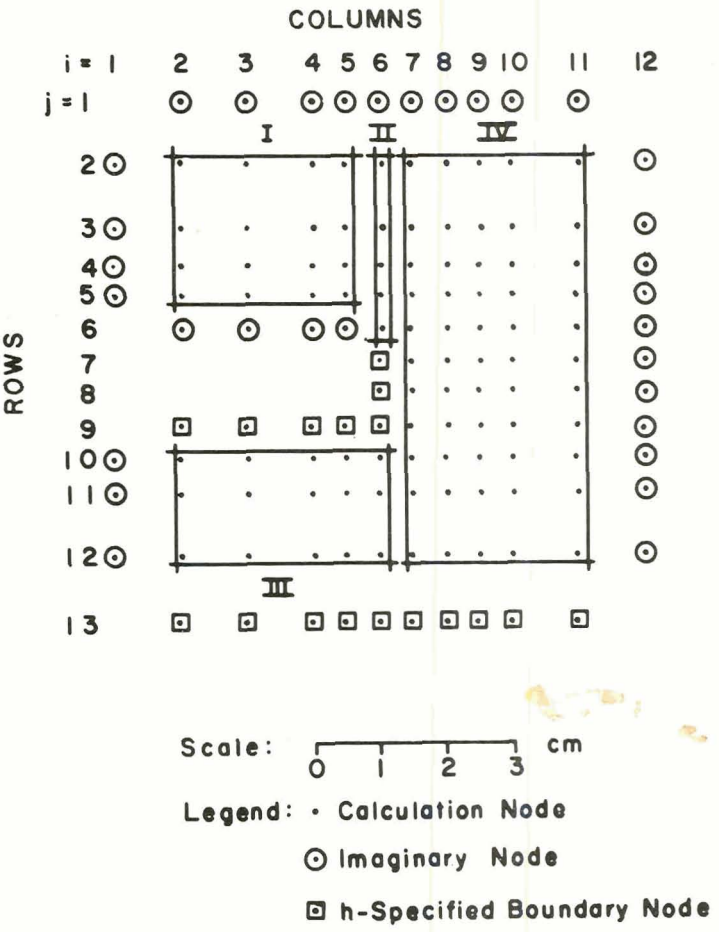

FIG. 4 Column subsections for Fig. 2.

Δy_+ = mesh increment below node, i,j.

Equation [3] does not apply at nodes for which pressure head is known. Otherwise, SOR methodology requires that equation [3] be solved for each node of the finite difference grid in some orderly sequence. The model begins at the left-hand end of the top row and processes each row in sequence from left to right. Pressure-head values calculated during an iteration become immediately available for use in calculating pressure heads for succeeding neighboring nodes. Thus, in equation [3], the nodes above and to the left of node i,j (nodes i-1,j and i,j-1) have the same superscrit as node i,j.

All K-values correspond with pressure head values from the previous iteration. Using new K-values at the nodes above and to the left of node i,j caused slower convergence rates, since the maximum overrelaxation factor (to be discussed later) was smaller than when using old K-values.

SUBSECTIONING

Generalization of the model was accomplished through the use of a technique called "subsectioning." Fig. 2 shows a section somewhat complex both in geometry and in the distribution of hydraulic boundary conditions. Figs. 3 and 4 illustrate how the section of Fig. 2 was subsectioned in row and column directions, respectively. The dots (Figs. 3 and 4) represent calculation nodes of the finite difference grid. The circled dots, labeled imaginary node in the figures' legends, were used to implement the impermeable condition of the boundaries to which they are adjacent.

As mentioned earlier, equation [3] applies to each node of the finite difference grid that does not have an h-value specified for it. Equation [3] does not apply outside the boundaries of the flow region; imaginary nodes are handled by special algorithms. One purpose of subsectioning, then, was simply to control which nodes are processed by equation [3]. Row subsectioning, in effect, specifies cross section geometry. The other purpose, accomplished by both row and column subsectioning, is to apply boundary conditions.

Rows 2 through 5 (Fig. 3) form a homogeneous set from the standpoint of both boundary conditions and pattern of nodes to be processed by equation [3], i.e., each row begins at column 2 and ends at column 11. Each row is impermeable on both the left and right ends. These rows form a subsection in that, for all of them, one set of data can be given the model to specify the end boundary conditions and to govern the processing of the nodes. Row 6 has the same beginning and ending boundary conditions as the rows above it, but the first node to be processed is on column 6. Row 7 is different again, so that row 6 is unique and forms a separate subsection. Rows 7, 8, and 9 are the same actual length as row 6, but the beginning boundary condition is one of pressure-head specified, so the node on the left end of the row is not to be processed. This calls for grouping them in a subsection separate from row 6.

