Documentation of a Computer Program to Simulate Transient Leakage from Confining Units Using the Modular Finite-Difference Ground-Water Flow Model

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PREFACE

This report presents a computer program for simulating transient leakage and ground-water storage changes in compressible confining units. A future formal release of this report is planned as a chapter in Techniques of Water-Resources Investigations of the U.S. Geological Survey. The performance of this computer program has been tested in models of hypothetical ground-water flow systems. Future applications of the programs could reveal errors that were not detected in the test simulations. Prior to the formal release of the report, users are requested to notify the originating office of any errors found in the report or in the computer program. Correspondence regarding the report or program should be sent to

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Copies of the computer program and test data sets on tape or diskette are available at cost of processing from

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CONVERSION FACTORS

Multiply	By	To obtain
centimeter (cm)	0.3937	inch
meter (m)	3.281	foot
per meter (m^{-1})	0.3048	per foot
meter per day (m/d)	3.281	foot per day
square meter (m^2)	10.76	square foot
square meter per day (m^2/d)	10.76	square foot per day
cubic meter (m^3)	35.33	cubic foot

Documentation of a Computer Program to Simulate Transient Leakage from Confining Units Using the Modular Finite-Difference Ground-Water Flow Model

By S.A. Leake, P. Patrick Leahy, *and* Anthony S. Navoy

Abstract

This report presents a new method of simulating transient leakage from confining units using the U.S. Geological Survey Modular Finite-Difference Ground-Water Flow Model. Transient leakage into or out of a compressible fine-grained confining unit results from ground-water storage changes within the unit. The importance of fine-grained units in analyses of transient ground-water flow is not always recognized. The new method of simulating transient leakage in the Modular Finite-Difference Ground-Water Flow Model is referred to as the Transient-Leakage Package, version 1, or the TLK1 Package.

The TLK1 Package solves integrodifferential equations that describe the flow components across the upper and lower boundaries of confining units. The exact equations are approximated to allow efficient solution for the flow components. The flow components are incorporated into the finite-difference equations for model cells that are adjacent to confining units. Vertical hydraulic conductivity, thickness, and specific storage are specified in input arrays for each confining unit. Confining-unit properties can differ from cell to cell and a confining unit need not be present at all locations; however, a confining unit must be bounded above and below by model layers in which head is calculated or specified.

The TLK1 Package was used for an example problem to simulate drawdown around a pumped well in a system with two aquifers separated by a confining unit. The pumping was limited to one of the two aquifers. The exact drawdown values determined from an analytical solution were compared with the simulated drawdown. The solution using the TLK1 Package closely matched the exact solution for drawdown values in excess of 1 centimeter in the pumped and unpumped aquifers. The problem also was simulated without the TLK1 Package by using a separate model layer to represent the confining unit. That simulation was further refined by using two model layers to represent the confining unit. The simulation made using the TLK1 Package was faster and more accurate than either of the simulations using model layers to represent the confining unit.

INTRODUCTION

Transient leakage into or out of a compressible fine-grained unit results from changes in ground-water storage within the unit. Aquifer systems commonly include fine-grained confining units and interbeds (fig. 1). Confining units are laterally extensive units that divide an aquifer system into individual aquifers. By definition, confining units are of lower permeability than adjacent aquifer material; however, many confining units are of high porosity and compressibility. Jacob (1940) recognized that release of water from storage in confined aquifers is derived from expansion of water, compression of the aquifer, and compression of clayey beds that are within or adjacent to an aquifer. Fine-grained beds are thought of as not being part of aquifers and their importance in analyses of transient ground-water flow is not always recognized.

Confining units can be represented in different ways in most ground-water models. The most common approach is to ignore storage changes in confining units and include vertical hydraulic conductivity and

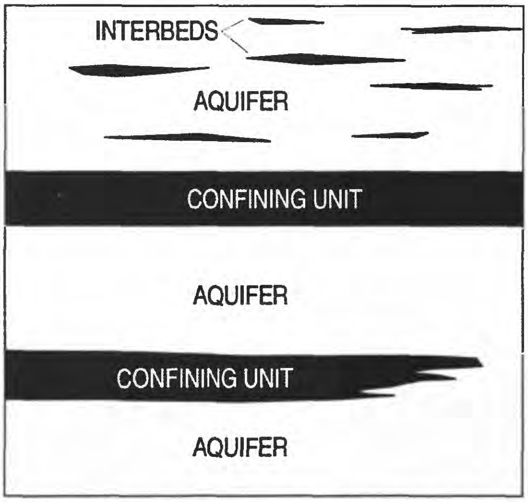


Figure 1. Types of fine-grained strata in aquifer systems. Confining units are laterally extensive and can divide coarse-grained material into individual aquifers. Fine-grained interbeds are laterally discontinuous beds within an aquifer.

thickness of confining units in vertical-conductance terms that couple the model layers. If storage changes are to be considered, the confining units can be represented with model layers. One consequence of this approach is that accurate simulation of complex vertical head distributions in confining units might require the use of many model layers for each confining unit. Also, use of model layers to simulate vertical flow in confining units can result in unnecessary computational effort spent in calculation of insignificant horizontal flow components.

Transient-leakage calculations are needed for analyses of aquifer systems in which changes in ground-water storage in confining units are a significant component of the total water budget or when accurate representation of drawdown is required at early times after the start of pumping. The significance of the storage changes can be dependent on scales of time and distance under consideration. For instance, results of an aquifer test can be dominated by effects of transient leakage immediately after the start of the test. As the test progresses, the effects of transient leakage diminish.

Storage changes in a confining unit are related directly to head changes in the unit. Nonlinear vertical head distributions develop in the unit in response to changes in head at the upper and lower boundaries of a confining unit (fig. 2). In the examples shown in figure 2, flow in the unit is vertical with initial steady-state flow from the upper to the lower aquifer. After an initial instantaneous head change in the adjacent aquifers, head and storage begin to change in the confining unit. If head in the aquifers is constant after an initial head change, the flow within the confining unit eventually will reach a new steady-state condition. The time at which a new steady-state condition will be reached depends on the thickness, vertical hydraulic conductivity, and specific storage of the confining unit. Storage changes in a confining unit are largest immediately following the head changes in the aquifers and diminish as head in the confining unit approaches the new steady-state distribution.

Purpose and Scope

This report documents a new method of simulating transient leakage from confining units using the U.S. Geological Survey Modular Finite-Difference Ground-Water Flow Model (MODFLOW) (McDonald and Harbaugh, 1988). The method presented here for simulating transient leakage is a new program for

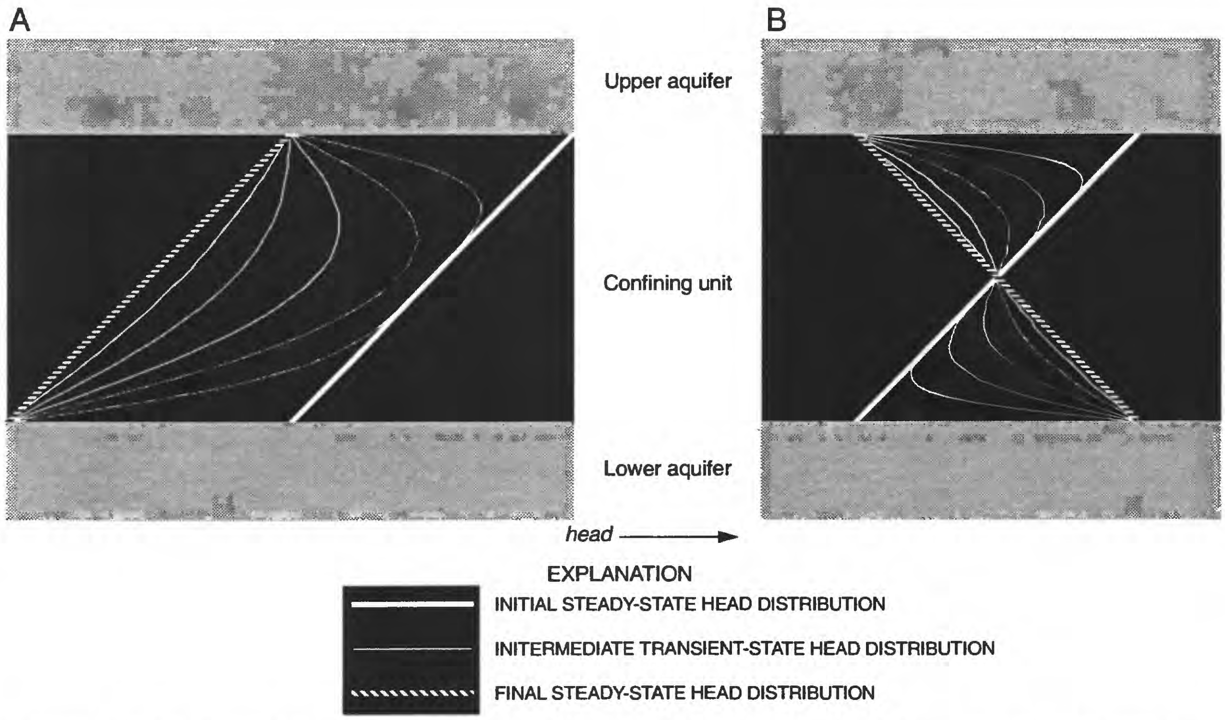


Figure 2. Distributions of head in a confining unit before and after head changes in overlying and underlying aquifers. Assumed initial conditions are steady-state flow from upper to lower aquifer. *A*, Head decreases equally in upper and lower aquifers. *B*, Head decreases in upper aquifer and increases in lower aquifer. Adapted from Trescott and others (1976).

MODFLOW referred to as the Transient-Leakage Package, version 1, or the TLK1 Package. The TLK1 Package includes six Fortran subroutines, or modules, that work as a part of MODFLOW. The method incorporated into the TLK1 Package is a solution of integrodifferential equations that describe flow at the upper and lower boundaries of confining units. The TLK1 Package allows simulation of transient leakage without use of additional model layers to simulate flow in confining units. Use of the new package generally is more accurate and computationally less intensive than use of model layers to simulate confining units. Confining units between model layers can be continuous or discontinuous (fig.1); however, the TLK1 Package cannot be used to simulate flow to or from interbeds within an aquifer. For details on simulation of flow to or from compressible interbeds, see Leake and Prudic (1991), Leake (1990), and Leake (1991).

Previous Investigations

A number of previous investigators have developed methods for solving for transient flow across the boundaries of confining units. Hantush (1960) formulated and developed a solution for radially symmetric flow in a two-aquifer system. He developed the solution for a pumped aquifer, an adjacent confining unit with storage, and an unpumped aquifer with a constant head on the distal side of the confining unit. Neuman and Witherspoon (1969) expanded the analytical solution to allow for drawdown in the unpumped aquifer. Bredehoeft and Pinder (1970) incorporated analytical solutions for early-time leakage into a finite-difference model for multiaquifer systems. Their model assumed for later times that leakage was proportional to head difference across the confining units. Their method was modified by Trescott and others (1976) to incorporate transient-leakage calculations in a widely used two-dimensional ground-water flow model. More complex integrodifferential equations describing flow across boundaries were developed by Herrera and Figueroa (1969), Herrera (1970), and Herrera and Rodarte (1973). Solution of the integrodifferential equations in a numerical model required head values to be known for all previous times. Solution of the equations also required evaluation of infinite series for which convergence was not necessarily rapid. Later work to simplify or approximate parts of the integrodifferential equations was carried out by Herrera and Yates (1977), De Marsily and others (1978), Premchitt (1981), Hennart and others (1981), Gambolati and others (1986), and Cooley (1992).

MATHEMATICAL DEVELOPMENT

Formulation of the equations for describing transient leakage in this report follows the mathematical development given by Cooley (1992). His work incorporates transient-leakage calculations in a two-dimensional finite-element model program. In his formulation, the confining unit is bounded on one side by an aquifer and on the other side by a source bed in which the head is specified. For the computer program presented in this report, the formulation developed by Cooley (1992) was modified for use with the finite-difference method and to allow variable-head aquifer layers above and below each confining unit. The presentation of the mathematical development parallels that given by Cooley (1992, p. 54-64).

The MODFLOW program solves a form of the three-dimensional ground-water flow equation

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)-W=S_s\frac{\partial h}{\partial t}, \tag{1}$$

where x, y, and z are cartesian coordinates, aligned along the major axes of the hydraulic-conductivity tensor; K_{xx}, K_{yy}, and K_{zz} are principal components of the hydraulic-conductivity tensor; h is hydraulic head; W is volumetric flux per unit volume of sources and (or) sinks of water; S_s is specific storage of the aquifer; and t is time. The finite-difference approximations for the flow equations are written in terms of volumetric flow for each model cell. If a model cell is above or below a confining unit, a term must be added to account for flow to or from the confining unit for the time step.

For this discussion, a simple two-aquifer model will be used to develop an expression for flow across the bottom of the confining unit into or out of the lower aquifer at grid location **i** (fig. 3). This location corresponds to a particular row, *i*, and column, *j*, in the finite-difference grid; for this example, **i** denotes the vertical stack of two finite-difference cells with an intervening confining unit. Flow in the confining unit is assumed to be vertical. Also, vertical hydraulic conductivity, specific storage, and thickness of the confining unit are assumed to be constant over the area covered by the cells at grid location **i**. With these assumptions, the problem can be formulated as

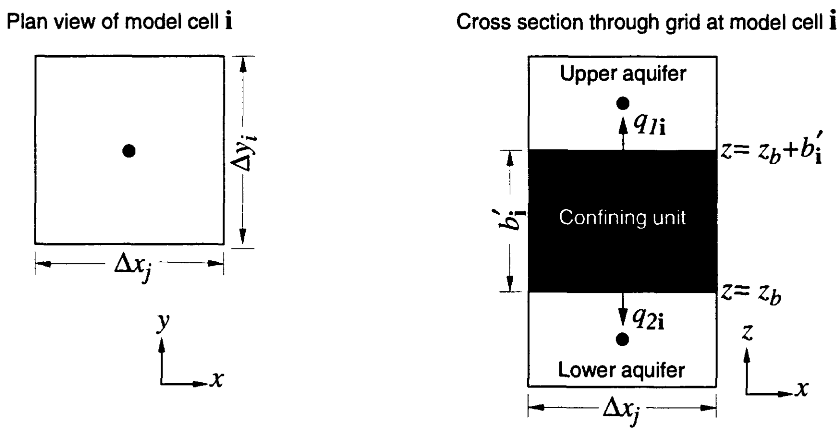
$$K'_{\mathbf{i}}\frac{\partial^2 h'_{\mathbf{i}}}{\partial z^2}=S'_{s\mathbf{i}}\frac{\partial h'_{\mathbf{i}}}{\partial t}, \tag{2}$$

subject to

$$h'_{\mathbf{i}}(z_b,t)=h_{2\mathbf{i}}(t),\ t\geq 0, \tag{3}$$

$$h'_{\mathbf{i}}(z_b+b'_{\mathbf{i}},t)=h_{1\mathbf{i}}(t),\ t\geq 0, \tag{4}$$

$$h'_{\mathbf{i}}(z,0)=\frac{z-z_b}{b'_{\mathbf{i}}}h_{1\mathbf{i}}(0)+\left[1-\frac{z-z_b}{b'_{\mathbf{i}}}\right]h_{2\mathbf{i}}(0),\ z_b\leq z\leq z_b+b'_{\mathbf{i}}. \tag{5}$$



Variables for confining unit

head: $h'_i(z, t)$

vertical hydraulic conductivity: K'_i

specific storage: S'_{si}

Variables for aquifers

head in upper aquifer: $h_{1i}(t)$

head in lower aquifer: $h_{2i}(t)$

Figure 3. Variables used in development of transient-leakage equations for model cell **i**.

Equation (5) describes the initial linear steady-state head distribution across the unit. The variables K'_i, $h'_i(z, t)$, S'_{si}, $h_{2i}(t)$, $h_{1i}(t)$, b'_i, and z_b are defined in figure 3.

The solution to this initial-value problem is given by Carslaw and Jaeger (1959). Using the variables defined here, the solution for head in the confining unit can be written as

$$h'_i(z,t) = 2\sum_{m=1}^{\infty}\frac{1}{m\pi}\sin\frac{m\pi(z-z_b)}{b'_i}\int_0^t\frac{d\eta_{mi}(\tau)}{d\tau}e^{-(m\pi)^2\gamma_i(t-\tau)}d\tau + \frac{h_{1i}(t)-h_{2i}(t)}{b'_i}(z-z_b)+h_{2i}(t), \quad (6)$$

where

$$\eta_{mi}(t) = (-1)^m h_{1i}(t) - h_{2i}(t), \quad (7)$$

and

$$\gamma_i = \frac{K'_i}{b'^2_i S'_{si}}. \quad (8)$$

The leakage rate per unit area at the bottom boundary of the unit, q_{2i}, is $K'_i\,\partial h'_i/\partial z$, evaluated at $z=z_b$. The sign convention for q_{1i} and q_{2i} is that a positive number denotes flow from the confining unit to the aquifer. By differentiating equation (6) with respect to z and evaluating the resulting function at $z=z_b$, q_{2i} at time t_{n+1} can be expressed as

$$q_{2i} = \frac{2K'_i}{b'_i} \sum_{m=1}^{\infty} (-1)^m \int_0^{t_{n+1}} \frac{dh_{1i}(\tau)}{d\tau} e^{-(m\pi)^2 \gamma_i (t_{n+1} - \tau)} d\tau - \frac{2K'_i}{b'_i} \sum_{m=1}^{\infty} \int_0^{t_{n+1}} \frac{dh_{2i}(\tau)}{d\tau} e^{-(m\pi)^2 \gamma_i (t_{n+1} - \tau)} d\tau$$

$$+ \frac{K'_i}{b'_i} [h_{1i}(t_{n+1}) - h_{2i}(t_{n+1})]. \tag{9}$$

To develop an approximation for a leakage term from equation (9) that can be included in the finite-difference equations, the integrals must be evaluated and the infinite series must be approximated. Cooley (1972) developed a procedure for evaluating the integrals at time level $t=t_{n+1}$ using the values of the integrals at time $t=t_n$. This procedure eliminates the need to store the head values for all previous times. For example, the second integral in equation (9) can be approximately evaluated as

$$\int_0^{t_{n+1}} \frac{dh_{2i}(\tau)}{d\tau} e^{-(m\pi)^2 \gamma_i (t_{n+1} - \tau)} d\tau = \int_0^{t_n} \frac{dh_{2i}(\tau)}{d\tau} e^{-(m\pi)^2 \gamma_i (t_n + \Delta t_{n+1} - \tau)} d\tau + \int_{t_n}^{t_{n+1}} \frac{dh_{2i}(\tau)}{d\tau} e^{-(m\pi)^2 \gamma_i (t_{n+1} - \tau)} d\tau$$

$$\approx e^{-(m\pi)^2 \gamma_i \Delta t_{n+1}} \int_0^{t_n} \frac{dh_{2i}(\tau)}{d\tau} e^{-(m\pi)^2 \gamma_i (t_n - \tau)} d\tau + \frac{h_{2i}^{n+1} - h_{2i}^n}{\Delta t_{n+1}} \int_{t_n}^{t_{n+1}} e^{-(m\pi)^2 \gamma_i (t_{n+1} - \tau)} d\tau \tag{10}$$

$$= e^{-(m\pi)^2 \gamma_i \Delta t_{n+1}} \int_0^{t_n} \frac{dh_{2i}(\tau)}{d\tau} e^{-(m\pi)^2 \gamma_i (t_n - \tau)} d\tau + \frac{h_{2i}^{n+1} - h_{2i}^n}{\Delta t_{n+1}} \frac{1}{(m\pi)^2 \gamma_i} \left(1 - e^{-(m\pi)^2 \gamma_i \Delta t_{n+1}}\right),$$

where $h_{2i}^{n+1} = h_{2i}(t_{n+1})$. To develop a recursive relation for updating the integrals, equation (10) is multiplied by 2 for convenience later and the resulting integral is denoted as

$$I_{mi}^{n+1} = 2 \int_0^{t_{n+1}} \frac{dh_{2i}(\tau)}{d\tau} e^{-(m\pi)^2 \gamma_i (t_{n+1} - \tau)} d\tau. \tag{11}$$

Using this notation, the recursive relation is defined as

$$I_{mi}^{n+1} = e^{-(m\pi)^2 \gamma_i \Delta t_{n+1}} I_{mi}^n + \frac{h_{2i}^{n+1} - h_{2i}^n}{\Delta t_{n+1}} \frac{2}{(m\pi)^2 \gamma_i} \left(1 - e^{-(m\pi)^2 \gamma_i \Delta t_{n+1}}\right), \tag{12}$$

where $I_{mi}^0 = 0$. Similarly, $2(-1)^m$ times the first integral in equation (9) is defined as

$$J_{mi}^{n+1} = 2(-1)^m \int_0^{t_{n+1}} \frac{dh_{1i}(\tau)}{d\tau} e^{-(m\pi)^2 \gamma_i (t_{n+1} - \tau)} d\tau. \tag{13}$$

The recursive relation for updating integral J_{mi}^{n+1} is

$$J_{mi}^{n+1} = e^{-(m\pi)^2 \gamma_i \Delta t_{n+1}} J_{mi}^n + \frac{h_{1i}^{n+1} - h_{1i}^n}{\Delta t_{n+1}} \frac{2(-1)^m}{(m\pi)^2 \gamma_i} \left(1 - e^{-(m\pi)^2 \gamma_i \Delta t_{n+1}}\right), \tag{14}$$

where $J^0_{mi} = 0$. With the recursive relations defined in equations (12) and (14), the integrals can be evaluated at time t_{n+1} using the values of the integrals at time t_n and the head values in the adjacent aquifers at times t_{n+1} and t_n.

Solution of equation (9) requires that the infinite series be approximated. As m increases, the absolute values of the series terms decrease. One method of approximation, therefore, is to truncate the series after some specified number of terms. The number of terms needed depends on the values of γ_i and Δt_{n+1}. Many terms might be required for some problems. This approach would be impractical because values of I^n_{mi} and J^n_{mi} must be stored for each term in the series. A better approach taken by Cooley (1992) is to approximate the infinite series with a finite series as follows:

$$2\sum_{m=1}^{\infty}\int_0^{t_{n+1}}\frac{dh_{2i}(\tau)}{d\tau}e^{-(m\pi)^2\gamma_i(t_{n+1}-\tau)}d\tau \approx \sum_{m=1}^{N_1}A'_m\int_0^{t_{n+1}}\frac{dh_{2i}(\tau)}{d\tau}e^{-\alpha_m\gamma_i(t_{n+1}-\tau)}d\tau, \qquad (15)$$

and

$$2\sum_{m=1}^{\infty}(-1)^m\int_0^{t_{n+1}}\frac{dh_{1i}(\tau)}{d\tau}e^{-(m\pi)^2\gamma_i(t_{n+1}-\tau)}d\tau \approx \sum_{m=1}^{N_2}B'_m\int_0^{t_{n+1}}\frac{dh_{1i}(\tau)}{d\tau}e^{-\beta_m\gamma_i(t_{n+1}-\tau)}d\tau, \qquad (16)$$

where A'_m, α_m, B'_m, and β_m are coefficients and N_1 and N_2 are the numbers of terms in the finite series. For values of N_1 and N_2, particular values of the coefficients can be determined to minimize the errors that result from using finite series in equation (9).

