The Transmissivity Iterative Calculation Routine - Theory and Numerical Implementation

1975

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THE TRANSMISSIVITY ITERATIVE CALCULATION
ROUTINE - THEORY AND NUMERICAL IMPLEMENTATION

by

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THE TRANSMISSIVITY ITERATIVE CALCULATION
ROUTINE - THEORY AND NUMERICAL IMPLEMENTATION

INTRODUCTION

Some of the most important input data to the Variable Thickenss Transient Flow Model¹ (VTT) are the aquifer property distributions. A great advantage of the VTT model simulation's numerical approach is its ability to handle heterogeneous distributions of aquifer properties. However, determination of the hydraulic conductivity and storage coefficient distributions is one of the more difficult tasks in the preparation of the input data. Since the VTT Model is two-dimensional, the two-dimensional areal distributions are needed. The values at any point represent the vertical average of that property over the aquifer's saturated thickness.

The classical approach to determine a heterogeneous hydraulic conductivity distribution has been to drill many wells and conduct many pump tests over the area being modeled. This approach has worked satisfactorily in areas where the aquifer properties are relatively uniform. However, the cost of doing this over a large, extremely heterogeneous aquifer such as the Hanford unconfined aquifer can be prohibitive. This is especially so, given the difficulty of extrapolating hydraulic conductivity values from point measurements to a uniform grid and the fact that reliable pump tests cannot be made in some areas because the high degree of heterogeneity invalidates the basic assumptions used in the pump test analysis models.

An alternate approach is to use mathematical modeling in conjunction with field data to deduce the hydraulic conductivity distribution. The Transmissivity Iterative Routine described in this report is a direct method of solving the

inverse problem using numerical simulation techniques to link the field-measured aquifer property data with the measured hydraulic potential data in order to derive a hydraulic conductivity distribution. Incorporation of the additional information from the hydraulic potential surface configuration produces a much more accurate hydraulic conductivity distribution than would be possible from measured conductivities and qualitative geological information alone.

The technique employed here to obtain a hydraulic conductivity distribution is based on numerical integration of the Boussinesq equation along instantaneous streamtubes of flow using a measured water table potential surface and solving for the conductivity. Since advantage is taken of the convergence properties of the streamtubes toward infiltration sites and channels of high transmissivity, only a small number of field-measured conductivities is required to obtain the entire distribution. Because it was not possible to use the same technique to obtain a storage coefficient distribution, it is necessary to either assume that it is constant or construct a distribution from available point measurements. The method, as used in the application to the Hanford unconfined aquifer, is very subjective and allows the hydrologist to use his knowledge on the hydrology of the aquifer in determining the hydraulic conductivity distribution.

The conductivity distribution is used as input to the Variable Thickness Transient Groundwater Flow Model.¹ The schematic diagram (Figure 1) illustrates the relationship of the Transmissivity Iterative Routine to the remainder of the Radionuclides in Soils program. The theoretical basis of the technique and its implementation on the Hanford Reservation's unconfined aquifer is described in this report.

HYDROLOGICAL MODELING PROGRAM COMPONENTS

FIGURE 1. Hydrological Modeling Program Components

SUMMARY AND CONCLUSIONS

A computer routine, the Transmissivity Iterative Routine (TIR), has been developed for calculating the hydraulic conductivity distribution in highly heterogeneous aquifers where characterization by field measurement methods alone would be prohibitive in cost. The method is based on the numerical integration of the Boussinesq equation for the hydraulic conductivity along instantaneous streamtubes of flow. Since advantage is taken of the convergence properties of streamtubes toward infiltration sites and channels of high transmissivity, only a small number of field measured transmissivities are required to obtain a hydraulic conductivity distribution. The routine yields the two-dimensional distribution of hydraulic conductivity averaged over the aquifer thickness. The agreement between the calculated and actual average conductivity is dependent on the degree to which the groundwater system satisfies the Dupuit assumption. The program was written for an interactive computer system with a light-pen, CRT display and graphical digitizer, which allow rapid reinterpretation and evaluation of groundwater contours.

Testing of the computer program on a synthetic surface identified a set of control parameters that resulted in a maximum computational error of ± 5 percent. This maximum error occurred as streamtubes passed near stagnation points where the groundwater hydraulic potential gradients and radii of curvature were small. Sensitivity tests on the Hanford unconfined aquifer indicated that the hydraulic conductivity calculation is not particularly sensitive to errors in the storage coefficient distribution over much of the aquifer. These tests also illustrated the power of the TIR method to evaluate the validity of field data.

The TIR was implemented on the Hanford unconfined aquifer and an approximation to the vertically averaged hydraulic conductivity distribution was calculated. The best way to determine the accuracy of the calculated conductivity distribution is to obtain enough additional measurements for comparisons to be of statistical significance. However, time and funding constraints have restricted this, so indirect methods of comparing calculated and observed groundwater changes and travel times were used. Preliminary verification of this distribution, accomplished by simulating the groundwater potential changes as functions of time for the period 1968 through 1973, was surprisingly good, considering the estimated accuracy of the input data, for those regions where enough data were available. Comparisons of calculated and observed travel times were also good in those regions. These results suggest that the method filters some of the errors in the data and that some of the data errors are compensating. A more rigorous analysis is required to quantify these effects.