Nodes are processed from left to right and from top to bottom within a subsection, and the subsections are processed in the order of their appearance in the input data deck. To maintain the orderly sequence of processing required by SOR, the row subsections must be properly ordered which means taking care that, for a given iteration, all nodes of a row have been processed before processing the

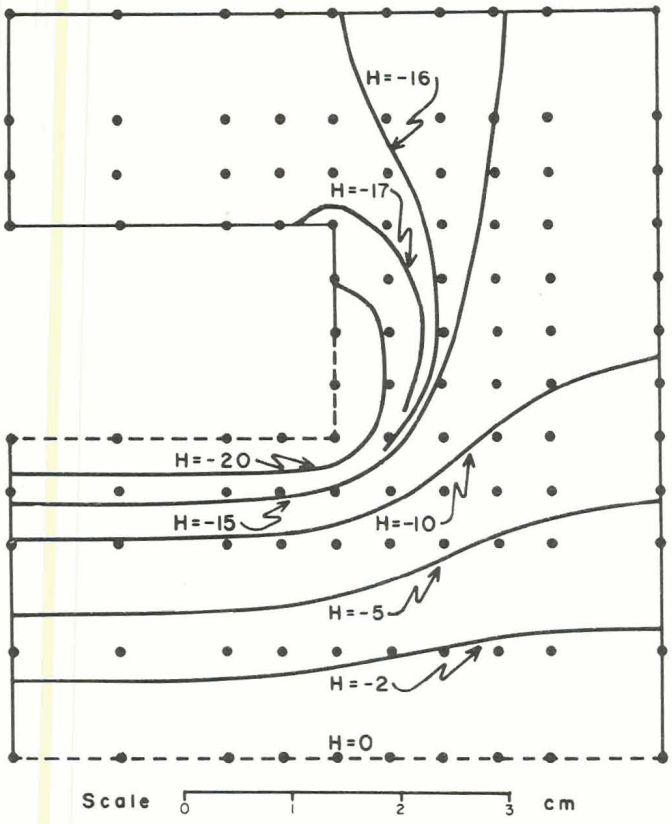

FIG. 5 Hydraulic head distribution for Fig. 2.

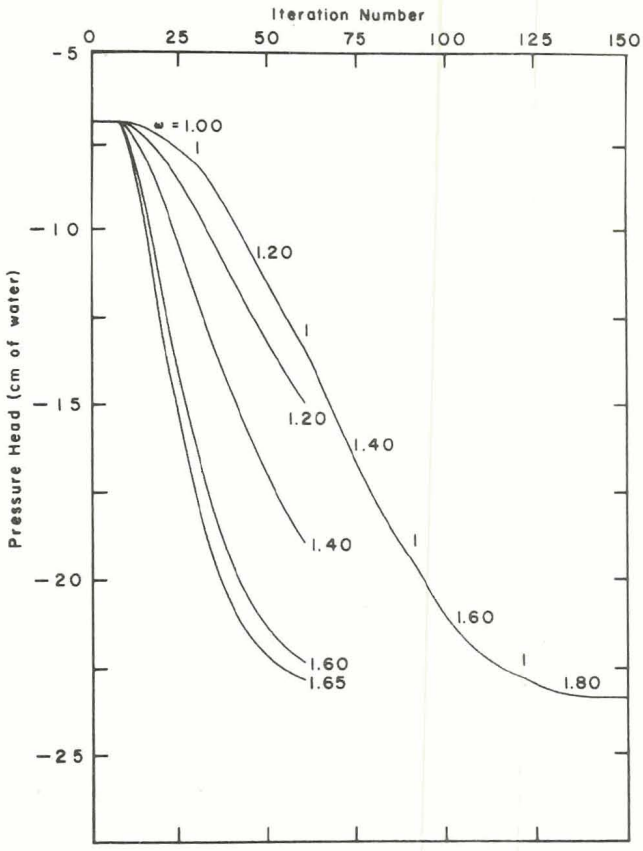

FIG. 6 Convergence rate as influenced by the over-relaxation factor, ω.

next lower row. Thus, if the cross section of Fig. 2 had a vertical notch or barrier halfway along its length and extending to some depth from the top boundary, some of the upper rows in Fig. 3 would be bisected. This would mean that the two parts of these rows would form two sub-sections. The data for both these subsections must precede data for the subsection that includes the first complete row of nodes below the notch or barrier.

A similar discussion can be given for defining column subsections in Fig. 4. Column subsections are used only to define boundary conditions at the ends of columns, however, and do not affect the order of processing. Therefore, the order of column subsection data can be arbitrary.

The subsectioning concept, with slight modifications, can be applied to other finite difference schemes. It was applied to a steady-state model using an alternating direction implicit (ADI) scheme, but the latter proved to be inferior to SOR for cross sections that were not perfectly square or rectangular. Convergence for ADI in these cases was many times slower than for SOR.