Using the terms in the finite series, the integral analogous to equation (11) can be defined as

$$\hat{I}^{n+1}_{mi} = A'_m\int_0^{t_{n+1}}\frac{dh_{2i}(\tau)}{d\tau}e^{-\alpha_m\gamma_i(t_{n+1}-\tau)}d\tau. \qquad (17)$$

Using the steps shown in equation (10), the recursive relation for approximately evaluating this integral at time t_{n+1} can be expressed as

$$\hat{I}^{n+1}_{mi} = e^{-\alpha_m\gamma_i\Delta t_{n+1}}\hat{I}^n_{mi} + \frac{h^{n+1}_{2i}-h^n_{2i}}{\Delta t_{n+1}}\frac{A'_m}{\alpha_m\gamma_i}(1-e^{-\alpha_m\gamma_i\Delta t_{n+1}}). \qquad (18)$$

Similarly, the integral analogous to equation (13) is defined as

$$\hat{J}^{n+1}_{mi} = B'_m\int_0^{t_{n+1}}\frac{dh_{1i}(\tau)}{d\tau}e^{-\beta_m\gamma_i(t_{n+1}-\tau)}d\tau \qquad (19)$$

and the recursive relation for approximately evaluating the integral is given by

$$\hat{J}^{n+1}_{mi} = e^{-\beta_m\gamma_i\Delta t_{n+1}}\hat{J}^n_{mi} + \frac{h^{n+1}_{1i}-h^n_{1i}}{\Delta t_{n+1}}\frac{B'_m}{\beta_m\gamma_i}(1-e^{-\beta_m\gamma_i\Delta t_{n+1}}). \qquad (20)$$

A method for determining the appropriate values of the coefficients A'_m, α_m, B'_m, and β_m can be developed by first substituting the finite series in equations (15) and (16) and the approximations given by equations (18) and (20) into the expression for q_{2i} given in equation (9). The resulting expression is most like the corresponding expression with infinite series if the following approximations are used:

$$2\sum_{m=1}^{\infty}\frac{1}{(m\pi)^2}\left(1-e^{-(m\pi)^2\gamma_i\Delta t_{n+1}}\right) \approx \sum_{m=1}^{N_1}\frac{A'_m}{\alpha_m}(1-e^{-\alpha_m\gamma_i\Delta t_{n+1}}), \qquad (21)$$

and

$$2\sum_{m=1}^{\infty}\frac{(-1)^m}{(m\pi)^2}\left(1-e^{-(m\pi)^2\gamma_i\Delta t_{n+1}}\right)\approx\sum_{m=1}^{N_2}\frac{B'_m}{\beta_m}(1-e^{-\beta_m\gamma_i\Delta t_{n+1}})\ . \quad (22)$$

For the best approximation of the flux term, the approximations in equations (21) and (22) should be exact when $\Delta t_{n+1} = 0$ and when $\Delta t_{n+1} \rightarrow \infty$. The first of these conditions helps to give accurate results for small time steps. This condition is automatically fulfilled because both the infinite and finite series are zero when $\Delta t_{n+1} = 0$. According to Herrera and Yates (1977, p. 726-727), the second condition ensures that the correct total yield from storage will be computed for a unit head change that is held indefinitely. If $\Delta t_{n+1} \rightarrow \infty$ in equations (21) and (22), the second condition is satisfied if

$$2\sum_{m=1}^{\infty}\frac{1}{(m\pi)^2}=\frac{1}{3}=\sum_{m=1}^{N_1}\frac{A'_m}{\alpha_m} \quad (23)$$

and

$$2\sum_{m=1}^{\infty}\frac{(-1)^m}{(m\pi)^2}=-\frac{1}{6}=\sum_{m=1}^{N_2}\frac{B'_m}{\beta_m}. \quad (24)$$

To further simplify the notation, Cooley (1992) defined a dimensionless time interval, Δt_D, as $\gamma_i\Delta t_n$. Using that variable, he defined the infinite and finite series in equations (21) and (22) as

$$S_1(\Delta t_D) = 2\sum_{m=1}^{\infty}\frac{1}{(m\pi)^2}(1-e^{-(m\pi)^2\Delta t_D}), \quad (25)$$

$$S_2(\Delta t_D) = 2\sum_{m=1}^{\infty}\frac{(-1)^m}{(m\pi)^2}(1-e^{-(m\pi)^2\Delta t_D}), \quad (26)$$

$$M_1(\Delta t_D) = \sum_{m=1}^{N_1}A_m(1-e^{-\alpha_m\Delta t_D}), \quad (27)$$

and

$$M_2(\Delta t_D) = \sum_{m=1}^{N_2}B_m(1-e^{-\beta_m\Delta t_D}), \quad (28)$$

where

$$A_m = \frac{A'_m}{\alpha_m}, \quad (29)$$

and

$$B_m = \frac{B'_m}{\beta_m}. \quad (30)$$

Both sets of series are functions of Δt_D only and therefore the coefficients A_m, B_m, α_m, and β_m can be obtained by fitting the approximate finite series $M_1(\Delta t_D)$ and $M_2(\Delta t_D)$ to the infinite series $S_1(\Delta t_D)$ and $S_2(\Delta t_D)$ over a range of Δt_D that includes most expected time-element sizes. Cooley (1992) used nonlinear least squares to calculate the coefficients that give the best fit. He used the weighted objective functions

$$SS_1 = \sum_{n=1}^{p_t} \frac{[S_1(\Delta t_D) - M_1(\Delta t_D)]^2}{|S_1(\Delta t_D)|}, \tag{31}$$

and

$$SS_2 = \sum_{n=1}^{p_t} \frac{[S_2(\Delta t_D) - M_2(\Delta t_D)]^2}{|S_2(\Delta t_D)|}, \tag{32}$$

where p_t is the number of Δt_D values used in the fitting process. Cooley (1992) carried out the nonlinear regression with 25 Δt_D values that were set to 1×10^{-6}, 2.5×10^{-6}, 5×10^{-6}, 1×10^{-5}, 2.5×10^{-5}, 5×10^{-5}, ..., 1×10^{2}. The infinite series generally are more difficult to fit at small values of Δt_D than at large values of Δt_D. The weights $1/|S_1(\Delta t_D)|$ and $1/|S_2(\Delta t_D)|$ help to improve the fit at small dimensionless-time intervals. The constraints given by equations 23 and 24 were satisfied by specifying

$$A_{N_1} = \frac{1}{3} - \sum_{m=1}^{N_1-1} A_m, \tag{33}$$

and

$$B_{N_2} = -\frac{1}{6} - \sum_{m=1}^{N_2-1} B_m. \tag{34}$$

The regression parameters, therefore, are N_1 values of α_m and N_1-1 values of A_m for equation (31), and N_2 values of β_m and N_2-1 values of B_m for equation (32).

Cooley (1992) found that good fits of the infinite series could be obtained with $N_1 = 3$ and $N_2 = 2$. Using those numbers of terms, he determined the values of A, α, B, and β shown in table 1. For this study,

Table 1. Values of parameters for finite series M_1 and M_2 that result in the best fit of infinite series S_1 and S_2 for N_1=3 and N_2=2 (from Cooley, 1992)

Parameter in finite series	m		
	1	2	3
A_m	0.26484	0.060019	0.0084740
α_m	13.656	436.53	49538.
B_m	-0.25754	0.090873	—
β_m	10.764	19.805	—

additional work was done to determine parameters for other values of N_1 and N_2. Nonlinear regressions were carried out using the SYSTAT software package (Wilkinson, 1990) to estimate parameters for the M_1 series for values of N_1 of 2, 3, 4, and 5. The parameters and values of the error function, SS_1, are given in table 2. The parameters for $N_1 = 3$ are almost identical to those estimated by Cooley (1992). Note that

Table 2. Values of parameters for finite series M_1 that result in the best fit of infinite series S_1 for values of N_1 of 2, 3, 4, and 5 terms

N_1	Parameter in finite series	m = 1	2	3	4	5	SS_1
2	A_m	0.28681	0.046523	—	—	—	0.019305
	α_m	16.351	1702.5	—	—	—	
3	A_m	0.26487	0.059994	0.0084659	—	—	0.0033526
	α_m	13.658	437.08	49639.	—	—	
4	A_m	0.23760	0.073663	0.018424	0.0036476	—	0.00053538
	α_m	11.464	151.83	3590.2	211280.	—	
5	A_m	0.22439	0.074416	0.025325	0.0073358	0.0018708	0.00008246
	α_m	10.701	94.307	1075.2	17848.	631120.	

increasing the number of terms decreases the error function and provides a better fit of the infinite series, particularly for small values of dimensionless time interval (fig. 4).

A similar analysis was attempted for the M_2 series, but increasing N_2 beyond the value of 2 that Cooley (1992) used did not significantly increase the goodness of fit. A graphical comparison of the S_2 series and M_2 series with two terms (fig. 5) confirms that the two series are virtually the same. The conclusion from this analysis was that no more than two terms are needed in the M_2 series over the range of Δt_D values included in the regression.

A new expression for q_{2i} can be developed using finite series M_1 and M_2. Substituting equations (15), (16), (17), and (19) into equation (9) results in

$$q_{2i} \approx \frac{K'_i}{b'_i}\left(\sum_{m=1}^{N_2} \hat{J}_{mi}^{n+1} - \sum_{m=1}^{N_1} \hat{I}_{mi}^{n+1} + h_{1i}^{n+1} - h_{2i}^{n+1}\right). \tag{35}$$

Substituting equations (18) and (20), the recursive relations for updating the integrals, provides a new expression for q_{2i} at time t_{n+1} that is written in terms of the integrals at time t_n. That expression is

$$q_{2i} \approx \frac{K'_i}{b'_i}\left(1 + \frac{M_2(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}}\right)h_{1i}^{n+1} - \frac{K'_i}{b'_i}\left(1 + \frac{M_1(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}}\right)h_{2i}^{n+1}$$

$$+ \frac{K'_i}{b'_i}\left(\sum_{m=1}^{N_2} e^{-\beta_m \gamma_i \Delta t_{n+1}} \hat{J}_{mi}^{n} - \frac{M_2(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}} h_{1i}^{n} - \sum_{m=1}^{N_1} e^{-\alpha_m \gamma_i \Delta t_{n+1}} \hat{I}_{mi}^{n} + \frac{M_1(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}} h_{2i}^{n}\right). \tag{36}$$

Equation (36) can be included into the finite-difference equations in MODFLOW with some minor adjustments.

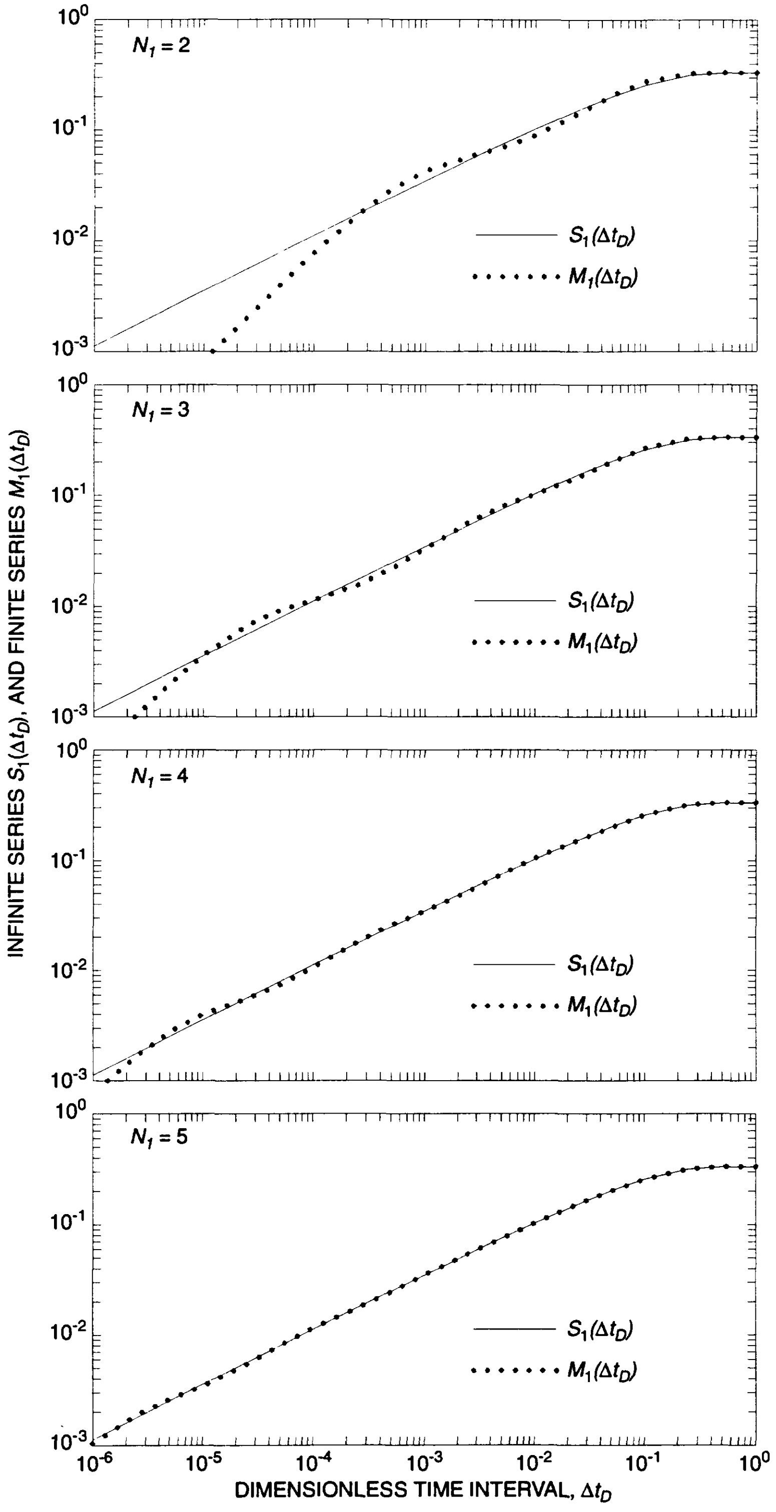


Figure 4. Relation between infinite series $S_1(\Delta t_D)$ and finite series $M_1(\Delta t_D)$ with 2, 3, 4, and 5 terms.

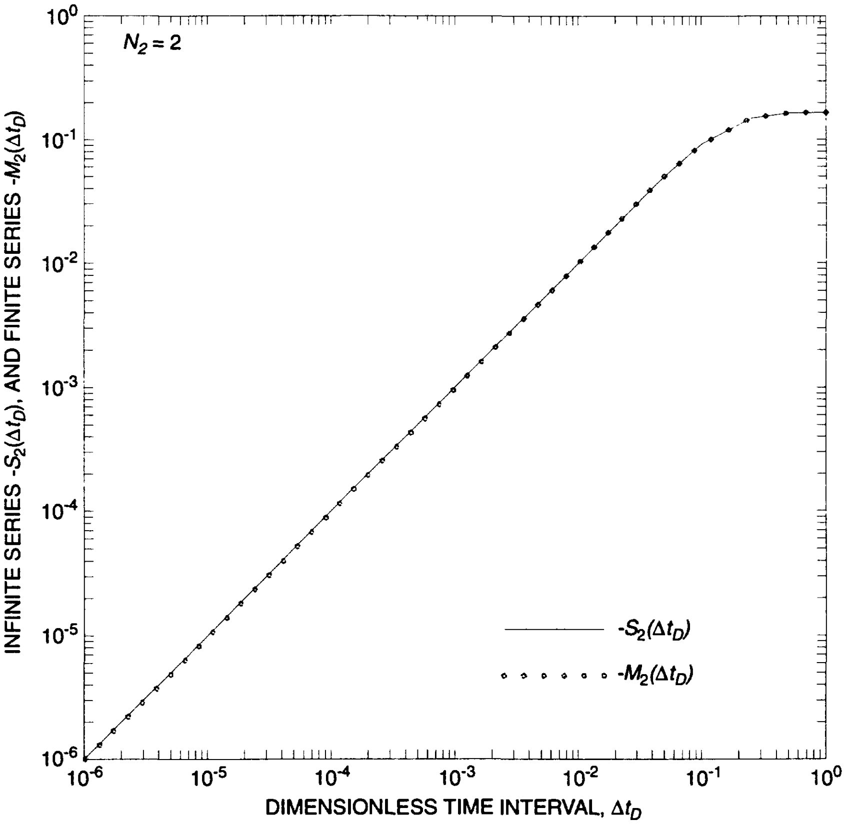


Figure 5. Relation between infinite series $-S_2(\Delta t_D)$ and finite series $-M_2(\Delta t_D)$ with two terms.

An expression similar to equation (36) is needed to describe q_{1i}, flow across the upper boundary of the confining unit. The expression for q_{1i} can be developed by repeating the steps used to develop q_{2i} starting with differentiating equation (6) with respect to z, multiplying by vertical hydraulic conductivity, K'_i, and evaluating the resulting expression at $z=z_b+b_i$. Carrying out the steps outlined for the derivation of q_{2i} in equation (36) results in

$$q_{1i} \approx \frac{K'_i}{b'_i}\left(1+\frac{M_2(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}}\right)h_{2i}^{n+1} - \frac{K'_i}{b'_i}\left(1+\frac{M_1(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}}\right)h_{1i}^{n+1}$$

$$+\frac{K'_i}{b'_i}\left(\sum_{m=1}^{N_2} e^{-\beta_m \gamma_i \Delta t_{n+1}} \hat{L}_{mi}^{n} - \frac{M_2(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}} h_{2i}^{n} - \sum_{m=1}^{N_1} e^{-\alpha_m \gamma_i \Delta t_{n+1}} \hat{K}_{mi}^{n} + \frac{M_1(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}} h_{1i}^{n}\right), \qquad (37)$$

where $\hat{L}_{mi}^{n}$ and $\hat{K}_{mi}^{n}$ are approximate integrals that are analogous to $\hat{J}_{mi}^{n}$ and $\hat{I}_{mi}^{n}$ given in equations (17) and (19). Integral $\hat{K}_{mi}^{n+1}$ is expressed as

$$\hat{K}_{mi}^{n+1} = A'_m \int_0^{t_{n+1}} \frac{dh_{1i}(\tau)}{d\tau} e^{-\alpha_m \gamma_i (t_{n+1}-\tau)} d\tau, \qquad (38)$$

and the recursive relation for evaluating the integral is

$$\hat{K}_{mi}^{n+1} = e^{-\alpha_m \gamma_i \Delta t_{n+1}} \hat{K}_{mi}^{n} + \frac{h_{1i}^{n+1} - h_{1i}^{n}}{\Delta t_{n+1}} \frac{A_m}{\gamma_i} (1 - e^{-\alpha_m \gamma_i \Delta t_{n+1}}) . \tag{39}$$

Similarly, integral $\hat{L}_{mi}^{n+1}$ is expressed as

$$\hat{L}_{mi}^{n+1} = B'_m \int_0^{t_{n+1}} \frac{dh_{2i}(\tau)}{d\tau} e^{-\beta_m \gamma_i (t_{n+1} - \tau)} d\tau , \tag{40}$$

and the recursive relation for evaluating the integral is given by

$$\hat{L}_{mi}^{n+1} = e^{-\beta_m \gamma_i \Delta t_{n+1}} \hat{L}_{mi}^{n} + \frac{h_{2i}^{n+1} - h_{2i}^{n}}{\Delta t_{n+1}} \frac{B_m}{\gamma_i} (1 - e^{-\beta_m \gamma_i \Delta t_{n+1}}) . \tag{41}$$

Equations (36) and (37) are the expressions needed to incorporate transient leakage into the finite-difference equations in MODFLOW. The procedure for formulating the finite-difference equations is described in the following sections.

IMPLEMENTATION OF TRANSIENT LEAKAGE IN THE GROUND-WATER MODEL

The Block-Centered Flow package in MODFLOW (McDonald and Harbaugh, 1988) calculates leakage terms between model layers. The terms are calculated as the product of head difference and vertical hydraulic conductance between the centers of vertically adjacent cells. Resulting calculated flow is referred to here as "steady leakage" because storage changes are ignored for sediments between model layers. If the sediments between model layers are a compressible confining unit, the steady-leakage approach is not necessarily appropriate.

Equations (36) and (37) form the basis for calculations carried out by the TLK1 Package. The formulation of those equations and their implementation in the package assumes that each confining unit is bounded above and below by model layers. The package cannot simulate confining units above the uppermost model layer or below the lowermost model layer; therefore, the number of confining units that the package can simulate is at most one fewer than the number of model layers. The transient-leakage equations do not have to be implemented over the entire horizontal area of the model grid. For a confining unit that pinches out (fig. 1), transient-leakage equations can be used where the confining unit exists and steady-leakage terms that are a standard part of the MODFLOW program can be used where the confining unit is absent. The TLK1 Package reads values of vertical hydraulic conductivity, specific storage, and thickness for each confining unit. If any of these properties are set to zero at a grid location, the confining unit is assumed to be absent and the steady-flow terms in MODFLOW will be used.

Flow calculations in the TLK1 Package use the M_1 and M_2 series described in equations (27) and (28) and shown on figures 4 and 5. The number of terms in the M_1 series, N_1, has a default value of 3 but any value from 2 to 5 can be used. Higher values result in better approximations of the infinite series for small dimensionless time intervals Δt_D; however, higher values require more computer memory to store values of integrals $\hat{I}_{mi}$, $\hat{J}_{mi}$, $\hat{K}_{mi}$, and $\hat{L}_{mi}$ for the series. The number of terms in the M_2 series is set to 2 and no other values can be used.

Formulation of Finite-Difference Equations

The MODFLOW program solves equation (1) using a block-centered finite-difference scheme. The finite-difference equations are developed by writing continuity equations for each active model cell for which head is unknown. The continuity equation for a model cell is written in terms of volumetric flow and includes terms for flow across each of six cell faces, sources or sinks within the cell, and storage change within the cell.

Modifications to the finite-difference equations in MODFLOW will be presented here for the case in which a confining unit with transient leakage is present between layers *k* and *k*+1 in the finite-difference grid. In their discussions of finite-difference equations for MODFLOW, McDonald and Harbaugh (1988) designate a model cell in the grid at row *i*, column *j*, and layer *k* as cell *i,j,k*. A variable or property for cell *i,j,k* includes these indices as a subscript. For properties that apply between the centers of two adjacent cells, the appropriate row, column, or layer index is incremented or decremented by 1/2. For example, $CV_{i,j,k+1/2}$ is the vertical conductance between the centers of cell *i,j,k*, and cell *i,j,k*+1, directly below. Previous discussions in this report have used the subscript **i** to denote a row and column location for a variable or property in a confining unit. In this discussion, **i** will be used in place of the longer subscript *i,j,k*+1/2 for selected quantities in the transient-leakage equations.

The finite-difference equation given by McDonald and Harbaugh (1988, equation 26) for cell *i,j,k* is

$$CV_{i,j,k-1/2}h^{n+1}_{i,j,k-1} + CC_{i-1/2,j,k}h^{n+1}_{i-1,j,k} + CR_{i,j-1/2,k}h^{n+1}_{i,j-1,k}$$

$$+(-CV_{i,j,k-1/2} - CC_{i-1/2,j,k} - CR_{i,j-1/2,k} - CR_{i,j+1/2,k} - CC_{i+1/2,j,k} - CV_{i,j,k+1/2} + HCOF_{i,j,k})h^{n+1}_{i,j,k} \quad (42)$$

$$+CV_{i,j,k+1/2}h^{n+1}_{i,j,k+1} + CC_{i+1/2,j,k}h^{n+1}_{i+1,j,k} + CR_{i,j+1/2,k}h^{n+1}_{i,j+1,k} = RHS_{i,j,k},$$

where *CV*, *CC*, and *CR* are conductance values between cell *i,j,k* and cells in adjacent layers, columns, and rows in the model grid, respectively; $h^{n+1}_{i,j,k}$ is head in cell *i,j,k* at time t_{n+1}; *HCOF* is the sum of all coefficients of the head value $h^{n+1}_{i,j,k}$; and *RHS* is the sum of all terms that do not include head at time t_{n+1}. The terms included in *HCOF* and *RHS* are given by McDonald and Harbaugh (1988, equation 26). The sign convention for flow rates in equation (42) is positive for flow being added to cell *i,j,k* and negative for flow removed from the cell. Using that convention, flow rates may be added to the left side or subtracted from the right side of the equation.

Formulation for Confined Conditions

Terms for the volumetric rate of flow to or from transient leakage can be derived from equations (36) and (37). Those equations are in terms of flow per unit area and must be converted to volumetric flow rates by multiplying by the cross-sectional area through which water is flowing between the confining unit and cells *i,j,k* and *i,j,k*+1. That area is the product of the width of row *i*, Δy_i (fig. 3), and the width of column *j*, Δx_j, and is denoted here as $A_{\mathbf{i}}$. The equations for volumetric flow can be expressed as

$$Q_{i,j,k+1} = b_{\mathbf{i}}h^{n+1}_{i,j,k} + a_{\mathbf{i}}h^{n+1}_{i,j,k+1} + c_{\mathbf{i}}, \quad (43)$$

and

$$Q_{i,j,k} = b_i h^{n+1}_{i,j,k+1} + a_i h^{n+1}_{i,j,k} + d_i, \tag{44}$$

where $Q_{i,j,k+1}$ and $Q_{i,j,k}$ are flow rates from the confining unit to the lower and upper aquifers, respectively; b_i and a_i are coefficients of head for time step n+1; and c_i and d_i are constants for time step n+1. The coefficients of head can be expressed as

$$b_i = \frac{A_i K'_i}{b'_i}\left(1 + \frac{M_2(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}}\right), \tag{45}$$

and

$$a_i = -\frac{A_i K'_i}{b'_i}\left(1 + \frac{M_1(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}}\right). \tag{46}$$

Constants for time step n+1 in equations (43) and (44) can be expressed as

$$c_i = \frac{A_i K'_i}{b'_i}\left(\sum_{m=1}^{N_2} e^{-\beta_m \gamma_i \Delta t_{n+1}} \hat{J}^n_{mi} - \frac{M_2(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}} h^n_{i,j,k} - \sum_{m=1}^{N_1} e^{-\alpha_m \gamma_i \Delta t_{n+1}} \hat{I}^n_{mi} + \frac{M_1(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}} h^n_{i,j,k+1}\right), \tag{47}$$

and

$$d_i = \frac{A_i K'_i}{b'_i}\left(\sum_{m=1}^{N_2} e^{-\beta_m \gamma_i \Delta t_{n+1}} \hat{L}^n_{mi} - \frac{M_2(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}} h^n_{i,j,k+1} - \sum_{m=1}^{N_1} e^{-\alpha_m \gamma_i \Delta t_{n+1}} \hat{K}^n_{mi} + \frac{M_1(\gamma_i \Delta t_{n+1})}{\gamma_i \Delta t_{n+1}} h^n_{i,j,k}\right). \tag{48}$$

The finite-difference equations for cells i,j,k and i,j,k+1 must be modified to include flow to or from the confining unit. The modifications involve removing existing terms for steady leakage between layers k and k+1 and substituting equations (43) and (44). In the finite-difference equation for cell i,j,k, the term that describes flow between layers k and k+1 is $CV_{i,j,k+1/2}h^{n+1}_{i,j,k+1} - CV_{i,j,k+1/2}h^{n+1}_{i,j,k}$. That term is cancelled and transient leakage is included by setting $CV_{i,j,k+1/2}$ equal to b_i, adding b_i to $HCOF_{i,j,k}$, adding a_i to $HCOF_{i,j,k}$, and subtracting d_i from $RHS_{i,j,k}$. Similarly, the term in the finite-difference equation for cell i,j,k+1 that describes flow between layers k and k+1 is $CV_{i,j,k+1/2}h^{n+1}_{i,j,k} - CV_{i,j,k+1/2}h^{n+1}_{i,j,k+1}$. With $CV_{i,j,k+1/2}$ already set to equal to b_i, transient leakage is included by adding b_i to $HCOF_{i,j,k+1}$, adding a_i to $HCOF_{i,j,k+1}$, and subtracting c_i from $RHS_{i,j,k+1}$. To carry out this procedure, values of a_i, b_i, c_i, and d_i are computed at the beginning of each model time step. For each iteration within a time step, $CV_{i,j,k+1/2}$ is set to equal b_i, values of a_i and b_i are added to $HCOF_{i,j,k}$ and $HCOF_{i,j,k+1}$, d_i is subtracted from $RHS_{i,j,k}$, and c_i is subtracted from $RHS_{i,j,k+1}$.