The tests and verification calculations performed demonstrated the usefulness of the TIR method for

- 1) generating hydraulic conductivity distributions for heterogeneous aquifers;
- 2) systematically evaluating the adequacy and reliability of existing data;
- 3) specifying the type, quantity and location of additional data that would be required to provide the desired accuracy and resolution of aquifer conductivity.

RECOMMENDATIONS

Time and funding constraints have prevented full utilization of the TIR on the Hanford unconfined aquifer. Because knowledge of the hydraulic conductivity distribution is important to effective waste management at Hanford, it is recommended that the method be systematically applied, in conjunction with a field data collection program, to calculate an accurate conductivity distribution for the unconfined aquifer. The TIR should be used to define the most cost-effective field data collection program possible for characterizing the unconfined aquifer, by identifying the density, location, and accuracy of field data needed.

To accomplish this objective, the following tasks should be completed:

- conduct a more complete and rigorous error and sensitivity analysis (including procedures that will enable a hydrologist to specify the accuracy and density of field data necessary to obtain a specified accuracy of the hydraulic conductivity distribution);
- improve the computer program to shorten the iterative loop calculation time (the hours presently necessary to compute a K distribution make it impractical to complete more than one or two iterations per year on the conductivity distribution); and
- verify the calculated hydraulic conductivity distributions by field measurements in new locations. It would also be productive to compute the K distribution from several different potential surfaces. A high degree of consistency would give added confidence in the results.

REVIEW OF PREVIOUS WORK

Solution of the differential equation of groundwater flow for hydraulic conductivity when the potential distribution is known is often referred to as the inverse problem. No attempt will be made here to summarize all the different approaches to the solution of this problem and associated model calibration techniques (a good summary appears in Sagar²). Only direct techniques (i.e., those that do not involve iterative solution of the flow simulation model equations to obtain the aquifer property distributions), and principally the direct technique upon which the Transmissivity Iterative Routine is based, are discussed in this report.

The iterations implied by the name, Transmissivity Iterative Routine, pertain to reworking of the hydraulic potential contour interpretations, to the reinterpretation of pump test conductivity data, and to iterations of the fitting of the conductivity distribution along the reference lines to obtain the most consistent hydraulic conductivity distribution over the entire aquifer.

WORK OF OTHER AUTHORS

The theory for the solution of the groundwater flow equation with the necessary boundary conditions for a unique hydraulic conductivity distribution along a streamline has been derived for the three-dimensional case by Nelson.^{3, 4, 5, 6} However, practical application of the results is difficult. The three-dimensional potential distribution and the hydraulic conductivity distribution with depth at a specific point are usually not available. In addition, in our opinion, there are apparently insurmountable difficulties in developing a sufficiently accurate numerical approximation of the gradient of the potential surface when only a few piezometer measurements are available to define that surface.

Prudhomme⁷ developed a theory analogous to Nelson's for a two-dimensional confined aquifer. In his paper he does not, however, describe the numerical technique used to approximate the gradient and Laplacian. He briefly describes a sample case in which the method was applied but presents no supportive data. Thus, it is difficult to evaluate the applicability of his method to an actual case study.

At the same time the work described in this report was progressing, Emsellem and deMarsily⁸ were formulating an alternate method for solving the inverse problem for transient flow in a confined aquifer. Their technique involves minimization of the flow imbalance over each subregion of flow by adjustment of the aquifer parameters so that the most "continuous" distribution of the properties is obtained. A successively finer division of the total flow region is made as the iterations progress. The division stops when no further improvement in potential calculation occurs or the scale of the spacing of the potential data is reached. The method has been tested on a relatively simple aquifer in Germany, but is still in its early stages of development, according to the authors. Witherspoon⁹ applied a version of the computer program to a heterogeneous aquifer but was not able to get satisfactory results.

Another approach to solving the inverse problem is the linear programming technique described by Kleinecke.¹⁰ The main drawback to this approach is that there is nothing to insure the presence of all the nodal aquifer parameter values in the solution.

Sagar² presented a direct method for solving the inverse problem that involves transformation of the partial differential equation of flow into algebraic equations using the known dependent variable derivatives. Subsequently, the equation system is solved by nonlinear optimization methods. Spline functions are used to evaluate the derivatives. Only

linear groundwater flow systems can be treated and one of the aquifer parameters must be specified.

Frind and Pinder¹¹ have applied the finite element method to the direct solution of the inverse problem under steady flow conditions using the Galerkin approach for the solution. They found that the transmissivity solution was most sensitive to the hydraulic potential approximation function. A similar sensitivity was found in the TIR technique discussed herein.

Finally, the introduction of uncertainty into the model calibration problem using direct methods of inverse problem solution is just beginning to be investigated. Neumann¹² presents arguments on the need to consider multiple objective criteria in view of the uncertainties involved.