Fig. 5 shows the hydraulic head distribution generated by the geometry and boundary conditions of Fig. 2. The direction of flow is from the water table boundary at the base of the cross section toward the -30 cm boundary in the notch.

OVERRELAXATION FACTOR

A considerable body of theory is available for applying SOR to linear problems. There is little theory applicable to nonlinear problems, but experience shows that SOR can be successfully applied to many of them. In developing this model, the biggest departure from extrapolation of linear techniques to nonlinear was encountered in applying the overrelaxation factor, ω. SOR with $0 < \omega < 2$ is convergent for problems involving linear partial differential equations regardless of boundary geometry and boundary hydraulic conditions. The optimum value of ω, ω_{opt}, causes the most rapid convergence possible using SOR. For linear problems, Forsythe and Wasow (1960) show that ω slightly greater than ω_{opt} causes more rapid convergence than ω slightly smaller than ω_{opt}.

In contrast with the linear case, a concept of optimum overrelaxation factor is not quite accurate when applied to equation [3]. For this equation, there seems to be a maximum ω-value, ω_{max}, at which convergence can be obtained. Reisenauer et al. (1963) apparently found this was true for a similar equation. For values greater than ω_{max}, the solution begins to diverge at some of the nodes of the finite difference grid. For a small range of $\omega > \omega_{max}$, minor fluctuations may slowly grow about a generally converging solution, and only a limited part of the grid may be affected. But for ω grossly larger than ω_{max}, the solution becomes unstable over the whole grid. The effects of small overestimations of ω_{max} are sometimes not discernible until considerable convergence has taken place.

Using textbook methods based on linear theory to estimate ω_{opt} as a first approximation to ω_{max} for rectangular geometry proved unsuccessful. The estimated values bore no discernible relation to the ω_{max} values obtained by trial and error. Furthermore, for linear problems ω_{opt} is usually larger than 1.0 (Forsythe and Wasow 1960). But ω_{max} often took on values less than 1.0, sometimes considerably less.

Fig. 6 shows that, like linear equations, convergence varies in a regular manner. The upper curve extending from 0 to 150 iterations was obtained at a representative node in a model for which ω was increased by 0.2 every 30 iterations. The limits of each 30 iterations are marked on the figure

by a tic mark above the curve. Inspection of the curve reveals that it steepened every time ω was increased; i.e., convergence rate increased as ω increased. This was true when $\omega = 1.80$ was used, even though this value was greater than ω_{max}. The shorter curves demonstrate convergence rate for each ω-value when starting at zero iterations. The maximum overrelaxation factor for which all nodes converged lay between 1.65 and 1.70.

As implied in the preceding discussion, the only known way to obtain a value for ω_{max} is by trial and error. STDY2 includes provision for trying different values of ω while advancing the solution. At the beginning of a computer run which models a given situation, the user may specify the ω-values to be tested during that run and may specify the number of iterations for each test. He may also specify certain nodes for which h is to be printed at the end of each iteration, after every other iteration or at some other frequency. When the run is finished, he may inspect the data for these nodes and determine whether fluctuation has begun or he may plot them in curves similar to the upper curve of Fig. 6. Restart data may be obtained at the end of each ω test so that, after selecting a value for ω, the solution may be continued from the most advanced data set that was not preceded by excessive fluctuation.

Strictly speaking, convergence may be obtained only using $\omega \leqslant \omega_{max}$, and fastest true convergence apparently occurs using ω_{max}. However, the import of the $\omega = 1.80$ portion of the upper curve of Fig. 6, as verified by experience with other cases, is that highest initial convergence rates can sometimes be obtained with ω-values that exceed ω_{max}. The magnitude by which ω exceeds ω_{max} and the number of iterations that can be run without excessively distorting the solution are, again, matters of trial and error. Final convergence, however, should be obtained using $\omega \leqslant \omega_{max}$.

SUMMARY

A concept called "subsectioning" was used to generalize the application of a steady-state, two-dimensional, finite difference model of porous media flow. Subsectioning allows generalization of the model to the extent that it can be applied to a wide variety of prototypes simply by changing specifications in input data. Although the flow equation modeled is nonlinear, experience shows that finite differencing by successive overrelaxation yields convergence. The primary departure from SOR linear theory appeared in connection with the overrelaxation factor, ω. This factor could not be estimated using the techniques of linear theory. For this nonlinear application, convergence rate increased as ω increased until some maximum was reached. Values of ω larger than this maximum led to instability in the solution. Experience indicates that the maximum ω-value is about as likely to take on a value less than 1.0 as it is to take on a value greater than 1.0.

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