Corrections for Dewatered Conditions

The formulation in the preceding section is valid as long as head in the underlying aquifer is above the base of the confining unit. If head falls below the confining unit, the leakage through the unit is no longer a function of head in the lower aquifer. McDonald and Harbaugh (1988, chap. 5, p. 19-14) described the calculations for steady vertical flow for the case in which head in the lower aquifer falls below the top of the aquifer or the base of the confining unit (fig. 6). For this situation, the pressure at the base of the confining unit is assumed to be zero and head is assumed to equal $TOP_{i,,j,k+1}$. The correct term for steady

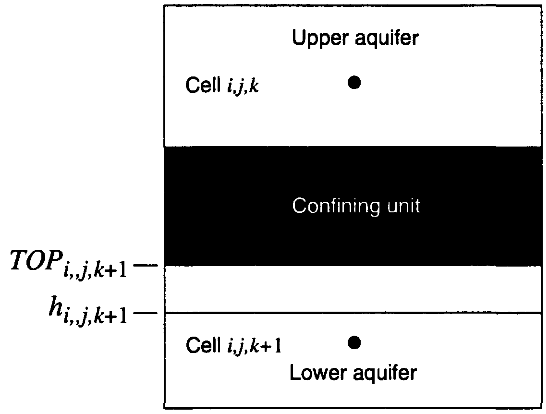


Figure 6. Situation in which a correction is needed to limit the downward flow into cell *i,j,k*+1. (From McDonald and Harbaugh, 1988).

flow across the lower face of cell *i,j,k* is $CV_{i,j,k+1/2}TOP_{i,j,k+1} - CV_{i,j,k+1/2}h^{n+1}_{i,j,k}$ (McDonald and Harbaugh, 1988, equation 56). This term could be substituted into the finite-difference equation for cell *i,j,k*, and the negative of this term could be substituted into the equation for cell *i,j,k*+1 to properly limit the leakage. McDonald and Harbaugh (1988) did not make these substitutions because the replaced terms would cause the coefficient matrix of the system of finite-difference equations to be unsymmetric. Solution with the unsymmetric coefficient matrix would be more difficult than solution with the existing symmetric matrix.

For cells *i,j,k*, and *i,j,k*+1, McDonald and Harbaugh (1988) retain the symmetry of the coefficient matrix by leaving existing flow terms on the left sides of the finite-difference equations and adding correction terms to the right sides. The correction term for cell *i,j,k*, $\Delta Q_{i,j,k}$, is the difference between the computed flow rate without limiting leakage and the "actual" flow rate using the correct leakage. The term is

$$\Delta Q_{i,j,k} = (CV_{i,j,k+1/2}h^{n+1}_{i,j,k+1} - CV_{i,j,k+1/2}h^{n+1}_{i,j,k}) - (CV_{i,j,k+1/2}TOP_{i,j,k+1} - CV_{i,j,k+1/2}h^{n+1}_{i,j,k})$$

$$= CV_{i,j,k+1/2}h^{n+1}_{i,j,k+1} - CV_{i,j,k+1/2}TOP_{i,j,k+1}. \qquad (49)$$

The procedure used in MODFLOW is to add the correction term to the right side of the finite-difference equation for cell *i,j,k* ($RHS_{i,j,k}$) whenever $h^{n+1}_{i,j,k+1}$ falls below $TOP_{i,j,k}$. Because $\Delta Q_{i,j,k}$ includes unknown head $h^{n+1}_{i,j,k+1}$, the term must be updated every iteration using the most recently computed head value.

When $h^{n+1}_{i,j,k+1}$ falls below $TOP_{i,j,k}$, a correction also must be added to the equation for cell *i,j,k*+1. The correction term is

$$\Delta Q_{i,j,k+1} = (CV_{i,j,k+1/2}h^{n+1}_{i,j,k} - CV_{i,j,k+1/2}h^{n+1}_{i,j,k+1}) - (CV_{i,j,k+1/2}h^{n+1}_{i,j,k} - CV_{i,j,k+1/2}TOP_{i,j,k+1})$$

$$= CV_{i,j,k+1/2}TOP_{i,j,k+1} - CV_{i,j,k+1/2}h^{n+1}_{i,j,k+1}. \qquad (50)$$

This term could be added to the right side of the finite-difference equation as was done for cell *i,j,k*; however, McDonald and Harbaugh (1988) noted that the coefficient of head in equation (50) can be included as part of the main diagonal of the coefficient matrix without destroying the symmetry of the matrix. They implemented the correction term by adding $CV_{i,j,k+1/2}$ to $HCOF_{i,j,k+1}$ and adding $CV_{i,j,k+1/2}TOP_{i,j,k+1}$ to $RHS_{i,j,k+1}$.

In the development of a preconditioned conjugate-gradient solver for MODFLOW, Hill (1990) found that the above procedure for cell *i,j,k*+1 can result in a coefficient matrix that is not diagonally dominant. Under this circumstance, the solver might not converge. Hill suggested that the correction be made by adding equation (50) to $RHS_{i,j,k+1}$, and she included necessary changes to subroutine BCF1FM of MODFLOW (Hill, 1990, p. 15). A.W. Harbaugh (U.S. Geological Survey, oral commun., 1993) indicated that the changes implemented by Hill (1990, p. 15) will be incorporated in any future releases of MODFLOW. The following development of corrections for transient-leakage components assumes that the modifications suggested by Hill (1990, p. 15) have been made to the MODFLOW program.

The corrections for the transient-leakage equation needed for dewatered conditions can be derived by replacing $h^{n+1}_{i,j,k+1}$ with $TOP_{i,j,k+1}$ in equations (43) and (44). The resulting expressions are

$$Q_{i,j,k+1} = b_i h^{n+1}_{i,j,k} + a_i TOP_{i,j,k+1} + c_i, \tag{51}$$

and

$$Q_{i,j,k} = b_i TOP_{i,j,k+1} + a_i h^{n+1}_{i,j,k} + d_i. \tag{52}$$

The same strategy used by McDonald and Harbaugh (1988) for correcting the steady-leakage components can be used to correct the transient-leakage components. The correction term for cell *i,j,k* can be derived by subtracting equation (52) from equation (44). The resulting expression is

$$\Delta Q_{i,j,k} = b_i h^{n+1}_{i,j,k+1} + a_i h^{n+1}_{i,j,k} + d_i - (b_i TOP_{i,j,k+1} + a_i h^{n+1}_{i,j,k} + d_i)$$

$$= b_i h^{n+1}_{i,j,k+1} - b_i TOP_{i,j,k+1}. \tag{53}$$

Equation (53) is the same correction that MODFLOW makes for steady leakage components in equation (49) because the TLK1 Package sets $CV_{i,j,k+1/2}$ equal to b_i. The correction outlined by equations (49) and (53) is made in the Block-Centered Flow package in MODFLOW and additional corrections in the TLK1 Package are not needed.

The correction term for cell *i,j,k*+1 can be derived by subtracting equation (51) from equation (43). The resulting expression is

$$\Delta Q_{i,j,k+1} = (b_i h^{n+1}_{i,j,k} + a_i h^{n+1}_{i,j,k+1} + c_i) - (b_i h^{n+1}_{i,j,k} + a_i TOP_{i,j,k+1} + c_i)$$

$$= a_i h^{n+1}_{i,j,k+1} - a_i TOP_{i,j,k+1}. \tag{54}$$

This term is not the same as the correction term applied by the Block-Centered Flow package in MODFLOW. The TLK1 Package therefore must cancel the correction term carried out by the Block-Centered Flow package and apply the correction term for transient leakage. The final correction term, $\Delta\hat{Q}_{i,j,k+1}$, to be added to the right side of the finite-difference equation for cell *i,j,k*+1 can be derived by subtracting equation (50) from equation (54). Using b_i in place of $CV_{i,j,k+1/2}$ in equation (50), the resulting expression is

$$\Delta\hat{Q}_{i,j,k+1} = (a_i h^{n+1}_{i,j,k+1} - a_i TOP_{i,j,k+1}) - (b_i TOP_{i,j,k+1} - b_i h^{n+1}_{i,j,k+1})$$

$$= (TOP_{i,j,k+1} - h^{n+1}_{i,j,k+1})\,(a_i + b_i)\,. \qquad (55)$$

This correction term is applied each iteration in the formulation of finite-difference equations for cells in which head is below the base of the confining unit.

Terms in c_i and d_i (equations (47) and (48)) include head in the layer below the confining unit. Also, terms in integrals $\hat{I}_{mi}$ and $\hat{L}_{mi}$ (equations (18) and (41)) include head in the layer below the confining unit. If head in that layer falls below the base of the confining unit in time step n, the TLK1 Package replaces head with the appropriate value of TOP for calculations of c_i, d_i, $\hat{I}_{mi}$, and $\hat{L}_{mi}$ for time step n+1.

Water-Budget Calculations

Each package in MODFLOW that adds flow components to finite-difference equations includes a procedure for incorporating the flow components in the water budget for the entire model. The components include flow volumes since the beginning of the simulation and flow rates for each time step. Rates and volumes calculated by the TLK1 Package account for (1) water flowing between boundaries and active model grid cells and (2) storage changes within active model grid cells.

The Transient-Leakage Package calculates flow components across the top and bottom faces of confining units. Flow between the confining unit and overlying or underlying active model cells is considered to be internal and therefore is not accounted for in calculations of inflow and outflow rates and volumes for the entire model. Flow components between a confining unit and overlying or underlying constant-head cells, however, are included in calculations of inflow and outflow rates and volumes for the entire model. For situations in which both underlying and overlying cells are constant head, the intervening confining unit is considered to be outside the active modeled area. In that case, flow components to the constant-head cells and storage changes in the confining unit are not included in the water budget.

The rate of change in storage in a confining unit at each row and column location is calculated for each time step by adding expressions corresponding to equations (36) and (37). This calculation is based on the condition that change in storage is equal to the difference between inflow and outflow to the confining unit. Rates and volumes of storage change for all cell locations and for confining units are summed to get inflow and outflow components of the water budget for the entire model.

For some problems, the preceding method of calculating storage changes in confining units can result in errors in volumes of water taken into or released from storage. The rates across the bottom and top boundaries of confining units are calculated on the basis of head values in the adjacent aquifers at the end of each time step. This formulation is consistent with the fully implicit or backward-difference form of equations in the MODFLOW program (McDonald and Harbaugh, 1988, equation 24). The calculations result in rates of change in storage that most closely approximate the conditions at the end of each time step. The TLK1 Package uses these rates for each time step to calculate change in storage volume for the entire simulation. If head in the aquifers is consistently increasing or decreasing throughout the simulation, then errors from the use of flow rates for the end of each time step can accumulate into an overall error in volume of storage change. The error in storage change is analogous to the error that results from using a rectangle rule for numerical integration (Conte and de Boor, 1972, p. 285-286). However, with the TLK1 Package, the error is likely to diminish with use of larger time steps for early simulation time. Large time steps result in exact representations of the infinite series by the finite series (equations (21) to (24)) and the correct total yield from storage for a head change that is held indefinitely (Herrera and Yates, 1977, p. 726-727). For further discussion of errors in computed storage changes, see section entitled "Problem 1—storage depletion in a multiaquifer system" (page 24).

Changes to the *MODFLOW* Program

To implement the Transient-Leakage Package, the MAIN program of MODFLOW must be modified to call the six modules (subroutines) of the package. The modifications to the MAIN program are the addition of the following six Fortran statements:

Add a new call statement for the TLK1AL module after comment C4 and within the group of statements that calls BCF1AL, WEL1AL, DRN1AL, and other space-allocation modules:

```
      IF(IUNIT(6).GT.0) CALL TLK1AL(ISUM,LENX,NCOL,NROW,NLAY,
     1           LCRAT,LCZCB,LCA1,LCB1,LCALPH,LCBET,LCRM1,LCRM2,LCRM3,
     2           LCRM4,LCTL,LCTLK,LCSLU,LCSLD,NODES1,NM1,NM2,NUMC,
     3           NTM1,ITLKSV,ITLKRS,ITLKCB,ISS,IUNIT(6),IOUT)
```

Add a new call statement for the TLK1RP module after comment C6 and within the group of statements that calls the BCF1RP, SIP1AL, and SOR1AL modules:

```
      IF(IUNIT(6).GT.0) CALL TLK1RP(X(LCRAT),X(LCZCB),X(LCA1),X(LCB1),
     1           X(LCALPH),X(LCBET),X(LCRM1),X(LCRM2),X(LCRM3),X(LCRM4),
     2           NODES1,NM1,NM2,NUMC,NTM1,ITLKRS,DELTM1,X(LCBUFF),
     3           X(LCDELC),X(LCDELR),TLKTIM,NROW,NCOL,IUNIT(6),IOUT)
```

Add a new call statement for the TLK1AD module after the statement that calls the BAS1AD module:

```
      IF(IUNIT(6).GT.0) CALL TLK1AD(X(LCRAT),X(LCZCB),X(LCA1),X(LCB1),
     1           X(LCALPH),X(LCBET),X(LCRM1),X(LCRM2),X(LCRM3),X(LCRM4),
     2           X(LCTL),X(LCTLK),X(LCSLU),X(LCSLD),NM1,NM2,NUMC,NTM1,
     3           DELTM1,X(LCHNEW),X(LCIBOU),X(LCTOP),
     4           NROW,NCOL,NLAY,DELT,TLKTIM,IUNIT(6),IOUT)
```

Add a new call statement for the TLK1FM module after comment C7C2A and within the group of statements that call BCF1FM, WEL1FM, DRN1FM, and other formulation modules:

```
      IF(IUNIT(6).GT.0) CALL TLK1FM(X(LCRAT),X(LCTL),X(LCTLK),X(LCSLU),
     1           X(LCSLD),NUMC,X(LCHNEW),X(LCIBOU),X(LCTOP),X(LCCV),
     2           X(LCHCOF),X(LCRHS),NROW,NCOL,NLAY)
```

Add a new call statement for the TLK1BD module after comment C7C4 and *immediately before* the statement that calls module BCF1BD:

```
      IF(IUNIT(6).GT.0) CALL TLK1BD(X(LCRAT),X(LCTL),X(LCTLK),
     1           X(LCSLU),X(LCSLD),NUMC,ITLKCB,X(LCHNEW),X(LCBUFF),
     2           X(LCIBOU),X(LCTOP),X(LCCV),VBNM,VBVL,MSUM,NCOL,NROW,
     3           NLAY,DELT,KSTP,KPER,ICBCFL,IOUT)
```

Add comment statements and a new call statement for the TLK1OT module immediately before comment C8:

```
C
C7C7----WRITE RESTART RECORDS
C7C7A---WRITE RESTART RECORDS FOR TRANSIENT-LEAKAGE PACKAGE
```

```
      IF(IUNIT(6).GT.0) CALL TLK1OT(X(LCRM1),X(LCRM2),
     1     X(LCRM3),X(LCRM4),NM1,NM2,ITLKSV,DELTM1,TLKTIM,IOUT)
```

Normally, the order of call statements in the MAIN program is unimportant for groups of modules performing the same function for different packages. The exception for the TLK1 Package is that the call to the TLK1BD module must precede the call to the BCF1BD module. The reason for this required order is that both budget modules make use of the CV array in calculations of vertical flow to constant-head cells. The TLK1BD module must use the CV array values for the calculations and enter zero values in the array so that incorrect quantities will not be calculated by the BCF1BD module.

Users of the TLK1 Package also should make sure that the BCF1FM module has been modified in accordance with the changes suggested by Hill (1990). If necessary, these changes can be carried out as follows (Hill, 1990, p. 15):

Replace statements in module BCF1FM

```
C7D-----WITH HEAD BELOW TOP ADD CORRECTION TERMS TO RHS AND HCOF.
      RHS(J,I,K)=RHS(J,I,K) + CV(J,I,K-1)*TOP(J,I,KT)
      HCOF(J,I,K)=HCOF(J,I,K) + CV(J,I,K-1)
  220 CONTINUE
```

with statements

```
C7D-----WITH HEAD BELOW TOP ADD CORRECTION TERMS TO RHS AND HCOF.
C7D-----MODIFIED TO PUT CORRECTION COMPLETELY ONTO RIGHT-HAND SIDE
      RHS(J,I,K)=RHS(J,I,K) + CV(J,I,K-1)*(TOP(J,I,KT)-HTMP)
  220 CONTINUE
```

For details on conditions under which these changes are necessary, see section entitled "Corrections for dewatered conditions," page 15.

The MODFLOW program with the modifications and the six modules for the TLK1 Package must be recompiled into a new executable program. The procedure for compiling the program is not addressed in this report.

APPLICABILITY AND LIMITATIONS

The TLK1 Package provides a relatively accurate and efficient way to simulate transient leakage in confining units between model layers. Before the package is applied for simulation of an aquifer system, users need to determine that (1) the capabilities of the TLK1 Package are needed and (2) the package is applicable to the hydrologic conditions being simulated.

The need for the TLK1 Package depends on the type of simulation being carried out. The package is not needed for any steady-state simulations. A common application in which the capabilities of the TLK1 Package is needed is simulation of transient flow in regional or large-scale aquifer systems. One way to assess the need for simulating transient-leakage components for this application is to compare storage coefficients of confining units (product of specific storage and thickness) with storage coefficients of adjacent aquifers. If the storage coefficients of the confining units are much smaller than those of the aquifers, then transient leakage resulting from storage changes in confining units will be much smaller than storage changes in aquifers.

Another potential application of the package is simulation of small-scale systems such as the radius of influence of a pumped well (see section entitled "Problem 2—Simulation of drawdown from pumping in a two-aquifer system," page 28). In these applications, transient-leakage effects are important immediately after a head change in aquifers and the effects diminish after head in the aquifers stabilizes. For example, Hanshaw and Bredehoeft (1968) presented a solution for one-dimensional flow through a confining unit in response to an instantaneous step change in head, H_0, in one adjacent aquifer and constant head in the other adjacent aquifer. Their solution is given in terms of dimensionless time, which is the product of time since the head change, and γ (equation (8), this report). Most flow from storage in the confining unit occurs between dimensionless-time values of 10^{-2} and 0.5. After a dimensionless time of 0.5, storage change in the confining unit is no longer significant.

Another method of assessing the importance of storage changes in confining units in a ground-water model is to compare results of simulations with and without transient leakage. The storage changes can be judged to be important if the volumes and rates in the budget are not small in relation to the total inflow and outflow rates for the entire model. Similarly, the storage changes are important if their inclusion in a model results in significant changes in computed head or drawdown in the aquifers.

The package is applicable to confining units in which (1) flow is nearly vertical, (2) aquifers are present above and below the confining unit, (3) confining unit properties do not vary vertically, and (4) specific storage of the confining unit is not a function of head. Neuman and Witherspoon (1969) addressed the consequences of the assumption of horizontal flow in aquifers and vertical flow in confining units. They report that errors in direction of flow introduced by the assumption generally are less than 5 percent if the hydraulic conductivities of the aquifers are more than two orders of magnitude greater than that of the confining unit. They indicate that the errors increase with time and decrease with distance from the pumped well.

Item 2 above limits the applicability of the package to the situation in which a confining unit is bounded above and below by aquifers. The TLK1 Package cannot simulate transient leakage in a confining unit that is bounded on the top or bottom by an impermeable boundary. This limitation means that confining units cannot be simulated above the uppermost layer or below the lowermost layer of a ground-water model. Furthermore, if cells above or below a confining unit are inactive, transient-leakage components are not computed. If cells above or below are inactive at the start of a simulation, then no transient-leakage components are computed for the entire simulation. If cells become inactive during the simulation, then transient-leakage components cease when the cells become inactive. An exception to the limitation requiring aquifers above and below each confining unit is the situation in which the confining unit is bounded above by a surface-water body or specified-head source. For that situation, the user could treat all or part of the upper model layer as a specified-head boundary and the TLK1 Package would compute transient leakage between the confining unit and the overlying boundary and between the confining unit and the underlying aquifer.

Leake and Prudic (1991) documented a package for MODFLOW to simulate flow in fine-grained beds in which specific storage is a function of head. Their package is applicable to the situation in which highly compressible interbeds and confining units compact inelastically when sediments are stressed beyond their previous maximum stress. The TLK1 Package cannot be used to simulate flow in confining units in which specific storage is not constant.

The alternative to the TLK1 Package for simulating transient leakage in MODFLOW is the use of model layers to represent the confining unit (McDonald and Harbaugh, 1988, fig. 11). For some problems, that approach might be better than use of TLK1. For example, if horizontal components of flow exist in the confining unit, those components can be simulated by discretizing the confining unit into one or more model layers. Also, use of model layers to simulate confining units might be needed if the model analysis involves particle tracking. The TLK1 Package computes flow rates at the boundaries of confining units but does not compute flow rates within the units. Also, model layers should be used to represent confining units if large areas of adjacent layers are dry or if the water table is within a confining unit.

INPUT INSTRUCTIONS

Input to the Transient-Leakage Package version 1 (TLK1) is read from the unit specified in IUNIT(6).

FOR EACH SIMULATION

TLK1AL

1.	Data:	NUMC	ITLKCB	NTM1	ITLKSV	ITLKRS
	Format:	I10	I10	I10	I10	I10

2. Data: IDCON(NUMC) (Maximum of 40 layers)
   Format: 40I2

TLK1RP

The following two-dimensional arrays are used to specify properties for each confining unit. The TLK1 Package reads NUMC sets of the three arrays (items 3-5). All three arrays are read for the confining unit specified in the first element of IDCON. If more than one confining unit is simulated, sets of three arrays are read for each subsequent confining unit specified in IDCON until properties for each confining unit have been read in.

3. Data: Vhcond(NCOL,NROW)
   Module: U2DREL

4. Data: Thick(NCOL,NROW)
   Module: U2DREL

5. Data: SS(NCOL,NROW)
   Module: U2DREL

Explanation of Fields Used in Input Instructions

NUMC is the total number of confining units with transient leakage simulated in the model.

ITLKCB is a flag and unit number.

If ITLKCB > 0, it is the unit number on which cell-by-cell flow terms will be recorded whenever ICBCFL is set (see McDonald and Harbaugh, 1988, chap. 4, p. 14-15).

If ITLKCB ≤ 0, cell-by-cell flow terms will not be recorded.

NTM1 is the number of terms in the M_1 finite series. If value entered is outside the range of 2 to 5, NTM1 will be set to the default of 3. For further information on the meaning of this term, see discussions of variable N_1 in sections entitled "Mathematical Development" (page 4), and "Implementation of Transient Leakage in the Ground-Water Model" (page 13).

ITLKSV is a flag and unit number.

If ITLKSV > 0, it is the unit number on which the restart record will be written for use by a later simulation.

If ITLKSV ≤ 0, a restart record will not be written.

ITLKRS is a flag and unit number.

If ITLKRS > 0, it is the unit number on which the restart record from a previous record will be read.

If ITLKRS ≤ 0, a restart record will not be read.

IDCON is an array that specifies the model layer for each of NUMC confining units with transient leakage. The value specified is layer number of the overlying model layer. For example, if the first confining unit with transient-leakage properties is between model layers 2 and 3, a value of 2 is specified for the first element of IDCON. The confining-unit identifier must be specified in ascending order.

Transient-leakage properties (vertical hydraulic conductivity, thickness, and specific storage) are specified in arrays, Vhcond, Thick, and SS. If a value of zero or less is entered for any element of the Vhcond, Thick, or SS arrays, TLK1 does not carry out transient-leakage calculations at the corresponding row and column location in the finite-difference grid. Instead, steady leakage will be calculated using the value of Vcont read by the Block-Centered Flow Package. For cells in which transient-leakage calculations are carried out, the value of Vcont is ignored.

Vhcond is the vertical hydraulic conductivity of the confining units with transient leakage.

Thick is the thickness of confining units with transient leakage.

SS is the specific storage of the confining units with transient leakage.