APPLICATIONS TO THE HANFORD GROUNDWATER SYSTEM

Nelson's energy dissipation approach, mentioned earlier, readily reduces to two-dimensions for the assumptions of a uniformly thick, confined aquifer. Nelson and Cearlock¹³ found that the two-dimensional version worked reasonably well for the portion of the Hanford unconfined aquifer for which adequate mathematical representations of the hydraulic potential surface could be obtained. However, they could not obtain adequate mathematical representations of the potential over the greater portion of the groundwater system.

Subsequent attempts by the senior author to obtain adequate representations over the entire Hanford aquifer using a variety of functional fitting and interpolation techniques were also unsuccessful. Interpolation techniques had the disadvantage that the magnitude of the computed Laplacian was a function of the technique used. He concluded that (1) methods for obtaining mathematical representations of the potential of the Hanford groundwater system consistent with the requirements of Nelson's approach did not exist; (2) there did not appear to be a rational

approach for significantly improving functional fitting methods to the level required; and (3) Nelson's approach is theoretically sound but of limited value when applied to complex groundwater systems because of functional fitting limitations.

Therefore, the Transmissivity Iterative Routine, described below, was developed to solve the inverse problem for complex, transient groundwater systems such as the one beneath the Hanford Reservation. The initial version of the program solved the inverse problem for the transmissivity, which was converted independently of the program to hydraulic conductivities by dividing the transmissivity by the aquifer thickness. Although in later versions the inverse problem was solved directly for the hydraulic conductivity, the original name of the computer program was retained.

THEORY OF THE TRANSMISSIVITY ITERATIVE ROUTINE

ASSUMPTIONS AND IMPLICATIONS

Most of the assumptions for the Transmissivity Iterative Routine are inherent in the Variable Thickness Transient Groundwater Flow Model (described in BNWL-1703¹) to which this routine applies. These basic assumptions include:

1. The groundwater flows as an incompressible fluid that saturates a rigid porous soil matrix.
2. Darcy's Law governs the flow.
3. The uppermost aquifer under the Hanford Reservation is unconfined.
4. The water table has only small inclinations and the slope of the aquifer bottom is slight.
5. Vertical velocities can be neglected so that the equations of flow can be averaged in the vertical direction (Dupuit or Boussinesq assumption).
6. Aquifer parameter distributions and the hydraulic potential are continuous over the region.
7. The hydraulic conductivity is isotropic but heterogeneous throughout the region.

That groundwater flow, for modeling purposes, is basically two dimensional is perhaps the most fundamental assumption. Although the transmissivity calculation technique could be extended to three dimensions without encountering theoretical or numerical problems, it is our opinion that the additional data and developments in measurement techniques that would be required make implementation of a three-dimensional solution to the inverse problem impractical at this time. Theory and techniques, presently under development, to measure conductivity and hydraulic potential with depth for sediments which

are inhomogeneous and cannot be divided into distinct, continuous layers would have to be proven. Furthermore, a three-dimensional analysis would require, in our opinion, an increase in the number of conductivity and hydraulic potential measurements by more than an order of magnitude.

Additional assumptions for the Transmissivity Iterative Routine, and comments about the assumptions, follow.

1. The storage coefficient for the unconfined aquifer is constant over the Reservation.

In view of the heterogeneity of the conductivity, there is little justification for a constant storage coefficient. However, a lack of data makes this assumption necessary. Techniques for computing a storage coefficient distribution simultaneously with the hydraulic conductivity distribution have not yet been developed. The assumed value of 0.1 is low for unconsolidated sediments and unconfined conditions, but it was selected for stability of the numerical calculation in the early phases of the model development. The error introduced by inaccuracies in the storage coefficient is proportional to the ratio of the rate of storage divided by the groundwater flux (transient ratio). The smaller the ratio, the less important storage is in the calculation of the conductivity.

2. The source term for recharge, leakage, and withdrawal is neglected.

Underflow at the boundaries of the groundwater system is automatically accounted for in the governing equations, since streamtubes either start or stop at these locations. Flow associated with major sources/sinks, which result in observable mounds or depressions in the water table, likewise is accounted for in the governing equations. Streamtubes are not generated in areas directly beneath these sites where infiltration occurs because the rapid rate of change in gradients introduces significant error into the calculations.

Thus, the source term is usually important only for diffuse sources/sinks, such as infiltration of precipitation, seepage from irrigation, interaquifer transfer and large numbers of small withdrawals or discharges.

Available data indicate that the diffuse sources/sinks are not important in the calculation of the hydraulic conductivity for the Hanford unconfined aquifer. For instance, there are no significant withdrawals of groundwater or irrigation developments on the Hanford Reservation. Present data indicate that infiltration from rainfall is negligible. The waste disposal discharge sites have so little flow in relation to the total groundwater flow through their local areas that no significant error results from neglecting them. Interchange between the unconfined and uppermost confined aquifers is probably small in most areas. However, further investigation is needed to substantiate this observation and obtain quantifiable data.

Although the source term has been neglected in work done to date, incorporating the term into the computer program presents no theoretical or numerical difficulty, as is shown in the subsection on Formulation of the Equations.

3. The hydraulic conductivity along a reference curve is relatively smooth.

Since the reference lines are short in relation to the aquifer length scale, it appears reasonable that a smooth, continuous hydraulic conductivity curve should exist across areas of streamline convergence. This assumption enables one to identify erratic conductivity values and attribute them to errors in potential contouring, in initial pump test values, or in the other parameter distributions. The essence of the iterative sequence is the extensive testing and adjusting that must be done to achieve the most consistent set of conductivity values and thus the best interpretation of the conductivity distribution along the reference curves.

4. The hydraulic conductivity distribution derived for a point in time is valid for all other times and associated water table configurations simulated by the VTT Model.

Since the vertical variation of the hydraulic conductivity is not known, the computed vertical average conductivity must be assumed independent of the saturated thickness when used in the VTT Model. If the vertical average conductivity significantly changes as the water table moves up from the finer silts and sands into the coarser and more permeable sands and gravels, the contribution of the zones of differing permeability should be weighted in proportion to their saturated thickness.

One possible way to evaluate the magnitude of vertical average conductivity changes with changes in aquifer saturated thickness would be to compute the conductivity distributions for two significantly different water table configurations. However, this type of data is not available for the Hanford unconfined aquifer.

Another estimate of the errors introduced by this assumption could be obtained by making in-place measurements of the permeability at selected points above and below the water table and determining how the value of the average permeability changes as the water table moves. However, a satisfactory procedure for making the in-place measurements must be developed. If the vertical average conductivity were found to be a strong function of saturated thickness, an extensive field measurement program would be required to obtain the data necessary to implement this feature into the VTT Model. This effort would be very expensive to implement.

FORMULATION OF THE EQUATIONS

The basic equation used for two-dimensional horizontal flow in an unconfined aquifer is the nonlinear Boussinesq¹⁴

equation used in the Variable Thickness Transient Ground-water Flow Model:¹

$$\underline{\nabla} \cdot K(h-h^0) \underline{\nabla} h = \sigma \frac{\partial h}{\partial t} - q \quad (1a)$$

where

K = vertically averaged hydraulic conductivity, ft/day

h = hydraulic potential, ft

h^0 = aquifer bottom elevation, ft

σ = storage coefficient

q = infiltration flux, ft/day

t = time, days

$\underline{\nabla}$ = two-dimensional (horizontal) gradient operator

It is assumed that the hydraulic potential, h, is known as a function of space and time for some period and that the boundary conditions and infiltration fluxes are also known.

Concern has been expressed by Nelson¹⁵ as to whether Equation 1a is the correct equation to use for the inverse problem. He suggests that Equation 1b may be more appropriate and avoids the difficulties associated with using the storage term in Equation 1a.

$$\underline{\nabla} \cdot K \underline{\nabla} h = 0 \quad (1b)$$

Nelson's assertion depends on whether the observed ground-water potentials used in the calculations are influenced by storage; however, data are not available at this time to assess these implications. In reality, conditions probably exist in which either equation may be more representative at different locations within the same aquifer. If Equation 1b is more representative at point, the effect of the storage term on the calculated conductivity would be small and would introduce little error into the calculations. For this reason and for consistency, Equation 1a was used as the basic storage equation for the inverse problem.

The objective is to solve Equation 1 for the hydraulic conductivity, given the storage coefficient distribution. In confined two-dimensional flow, the transmissivity term, T , is proportional to the hydraulic conductivity, K . The formal relationship that can be defined for unconfined flow is $T = K(h-h^0)$. Note the very important fact that the transmissivity in unconfined flow is a function of time due to the dependence on the hydraulic potential, h .

Equation 1 is a first order partial differential equation for the hydraulic conductivity which can be written as

$$K(h-h^0) \nabla^2 h + (h-h^0) \underline{\nabla} K \cdot \underline{\nabla} h + K \underline{\nabla} (h-h^0) \cdot \underline{\nabla} h - \sigma \frac{\partial h}{\partial t} + q = 0 \quad (2)$$

By the methods presented in Goursat¹⁶ and Hildebrand,¹⁷ the above partial differential equation can be reduced to a system of ordinary differential equations:

$$\frac{dx}{ds} = - \frac{\partial h}{\partial x} \quad (3a)$$

$$\frac{dy}{ds} = - \frac{\partial h}{\partial y} \quad (3b)$$

$$\frac{dK}{ds} = K(\nabla^2 h + \frac{1}{h-h^0} \underline{\nabla} (h-h^0) \cdot \underline{\nabla} h) - \frac{\sigma}{h-h^0} \frac{\partial h}{\partial t} + \frac{q}{h-h^0} \quad (3c)$$

The first two equations give the characteristic curves of the solution region and the last is the ordinary differential equation for K along those curves.