PROGRAM OUTPUT

Standard program output from the TLK1 Package consists of flow rates and volumes included in the overall volumetric budget. The budget is printed by MODFLOW and includes flow rates and volumes for all flow-component and stress packages used in a simulation. For the TLK1 Package, two flow components are included in the volumetric budget. The first component is storage change for all confining units with transient leakage. Entries in the budget for this component are designated "`C.B. STORAGE`." Values for storage change in confining units are included for total net inflow and total net outflow. Also, values are given for the net volume of storage change since the start of the simulation and for the volumetric rate of storage change over the most recent time step. The sign convention for storage change in confining units is the same as is used for storage changes computed by the Block-Centered Flow Package. If head declines, the release of water from storage is treated as a component of inflow in the budget. If head increases, the storage change is treated as a component of outflow. The TLK1 Package also includes flow from confining units to constant-head cells as inflow and outflow components in the budget. Those components are designated "`C.H. LEAKAGE`." If both overlying and underlying cells are constant-head cells, the TLK1 Package treats that part of the confining unit as being outside of the active modeled area. Storage changes and constant-head flow rates will not be included in the budget for that area.

The TLK1 Package also can record cell-by-cell flow rates for any or all model time steps. The flow components are storage change in the confining unit, flow across the top face of the confining unit, and flow across the bottom face of the confining unit. Unformatted records that include all values of each flow component are written with module ULASAV using the identifiers given in table 3. Each record includes a value for each cell in the model grid. The flow components are recorded in the location of the model cell overlying the confining unit. Zero values are recorded for cell locations with no underlying confining unit.

Table 3. Identifiers for cell-by-cell flow components

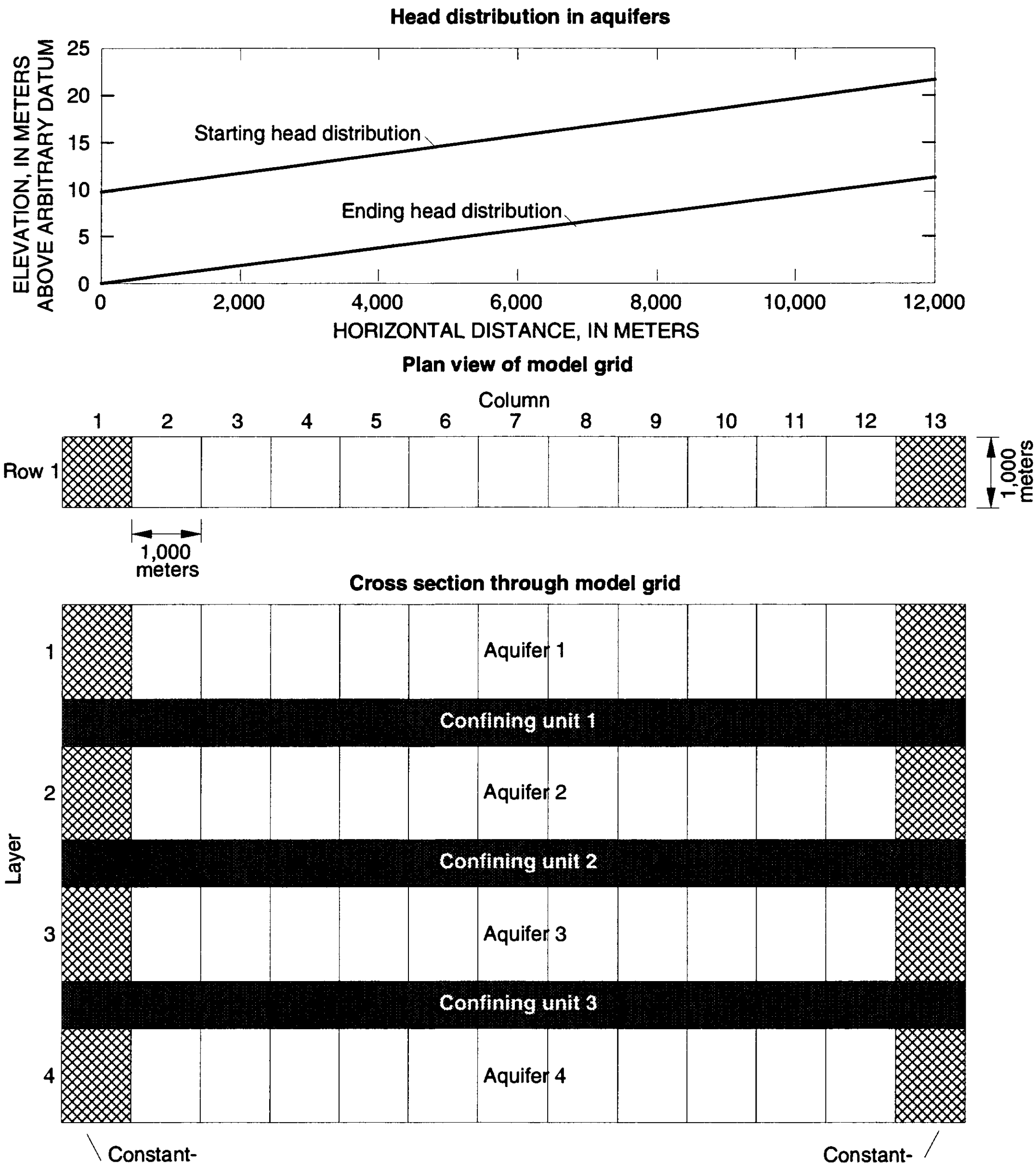
Flow Component	Identifier
Storage change in the confining unit	`C.B. STORAGE`
Flow across top face of the confining unit	`FLOW IN TOP`
Flow across bottom face of the confining unit	`FLOW IN BASE`

EXAMPLE PROBLEMS

Two example problems are presented to illustrate data input and program output of the TLK1 Package. Another purpose of the example problems is to demonstrate the validity of results from the TLK1 Package. In the first example problem, the ultimate or long-term volume of storage change in two confining units is calculated using the TLK1 Package. That value is compared with the exact manually calculated volume. In the second example problem, drawdown around a pumped well is calculated in a two-aquifer system with a single confining unit. The values are compared with results from an exact analytical solution.

Problem 1—Simulation of Storage Depletion in a Multiaquifer System

Example problem 1 illustrates use of the TLK1 Package in a ground-water flow system with four aquifers and three confining units (fig. 7). In response to head changes, transient leakage can occur in the upper and lower confining units. Storage changes in the middle confining unit are assumed to be small; therefore, steady-leakage components through that unit can be simulated using the Block-Centered Flow Package.



Properties for aquifers 1, 2, 3, and 4

Transmissivity:	2,500 meters squared per day
Storage coefficient:	2×10^{-4}

Properties for confining units

	Confining units 1 and 3	Confining unit 2
Vertical hydraulic conductivity:	1×10^{-2} meters per day	1×10^{-2} meters per day
Specific storage:	1×10^{-5} per meter	0 per meter
Thickness:	25 meters	25 meters

Figure 7. Head distribution, model grid, boundary conditions, aquifer properties, and confining-unit properties for problem 1.

The problem simulates flow in a cross section with no initial vertical gradients and an initial horizontal gradient of 0.001 in all aquifers. Horizontal gradients are specified by initial head values for cells in four model layers representing the aquifers. The first and last cells in each layer are constant-head boundaries that are set to 10 m below the starting head distribution. That configuration results in an instantaneous head drop of 10 m at the lateral edges of the system at the start of the simulation. Subsequently, head will decline in all four aquifers and water will be released from storage in the aquifers and in the upper and lower confining units. Input data sets for the TLK1 Package and other MODFLOW packages are given in the appendix.

The problem used a value of 3 for NTM1. After sufficient simulation time, heads throughout the aquifer system will decline by 10 m and a new steady-state flow system will be established. For the aquifer and confining-unit properties shown on figure 7, a new steady-state condition is established within 100 days of the initial change in boundary conditions. Simulation of 100 days with 40 equal time steps of 2.5 days in length results in the volumetric balance shown in table 4. The calculated volume of inflow of water from storage is 88,000 m^3 for all four aquifers and 54,998 m^3 for both confining units with transient leakage.

Because head change and storage properties are known, the volume of water released from storage in the aquifers and confining units can be calculated manually. Change in storage, ΔS, can be computed as

$$\Delta S = A S_s b \Delta h, \tag{56}$$

where A is area over which head change, Δh, occurs, S_s is specific storage, and b is thickness of sediments. For the aquifers in this problem, the storage coefficient can be substituted for $S_s b$ in equation (56). Head change is zero at constant head cells and therefore the area over which the head change of -10 m occurs is 1,000 m by 11,000 m or 1.1×10^7 m^2. Using equation (56), the change in storage for each aquifer is computed as $(1.1\times10^7\ m^2)(2\times10^{-4})(-10\ m)$ or -2.2×10^4 m^3, and the storage change for all four aquifers is -8.8×10^4 m^3. The model-calculated inflow from storage of 88,000 m^3 (table 4) agrees with the manually calculated value of storage change in the four aquifers.

The confining units extend between constant-head boundary cells at the edges of the each aquifer (fig. 7). The TLK1 Package, however, ignores calculations for parts of confining units with constant-head cells in overlying and underlying cells. Therefore, the area over which the head decline occurs in confining units is 1.1×10^7 m^2. Storage change in each confining unit is $(1.1\times10^7\ m^2)(1\times10^{-5}\ m^{-1})(25\ m)(-10\ m)$ or -2.75×10^4 m^3. The storage change for both confining units with transient leakage is -5.5×10^4 m^3. The model-calculated inflow from storage of 54,998 m^3 (table 4) is nearly identical to this manually calculated value.

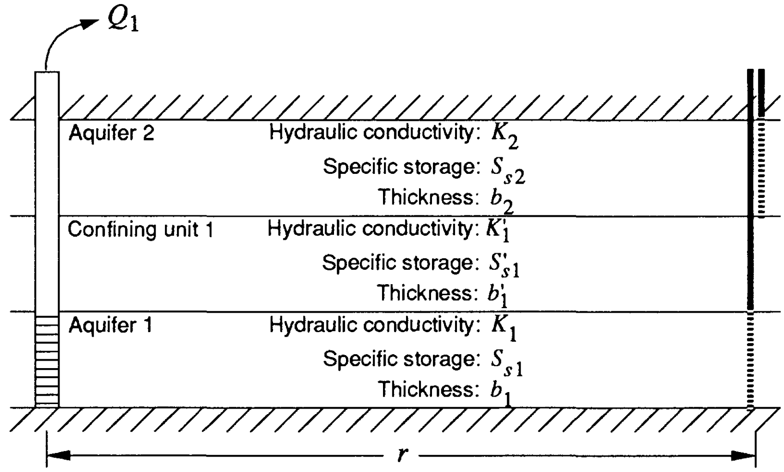
The confining unit properties selected for this problem result in a value of $\gamma_{\mathbf{i}}$ of 1.6 day^{-1} (equation (8)) for all locations **i**. Use of this $\gamma_{\mathbf{i}}$ with time steps of 2.5 days results in dimensionless time intervals, Δt_D, of 4.0 for each of the 40 time steps. That value of Δt_D is in the range of values in which the approximate M_1 series matches the exact S_1 series regardless of the number of terms used in the M_1 series (fig. 4). Use of smaller time steps will result in a less accurate approximation of the total storage change. To test the effect of time step length and variation on the results, the data sets were modified to simulate the 100-day period with 40 successive time steps that expand by a factor of 1.5. That expansion factor results in an initial time step of 4.52×10^{-6} days and a final time step of 33.3 days. With this series of time steps, inflow from storage in confining units computed by the model is 53,401 m^3, which is in error by about 3 percent. The deviation of the computed storage from the true value of 55,000 m^3 is result of the implicit formulation of the TLK1 Package in which rates of storage change at the end of each time step are used to calculate storage volumes. Increasing the number of terms in the M_1 series does not reduce the error in computed storage change for this problem.

Table 4. Volumetric budget from simulation of problem 1

```
          VOLUMETRIC BUDGET FOR ENTIRE MODEL AT END OF TIME STEP 40 IN STRESS PERIOD  1
          ----------------------------------------------------------------------------

     CUMULATIVE VOLUMES      L**3            RATES FOR THIS TIME STEP      L**3/T
     ------------------                      ------------------------

               IN:                                      IN:
               ---                                      ---
        C.B. STORAGE =    54998.                 C.B. STORAGE =   0.00000
        C.H. LEAKAGE =   0.00000                 C.H. LEAKAGE =   0.00000
             STORAGE =    88000.                      STORAGE =   0.00000
       CONSTANT HEAD =   0.94736E+06            CONSTANT HEAD =    10000.

            TOTAL IN =   0.10904E+07                 TOTAL IN =    10000.

              OUT:                                     OUT:
              ----                                     ----
        C.B. STORAGE =    2.3366                 C.B. STORAGE =   0.39971E-01
        C.H. LEAKAGE =   0.00000                 C.H. LEAKAGE =   0.00000
             STORAGE =   0.00000                      STORAGE =   0.00000
       CONSTANT HEAD =   0.10904E+07            CONSTANT HEAD =    10000.

           TOTAL OUT =   0.10904E+07                TOTAL OUT =    10000.

            IN - OUT =  -0.50000                     IN - OUT =  -0.78125E-02

     PERCENT DISCREPANCY =              0.00     PERCENT DISCREPANCY =              0.00
```

Problem 2—Simulation of Drawdown from Pumping in a Two-Aquifer System

Problem 2 demonstrates application of the TLK1 Package to simulate drawdown in a system with two aquifers separated by a confining unit (fig. 8). Pumping from one of the aquifers can cause drawdown in both aquifers and in the confining unit. For idealized conditions such as homogeneous aquifer and confining-unit properties, Neuman and Witherspoon (1969) developed an analytical solution for drawdown, s, in the system. Their solution provides a standard for comparison of results of drawdown calculations in a model that uses the TLK1 Package to simulate flow and storage changes in the confining unit.



DIMENSIONLESS VARIABLES

$$t_{D1} = \frac{K_1 t}{S_{s1} r^2} \qquad s_{D1} = \left(\frac{4\pi K_1 b_1}{Q_1}\right) s$$

$$\beta_{11} = \frac{K'_1\, r}{4K_1 b_1}\left(\frac{K_1 S'_{s1}}{S_{s1} K'_1}\right)^{1/2} \qquad \beta_{21} = \frac{K'_1\, r}{4K_2 b_2}\left(\frac{K_2 S'_{s1}}{S_{s2} K'_1}\right)^{1/2}$$

$$\frac{r}{B_{11}} = \frac{r}{b_1}\left(\frac{K'_1\, b_1}{b'_1\, K_1}\right)^{1/2} \qquad \frac{r}{B_{21}} = \frac{r}{b_2}\left(\frac{K'_1\, b_2}{b'_1\, K_2}\right)^{1/2}$$

Figure 8. Conceptual model and dimensionless variables for analytical solution for drawdown in a two-aquifer system (Neuman and Witherspoon,1969).

Problem 2 is based on the analytical solution given in figure 3 of Neuman and Witherspoon (1969). Aquifer and confining-unit properties and results of the analytical solution are specified in terms of dimensionless variables shown in figure 8. The dimensionless variables that specify aquifer and confining-unit properties are $\beta_{11} = \beta_{21} = r/B_{11} = r/B_{21} = 0.1$. The value of 0.1 for the dimensionless variables can be achieved with different combinations of aquifer and confining-unit properties. To implement this problem using MODFLOW with the TLK1 Package, radial distance from the well, r, was 100 m; hydraulic conductivity of aquifers 1 and 2, K_1 and K_2, were 500 m/d; specific storage of aquifers 1 and 2, S_{s1} and S_{s2}, were 5×10^{-6} m^{-1}; thickness of aquifers 1 and 2, b_1 and b_2, were 5 m; hydraulic conductivity of confining unit 1, K'_1, was 0.01 m/d; specific storage of confining unit 1, S'_{s1}, was 1×10^{-4} m^{-1}; and thickness of confining unit 1, b'_1, was 4 m. The value for pumpage, Q_1, was 3.14×10^4 m^3/d. With those values, the relation between dimensionless time, t_{D1}, and time, t, is $t_{D1} = 10^4 t$; and the relation between dimensionless drawdown, s_{D1}, and drawdown, s, is $s_{D1} = s$.

Because flow to the well is radially symmetric, results can be obtained by simulating only one of the four quadrants of area around the well. Data sets for MODFLOW were constructed to simulate the area shown in figure 9A. The model grid includes two layers; the upper layer represents aquifer 2 and the lower layer represents aquifer 1. The upper-left corner of the grid is row 1 and column 1 and is the location of the pumped well (fig. 9B). The grid dimensions are 1 m by 1 m, and subsequent rows and columns expand by a factor of about 1.5. With 30 rows and 30 columns in the grid, the lateral dimensions of the flow region are about 2×10^5 m by 2×10^5 m. The large dimensions of the flow region approximate an infinite aquifer for simulated responses in cells near the pumped well. One-fourth of the total pumpage or 7.85×10^3 m^3/d was simulated at the pumping well location. The model cell in row 10, column 10, is 100 m from the pumped well and the computed drawdown there can be used for comparison with the analytical solution shown in figure 3 of Neuman and Witherspoon (1969).

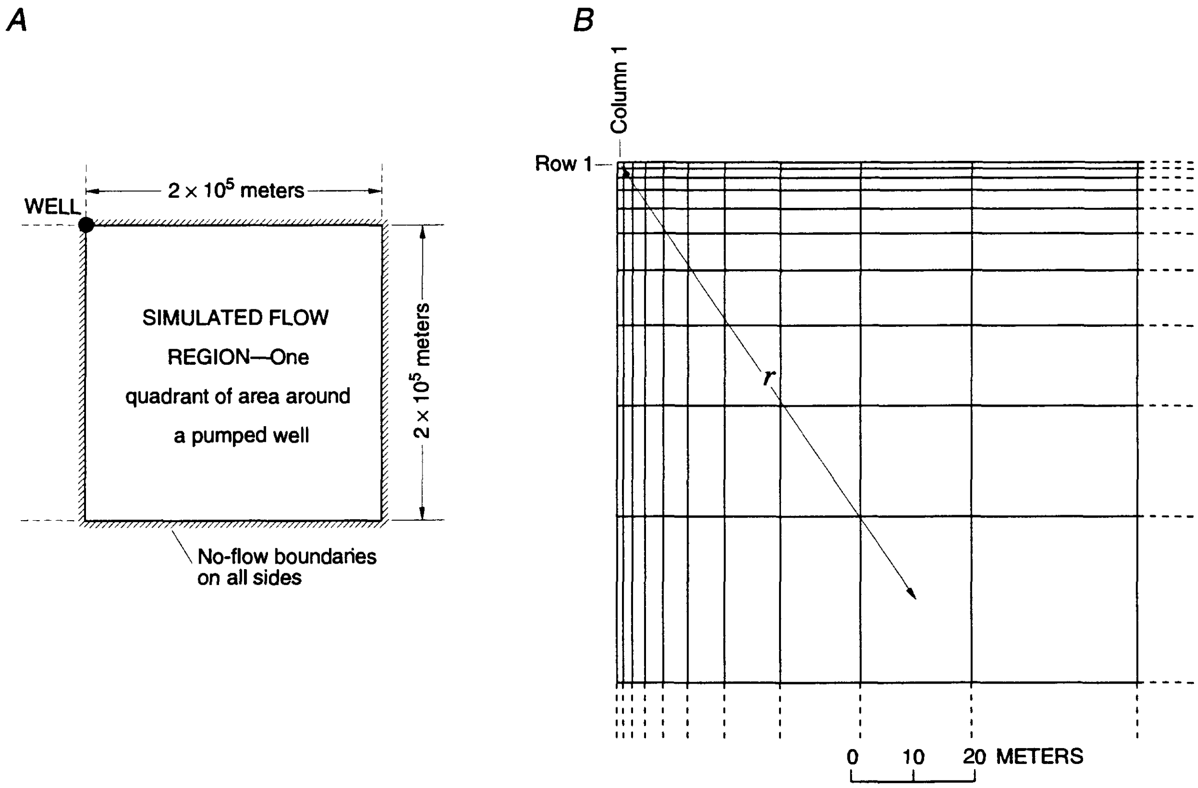


Figure 9. Modeled area for problem 2. *A*, Dimensions and boundary conditions for quadrant of area around pumped well. *B*, Part of model grid near pumped well.

Values of t_{D1} in figure 3 of Neuman and Witherspoon (1969) range from 10^{-1} to 10^6. With the values of K_1, S_{s1} and r selected for the simulation, the maximum dimensionless time of 10^6 is reached in 100 days of pumping. For this problem, 60 time steps were used with a multiplication factor for successive time steps of 1.5. The default value of three terms in the M_1 series was selected. The results of the simulation in terms of dimensionless time and dimensionless drawdown are shown in figure 10. Values of drawdown for small dimensionless times are in error; however, dimensionless drawdown values in the range of 10^{-2} or greater closely approximate the analytical solution by Neuman and Witherspoon (1969, fig. 3). That range of dimensionless drawdown corresponds to actual drawdown of 1 cm or greater.

The accuracy and computational efficiency of the TLK1 Package can be demonstrated by using the Block-Centered Flow Package (BCF1) instead of the TLK1 Package to simulate flow and storage changes in the confining unit. McDonald and Harbaugh (1988, fig. 11) noted that low-conductivity units such as confining units can be simulated as one or more individual model layers. Use of one model layer to represent a confining unit results in the vertical distribution of head in the unit approximated with a single head value at the center of the unit. Addition of model layers to represent the unit adds detail to the approximation of the head distribution but increases the computation time and storage requirements for the simulation. Two simulations of problem 2 were carried out using the BCF1 Package. The unit was simulated using one model layer for the first simulation and two model layers for a second simulation. Properties of the confining unit for both simulations were specified in the input data sets for the BCF1 Package.

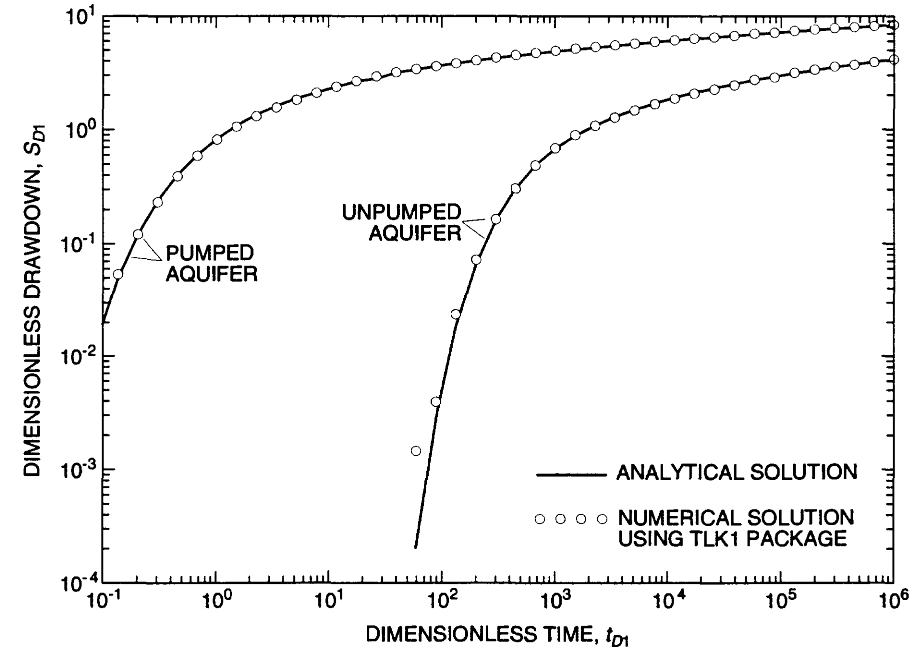


Figure 10. Results of problem 2 using the TLK1 Package to simulate the confining unit.

Results of the simulations using the BCF1 Package deviate from the analytical solutions for the pumped and unpumped aquifers at early dimensionless times (fig. 11). Increasing the number of layers representing the confining unit from one to two significantly improves results for early dimensionless times; however, use of two layers does not produce results that are as accurate as results using the TLK1 Package. Increasing the number of layers beyond two probably would result in further improvements in the solution at early dimensionless times. Each added layer, however, increases the computational resources required to carry out the simulation. The computation time and computer storage requirements for the three methods of simulating the problem are presented in table 5. The simulation with TLK1 was significantly faster than either of the simulations using the BCF1 Package. Use of two layers to represent the confining unit required almost twice the computation time as the simulation using the TLK1 Package. Array storage requirements for the TLK1 simulation were between the requirements for the two BCF1 simulations.

In conclusion, simulation of problem 2 with the TLK1 Package results in drawdown that closely matches the analytical solution for drawdown in excess of 1 cm. Similar results might be attainable using the BCF1 Package to simulate the confining unit; however, more than two model layers would be needed to represent flow in the confining unit. The computation time and storage requirements using two layers are significantly greater than time and storage requirements using the TLK1 Package.