A streamline is a curve which is tangent to the local velocity vector at each point. In a transient system, there are instantaneous streamlines with different configurations for different points in time. At a given point in time they have the properties of streamlines for steady flow; i.e., they

do not cross, they begin and end at boundaries of the region or point sources and sinks, and they are orthogonal to the equipotential lines when isotropic flow is assumed. When t is set to a constant, t' , the following equation defines the instantaneous streamline pattern:

$$\frac{K(h-h^0)}{\sigma} \nabla h \cdot \nabla \Psi = 0 \quad \text{at } t = t'$$

where $\Psi(x, y, t') = C$ is the stream function.

By the method of characteristics, it can be shown that the instantaneous streamlines are identical to the characteristic curves for Equations 3a-3c. When these equations are solved from an initial point (x_0, y_0) the streamline for $t = t'$ is obtained. Other starting points give other instantaneous streamlines. The differential equation for K can be solved along these streamlines when the appropriate initial conditions are known.

It has been shown by Nelson^{5,6} that the necessary condition for a unique solution for K is a single value of hydraulic conductivity on each streamline at time t' . In other words, the hydraulic conductivity must be known along a curve $\Gamma(x, y)$ that is not a characteristic curve (streamline) and that intersects every streamline of the region at time t' . This curve may be piecewise continuous. Using the chain rule, Equations 3a and 3b give:

$$\frac{dh}{ds} = \frac{\partial h}{\partial x} \frac{dx}{ds} + \frac{\partial h}{\partial y} \frac{dy}{ds} = -\nabla h \cdot \nabla h \quad \text{along a streamline so}$$

$$\frac{dK}{ds} = \frac{dK}{dh} \frac{dh}{ds} = - \frac{dK}{dh} (\nabla h)^2$$

where $(\nabla h)^2 = \nabla h \cdot \nabla h$

Thus, Equation 3c becomes:

$$\frac{dK}{dh} + K \frac{\nabla^2 h + \nabla \ln(h-h^0) \cdot \nabla h}{(\nabla h)^2} = \frac{\frac{\sigma}{h-h^0} \frac{\partial h}{\partial t} \Big|_{t'} - \frac{q}{h-h^0}}{(\nabla h)^2} \quad (4)$$

on each streamline.

Now that the parameter, s , that measures distance along the streamline has been eliminated, the solution to Equation 4 follows directly:

$$K(x,y) = K_o(h_o) e^{\int_{h_o}^h A' dn} + \left[e^{\int_{h_o}^h A' dh} \right] \left[\int_{h_o}^h e^{\int_{h_o}^h A' dh} B' dh \right] \quad (5)$$

where

$$A' = \frac{\nabla^2 h + \nabla \ln(h-h^o) \cdot \nabla h}{(\nabla h)^2} \quad \text{and} \quad B' = \frac{\sigma \frac{\partial h}{\partial t} \Big|_{t'} - q}{(h-h^o) (\nabla h)^2}$$

Note that h^o is the aquifer bottom surface and h_o is the point at which hydraulic conductivity K_o is known on the streamline under consideration.

An entirely equivalent formulation can be made in terms of the transmissivity $T = K(h-h^o)$ for any instant in time. The corresponding analytical solution⁷ is

$$K(x,y) = T_o e^{\int_{h_o}^h A dh} + \left[e^{\int_{h_o}^h A dh} \right] \left[\int_{h_o}^h e^{\int_{h_o}^h A dh} B dh \right] \quad (6)$$

where

$$A = \frac{\nabla^2 h}{(\nabla h)^2} \quad \text{and} \quad B = \frac{\sigma \frac{\partial h}{\partial t} \Big|_{t'} - q}{(\nabla h)^2}$$

and T_o is known at a point, $h_o(s_o)$, on each streamline.

Unfortunately, it is not practically feasible to use Equations 5 or 6 directly in determining the hydraulic conductivity distribution because the Laplacians and the product of the gradients of the potential surface need to be calculated. Previous work demonstrated that this cannot be done with sufficient accuracy in a numerical procedure, particularly when the surface of h is determined from field measurements.

For these reasons a slightly modified approach is taken by returning to the original Boussinesq equation and integrating it over the sub-element area (streamtube element) between two streamlines, as shown in Figure 2 and given in Equation 7.

$$\iint_{\psi s} (\nabla \cdot K(h-h^0) \nabla h - \sigma \frac{\partial h}{\partial t} + q) dsdn = 0 \quad \text{at } t=t' \quad (7)$$

FIGURE 2. Streamtube Element Between Two Instantaneous Streamlines

The integrals are approximated by the following procedure.

By Green's first theorem

$$\iint_{r_{ij}} (\nabla \cdot K(h-h^0) \nabla h) dsdn = \int_{\Gamma_{ij}} K(h-h^0) \frac{\partial h}{\partial \hat{n}} d\Gamma$$

where $\hat{n}$ is the outward normal to r_{ij} on Γ_{ij} .

Since $\frac{\partial h}{\partial \hat{n}} = 0$ along Ψ_j

$$\int_{i,j}^{i+1,j} K(h-h^0) \frac{\partial h}{\partial \hat{n}} d\Gamma = \int_{i,j+1}^{i+1,j+1} K(h-h^0) \frac{\partial h}{\partial \hat{n}} d\Gamma = 0.$$

Integrating along the other two sides gives

$$\int_{i+1,j}^{i+1,j+1} K(h-h^0) \frac{\partial h}{\partial \hat{n}} d\Gamma \approx$$

$$K_{i+1,j+1/2} (h_{i+1,j+1/2} - h_{i+1,j+1/2}^0) \frac{\partial h}{\partial s} \Big|_{i+1,j+1/2} w_{i+1}$$

and

$$\int_{i,j}^{i,j+1} K(h-h^0) \frac{\partial h}{\partial \hat{n}} d\Gamma \approx$$

$$K_{i,j+1/2} (h_{i,j+1/2} - h_{i,j+1/2}^0) \frac{\partial h}{\partial s} \Big|_{i,j+1/2} w_i$$

Integrating the volume integral gives

$$\iint_{\Psi_{ij}} (-\sigma \frac{\partial h}{\partial t} \Big|_{t'} + q) dsdn \approx \left[-1/2 (\sigma_{i+1,j+1/2} \frac{\partial h}{\partial t} \Big|_{i+1,j+1/2} + \sigma_{i,j+1/2} \frac{\partial h}{\partial t} \Big|_{i,j+1/2}) \right. \\ \left. + \frac{1}{2} (q_{i+1,j+1/2} w_{i+1} + q_{i,j+1/2} w_i) \right] \left[s_{i+1,j+1/2} - s_{i,j+1/2} \right]$$

Combining the equations above and solving for K_{i+1} gives the finite-difference equation for calculating the conductivity along a given streamtube. Since all of the terms are evaluated at $j+1/2$, and $t=t'$, for convenience these subscripts are dropped.

$$K_{i+1} = \left[\frac{1}{\left. \frac{\partial h}{\partial s} \right|_{i+1} w_{i+1} (h_{i+1} - h_{i+1}^o)} \right] \left[K_i (h_i - h_i^o) \left. \frac{\partial h}{\partial s} \right|_i w_i - \left(\frac{s_{i+1} - s_i}{2} \right) \right. \\ \left. \left[\sigma_{i+1} \left. \frac{\partial h}{\partial t} \right|_{i+1} w_{i+1} + \sigma_i \left. \frac{\partial h}{\partial t} \right|_i w_i - q_{i+1} w_{i+1} - q_i w_i \right] \right] \quad (8)$$

The boundary condition required is the value of K at any point on the centerline of each streamtube that one desires to calculate. With this starting value, K at any point along the streamtube centerline can be computed using Equation 8.

For the analyses conducted to date, the infiltration term, q , has been considered negligible and the storage coefficient has been treated as a constant (see subsection on Assumptions and Implications). Under these two assumptions, Equation 8 reduces to

$$K_{i+1} = \left\{ \frac{1}{\left. \frac{\partial h}{\partial s} \right|_{i+1} w_{i+1} (h_{i+1} - h_{i+1}^o)} \right\} \left\{ K_i (h_i - h_i^o) \left. \frac{\partial h}{\partial s} \right|_i w_i - \sigma \left[\frac{s_{i+1} - s_i}{2} \right] \right. \\ \left. \left[\left. \frac{\partial h}{\partial t} \right|_{i+1} w_{i+1} + \left. \frac{\partial h}{\partial t} \right|_i w_i \right] \right\} \quad (9)$$

For analyses under steady state assumptions, Equation 9 reduces to

$$K_{i+1} = \frac{K_i (h_i - h_i^O) \left. \frac{\partial h}{\partial s} \right|_i w_i}{\left. \frac{\partial h}{\partial s} \right|_{i+1} w_{i+1} (h_{i+1} - h_{i+1}^O)} \quad (10)$$

Equations 9 and 10 can be recast so that the hydraulic conductivity can be calculated at any point along the stream-tube with respect to the starting point. Equation 9 becomes

$$K_{n+1} = \left(\prod_{i=1}^{n+1} \delta_i \right) K_O - \sum_{i=1}^{n+1} \epsilon_i \quad (11)$$

where

$$\delta_j = \delta_i = \frac{w_{i-1} \left. \frac{\partial h}{\partial s} \right|_{i-1} (h_{i-1} - h_{i-1}^O)}{w_i \left. \frac{\partial h}{\partial s} \right|_i (h_i - h_i^O)} \quad \text{and} \quad (12a)$$

$$\epsilon_i = \frac{\left[\sigma \left(\frac{s_i - s_{i-1}}{2} \right) \right] \left[\left. \frac{\partial h}{\partial t} \right|_i (h_i - h_i^O) w_i + \left. \frac{\partial h}{\partial t} \right|_{i-1} (h_{i-1} - h_{i-1}^O) w_{i-1} \right]}{w_i \left. \frac{\partial h}{\partial s} \right|_i (h_i - h_i^O)} \quad (12b)$$

Equation 10 becomes

$$K_{n+1} = \left(\prod_{i=1}^{n+1} \delta_i \right) K_O \quad (13)$$

where δ_i is defined by Equation 12a.