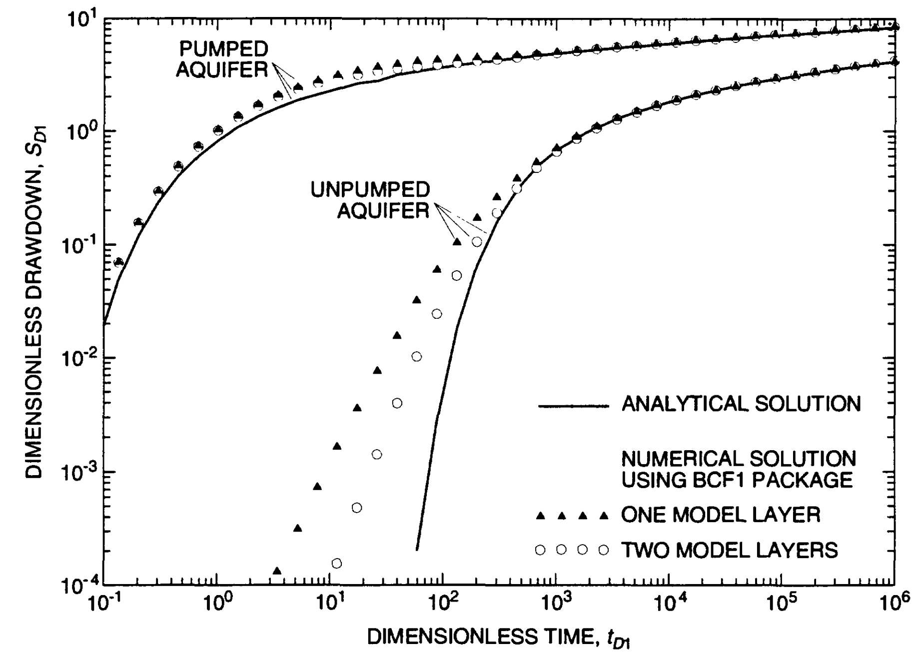


Figure 11. Results of problem 2 using the BCF1 Package with one and two model layers to simulate the confining unit.

Table 5. Computation time and storage requirements for solution of problem 2 using three different methods of simulating the confining unit

Method of simulating confining unit	Computation time, in seconds[1]	Storage requirements, in elements of X array[2]
TLK1 Package with three terms in M_1 series	254	16
BCF1 Package with one model layer to simulate confining unit	344	11
BCF1 Package with two model layers to simulate confining unit	501	22

[1] Simulations were carried out on a Data General AViiON AV/300D computer.

[2] Storage requirements are in terms of single-precision real numbers stored in the X array of MODFLOW. Values given are additional array elements needed for the confining unit per model row and column.

MODULE DOCUMENTATION

The Transient-Leakage Package (TLK1) contains six modules (subroutines). Each of the six modules is called by the main program of MODFLOW. Required changes to the main program are given in the section entitled "Changes to the MODFLOW program" (page 19). The modules in the TLK1 Package are

TLK1AL Reads package options and flags and allocates space for data arrays.

TLK1RP Reads arrays of hydraulic conductivity, thickness, and specific storage for each confining unit; reads restart record if restart option is selected; initializes arrays containing cumulative memory functions; computes time constants; and selects constants for M_1 and M_2 series.

TLK1AD Updates cumulative memory functions for each time step, and computes coefficients and terms in equations for flow at top and bottom of confining unit for each time step.

TLK1FM Formulates terms for the finite-difference equations, sets vertical conductance array elements to the appropriate term, and adds terms to the main diagonal of the head-coefficient matrix (HCOF) and to the right-hand-side matrix (RHS).

TLK1BD Computes flow rates and cumulative storage changes for all confining units and writes cell-by-cell flow rates if option is selected.

TLK1OT Writes a restart record containing cumulative memory arrays if option is selected.

The last two characters in the names of each of the modules are an abbreviation for the procedure that the module carries out. Most flow-component and stress packages in MODFLOW use only four procedures—Allocate (AL), Read and Prepare (RP), Formulate (FM), and Budget (BD) (table 6). In addition to these basic procedures, the TLK1 Package uses the Advance procedure (AD) to calculate terms in the equations that are held as constants within each time step and the Output (OT) procedure to save information for continuation of a model run.

Table 6. Primary modules of MODFLOW organized by procedure and package (modified from McDonald and Harbaugh, 1988, fig. 15)

Procedure	Packages										
	BAS1	BCF1	WEL1	RCH1	RIV1	DRN1	EVT1	GHB1	SIP1	SOR1	TLK1
Define (DF)	BAS1DF										
Allocate (AL)	BAS1AL	BCF1AL	WEL1AL	RCH1AL	RIV1AL	DRN1AL	EVT1AL	GHB1AL	SIP1AL	SOR1AL	TLK1AL
Read and prepare (RP)	BAS1RP	BCF1RP							SIP1RP	SOR1RP	TLK1RP
Stress (ST)	BAS1ST										
Read and prepare (RP)			WEL1RP	RCH1RP	RIV1RP	DRN1RP	EVT1RP	GHB1RP			
Advance (AD)	BAS1AD										TLK1AD
Formulate (FM)	BAS1FM	BCF1FM	WEL1FM	RCH1FM	RIV1FM	DRN1FM	EVT1FM	GHB1FM			TLK1FM
Approximate (AP)									SIP1AP	SOR1AP	
Output Control (OC)	BAS1OC										
Budget (BD)		BCF1BD	WEL1BD	RCH1BD	RIV1BD	DRN1BD	EVT1BD	GHB1BD			TLK1BD
Output (OT)	BAS1OT										TLK1OT

TLK1AL

Narrative for Module TLK1AL

This module reads package options and flags and allocates space in the X array (McDonald and Harbaugh, 1988, chap. 3, p. 22-23) for arrays in the TLK1 Package. Operations are carried out in the following order:

1. Print a message identifying the package.

2. Check to see that transient-leakage option is appropriate.

3. If simulation is steady state, cancel the transient-leakage option and continue the simulation.

4. Read number of confining units, NUMC; unit number for cell-by-cell flow terms, ITLKCB; number of terms in M_1 series, NTM1; and unit numbers for saving and reading restart information, ITLKSV and ITLKRS.

5. If the number of confining units specified for simulation exceeds the intervals between model layers, stop the simulation.

6. If cell-by-cell flow terms are to be saved, then print unit number.

7. If number of terms in M_1 series, NTM1, is outside the range from 2 to 5, set to a default value of 3.

8. If restart information is to be saved or read, print unit numbers for input and (or) output.

9. For each confining unit, read the number of model layer above the unit.

10. Allocate storage for the following arrays:

RATE	Reciprocal of the time constant of the confining unit,
ZCB	Thickness of the confining unit,
TLK	Coefficient of head in transient-leakage equations,
TL	Coefficient of head in transient-leakage equations,
SLU	Explicit term in equation for flow at top boundary of confining unit, and
SLD	Explicit term in equation for flow at bottom boundary of confining unit.

11. Allocate storage for coefficients in the M_1 and M_2 series in arrays A1, B1, ALPH, and BET.

12. Allocate storage for cumulative memory arrays RM1, RM2, RM3, and RM4.

13. Calculate and print the amount of space used by the TLK1 Package.

14. RETURN.

Flowchart for Module TLK1AL

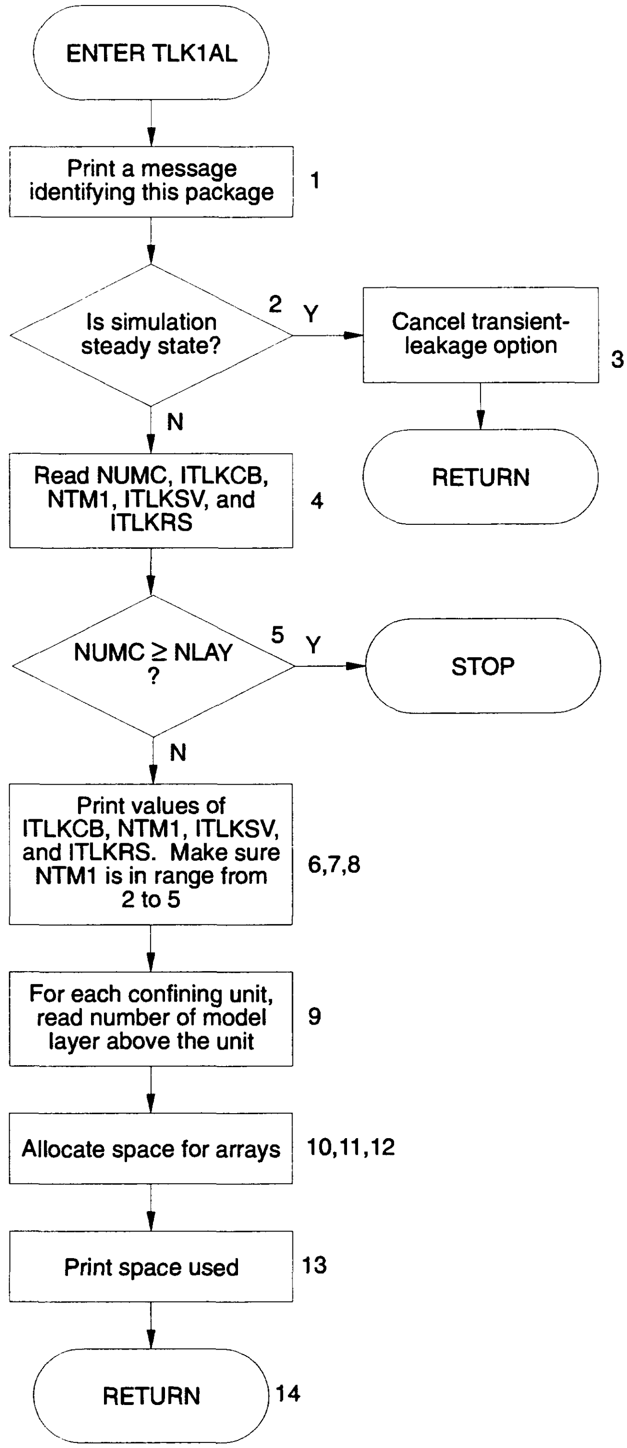
NUMC is the number of confining units.

ITLKCB is the unit number for saving cell-by-cell flow terms.

NTM1 is the number of terms in the M_1 series.

ITLKSV is the unit number for saving restart information.

ITLKRS is the unit number for reading restart information.



Program Listing for Module TLK1AL

```
      SUBROUTINE TLK1AL(ISUM,LENX,NCOL,NROW,NLAY,LCRAT,LCZCB,
     1 LCA1,LCB1,LCALPH,LCBET,LCRM1,LCRM2,LCRM3,LCRM4,LCTL,LCTLK,LCSLU,
     2 LCSLD,NODES1,NM1,NM2,NUMC,NTM1,ITLKSV,ITLKRS,ITLKCB,ISS,IN,IOUT)
C
C-----VERSION 1100 06JAN1994 TLK1AL
C     ******************************************************************
C     ALLOCATE ARRAY STORAGE FOR TRANSIENT LEAKAGE PACKAGE
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      COMMON /FLWCOM/ LAYCON(80)
      COMMON /TLEAK/ IDCON(80),NTOP(80)
C     ------------------------------------------------------------------
C
C1------IDENTIFY PACKAGE
      WRITE(IOUT,1)
    1 FORMAT(1H0,'TLK1--TRANSIENT LEAKAGE PACKAGE, VERSION 1, 04/07/93')
C
C2------CHECK TO SEE THAT TRANSIENT-LEAKAGE OPTION IS APPROPRIATE
      IF(ISS.EQ.0) GO TO 8
C
C3------IF INAPPROPRIATE PRINT A MESSAGE & CANCEL OPTION.
      WRITE(IOUT,5)
    5 FORMAT(1X,'TRANSIENT-LEAKAGE INAPPROPRIATE FOR STEADY-STATE',
     1 ' PROBLEM.',/,1X,'OPTION CANCELLED, SIMULATION CONTINUING.')
      IN=0
      RETURN
C
C4------READ NUMBER OF CONFINING UNITS, FLAG FOR CELL-BY-CELL FLOW
C4------TERMS, NUMBER OF TERMS IN M1 SERIES, AND UNIT NUMBERS FOR
C4------SAVING AND READING RESTART INFORMATION
    8 READ(IN,10) NUMC,ITLKCB,NTM1,ITLKSV,ITLKRS
   10 FORMAT(8I10)
C
C5------IF NUMBER OF CONFINING UNITS EXCEEDS NUMBER OF INTERVALS
C5------BETWEEN MODEL LAYERS, STOP THE SIMULATION
      IF(NUMC.GE.NLAY) THEN
       WRITE(IOUT,20) NUMC
   20  FORMAT(1X,I3,' CONFINING UNITS EXCEED THE MAXIMUM ALLOWABLE FOR',
     1 ' THIS PROBLEM')
       STOP
      ELSE
       WRITE(IOUT,30) NUMC
   30  FORMAT(1X,I3,' CONFINING UNITS INCLUDE TRANSIENT LEAKAGE')
      ENDIF
C
C6------IF CELL-BY-CELL FLOW TERMS ARE TO BE SAVED THEN PRINT UNIT #
      IF(ITLKCB.GT.0) THEN
       WRITE(IOUT,40) ITLKCB
   40  FORMAT(1X,'CELL-BY-CELL FLOWS WILL BE RECORDED ON UNIT',I3)
      ELSE IF(ITLKCB.LT.0) THEN
       WRITE(IOUT,50)
```

```
   50  FORMAT(1X,'CELL-BY-CELL FLOWS WILL BE PRINTED WHEN ICBCFL NOT 0')
      ELSE
       WRITE(IOUT,60)
   60  FORMAT(1X,'CELL-BY-CELL FLOWS WILL NOT BE PRINTED OR RECORDED')
      ENDIF
C
C7------IF NTM1 OUTSIDE OF RANGE FROM 2 TO 5, SET TO DEFAULT VALUE OF 3
      IF(NTM1.LT.2.OR.NTM1.GT.5) THEN
       NTM1=3
       WRITE(IOUT,70)
   70  FORMAT(1X,'DEFAULT OF 3 TERMS WILL BE USED IN M1 SERIES')
      ELSE
       WRITE(IOUT,80) NTM1
   80  FORMAT(1X,'NUMBER OF TERMS IN M1 SERIES IS',I2)
      ENDIF
C
C8------IF RESTART INFORMATION IS TO BE SAVED OR READ, PRINT UNIT
C8------NUMBERS
      IF (ITLKSV.GT.0) THEN
       WRITE(IOUT,90) ITLKSV
   90  FORMAT(1X, 'RESTART RECORDS WILL BE SAVED AT END OF SIMULATION',
     1 ' ON UNIT',I4)
      ENDIF
      IF (ITLKRS.GT.0) THEN
       WRITE(IOUT,100) ITLKRS
  100  FORMAT(1X, 'RESTART RECORDS WILL BE READ AT START OF SIMULATION',
     1 ' ON UNIT',I4)
      ENDIF
C
C9------FOR EACH CONFINING UNIT, READ NUMBER OF MODEL LAYER ABOVE UNIT
      READ(IN,110) (IDCON(ILCB),ILCB=1,NUMC)
  110 FORMAT(40I2)
C
C10-----IDENTIFY LAYERS FOR WHICH THE TOP ARRAY IS AVAILABLE AND SAVE
C10-----SEQUENCE NUMBER OF TOP ARRAY
      NUMTOP=0
      DO 120 K=1,NLAY
      NTOP(K)=0
      IF(LAYCON(K).EQ.2 .OR. LAYCON(K).EQ.3) THEN
       NUMTOP=NUMTOP+1
       NTOP(K)=NUMTOP
      ENDIF
  120 CONTINUE
C11-----ALLOCATE STORAGE FOR RATE, ZCB, TLK, TL, SLU, AND SLD ARRAYS
      ISP=ISUM
      NODES1=NCOL*NROW*NUMC
      LCRAT=ISUM
      ISUM=ISUM + NODES1
      LCZCB=ISUM
      ISUM=ISUM + NODES1
      LCTLK=ISUM
      ISUM=ISUM + NODES1
      LCTL=ISUM
      ISUM=ISUM + NODES1
      LCSLU=ISUM
```

```
      ISUM=ISUM + NODES1
      LCSLD=ISUM
      ISUM=ISUM + NODES1
C
C12----- ALLOCATE STORAGE FOR A1, B1, ALPH, BET ARRAYS
      LCA1=ISUM
      ISUM=ISUM + NTM1
      LCB1=ISUM
      ISUM=ISUM + 2
      LCALPH=ISUM
      ISUM=ISUM + NTM1
      LCBET=ISUM
      ISUM=ISUM + 2
C
C12-----ALLOCATE STORAGE FOR RM1, RM2, RM3, AND RM4 ARRAYS
      NM1=NTM1*NODES1
      NM2=2*NODES1
      LCRM1=ISUM
      ISUM=ISUM + NM1
      LCRM2=ISUM
      ISUM=ISUM + NM2
      LCRM3=ISUM
      ISUM=ISUM + NM1
      LCRM4=ISUM
      ISUM=ISUM + NM2
C
C13-----CALCULATE AND PRINT AMOUNT OF SPACE USED BY TRANSIENT LEAKAGE
      ISP=ISUM - ISP
      WRITE(IOUT,130) ISP
  130 FORMAT(1X,I6,'ELEMENTS IN X ARRAY ARE USED FOR TRANSIENT LEAKAGE')
      ISUM1=ISUM-1
      WRITE(IOUT,140) ISUM1,LENX
  140 FORMAT(1X,I6,'ELEMENTS OF X ARRAY USED OUT OF ',I7)
      IF(ISUM1.GT.LENX) WRITE(IOUT,150)
  150 FORMAT(1X,'   *** X ARRAY MUST BE DIMENSIONED LARGER ***')
C14-----RETURN
      RETURN
      END
```

List of Variables for Module TLK1AL

Variable	Range	Definition
IDCON	Package	DIMENSION(80), Number of the model layer above each confining unit.
ILCB	Module	Index for confining units.
IN	Package	Primary unit number from which input from this package will be read.
IOUT	Global	Primary unit number for all printed output.
ISP	Module	Number of elements in the X array allocated by this package.
ISS	Global	Steady-state flag: = 0 Simulation is transient. ≠ 0 Simulation is steady state.
ISUM	Global	Element number of the lowest element in the X array that has not yet been allocated. When space is allocated in the X array, the size of the allocation is added to ISUM.
ISUM1	Module	ISUM-1
ITLKCB	Package	Flag and a unit number: > 0 Unit number on which cell-by-cell flow terms will be recorded whenever ICBCFL is set. ≤ 0 Cell-by-cell flow terms will not be printed.
ITLKRS	Package	Flag and a unit number: > 0 Unit number from which restart information will be read. ≤ 0 Restart information will not be read.
ITLKSV	Package	Flag and a unit number: > 0 Unit number on which restart information will be recorded. ≤ 0 Restart information will not be recorded.
K	Module	Index for layers.
LAYCON	Global	DIMENSION(80), Layer-type code: 0 Layer is strictly confined. 1 Layer is strictly unconfined. 2 Layer is convertible between confined and unconfined (saturated thickness is constant). 3 Layer is convertible between confined and unconfined (saturated thickness varies).
LCA1	Package	Location in the X array of the first element of array A1.
LCALPH	Package	Location in the X array of the first element of array ALPH.
LCB1	Package	Location in the X array of the first element of array B1.
LCBET	Package	Location in the X array of the first element of array BET.
LCRAT	Package	Location in the X array of the first element of array RATE.
LCRM1	Package	Location in the X array of the first element of array RM1.
LCRM2	Package	Location in the X array of the first element of array RM2.
LCRM3	Package	Location in the X array of the first element of array RM3.
LCRM4	Package	Location in the X array of the first element of array RM4.
LCSLD	Package	Location in the X array of the first element of array SLD.
LCSLU	Package	Location in the X array of the first element of array SLU.
LCTL	Package	Location in the X array of the first element of array TL.
LCTLK	Package	Location in the X array of the first element of array TLK.
LCZCB	Package	Location in the X array of the first element of array ZCB.
LENX	Global	Number of elements in the X array. Value should always equal the dimension of the X array specified in the MAIN program.
NCOL	Global	Number of columns in the model grid.
NLAY	Global	Number of layers in the model grid.
NM1	Package	Number of elements in arrays RM1 and RM3.

Variable	Range	Definition
NM2	Package	Number of elements in arrays RM2 and RM4.
NODES1	Package	Number of elements in arrays RATE and ZCB. Equal to product of number of confining units, number of rows, and number of columns.
NROW	Global	Number of rows in the model grid.
NTM1	Package	Number of terms in the M_1 series.
NTOP	Package	DIMENSION(80), Sequence number of the TOP array for each layer in the model grid. Set to 0 for model layers without a top array.
NUMC	Package	Number of confining units with transient leakage.
NUMTOP	Module	Temporary counter for sequence numbers of TOP arrays.

TLK1RP

Narrative for Module TLK1RP

This module reads arrays of hydraulic conductivity, thickness, and specific storage for each confining unit. If the restart option is selected, the module reads a restart record containing the values of the cumulative memory functions. Otherwise, the module initializes the memory functions to zero. The module also computes and stores γ_i, the reciprocal of the time constant, for each location in each confining unit. Finally, the module initializes arrays that contain constants for the M_1 and M_2 series. Operations are carried out in the following order:

1. Print a table showing locations of confining units with respect to model layers.

2. Read hydraulic conductivity, thickness, and specific storage for each confining unit. All three arrays are read using utility module U2DREL. Hydraulic conductivity is read into array RATE and thickness is read in to array ZCB. Specific storage is read in to temporary storage in array BUFF.

3. Initialize cumulative memory arrays RM1, RM2, RM3, and RM4. If the restart option is selected, values for all four arrays are read from the restart record. Otherwise, values in each array are set to zero.

4. Use hydraulic conductivity, thickness, and specific storage to define properties for use in later computations. If the value of hydraulic conductivity, thickness, or specific storage is zero at a location in the model grid, values of the other properties are set to zero and transient-leakage calculations will not be carried out for the confining unit at that location. The array that originally contained hydraulic conductivity, RATE, is converted to a conductance value for each location with transient leakage. Similarly, the array that originally contained thickness, ZCB, is converted to the reciprocal of the time constant, defined in equation (8) of this report.

5. Define constants for the approximate series M_1 and M_2.

6. RETURN.

Flowchart for Module TLK1RP

ITLKRS is a flag and a unit number.
  > 0, restart record will be read on unit ITLKRS
  ≤ 0, restart record will not be read

RM1 is a cumulative memory function that is updated each time step to equal the integral $\hat{K}$ given in equations (38) and (39).

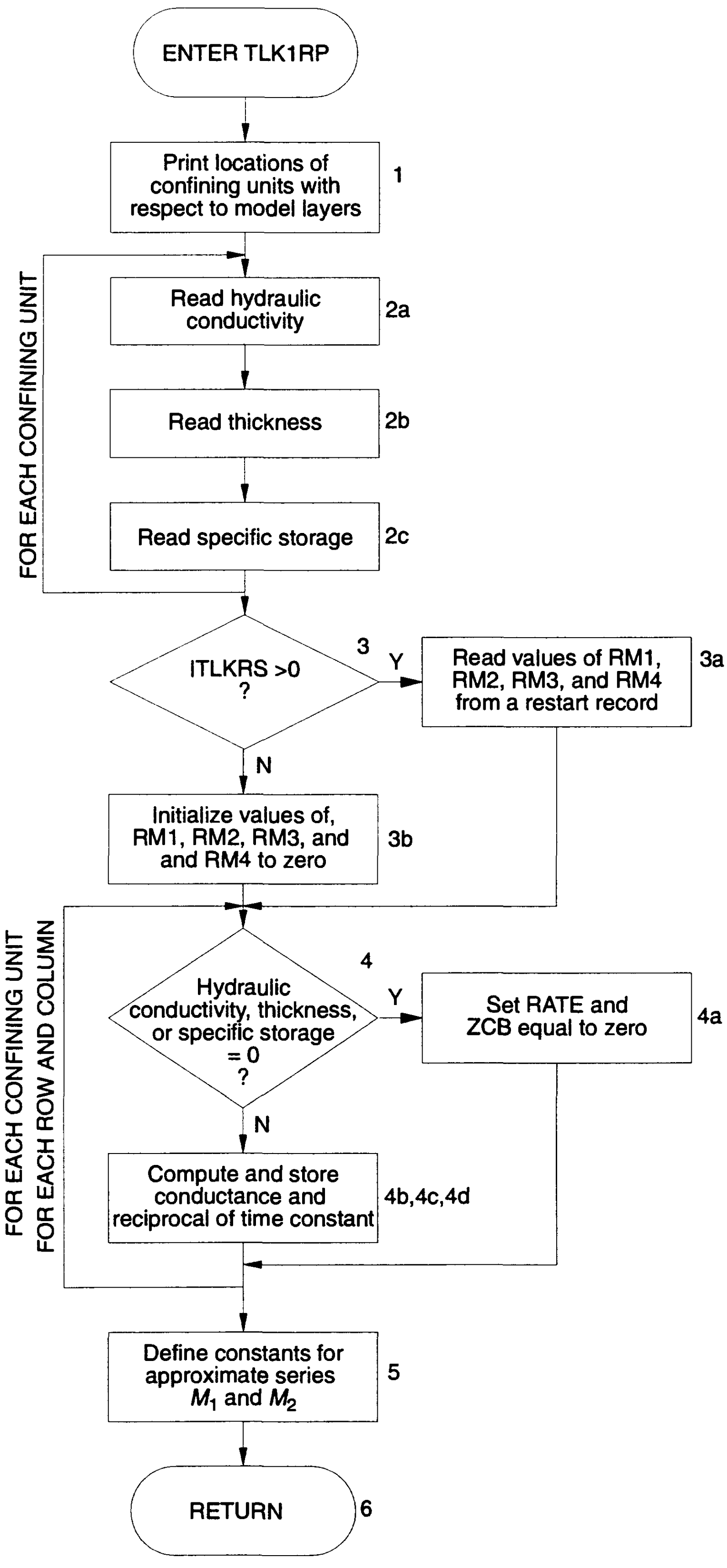
RM2 is a cumulative memory function that is updated each time step to equal the integral $\hat{L}$ given in equations (40) and (41).