OVERVIEW OF CALCULATION PROCEDURE

To obtain the hydraulic conductivity distribution over a discrete set of nodes, Equation 7 must be integrated along a set of streamtubes which contains each node point. This is accomplished by solving either Equation 8, 9 or 10 as follows.

The streamtube is defined by two streamlines generated from a point where the vertically averaged conductivity is known (Figure 2). The streamtube is generated both up- and down-gradient in incremental steps until boundaries are reached, the conductivity being calculated at the center of the streamtube for each step. Parameters are input for controlling the streamtube so that width, step size and angular adjustments are maintained within specified limits.

The conductivity values at nodes not contained in one of these tubes can be obtained by exploiting the convergence properties of the streamtubes toward points of infiltration or areas of high conductivity. At a convergence region a reference line can be drawn to intersect the streamtubes and values of conductivity calculated at the location where each streamtube intersects the reference line. It is physically reasonable that there should be a smooth variation of conductivity along a reference line crossing a group of adjacent streamtubes. Thus, the hydrologist draws what he feels is the best curve defining the conductivity values along the reference line using all of the data he has available to him.

Using the conductivity curve at the reference line, Equation 9 can be solved to obtain the conductivity at any node contained within the streamtubes which intersect the reference line. However, since it is difficult to select the correct starting location at the reference line for the streamtube which contains a specific node, an indirect procedure has been devised which is based on Equation 11.

An initial value K_0 is assumed at a node and the streamtube is generated to the reference line. Using the fit curve value K'_{n+1} and the calculated value, K_{n+1} , both determined at the point the streamtube intersects the reference line, the initial value of conductivity, K , at the node in question is corrected by the following equation:

$$K'_O = \frac{1}{\prod_{i=1}^{n+1} \delta_i} (K'_{n+1} - K_{n+1}) + K_O \quad (14)$$

where δ_i is defined by Equation 12a.

Values of the coefficients needed for solving Equations 8, 9 or 10, (such as $\frac{\partial h}{\partial t}$, $\frac{\partial h}{\partial x}$, $\frac{\partial h}{\partial y}$) are obtained by linear interpolation from the four rectangular grid points which define the cell containing the calculation point. This approach therefore necessitates that all input data be defined on a uniform grid. The spatial gradients are generated using central difference approximations on the hydraulic potential distribution.

The numerical technique used to solve Equations 8, 9 and 10 is described in greater detail in BNWL-1707, "The Transmissivity Iterative Programs on the PDP-9 Computer - A Man-Machine Interactive System."

TESTING THE TRANSMISSIVITY ITERATIVE ROUTINE

The Transmissivity Iterative Routine was tested on both a synthetic surface and the Hanford unconfined aquifer. The results of these analyses are summarized below and presented in detail in Appendices A and B.

Test on a Synthetic Surface

The program was tested on a steady state synthetic potential surface (Figure 3) to determine the best combination of control parameters within the constraints of accuracy and computational time. Accuracy was the dominant consideration, because identification of inconsistencies which may occur in the construction of the hydraulic conductivity reference curves is easier if the inconsistencies are a result of data or data interpretation errors, rather than computational errors.

The scale of the test surface was representative of the hydraulic gradients observed in the Hanford unconfined aquifer. Several test series with three different streamtubes were run to determine the optimum values of the seven control parameters. As a result of these tests the optimum parameter values for minimizing computational errors and times were identified (Table 1). Using these control parameters, four additional streamtubes were generated. The paths of the streamtubes are shown in Figure 3 and the calculated error in hydraulic conductivity along these streamtubes is shown in Figures 4 through 10. The error is calculated by the following equation:

$$\text{error} = \frac{K_c - K_n}{K_n} 100$$

where K_n = known conductivity

K_c = calculated conductivity

TABLE 1. Optimum Control Parameter Values

Starting Width (ft)	1.25
Minimum Width (ft)	0.5
Maximum Width (ft)	2.0
Width Adjustment Factor (%)	0.4
Starting Step Size (ft)	1.25
Step Adjustment Factor (%)	0.05
Maximum Angle of Deviation (Degrees)	5.0

FIGURE 3. Synthetic Groundwater Potential Surface and Streamtubes Used in Sensitivity Tests of the TIR Method

FIGURE 4. Calculation Error in Hydraulic Conductivity Along Streamtube #1 Using Optimum Control Parameters

FIGURE 5. Calculation Error in Hydraulic Conductivity Along Streamtube #2 Using Optimum Control Parameters

ERROR ANALYSIS

FIGURE 6. Calculation Error in Hydraulic Conductivity Along Streamtube #3 Using Optimum Control Parameters

ERROR ANALYSIS

FIGURE 7. Calculation Error in Hydraulic Conductivity Along Streamtube #4 Using Optimum Control Parameters

ERROR ANALYSIS

FIGURE 8. Calculation Error in Hydraulic Conductivity Along Streamtube #5 Using Optimum Control Parameters

ERROR ANALYSIS

FIGURE 9. Calculation Error in Hydraulic Conductivity Along Streamtube #6 Using Optimum Control Parameters

ERROR ANALYSIS

FIGURE 10. Calculation Error in Hydraulic Conductivity Along Streamtube #7 Using Optimum Control Parameters

The maximum calculation error for any of these streamtubes is approximately 5 percent, which is considered very good.