RM3 is a cumulative memory function that is updated each time step to equal the integral $\hat{I}$ given in equations (17) and (18).

RM4 is a cumulative memory function that is updated each time step to equal the integral $\hat{J}$ given in equations (19) and (20).

RATE is an array used to store vertical hydraulic conductance for confining units.

ZCB is an array used to store the reciprocal of the time constant for confining units.



Program Listing for Module TLK1RP

```
      SUBROUTINE TLK1RP(RATE,ZCB,A1,B1,ALPH,BET,RM1,RM2,RM3,RM4,
     1 NODES1,NM1,NM2,NUMC,NTM1,ITLKRS,DELTM1,BUFF,DELC,DELR,TLKTIM,
     2 NROW,NCOL,IN,IOUT)
C
C-----VERSION 1100 06JAN1994 TLK1RP
C     ****************************************************************
C     READ AND INITIALIZE TRANSIENT LEAKAGE ARRAYS
C     ****************************************************************
C
C        SPECIFICATIONS:
C     ----------------------------------------------------------------
      CHARACTER*4 ANAME
C
      DIMENSION RATE(NODES1),ZCB(NODES1),A1(NTM1),B1(2),ALPH(NTM1),
     1 BET(2),RM1(NM1),RM2(NM2),RM3(NM1),RM4(NM2),BUFF(NODES1),
     2 DELC(NROW),DELR(NCOL),ANAME(6,3)
C
      COMMON /TLEAK/ IDCON(80),NTOP(80)
C
      DATA ANAME(1,1),ANAME(2,1),ANAME(3,1),ANAME(4,1),ANAME(5,1),
     1ANAME(6,1)/'   V','ERTI','CAL ','COND','UCTI','VITY'/
      DATA ANAME(1,2),ANAME(2,2),ANAME(3,2),ANAME(4,2),ANAME(5,2),
     1ANAME(6,2)/' CON','FINI','NG B','ED T','HICK','NESS'/
      DATA ANAME(1,3),ANAME(2,3),ANAME(3,3),ANAME(4,3),ANAME(5,3),
     1ANAME(6,3)/'    ','    ','SPEC','IFIC',' STO','RAGE'/
C     ----------------------------------------------------------------
C
C1------PRINT LOCATIONS OF CONFINING UNITS WITH RESPECT TO MODEL LAYERS
      WRITE(IOUT,20) (ILCB,IDCON(ILCB),IDCON(ILCB)+1,ILCB=1,NUMC)
   20 FORMAT('0',5X,'The following confining units with transient ',
     1 'leakage are active:',/,23X,'Model     Model',/,
     2 8X,'Confining      layer     layer',/,11X,
     3 'unit        above     below',/,6X,34('-'),/,80(2I13,I10,/))
C
C2------READ ARRAYS FOR EACH CONFINING UNIT
      NCR=NCOL*NROW
      DO 50 I=1,NUMC
      LOC=1 + (I-1)*NCR
C
C2A-----READ VERTICAL HYDRAULIC CONDUCTIVITY
      CALL U2DREL(RATE(LOC),ANAME(1,1),NROW,NCOL,IDCON(I),IN,IOUT)
C
C2B-----READ THICKNESS
      CALL U2DREL(ZCB(LOC),ANAME(1,2),NROW,NCOL,IDCON(I),IN,IOUT)
C
C2C-----READ SPECIFIC STORAGE
      CALL U2DREL(BUFF(LOC),ANAME(1,3),NROW,NCOL,IDCON(I),IN,IOUT)
   50 CONTINUE
C
C3------INITIALIZE ARRAYS WITH CUMULATIVE MEMORY FUNCTIONS
      IF(ITLKRS.GT.0) THEN
C3A-----READ VALUES FOR RM1, RM2, RM3, AND RM4 FROM A RESTART RECORD
        READ(ITLKRS) DELTM1,TLKTIM,(RM1(J),J=1,NM1),(RM2(J),J=1,NM2),
```

```
     1                            (RM3(J),J=1,NM1),(RM4(J),J=1,NM2)
       WRITE(IOUT,60) TLKTIM
   60  FORMAT(1X,'A RESTART RECORD FOR TRANSIENT LEAKAGE HAS BEEN READ',
     1 ' FOR TIME=',G15.7)
       WRITE(IOUT,70)
   70  FORMAT(1X,'TIME SUMMARY WILL REFLECT TIME SINCE START OF ',
     1 'THIS CONTINUATION OF A PREVIOUS SIMULATION.')
      ELSE
C3B-----INITIALIZE RM1, RM2, RM3, AND RM4 TO ZERO
       DO 90 J=1,NM1
       RM1(J)=0.0
       RM3(J)=0.0
   90  CONTINUE
       DO 92 J=1,NM2
       RM2(J)=0.0
       RM4(J)=0.0
   92  CONTINUE
       TLKTIM=0.0
      ENDIF
C
C4------USE HYDRAULIC CONDUCTIVITY, THICKNESS, AND SPECIFIC STORAGE TO
C4------DEFINE PROPERTIES FOR USE IN LATER COMPUTATIONS
      DO 210 I=1,NODES1
C
C4A------SKIP COMPUTATIONS IF HYDRAULIC CONDUCTIVITY, THICKNESS, OR
C4A------OR SPECIFIC STORAGE EQUAL ZERO
      IF(RATE(I).LE.0..OR.ZCB(I).LE.0..OR.BUFF(I).LE.0.) THEN
       RATE(I)=0.0
       ZCB(I)=0.0
      ELSE
       K=1 + (I-1)/NCR
       IR=1 + ((I-1)-(K-1)*NCR)/NCOL
       IC=I - NCOL*(IR-1) - NCR*(K-1)
       AREA=DELR(IC)*DELC(IR)
C
C4B------COMPUTE LEAKANCE
       RATE(I) = RATE(I)/ZCB(I)
C
C4C------COMPUTE RECIPROCAL OF TIME CONSTANT
       ZCB(I) = RATE(I)/(ZCB(I)*BUFF(I))
C
C4D------CONVERT LEAKANCE TO CONDUCTANCE
       RATE(I)=RATE(I)*AREA
      ENDIF
  210 CONTINUE
C
C5------DEFINE CONSTANTS FOR APPROXIMATE SERIES M1 AND M2
      IF(NTM1.EQ.2) THEN
       A1(1)=0.2868101
       A1(2)=0.0465232
       ALPH(1)=16.3515574
       ALPH(2)=1702.46
      ELSE IF(NTM1.EQ.3) THEN
       A1(1)=0.2648731
       A1(2)=0.0599943
```

```
         A1(3)=0.0084659
         ALPH(1)=13.6575887
         ALPH(2)=437.0762325
         ALPH(3)=49639.1
        ELSE IF(NTM1.EQ.4) THEN
         A1(1)=0.2375983
         A1(2)=0.0736630
         A1(3)=0.0184244
         A1(4)=0.0036476
         ALPH(1)=11.4642958
         ALPH(2)=151.8318702
         ALPH(3)=3590.24
         ALPH(4)=211276.
        ELSE
         A1(1)=0.2243858
         A1(2)=0.0744159
         A1(3)=0.0253250
         A1(4)=0.0073358
         A1(5)=0.0018708
         ALPH(1)=10.7005496
         ALPH(2)=94.3072975
         ALPH(3)=1075.20
         ALPH(4)=17848.6
         ALPH(5)=631121.0
        ENDIF
        B1(1)     = -0.25754
        B1(2)     =  0.090873
        BET(1)  =  10.764
        BET(2)  =  19.805
C
C6------RETURN
        RETURN
        END
```

List of Variables for Module TLK1RP

Variable	Range	Definition
A1	Package	DIMENSION(NTM1), Constant *A* in the M_1 series.
ALPH	Package	DIMENSION(NTM1), Constant α in the M_1 series.
ANAME	Module	DIMENSION(6,3), Labels for input arrays.
AREA	Module	Area of upper and lower faces of finite-difference cell.
B1	Package	DIMENSION(2), Constant *B* in the M_2 series.
BET	Package	DIMENSION(2), Constant β in the M_2 series.
BUFF	Global	DIMENSION(NODES1) Buffer used for temporary storage of specific-storage array.
DELC	Global	DIMENSION(NROW), Cell dimensions in the column direction. DELC(I) contains the width of row I.
DELR	Global	DIMENSION(NCOL), Cell dimensions in the row direction. DELR(J) contains the width of column J.
DELTM1	Package	Length of the previous time step.
I	Module	Index for elements in RATE and ZCB arrays.
IC	Module	Index for columns.
IDCON	Package	DIMENSION(80), Number of the model layer above each confining unit.
ILCB	Module	Index for confining units.
IN	Package	Primary unit number from which input from this package will be read.
IOUT	Global	Primary unit number for all printed output.
IR	Module	Index for rows.
ITLKRS	Package	Flag and a unit number: > 0 Unit number from which restart information will be read. ≤ 0 Restart information will not be read.
J	Module	Index for RM1, RM2, RM3, and RM4 arrays.
K	Module	Index for layers.
LOC	Module	Pointer for starting locations of information for each confining unit in arrays storing hydraulic conductivity, thickness, and specific storage.
NCOL	Global	Number of columns in the model grid.
NCR	Module	Number of cells in each layer of the model grid.
NM1	Package	Number of elements in arrays RM1 and RM3.
NM2	Package	Number of elements in arrays RM2 and RM4.
NODES1	Package	Number of elements in arrays RATE and ZCB. Equal to product of number of confining units, number of rows, and number of columns.
NROW	Global	Number of rows in the model grid.
NTM1	Package	Number of terms in the M_1 series.
NTOP	Package	DIMENSION(80), Sequence number of the TOP array for each layer in the model grid. Set to 0 for model layers without a top array.
NUMC	Package	Number of confining units with transient leakage.
RATE	Package	DIMENSION(NODES1), Hydraulic conductance of confining units.
RM1	Package	DIMENSION(NM1), Cumulative memory function. Value is updated each time step to equal the integral $\hat{K}$ given in equations (38) and (39).
RM2	Package	DIMENSION(NM2), Cumulative memory function. Value is updated each time step to equal the integral $\hat{L}$ given in equations (40) and (41).
RM3	Package	DIMENSION(NM1), Cumulative memory function. Value is updated each time step to equal the integral $\hat{I}$ given in equations (17) and (18).
RM4	Package	DIMENSION(NM2), Cumulative memory function. Value is updated each time step to equal the integral $\hat{J}$ given in equations (19) and (20).
TLKTIM	Package	Simulation time since start of first model run in a series of continuation runs. If restart option is not selected, value equals simulation time since start of run.
ZCB	Package	DIMENSION(NODES1), Reciprocal of the time constant of confining units.

TLK1AD

Narrative for Module TLK1AD

This module formulates coefficients of head and constants in transient-leakage equations (43) and (44). Coefficients of head are b_i and a_i in equations (45) and (46) and constants are c_i and d_i in equations (47) and (48). The values are calculated at the beginning of each time step for later use in formulating the finite-difference equations. To calculate c_i and d_i, the module updates the cumulative memory functions RM1, RM2, RM3, and RM4 to equal convolution integrals $\hat{K}$, $\hat{L}$, $\hat{I}$, and $\hat{J}$ using recursive relations given in equations (39), (41), (18), and (20). Operations are carried out in the following order:

1. Initialize variables that contain length of the current and previous time steps.

2. Compute implicit components (coefficients of head) and explicit components (constants) for transient-leakage equations. For each confining unit and for each location in the model grid, the following steps 3-12 are carried out.

3. Compute dimensionless time interval, XLMT, for current time step and dimensionless time interval, XLMT0, for previous time step.

4. If dimensionless time interval XLMT is large, treat leakage as steady and skip the calculations in steps 5-11.

5. Compute and sum terms in M_1 and M_2 series, update cumulative memory functions, and add cumulative memory to explicit terms in transient-leakage equations (steps 6-10).

6. Compute arguments of exponential functions for current and previous time steps.

7. Compute complimentary exponential functions and exponential functions for current and previous time steps. If argument of function, $\alpha \Delta t_D$ or $\beta \Delta t_D$, is 0.01 or less, use a Taylor's series approximation of the complimentary exponential function. For arguments larger than 0.01, use the intrinsic function EXP.

8. Update cumulative memory functions RM1, RM2, RM3, and RM4 to equal convolution integrals $\hat{K}$, $\hat{L}$, $\hat{I}$, and $\hat{J}$.

9. Update cumulative memory functions RM1, RM2, RM3, and RM4 to equal parts of the explicit terms in the transient-leakage equations.

10. Add negative cumulative memory functions RM1, RM2, RM3, and RM4 to explicit terms.

11. Complete assembly of explicit terms by multiplying by vertical conductance.

12. Compute and assemble implicit coefficients of head in arrays TLK and TL.

13. Set previous time-step length equal to the length of the current time step.

14. RETURN.

Flowchart for Module TLK1AD

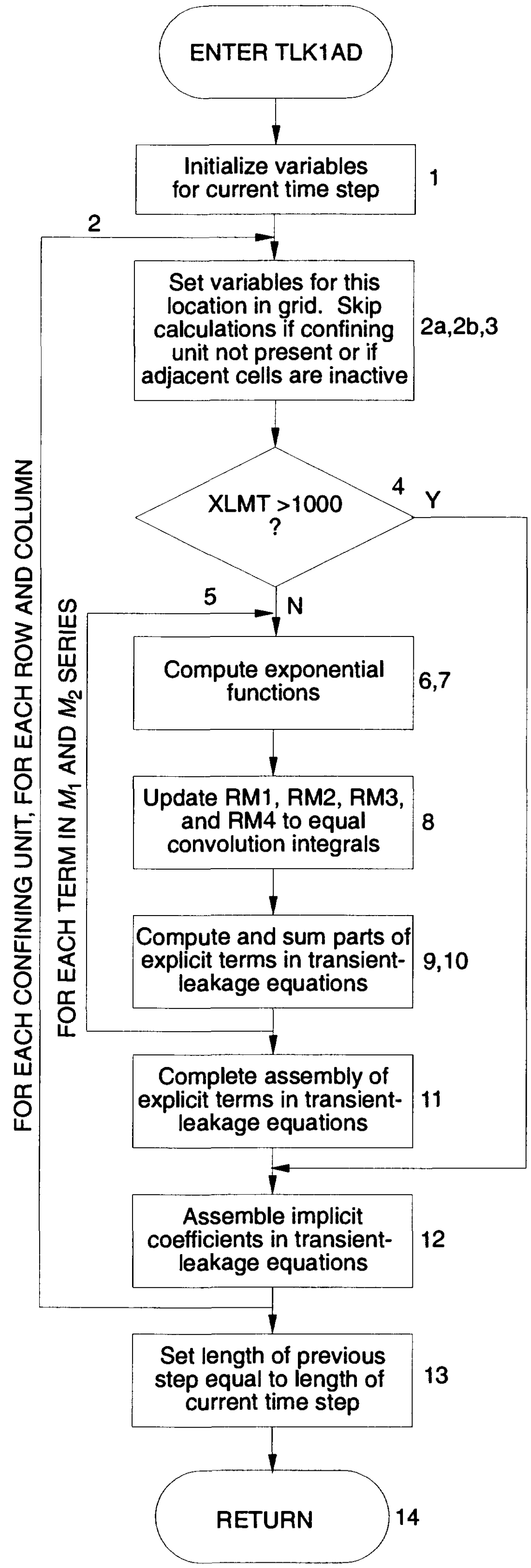
XLMT is dimensionless time interval for current time step and current location in the confining unit.

RM1 is a cumulative memory function that is updated each time step to equal the integral $\hat{K}$ given in equations (38) and (39).

RM2 is a cumulative memory function that is updated each time step to equal the integral $\hat{L}$ given in equations (40) and (41).

RM3 is a cumulative memory function that is updated each time step to equal the integral $\hat{I}$ given in equations (17) and (18).

RM4 is a cumulative memory function that is updated each time step to equal the integral $\hat{J}$ given in equations (19) and (20).



Program Listing for Module TLK1AD

```
      SUBROUTINE TLK1AD(RATE,ZCB,A1,B1,ALPH,BET,RM1,RM2,RM3,RM4,
     1 TL,TLK,SLU,SLD,NM1,NM2,NUMC,NTM1,DELTM1,HNEW,IBOUND,TOP,
     2 NROW,NCOL,NLAY,DELT,TLKTIM,IN,IOUT)
C
C-----VERSION 1100 06JAN1994 TLK1AD
C     ******************************************************************
C     COMPUTE TRANSIENT LEAKAGE TERMS AT EVERY TIME STEP
C     ******************************************************************
C
C     SPECIFICATIONS:
C     ------------------------------------------------------------------
      DOUBLE PRECISION HNEW
C
      DIMENSION HNEW(NCOL,NROW,NLAY),TOP(NCOL,NROW,NLAY),
     1 RATE(NCOL,NROW,NUMC),ZCB(NCOL,NROW,NUMC),TLK(NCOL,NROW,NUMC),
     2 TL(NCOL,NROW,NUMC),SLU(NCOL,NROW,NUMC),SLD(NCOL,NROW,NUMC),
     3 RM1(NM1),RM2(NM2),RM3(NM1),RM4(NM2),A1(NTM1),B1(2),
     4 ALPH(NTM1),BET(2),IBOUND(NCOL,NROW,NLAY)
C
      COMMON /TLEAK/ IDCON(80),NTOP(80)
C
C     ------------------------------------------------------------------
C
C1------INITIALIZE VARIABLES FOR CURRENT TIME STEP
      TLKTIM=TLKTIM+DELT
      IF(TLKTIM.LE.DELT) DELTM1=1.0
      NQ=0
C
C2------FOR EACH CONFINING UNIT, ROW, AND COLUMN, COMPUTE IMPLICIT TERMS
C2------TL, AND TLK, AND EXPLICIT TERMS SLU AND SLD
      DO 50 ILCB=1,NUMC
      IL = IDCON(ILCB)
      IL1=IL+1
      NTP=NTOP(IL1)
      DO 41 IR=1,NROW
      DO 40 IC=1,NCOL
      NQ=NQ+1
      TL(IC,IR,ILCB)=0.0
      TLK(IC,IR,ILCB)=0.0
C2A-----SKIP COMPUTATIONS IF (1)CONFINING UNIT NOT PRESENT, (2)CELL
C2A-----ABOVE OR BELOW IS NOT ACTIVE, OR (3) CELLS BOTH ABOVE AND
C2A-----BELOW ARE CONSTANT-HEAD CELLS
      IF(RATE(IC,IR,ILCB).LE.0.0) GO TO 40
      IF(IBOUND(IC,IR,IL).EQ.0) GO TO 40
      IF(IBOUND(IC,IR,IL1).EQ.0) GO TO 40
      IF(IBOUND(IC,IR,IL).LT.0.AND.IBOUND(IC,IR,IL1).LT.0) GO TO 40
C2B-----SET TEMPORARY VARIABLES EQUAL TO CONDUCTANCE, RECIPROCAL OF
C2B-----TIME CONSTANT, AND HEAD ABOVE AND BELOW UNIT.  IF HEAD
C2B-----BELOW IS BENEATH BOTTOM OF UNIT, USE TOP AS HEAD VALUE
      TLN = RATE(IC,IR,ILCB)
      XLM = ZCB(IC,IR,ILCB)
      HT = HNEW(IC,IR,IL)
```

```
      HB = HNEW(IC,IR,IL1)
      IF(NTP.GT.0) THEN
       TOP2=TOP(IC,IR,NTP)
       IF(HB.LT.TOP2) HB=TOP2
      ENDIF
C
C3------COMPUTE DIMENSIONLESS TIME INTERVAL AT CURRENT TIME STEP, XLMT,
C3------AND DIMENSIONLESS TIME INTERVAL AT PREVIOUS TIME STEP, XLMTO
      XLMT = XLM*DELT
      XLMTO = XLM*DELTM1
C
C4------IF STEADY LEAKAGE ONLY, SKIP PROCESSING OF CONVOLUTION TERMS
      XTA = 0.0
      XTB = 0.0
      SLB = 0.0
      SLT = 0.0
      IF(XLMT.GT.1000.) GO TO 30
      RDELT = 1./XLMT
      RDELT1 = 1./XLMTO
C
C5------COMPUTE AND SUM TERMS IN M1 AND M2 SERIES AND IN EXPLICIT
C5------COMPONENTS OF FLOW EQUATIONS
      DO 20 M=1,NTM1
      NQ1=(NQ-1)*NTM1+M
      IF(M.LT.3) NQ2=(NQ-1)*2+M
C
C6------COMPUTE ARGUMENTS OF EXPONENTIAL FUNCTIONS FOR CURRENT AND
C6------PREVIOUS TIME STEPS
      XPA = ALPH(M)*XLMT
      XPB = BET(M)*XLMT
      XPAO = ALPH(M)*XLMTO
      XPBO = BET(M)*XLMTO
C
C7-----EVALUATE COMPLEMENTARY EXPONENTIAL FUNCTIONS USING TAYLOR
C7-----SERIES FOR ARGUMENTS OF MAGNITUDE 0.01 OR LESS AND USING THE
C7-----FORTRAN EXP FUNCTION OTHERWISE
C7A----COMPUTE EXPONENTIAL FUNCTIONS FOR TERMS IN M1 SERIES
      XXA = XPA*(24.+XPA*(-12.+XPA*(4.-XPA)))/24.
      IF(XPA.GT.0.1) XXA = 1.0 - EXP(-XPA)
      ATEX = 1.0 - XXA
      XXA1 = RDELT*A1(M)*XXA
      XTA = XTA + XXA1
      XXAO = XPAO*(24.+XPAO*(-12.+XPAO*(4.-XPAO)))/24.
      IF(XPAO.GT.0.1) XXAO = 1.0 - EXP(-XPAO)
      XXAO1 = RDELT1*A1(M)*XXAO
C7B-----COMPUTE EXPONENTIAL FUNCTIONS FOR TERMS IN M2 SERIES
C7B-----SKIP COMPUTATIONS IF TERM COUNTER M IS GREATER THAN 2
      IF(M.LT.3) THEN
       XXB = XPB*(24.+XPB*(-12.+XPB*(4.-XPB)))/24.
       IF(XPB.GT.0.1) XXB = 1.0 - EXP(-XPB)
       BTEX = 1.0 - XXB
       XXB1 = RDELT*B1(M)*XXB
       XTB = XTB + XXB1
       XXBO = XPBO*(24.+XPBO*(-12.+XPBO*(4.-XPBO)))/24.
       IF(XPBO.GT.0.1) XXBO = 1.0 - EXP(-XPBO)
```

```
         XXBO1 = RDELT1*B1(M)*XXBO
        ENDIF
C
C8------UPDATE CUMULATIVE MEMORY TERMS RM1, RM2, RM3 AND RM4 TO EQUAL
C8------THE CONVOLUTION INTEGRALS FOR THE PREVIOUS TIME STEP
      IF(TLKTIM.LE.DELT) GO TO 10
      RM1(NQ1) = RM1(NQ1) + XXAO1*HT
      RM3(NQ1) = RM3(NQ1) + XXAO1*HB
      IF(M.LT.3) THEN
       RM2(NQ2) = RM2(NQ2) + XXBO1*HB
       RM4(NQ2) = RM4(NQ2) + XXBO1*HT
      ENDIF
   10 CONTINUE
C
C9------UPDATE CUMULATIVE MEMORY TERMS TO EQUAL PARTS OF EXPLICIT
C9------TERMS FOR THE CURRENT TIME STEP
      RM1(NQ1) = RM1(NQ1)*ATEX - XXA1*HT
      RM3(NQ1) = RM3(NQ1)*ATEX - XXA1*HB
      IF(M.LT.3) THEN
       RM2(NQ2) = RM2(NQ2)*BTEX - XXB1*HB
       RM4(NQ2) = RM4(NQ2)*BTEX - XXB1*HT
      ENDIF
C
C10-----ADD CUMULATIVE MEMORY TO EXPLICIT TERMS FOR CURRENT TIME STEP
      SLT = SLT - RM1(NQ1)
      SLB = SLB - RM3(NQ1)
      IF(M.LT.3) THEN
       SLT = SLT  + RM2(NQ2)
       SLB = SLB  + RM4(NQ2)
      ENDIF
   20 CONTINUE
C
C11-----ASSEMBLE EXPLICIT TRANSIENT-LEAKAGE TERMS
      SLB = TLN*SLB
      SLT = TLN*SLT
C
C12-----ASSEMBLE IMPLICIT COEFFICIENTS OF HEAD IN ARRAYS TLK AND
C12-----TL, AND EXPLICIT TERMS IN ARRAYS SLU AND SLD
   30 CONTINUE
      TLK(IC,IR,ILCB) = TLN*(       1. + XTB)
      TL(IC,IR,ILCB) = TLN*(-XTA - 1.       )
      SLU(IC,IR,ILCB) = SLT
      SLD(IC,IR,ILCB) = SLB
   40 CONTINUE
   41 CONTINUE
   50 CONTINUE
C
C13-----SET PREVIOUS TIME STEP EQUAL TO CURRENT TIME STEP
      DELTM1=DELT
C
C14-----RETURN
      RETURN
      END
```

List of Variables for Module TLK1AD

Variable	Range	Definition
A1	Package	DIMENSION(NTM1), Constant A in the M_1 series.
ALPH	Package	DIMENSION(NTM1), Constant α in the M_1 series.
ATEX	Module	Exponential function of $\alpha\Delta t_D$.
B1	Package	DIMENSION(2), Constant B in the M_2 series.
BET	Package	DIMENSION(2), Constant β in the M_2 series.
BTEX	Module	Exponential function of $\beta\Delta t_D$.
DELT	Global	Length of current time step.
DELTM1	Package	Length of the previous time step.
HB	Module	Temporary single-precision equivalent of element in HNEW array corresponding to the aquifer below the confining unit. If head below confining unit is below the top of the aquifer, HB will be set to the appropriate value in the TOP array.
HNEW	Global	DIMENSION(NCOL,NROW,NLAY), Most recent estimate of head in each cell.
HT	Module	Temporary single-precision equivalent of element in HNEW array corresponding to the aquifer above the confining unit.
IBOUND	Global	DIMENSION(NCOL,NROW,NLAY), Status of each cell < 0 Constant-head cell. $= 0$ No-flow cell. > 0 Variable-head cell.
IC	Module	Index for columns.
IDCON	Package	DIMENSION(80), Number of the model layer above each confining unit.
IL	Module	Index for layers.
IL1	Module	Index for layer below confining unit.
ILCB	Module	Index for confining units.
IN	Package	Primary unit number from which input from this package will be read.
IOUT	Global	Primary unit number for all printed output.
IR	Module	Index for rows.
M	Module	Index for terms in M_1 and M_2 series.
NCOL	Global	Number of columns in the model grid.
NLAY	Global	Number of layers in the model grid.
NM1	Package	Number of elements in arrays RM1 and RM3.
NM2	Package	Number of elements in arrays RM2 and RM4.
NQ	Module	Counter used in computing NQ1 and NQ2.
NQ1	Module	Index for RM1 and RM3 arrays.
NQ2	Module	Index for RM2 and RM4 arrays.
NROW	Global	Number of rows in the model grid.
NTM1	Package	Number of terms in the M_1 series.
NTOP	Package	DIMENSION(80), Sequence number of the TOP array for each layer in the model grid. Set to 0 for model layers without a top array.
NTP	Module	Temporary equivalent of NTOP(IL).
NUMC	Package	Number of confining units with transient leakage.
RATE	Package	DIMENSION(NODES1), Hydraulic conductance of confining units.
RDELT	Module	Reciprocal of dimensionless time interval for current time step.
RDELT1	Module	Reciprocal of dimensionless time interval for previous time step.
RM1	Package	DIMENSION(NM1), Cumulative memory function. Value is updated each time step to equal the integral $\hat{K}$ given in equations (38) and (39).
RM2	Package	DIMENSION(NM2), Cumulative memory function. Value is updated each time step to equal the integral $\hat{L}$ given in equations (40) and (41).
RM3	Package	DIMENSION(NM1), Cumulative memory function. Value is updated each time step to equal the integral $\hat{I}$ given in equations (17) and (18).

Variable	Range	Definition
RM4	Package	DIMENSION(NM2), Cumulative memory function. Value is updated each time step to equal the integral $\hat{J}$ given in equations (19) and (20).
SLB	Module	Temporary accumulator for components in explicit term in transient-leakage equation for flow across bottom of confining unit.
SLD	Package	DIMENSION(NCOL,NROW,NUMC), Explicit term in transient-leakage equation for flow across bottom of confining unit. Equivalent to c_i in equation (47).
SLT	Module	Temporary accumulator for components in explicit term in transient-leakage equation for flow across top of confining unit.
SLU	Package	DIMENSION(NCOL,NROW,NUMC), Explicit term in transient-leakage equation for flow across top of confining unit. Equivalent to d_i in equation (48).
TL	Package	DIMENSION(NCOL,NROW,NUMC), Coefficient of head in transient-leakage equations for flow across top and bottom of confining unit. Equivalent to a_i in equation (46).
TLK	Package	DIMENSION(NCOL,NROW,NUMC), Coefficient of head in transient-leakage equations for flow across top and bottom of confining unit. Equivalent to b_i in equation (45).
TLKTIM	Package	Simulation time since start of first model run in a series of continuation runs. If restart option is not selected, value equals simulation time since start of run.
TLN	Module	Temporary equivalent of RATE(IC,IR,ILCB).
TOP	Global	DIMENSION(NCOL,NROW,NLAY), Elevation of the aquifer top. The TLK1 Package treats this as the elevation of the base of the confining unit. Although TOP is dimensioned to the size of the grid, space exists only for cells that can convert between confined and unconfined.
TOP2	Module	Temporary equivalent of TOP(IC,IR,NTP).
XLM	Module	Temporary equivalent of ZCB(IC,IR,ILCB).
XLMT	Module	Dimensionless time interval for current time step.
XLMTO	Module	Dimensionless time interval for previous time step.
XPA	Module	Argument of exponential functions. Equivalent to product of parameter α and dimensionless time interval for current time step.
XPAO	Module	Argument of exponential functions. Equivalent to product of parameter α and dimensionless time interval for previous time step.
XPB	Module	Argument of exponential functions. Equivalent to product of parameter β and dimensionless time interval for current time step.
XPBO	Module	Argument of exponential functions. Equivalent to product of parameter β and dimensionless time interval for previous time step.
XTA	Module	Accumulator for exponential terms.
XTB	Module	Accumulator for exponential terms.
XXA	Module	Complimentary exponential function of XPA.
XXA1	Module	Product of XXA, parameter α, and RDELT.
XXAO	Module	Complimentary exponential function of XPAO.
XXAO1	Module	Product of XXAO, parameter α, and RDELT1.
XXB	Module	Complimentary exponential function of XPB.
XXB1	Module	Product of XXB, parameter β, and RDELT.
XXBO	Module	Complimentary exponential function of XPBO.
XXBO1	Module	Product of XXBO, parameter β, and RDELT1.
ZCB	Package	DIMENSION(NCOL,NROW,NUMC), Reciprocal of the time constant of confining units.

TLK1FM

Narrative for Module TLK1FM

This module incorporates flow equations for transient leakage into the finite-difference equations in MODFLOW. The process involves assigning the proper values to the vertical conductance array, CV, adding terms to the main-diagonal array, HCOF, and adding terms to the right-hand-side array, RHS. If head in the aquifer under the confining unit is below the base of the unit, a correction term is added to the appropriate element in the RHS array. Operations are carried out in the following order:

1. Assign coefficient of head, TLK, to appropriate elements of the vertical conductance array, CV.
2. For each confining unit, formulate equations for finite-difference cells above and below the unit. The formulation is carried out in following steps 3-7.
3. Add coefficients of head, TL and TLK, to main-diagonal array HCOF for cell above confining unit.
4. Add coefficients of head, TL and TLK, to main-diagonal array HCOF for cell below confining unit.
5. Subtract explicit term SLU from right-hand-side array, RHS, for cell above confining unit.
6. Subtract explicit term SLD from right-hand-side array, RHS, for cell below confining unit.
7. If head in aquifer under the confining unit is below the base of the unit, make corrections to RHS array for cell below the confining unit.
8. RETURN.

Flowchart for Module TLK1FM

TLK is a coefficient of head in transient-leakage equations for flow across top and bottom of confining unit.

CV is conductance in the vertical direction in the original MODFLOW program.

TL is a coefficient of head in transient-leakage equations for flow across top and bottom of confining unit.

HCOF is coefficient of head in the finite-difference equation.

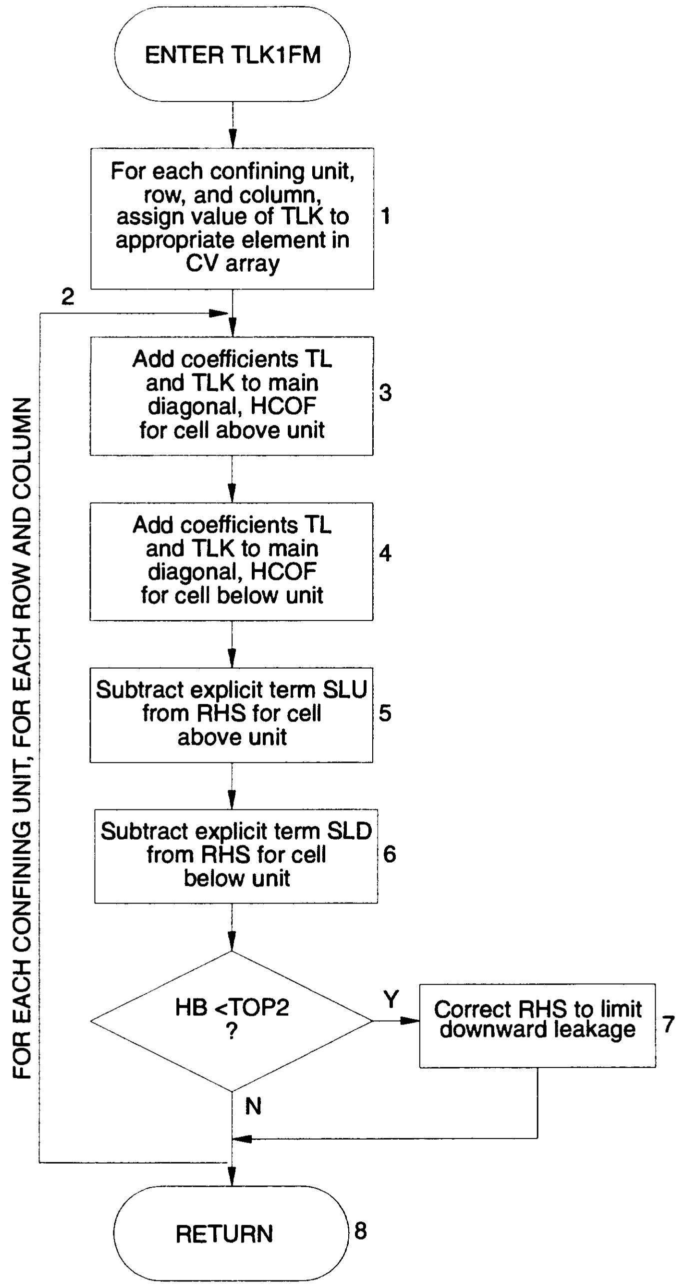
SLU is the explicit term in transient-leakage equation for flow across top of confining unit.

RHS is right-hand side of the finite-difference equation.

SLD is the explicit term in transient-leakage equation for flow across bottom of confining unit.

HB is head in aquifer below confining unit.

TOP2 is top of aquifer below confining unit.



Program Listing for Module TLK1FM

```
      SUBROUTINE TLK1FM(RATE,TL,TLK,SLU,SLD,NUMC,
     1 HNEW,IBOUND,TOP,CV,HCOF,RHS,NROW,NCOL,NLAY)
C
C-----VERSION 1100 06JAN1994 TLK1FM
C     ******************************************************************
C     ADD TRANSIENT LEAKAGE TO RHS AND HCOF
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      DOUBLE PRECISION HNEW
C
      DIMENSION HNEW(NCOL,NROW,NLAY),TOP(NCOL,NROW,NLAY),
     1 TL(NCOL,NROW,NUMC),TLK(NCOL,NROW,NUMC),SLU(NCOL,NROW,NUMC),
     2 SLD(NCOL,NROW,NUMC),CV(NCOL,NROW,NLAY),HCOF(NCOL,NROW,NLAY),
     3 RHS(NCOL,NROW,NLAY),IBOUND(NCOL,NROW,NLAY),RATE(NCOL,NROW,NUMC)
C
      COMMON /TLEAK/ IDCON(80),NTOP(80)
C     ------------------------------------------------------------------
C
C1------ASSIGN VALUE OF IMPLICIT COEFFICIENT, TLK, TO VERTICAL
C1------HYDRAULIC CONDUCTANCE ARRAY, CV
      DO 10 ILCB=1,NUMC
      IL=IDCON(ILCB)
      DO 10 IC=1,NCOL
      DO 10 IR=1,NROW
      IF(RATE(IC,IR,ILCB).GT.0.0) THEN
       CV(IC,IR,IL)=TLK(IC,IR,ILCB)
      ENDIF
   10 CONTINUE
C
C2------FOR EACH CONFINING UNIT, FORMULATE EQUATIONS FOR CELLS IN MODEL
C2------LAYERS ABOVE AND BELOW
      DO 30 ILCB=1,NUMC
      IL=IDCON(ILCB)
      IL1=IL+1
      NTP=NTOP(IL1)
      DO 21 IC=1,NCOL
      DO 20 IR=1,NROW
C
C2A-----SKIP PROCESSING IF CELL IS INACTIVE
      IF(IBOUND(IC,IR,IL).EQ.0) GO TO 20
      IF(IBOUND(IC,IR,IL1).EQ.0) GO TO 20
      IF(RATE(IC,IR,ILCB).LE.0.0) GO TO 20
C
C3------ADD COEFFICIENTS TL AND TLK TO DIAGONAL, HCOF, FOR MODEL LAYER
C3------ABOVE CONFINING UNIT
      TLX  =  TL(IC,IR,ILCB)
      TLKX = TLK(IC,IR,ILCB)
      HCOF(IC,IR,IL)=HCOF(IC,IR,IL) + TLX + TLKX
C
C4------ADD COEFFICIENTS TL AND TLK TO DIAGONAL, HCOF, FOR MODEL LAYER
```

```
C4------BELOW CONFINING UNIT
      HCOF(IC,IR,IL1)=HCOF(IC,IR,IL1) + TLX + TLKX
C
C5------SUBTRACT EXPLICIT TERM SLU FROM RHS ACCUMULATOR FOR MODEL
C5------LAYER ABOVE CONFINING UNIT
      RHS(IC,IR,IL)=RHS(IC,IR,IL) - SLU(IC,IR,ILCB)
C
C6------SUBTRACT EXPLICIT TERM SLD FROM RHS ACCUMULATOR FOR MODEL
C6------LAYER BELOW CONFINING UNIT
      RHS(IC,IR,IL1)=RHS(IC,IR,IL1) - SLD(IC,IR,ILCB)
C
C7------MAKE CORRECTIONS FOR CASE WHERE HEAD IN LAYER BELOW CONFINING
C7------UNIT FALLS BELOW BOTTOM OF UNIT (TOP OF AQUIFER)
      IF(NTP.LE.0) GO TO 20
      HB=HNEW(IC,IR,IL1)
      TOP2=TOP(IC,IR,NTP)
      IF(HB.GT.TOP2) GO TO 20
       RHS(IC,IR,IL1)=RHS(IC,IR,IL1) - (TOP2-HB)*(TLX+TLKX)
   20 CONTINUE
   21 CONTINUE
   30 CONTINUE
C
C7------RETURN
      RETURN
      END
```

List of Variables for Module TLK1FM

Variable	Range	Definition
CV	Global	DIMENSION(NCOL,NROW,NLAY), Conductance in the vertical direction in the original MODFLOW program. The TLK1 Package uses this array for coefficients of head where confining units exist. Although CV is dimensioned to the size of the grid, space exists only for NLAY-1 layers.
HB	Module	Temporary single-precision equivalent of element in HNEW array corresponding to the aquifer below the confining unit. If head below confining unit is below the top of the aquifer, HB will be set to the appropriate value in the TOP array.
HCOF	Global	DIMENSION(NCOL,NROW,NLAY), Coefficient of head in the finite-difference equations.
HNEW	Global	DIMENSION(NCOL,NROW,NLAY), Most recent estimate of head in each cell.
IBOUND	Global	DIMENSION(NCOL,NROW,NLAY), Status of each cell < 0 Constant-head cell. = 0 No-flow cell. > 0 Variable-head cell.
IC	Module	Index for columns.
IDCON	Package	DIMENSION(80), Number of the model layer above each confining unit.
IL	Module	Index for layers.
IL1	Module	Index for layer below confining unit.
ILCB	Module	Index for confining units.
IR	Module	Index for rows.
NCOL	Global	Number of columns in the model grid.
NLAY	Global	Number of layers in the model grid.
NROW	Global	Number of rows in the model grid.
NTOP	Package	DIMENSION(80), Sequence number of the TOP array for each layer in the model grid. Set to 0 for model layers without a top array.
NTP	Module	Temporary equivalent of NTOP(IL).
NUMC	Package	Number of confining units with transient leakage.
RATE	Package	DIMENSION(NODES1), Hydraulic conductance of confining units.
RHS	Global	DIMENSION(NCOL,NROW,NLAY), Right-hand side of finite-difference equation.
SLD	Package	DIMENSION(NCOL,NROW,NUMC), Explicit term in transient-leakage equation for flow across bottom of confining unit. Equivalent to c_i in equation (47).
SLU	Package	DIMENSION(NCOL,NROW,NUMC), Explicit term in transient-leakage equation for flow across top of confining unit. Equivalent to d_i in equation (48).
TL	Package	DIMENSION(NCOL,NROW,NUMC), Coefficient of head in transient-leakage equations for flow across top and bottom of confining unit. Equivalent to a_i in equation (46).
TLK	Package	DIMENSION(NCOL,NROW,NUMC), Coefficient of head in transient-leakage equations for flow across top and bottom of confining unit. Equivalent to b_i in equation (45).
TLKX	Module	Temporary equivalent of TLK(IC,IR,ILCB).
TLX	Module	Temporary equivalent of TL(IC,IR,ILCB).
TOP	Global	DIMENSION(NCOL,NROW,NLAY), Elevation of the aquifer top. The TLK1 Package treats this as the elevation of the base of the confining unit. Although TOP is dimensioned to the size of the grid, space exists only for cells that can convert between confined and unconfined.
TOP2	Module	Temporary equivalent of TOP(IC,IR,NTP).

TLK1BD

Narrative for Module TLK1BD

This module calculates flow rates and quantities of water for flow across the top and bottom of each confining unit and storage changes within the confining units. Storage changes in the confining unit are calculated as the difference between flow across the top and bottom faces at each location. Rates and volumes of storage change in the confining unit are included in the overall volumetric budget for the model. Rates and volumes of flow to constant-head cells above and below confining units also are calculated and included in the overall volumetric budget. The module also saves cell-by-cell flow rates. Operations are carried out in the following order:

1. Clear the accumulators for flow rate across top of unit, flow rate across bottom of unit, flow rate to constant-head cells, and flow rate from constant head cells.

2. If cell-by-cell flow terms are to be saved, clear the buffer (BUFF) in which they will be accumulated prior to saving.

3. For each confining unit, row, and column, calculate flow rates and storage changes for this time step. (steps 4-10).

4. Set vertical conductance (CV) to zero so the Block-Centered Flow Package will not compute vertical flow to constant-head cells adjacent to confining unit with transient leakage.

5. Set temporary variables for head above and below confining unit. If head in underlying aquifer is below the base of the unit (top of the aquifer), use TOP as head at bottom boundary of unit.

6. Calculate the flow rate across top and bottom boundaries of the unit. Calculate rate of flow to or from storage as the net flow rate across the upper and lower boundaries.

7. If the cell above or below is constant-head, save the flow rate in variable CHFL.

8. If cell-by-cell flow terms are to be saved, put rate of change of storage in BUFF array, put flow across top face in TL array, and put flow across bottom face in TLK array.

9. Include storage and constant-head flow rates in appropriate inflow and outflow accumulators for overall volumetric budget.

10. Save cell-by-cell flow rates if requested. Rates to be saved for each confining unit are storage change, flow across the top face, and flow across bottom face.

11. Calculate volumes and move rates, volumes, and labels into arrays for printing volumetric budget.

12. Increment budget term counter, MSUM.

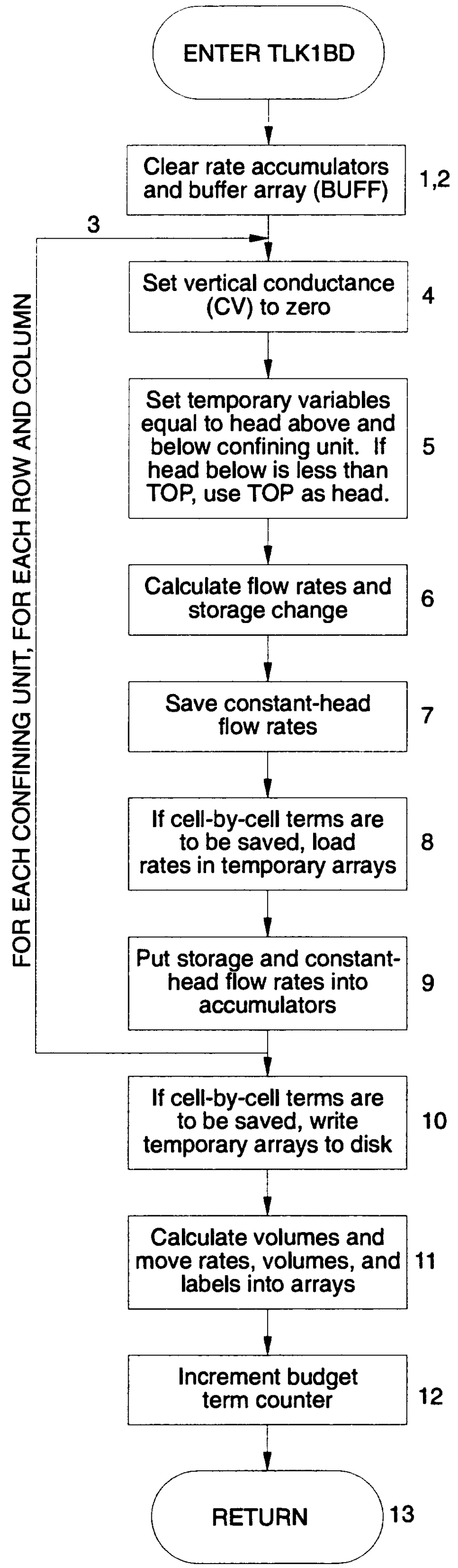
13. RETURN.

Flowchart for Module TLK1BD

BUFF is an array in which values are stored as they are being gathered for printing.

CV is conductance in the vertical direction in the original MODFLOW program.

TOP is the elevation of the aquifer top.



Program Listing for Module TLK1BD

```
      SUBROUTINE TLK1BD(RATE,TL,TLK,SLU,SLD,NUMC,ITLKCB,
     1 HNEW,BUFF,IBOUND,TOP,CV,VBNM,VBVL,MSUM,NCOL,NROW,NLAY,
     2 DELT,KSTP,KPER,ICBCFL,IOUT)
C
C-----VERSION 1100 06JAN1994 TLK1BD
C     ******************************************************************
C     VOLUMETRIC BUDGET FOR TRANSIENT LEAKAGE
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      CHARACTER*4 VBNM,TEXT1,TEXT2,TEXT3,TEXT4
      DOUBLE PRECISION HNEW
      DIMENSION HNEW(NCOL,NROW,NLAY),TOP(NCOL,NROW,NLAY),
     1 TLK(NCOL,NROW,NUMC),TL(NCOL,NROW,NUMC),SLU(NCOL,NROW,NUMC),
     2 SLD(NCOL,NROW,NUMC),RATE(NCOL,NROW,NUMC),CV(NCOL,NROW,NLAY),
     3 VBNM(4,20),VBVL(4,20),IBOUND(NCOL,NROW,NLAY),BUFF(NCOL,NROW,NLAY)
C
      COMMON /TLEAK/ IDCON(80),NTOP(80)
C
      DIMENSION TEXT1(4),TEXT2(4),TEXT3(4),TEXT4(4)
C
      DATA TEXT1(1),TEXT1(2),TEXT1(3),TEXT1(4)/'    ','C.B.',' STO',
     1'RAGE'/
      DATA TEXT2(1),TEXT2(2),TEXT2(3),TEXT2(4)/'    ','C.H.',' LEA',
     1'KAGE'/
      DATA TEXT3(1),TEXT3(2),TEXT3(3),TEXT3(4)/'    ',' FLO','W IN',
     1' TOP'/
      DATA TEXT4(1),TEXT4(2),TEXT4(3),TEXT4(4)/'    ','FLOW',' IN ',
     1'BASE'/
C     ------------------------------------------------------------------
C
C1------CLEAR THE RATE ACCUMULATIONS
      RATOUT=0.0
      RATIN=0.0
      CRATOUT=0.0
      CRATIN=0.0
      IBD=0
C
C2------IF CELL-BY-CELL FLOWS WILL BE SAVED,THEN CLEAR THE BUFFER
      IF(ICBCFL.EQ.0 .OR. ITLKCB.LE.0) GO TO 20
      IBD=1
      DO 10 IL=1,NLAY
      DO 10 IR=1,NROW
      DO 10 IC=1,NCOL
      BUFF(IC,IR,IL)=0.
   10 CONTINUE
C
C3------CALCULATE RATES FOR THIS TIME STEP
   20 DO 40 ILCB=1,NUMC
      IL=IDCON(ILCB)
      IL1=IL+1
      NTP=NTOP(IL1)
```

```
      DO 31 IC=1,NCOL
      DO 30 IR=1,NROW
C
C3A-----IF CELL IS EXTERNAL OR CONFINING UNIT DOES NOT EXIST,
C3A-----DO NOT DO BUDGET FOR IT
      IF(RATE(IC,IR,ILCB).LE.0.0) GO TO 30
      IF(IBOUND(IC,IR,IL).EQ.0) GO TO 30
      IF(IBOUND(IC,IR,IL1).EQ.0) GO TO 30
      IF(IBOUND(IC,IR,IL).LE.0.AND.IBOUND(IC,IR,IL1).LE.0) GO TO 30
C
C3B-----INITIALIZE TEMPORARY VARIABLES
      RATT=0.0
      RATB=0.0
      CHFL=0.0
C
C4------SET VERTICAL CONDUCTANCE (CV) TO ZERO TO AVOID COMPUTING
C4------FLOW FROM CONSTANT HEAD CELLS TWICE
      CV(IC,IR,IL)=0.
C
C5------GET HEAD VALUES IN MODEL LAYERS ABOVE AND BELOW CONFINING UNIT
C5------IF HEAD IN LAYER BELOW CONFINING UNIT FALLS BELOW BOTTOM OF
C5------UNIT (TOP OF AQUIFER), SET HEAD EQUAL TO TOP
      HT=HNEW(IC,IR,IL)
      HB=HNEW(IC,IR,IL1)
      IF(NTP.GT.0) THEN
       IF(HB.LT.TOP(IC,IR,NTP)) HB=TOP(IC,IR,NTP)
      ENDIF
C
C6------CALCULATE THE NET FLOW RATE INTO CELL
      RATT = TL(IC,IR,ILCB)*HT+SLU(IC,IR,ILCB)+TLK(IC,IR,ILCB)*HB
      RATB = TL(IC,IR,ILCB)*HB+SLD(IC,IR,ILCB)+TLK(IC,IR,ILCB)*HT
      SRAT = RATT + RATB
C7------SAVE RATES FOR FLOW FROM CONSTANT-HEAD CELLS THROUGH CONFINING
C7------UNITS.
      IF(IBOUND(IC,IR,IL).LT.0) THEN
       CHFL=RATT
      ENDIF
      IF(IBOUND(IC,IR,IL1).LT.0) THEN
       CHFL=RATB
      ENDIF
C
C8------IF CELL-BY-CELL BUDGET IS REQUESTED,THEN PUT RATES IN BUFFER
      IF(IBD.EQ.1) THEN
       BUFF(IC,IR,IL)=-SRAT
       TL(IC,IR,ILCB)=-RATT
       TLK(IC,IR,ILCB)=-RATB
      ENDIF
C
C9------INCLUDE STORAGE AND CONSTANT-HEAD FLOW RATES IN APPROPRIATE
C9------OUTFLOW OR INFLOW ACCUMULATOR
      IF(SRAT.LT.0.0) THEN
       RATOUT=RATOUT - SRAT
      ELSE
       RATIN=RATIN + SRAT
      ENDIF
```

```
      IF(CHFL.LT.0.0) THEN
       CRATIN=CRATIN - CHFL
      ELSE
       CRATOUT=CRATOUT + CHFL
      ENDIF
   30 CONTINUE
   31 CONTINUE
   40 CONTINUE
C
C10-----SAVE THE FOLLOWING CELL-BY-CELL RATES IF REQUESTED: STORAGE
C10-----IN EACH CONFINING UNIT, FLOW ACROSS THE TOP OF EACH UNIT, AND
C10-----FLOW ACROSS BOTTOM OF EACH UNIT
      IF(IBD.EQ.1) THEN
       CALL UBUDSV(KSTP,KPER,TEXT1,ITLKCB,BUFF,NCOL,NROW,NLAY,IOUT)
       DO 60 ILCB=1,NUMC
       IL=IDCON(ILCB)
       DO 60 IC=1,NCOL
       DO 60 IR=1,NROW
       BUFF(IC,IR,IL)=TL(IC,IR,ILCB)
   60  CONTINUE
       CALL UBUDSV(KSTP,KPER,TEXT3,ITLKCB,BUFF,NCOL,NROW,NLAY,IOUT)
       DO 70 ILCB=1,NUMC
       IL=IDCON(ILCB)
       DO 70 IC=1,NCOL
       DO 70 IR=1,NROW
       BUFF(IC,IR,IL)=TLK(IC,IR,ILCB)
   70  CONTINUE
       CALL UBUDSV(KSTP,KPER,TEXT4,ITLKCB,BUFF,NCOL,NROW,NLAY,IOUT)
      ENDIF
C
C11-----CALCULATE VOLUMES, AND MOVE RATES, VOLUMES, AND LABELS
C11-----INTO ARRAYS FOR PRINTING
      VBVL(1,MSUM)=VBVL(1,MSUM)+RATIN*DELT
      VBVL(2,MSUM)=VBVL(2,MSUM)+RATOUT*DELT
      VBVL(3,MSUM)=RATIN
      VBVL(4,MSUM)=RATOUT
      VBVL(1,MSUM+1)=VBVL(1,MSUM+1)+CRATIN*DELT
      VBVL(2,MSUM+1)=VBVL(2,MSUM+1)+CRATOUT*DELT
      VBVL(3,MSUM+1)=CRATIN
      VBVL(4,MSUM+1)=CRATOUT
      VBNM(1,MSUM)=TEXT1(1)
      VBNM(2,MSUM)=TEXT1(2)
      VBNM(3,MSUM)=TEXT1(3)
      VBNM(4,MSUM)=TEXT1(4)
      VBNM(1,MSUM+1)=TEXT2(1)
      VBNM(2,MSUM+1)=TEXT2(2)
      VBNM(3,MSUM+1)=TEXT2(3)
      VBNM(4,MSUM+1)=TEXT2(4)
C
C12-----INCREMENT BUDGET TERM COUNTER
      MSUM=MSUM+2
C
C13-----RETURN
      RETURN
      END
```

List of Variables for Module TLK1BD

Variable	Range	Definition
BUFF	Global	DIMENSION(NODES1), Buffer used for temporary storage of flow rates prior to recording cell-by-cell budgets.
CHFL	Module	Rate of flow to or from constant-head cell adjacent to confining unit.
CRATIN	Module	Total inflow from constant-head cells to confining units.
CRATOUT	Module	Total outflow to constant-head cells from confining units.
CV	Global	DIMENSION(NCOL,NROW,NLAY), Conductance in the vertical direction in the original MODFLOW program. The TLK1 Package uses this array for coefficients of head where confining units exist. Although CV is dimensioned to the size of the grid, space exists only for NLAY-1 layers.
DELT	Global	Length of current time step.
HB	Module	Temporary single-precision equivalent of element in HNEW array corresponding to the aquifer below the confining unit. If head below confining unit is below the top of the aquifer, HB will be set to the appropriate value in the TOP array.
HNEW	Global	DIMENSION(NCOL,NROW,NLAY), Most recent estimate of head in each cell.
HT	Module	Temporary single-precision equivalent of element in HNEW array corresponding to the aquifer above the confining unit.
IBD	Module	Flag: $= 0$ Cell-by-cell terms for this package will not be recorded. $\neq 0$ Cell-by-cell terms for this package will be recorded.
IBOUND	Global	DIMENSION(NCOL,NROW,NLAY), Status of each cell < 0 Constant-head cell. $= 0$ No-flow cell. > 0 Variable-head cell.
IC	Module	Index for columns.
ICBCFL	Global	Flag: $= 0$ Cell-by-cell terms will not be recorded for the current time step. $\neq 0$ Cell-by-cell terms will be recorded for the current time step.
IDCON	Package	DIMENSION(80), Number of the model layer above each confining unit.
IL	Module	Index for layers.
IL1	Module	Index for layer below confining unit.
ILCB	Module	Index for confining units.
IOUT	Global	Primary unit number for all printed output.
IR	Module	Index for rows.
ITLKCB	Package	Flag and a unit number: > 0 Unit number on which cell-by-cell flow terms will be recorded whenever ICBCFL is set. ≤ 0 Cell-by-cell flow terms will not be printed.
KPER	Global	Stress period counter.
KSTP	Global	Time step counter. Reset at the start of each stress period.
MSUM	Global	Counter for budget entries in VBVL and VBNM.
NCOL	Global	Number of columns in the model grid.
NLAY	Global	Number of layers in the model grid.
NROW	Global	Number of rows in the model grid.
NTOP	Package	DIMENSION(80), Sequence number of the TOP array for each layer in the model grid. Set to 0 for model layers without a top array.
NTP	Module	Temporary equivalent of NTOP(IL).
NUMC	Package	Number of confining units with transient leakage.
RATB	Module	Rate of flow from confining unit to underlying cell, positive for flow into cell.
RATE	Package	DIMENSION(NODES1), Hydraulic conductance of confining units.

Variable	Range	Definition
RATIN	Module	Total rate of inflow to aquifers from storage changes in confining units.
RATOUT	Module	Total rate of outflow from aquifers to storage changes in confining units.
RATT	Module	Rate of flow from confining unit to overlying cell, positive for flow into cell.
SLD	Package	DIMENSION(NCOL,NROW,NUMC), Explicit term in transient-leakage equation for flow across bottom of confining unit. Equivalent to c_i in equation (47).
SLU	Package	DIMENSION(NCOL,NROW,NUMC), Explicit term in transient-leakage equation for flow across top of confining unit. Equivalent to d_i in equation (48).
SRAT	Module	Rate of change of storage in confining unit.
TEXT1	Module	DIMENSION(4), Label for volumetric budget and cell-by-cell budget.
TEXT2	Module	DIMENSION(4), Label for volumetric budget.
TEXT3	Module	DIMENSION(4), Label for cell-by-cell budget.
TEXT4	Module	DIMENSION(4), Label for cell-by-cell budget.
TL	Package	DIMENSION(NCOL,NROW,NUMC), Coefficient of head in transient-leakage equations for flow across top and bottom of confining unit. Equivalent to a_i in equation (46). Also used in this module to store flow rate across top of confining units prior to recording cell-by-cell budget.
TLK	Package	DIMENSION(NCOL,NROW,NUMC), Coefficient of head in transient-leakage equations for flow across top and bottom of confining unit. Equivalent to b_i in equation (45). Also used in this module to store flow rate across bottom of confining units prior to recording cell-by-cell budget.
TOP	Global	DIMENSION(NCOL,NROW,NLAY), Elevation of the aquifer top. The TLK1 Package treats this as the elevation of the base of the confining unit. Although TOP is dimensioned to the size of the grid, space exists only for cells that can convert between confined and unconfined.
VBNM	Global	DIMENSION(4,20), Labels for entries in volumetric budget.
VBVL	Global	DIMENSION(4,20), Entries for the volumetric budget. For flow component N, the values in VBVL are (1,N), Rate for current time step into the flow field. (2,N), Rate for current time step out of the flow field. (3,N), Volume into the flow field during the simulation. (4,N), Volume out of the flow field during the simulation.

TLK1OT

Narrative for Module TLK1OT

This module records a restart record for later use in continuing the simulation in a new model run. Operations are carried out in the following order:

1. Return if save option is not selected. Save option is selected by setting ITLKSV to a value greater than zero. If ITLKSV is greater than zero, the value is a unit number for recording the restart information.

2. Write an unformatted restart record on unit ITLKSV. The restart record contains the length of the previous time step, the total simulation time (TLKTIM), and the contents of the cumulative memory functions RM1, RM2, RM3, and RM4.

3. Print a message noting the creation of a restart record.

4. RETURN.

Flowchart for Module TLK1OT

ITLKSV is a flag and a unit number.

> 0 Restart record will be recorded on unit ITLKRS.

≤ 0 Restart record will not be recorded.

DELTM1 is length of preceding time step.

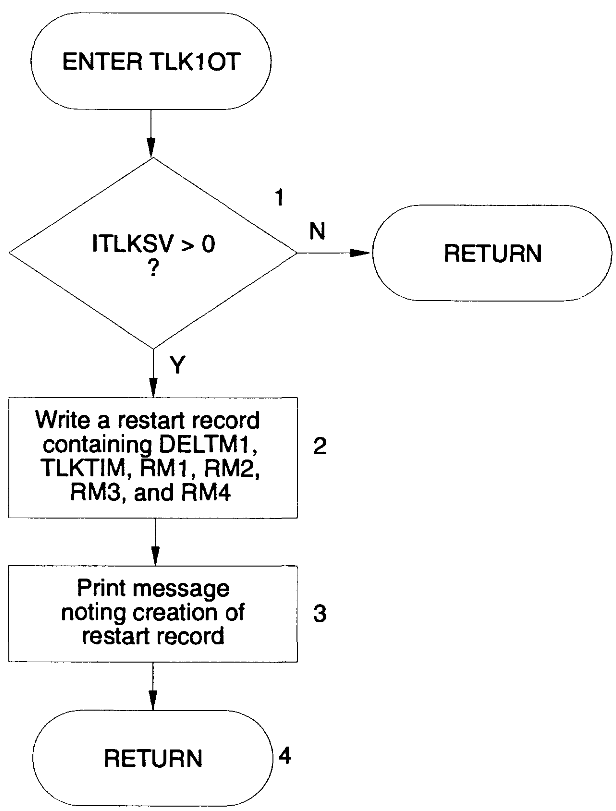
TLKTIM is simulation time since start of first model run in a series of continuation runs.

RM1 is a cumulative memory function that is updated each time step to equal the integral $\hat{K}$ given in equations (38) and (39).

RM2 is a cumulative memory function that is updated each time step to equal the integral $\hat{L}$ given in equations (40) and (41).

RM3 is a cumulative memory function that is updated each time step to equal the integral $\hat{I}$ given in equations (17) and (18).

RM4 is a cumulative memory function that is updated each time step to equal the integral $\hat{J}$ given in equations (19) and (20).



Program Listing for Module TLK1OT

```
      SUBROUTINE TLK1OT(RM1,RM2,RM3,RM4,NM1,NM2,ITLKSV,DELTM1,TLKTIM,
     1 IOUT)
C
C-----VERSION 1100 06JAN1994 TLK1OT
C     ******************************************************************
C     CREATE AN UNFORMATTED RESTART FILE FOR CUMULATIVE MEMORY (RM)
C     IN TRANSIENT-LEAKAGE PACKAGE
C     ******************************************************************
C
C        SPECIFICATIONS:
C     ------------------------------------------------------------------
      DIMENSION RM1(NM1),RM2(NM2),RM3(NM1),RM4(NM2)
C     ------------------------------------------------------------------
C
C1------RETURN IF SAVE OPTION IS NOT SELECTED
      IF(ITLKSV.LE.0) RETURN
C2------WRITE RESTART RECORD
      WRITE(ITLKSV) DELTM1,TLKTIM,(RM1(J),J=1,NM1),(RM2(J),J=1,NM2),
     1                          (RM3(J),J=1,NM1),(RM4(J),J=1,NM2)
C
C3------PRINT MESSAGE NOTING THE CREATION OF A RESTART FILE
      WRITE(IOUT,20) TLKTIM
   20 FORMAT(1X,'A RESTART RECORD FOR TRANSIENT LEAKAGE HAS BEEN CREATED
     1 FOR TIME=',G15.7)
C
C4------RETURN
      RETURN
      END
```

List of Variables for Module TLK1OT

Variable	Range	Definition
DELTM1	Package	Length of the previous time step.
IOUT	Global	Primary unit number for all printed output.
ITLKSV	Package	Flag and a unit number: > 0 Unit number on which restart information will be recorded. ≤ 0 Restart information will not be recorded.
J	Module	Index for RM1, RM2, RM3, and RM4.
NM1	Package	Number of elements in arrays RM1 and RM3.
NM2	Package	Number of elements in arrays RM2 and RM4.
RM1	Package	DIMENSION(NM1), Cumulative memory function. Value is updated each time step to equal the integral $\hat{K}$ given in equations (38) and (39).
RM2	Package	DIMENSION(NM2), Cumulative memory function. Value is updated each time step to equal the integral $\hat{L}$ given in equations (40) and (41).
RM3	Package	DIMENSION(NM1) Cumulative memory function. Value is updated each time step to equal the integral $\hat{I}$ given in equations (17) and (18).
RM4	Package	DIMENSION(NM2) Cumulative memory function. Value is updated each time step to equal the integral $\hat{J}$ given in equations (19) and (20).
TLKTIM	Package	Simulation time since start of first model run in a series of continuation runs. If restart option is not selected, value equals simulation time since start of run.

REFERENCES CITED

Bredehoeft, J.D., and Pinder, G.F., 1970, Digital analysis of areal flow in multiaquifer groundwater systems—a quasi three-dimensional model: Water Resources Research, v. 6, no. 3, p. 883–888.

Carslaw, H.S., and Jaeger, J.C., 1959, Conduction of heat in solids: Oxford, Great Britain, Clarendon, 510 p.

Conte, S.D., and de Boor, Carl, 1972, Elementary Numerical Analysis, 2d ed.: New York, McGraw-Hill Book Company, 396 p.

Cooley, R.L., 1972, Numerical simulation of flow in an aquifer overlain by a water-table aquitard: Water Resources Research, v. 8, no. 4, p. 1046–1050.

Cooley, R.L., 1992, A modular finite-element model (MODFE) for areal and axisymmetric ground-water flow problems, Part 2—Derivation of finite-element equations and comparisons with analytical solutions: U.S. Geological Survey Techniques of Water-Resources Investigations, book 6, chap. A4, 108 p.

De Marsily, G., Ledoux, E., Levassor, A.,Poitrinal, D., and Salem, A., 1978, Modelling of large multilayered aquifer systems—Theory and applications: Journal of Hydrology, v. 36, p. 1–34.

Gambolati, Giuseppe, Sartoretto, Flavio, and Uliana, Fiore, 1986, A conjugate gradient finite element model of flow for large multiaquifer systems: Water Resources Research, v. 22, no. 7, p. 1003–1015.

Hanshaw, B.B., and Bredehoeft, J.D., 1968, On the maintenance of anomalous fluid pressures—II. Source layer at depth: Geological Society of America Bulletin, v. 79, p. 1107–1122.

Hantush, M.S., 1960, Modification of the theory of leaky aquifers: Journal of Geophysical Research, v. 65, no. 11, p. 3713–3725.

Hennart, J.P, Yates, Robert, and Herrera, Ismael, 1981, Extension of the integrodifferential approach to inhomogeneous multiaquifer systems: Water Resources Research, v. 17, no. 4, p. 1044–1050.

Herrera, Ismael, 1970, Theory of multiple leaky aquifers: Water Resources Research, v. 6, no. 1, p. 185–193.

Herrera, Ismael, and Figueroa V., G.E., 1969, A correspondence principle for the theory of leaky aquifers: Water Resources Research, v. 5, no. 4, p. 900–904.

Herrera, Ismael, and Rodarte, Leopoldo, 1973, Integrodifferential equations for systems of leaky aquifers and applications—1, The nature of approximate theories: Water Resources Research, v. 9, no. 4, p. 995–1005.

Herrera, Ismael, and Yates, Robert, 1977, Integrodifferential equations for systems of leaky aquifers and applications—3, A numerical method of unlimited applicability: Water Resources Research, v. 13, no. 4, p. 725–732.

Hill, M.C., 1990, Preconditioned conjugate-gradient 2 (PCG2), a computer program for solving ground-water flow equations: U.S. Geological Survey Water-Resources Investigations Report 90—4048, 43 p.

Jacob, C.E., 1940, On the flow of water in an elastic artesian aquifer: American Geophysical Union Transmittal 21st Annual Meeting, part 2, p. 574–586.

Leake, S.A., 1990, Interbed storage changes and compaction in models of regional ground-water flow: Water Resources Research, v. 26, no. 9, p. 1939–1950.

Leake, S.A., 1991, Simulation of vertical compaction in models of regional ground-water flow, *in* Johnson, Ivan, ed., Land Subsidence—Proceedings of the Fourth International Symposium on Land Subsidence, May 1991, Houston, Texas: International Association of Hydrological Sciences Publication No. 200, p. 565–574.

Leake, S.A., and Prudic, D.E., 1991, Documentation of a computer program to simulate aquifer-system compaction using the modular finite-difference ground-water flow model: U.S. Geological Survey Techniques of Water-Resources Investigations, book 6, chap. A2, 68 p.

McDonald, M.G., and Harbaugh, A.W., 1988, A modular three-dimensional finite-difference ground-water flow model: U.S. Geological Survey Techniques of Water-Resources Investigations, book 6, chap. A1, 586 p.

Neuman, S.P., and Witherspoon, P.A., 1969, Theory of flow in a confined two-aquifer system: Water Resources Research, v. 5, no. 4, p. 803–816.

Premchitt, Jerasak, 1981, A technique using integrodifferential equations for model simulation of multiaquifer systems: Water Resources Research, v. 17, no. 1, p. 162–168.

Trescott, P.C., Pinder, G.F., and Larson, S.P., 1976, Finite-difference model for aquifer simulation in two dimensions with results of numerical experiments: U.S. Geological Survey Techniques of Water-Resources Investigations, book 7, chap. C1, 116 p.

Wilkinson, Leland, 1990, SYSTAT—The system for statistics: Evanston, Illinois, SYSTAT, Inc., 677 p.

APPENDIX

Input Data Sets for Example Problem 1

This problem simulates storage depletion in a multiaquifer system. Data sets are needed for the Basic Package, BAS1; the Output-Control option; the Block-Centered Flow Package, BCF1; the Strongly Implicit Procedure Package, SIP1; and the Transient-Leakage Package, TLK1.

Basic Package input data set

The Basic Package input data set consists of 23 records, all of which are shown below. The input is read from Fortran unit 5.

```
Example problem for use of TLK1 Package:
Problem 1—Storage depletion
         4         1        13         1         4
  7 00 00 00 00 09 00 00 12 00 00 60 00 00 00 00 00 00 00 00 00 00
         0         1
         5         1(13I3)                                  IBOUND        L1
 -1  1  1  1  1  1  1  1  1  1  1  1 -1
         5         1(13I3)                                  IBOUND        L2
 -1  1  1  1  1  1  1  1  1  1  1  1 -1
         5         1(13I3)                                  IBOUND        L3
 -1  1  1  1  1  1  1  1  1  1  1  1 -1
         5         1(13I3)                                  IBOUND        L4
 -1  1  1  1  1  1  1  1  1  1  1  1 -1
         0
         5        1.(13F5.0)                                ST HEAD       L1
   0.  11.  12.  13.  14.  15.  16.  17.  18.  19.  20.  21.  12.
         5        1.(13F5.0)                                ST HEAD       L2
   0.  11.  12.  13.  14.  15.  16.  17.  18.  19.  20.  21.  12.
         5        1.(13F5.0)                                ST HEAD       L3
   0.  11.  12.  13.  14.  15.  16.  17.  18.  19.  20.  21.  12.
         5        1.(13F5.0)                                ST HEAD       L4
   0.  11.  12.  13.  14.  15.  16.  17.  18.  19.  20.  21.  12.
      100.        40       1.0
```

Output Control input data set

The Output Control input data set consists of 49 records, 12 of which are shown below. The input is read from Fortran unit 60 as specified in the data set for the Basic Package.

```
         6         6        61        61
         1         1         0         1         INCODE IHDDFL IBUDFL ICBCFL
         0         0         0         0         Hdpr   Ddpr   Hdsv   Ddsv   L1
         0         0         0         1         Hdpr   Ddpr   Hdsv   Ddsv   L2
         0         0         0         0         Hdpr   Ddpr   Hdsv   Ddsv   L3
         0         0         0         0         Hdpr   Ddpr   Hdsv   Ddsv   L4
        -1         1         0         1         INCODE IHDDFL IBUDFL ICBCFL  2
```

(include 37 additional records identical to the preceding record)

```
         1         1         1         1         INCODE IHDDFL IBUDFL ICBCFL
         0         1         0         1         Hdpr   Ddpr   Hdsv   Ddsv   L1
         0         1         0         1         Hdpr   Ddpr   Hdsv   Ddsv   L2
         0         1         0         1         Hdpr   Ddpr   Hdsv   Ddsv   L3
         0         1         0         1         Hdpr   Ddpr   Hdsv   Ddsv   L4
```

Block-Centered Flow input data set

The Block-Centered Flow input data set consists of 17 records, all of which are shown below. The input is read from Fortran unit 7 as specified in the data set for the Basic Package.

```
         0         0
 0 0 0 0
         0        1.                                       TRPY
         0     1000.                                       DELR
         0     1000.                                       DELC
         0   2.00E-4                                       layer 1 Sf1
         0     2500.                                       layer 1 Tran
         0     0.000                                       layer 1 Vcont
         0   2.00E-4                                       layer 2 Sf1
         0     2500.                                       layer 2 Tran
         0    0.0004                                       layer 2 Vcont
         0   2.00E-4                                       layer 3 Sf1
         0     2500.                                       layer 3 Tran
         0     0.000                                       layer 3 Vcont
         0   2.00E-4                                       layer 4 Sf1
         0     2500.                                       layer 4 Tran
```

Strongly Implicit Procedure Package input data set

The Strongly Implicit Procedure Package input data set consists of two records, both of which are shown below. The input is read from Fortran unit 12 as specified in the data set for the Basic Package.

```
       120         5   MXITER  NPARM
        1.    1.0E-5         1         0         5
```

Transient-Leakage Package input data set

The Transient-Leakage Package input data set consists of eight records, all of which are shown below. The input is read from Fortran unit 9 as specified in the data set for the Basic Package.

```
         2        63         2         0         0
 1 3
         0    0.0100(13F5.0)                     confining unit 1 RATE
         0       25.                             confining unit 1 ZCB
         0    1.0E-5                             confining unit 1 SS
         0    0.0100(13F5.0)                     confining unit 3 RATE
         0       25.                             confining unit 3 ZCB
         0    1.0E-5                             confining unit 3 SS
```