The results showed that the largest errors occur as streamtubes approach stagnation points and that the calculational error is most sensitive to the control parameters for streamtubes which pass through these areas.

Tests on the Hanford Unconfined Aquifer

Since negative hydraulic conductivities were calculated for some streamtubes when a storage coefficient value of 0.2 was assumed, a limited sensitivity analysis for the storage coefficient was conducted on the southeastern portion of the

aquifer, the only region in which field data were sufficient to make meaningful observations. The optimum control parameters determined by the synthetic tests were used in these tests.

The results showed that the hydraulic conductivity calculations for over half of the streamtubes were relatively insensitive to variations in the storage coefficient (see Table B-1, Appendix B). A typical result showed that a 100 percent change in the storage coefficient resulted in less than a 20 percent change in the calculated hydraulic conductivity at the reference line. For those streamtubes in which the calculated hydraulic conductivities were sensitive to changes in storage coefficient, it appeared that the starting conductivities used in the analysis were low. Reanalysis of the pump test data for these measurements supported this observation.

It should be emphasized that these results are representative for a given region where the groundwater flow is large compared to the rate of storage. Preliminary tests with limited data for other portions of the aquifer indicate that the conductivity calculations are more sensitive to changes in the storage coefficient. This is to be expected since the ratio of groundwater flow to rate of storage is less in these regions than in the southeastern portion of the aquifer.

The sensitivity analysis illustrates the usefulness of the TIR method to evaluate the validity of data and derive the most realistic aquifer parameter distributions. Its full potential will be realized only by a time-consuming, systematic analysis coordinated with a good field data collection program.

NUMERICAL IMPLEMENTATION OF THE TRANSMISSIVITY
ITERATIVE ROUTINE ON THE HANFORD UNCONFINED AQUIFER

The Transmissivity Iterative Routine was implemented on the Hanford unconfined aquifer in three sequential steps: preparation of input data, calculation of the conductivity reference lines, and calculation of the conductivity distribution.

INPUT DATA REQUIREMENTS

The method requires the following input data:

- 1) the grid origin, grid size, node size, and location of boundaries;
- 2) the location and flow rates of infiltration sources and discharge sinks;
- 3) the measured potential distribution for a point in time, $t=t'$, for which the instantaneous streamlines are to be calculated;
- 4) the distribution of $\left. \frac{\partial h}{\partial t} \right|_{t'}$; i.e., the rate of change of potential with time for $t=t'$;
- 5) the aquifer bottom surface;
- 6) the measured conductivity values at various points over the aquifer being modeled; and
- 7) the storage coefficient distribution.

There are many methods for obtaining the values of data points for the various parameters. For instance, the hydraulic conductivity boundary condition (K_0) values are presently known from field tests at 46 points over the Hanford Reservation (see Figure 14). Likewise, methods vary for transferring the point measurement data onto a uniform grid. Experience has indicated that this can be done more accurately by hand drawing of contours using graphical interpolation techniques than by functional fitting or computer-oriented interpolation techniques. In drawing the

contours, the analyst can take into account his knowledge of the groundwater flow system, the geology and related theory. The contour maps are then digitized to transfer the data to the required uniform grid. In other words, the irregularly spaced digital data are converted to continuous analog data which are in turn converted to uniformly spaced digital data.

For the Hanford unconfined aquifer the sources and sinks were neglected, as described in the assumptions. The measured potential distribution (Figure 11) was taken to be the water table contour map, due to the assumption of basically horizontal flow. This map was hand-contoured from field measurements and digitized. The temporal rate-of-change map (Figure 12) was developed from a series of five bi-weekly measurements from which the rates of change at each well were determined by a linear least-squares fit of the data. Again, hand contouring was used to produce the map, which was then digitized.

The aquifer bottom is not well defined or necessarily continuous over the extent of the aquifer. In many locations the aquifer bottom is a clay layer while in other instances it is the uppermost continuous basalt flow. In constructing the aquifer bottom map, consideration was given to discontinuities in hydraulic potentials, significant changes in clay content and noticeable loss of water during drilling. These data were used in conjunction with geological cross sections and driller's log data to produce the aquifer bottom surface shown in Figure 13.

The input hydraulic conductivity values (Figure 14) at various wells were derived from analyses of pump test data. The K values shown in Figure 14 represent the starting values for the streamtubes. This data preparation step is described in BNWL-1709.

FIGURE 11. Groundwater Potentials Used in Calculating the Hydraulic Conductivity Distribution

FIGURE 13. Elevation of the Hanford Unconfined Aquifer Bottom Used in Calculating the Hydraulic Conductivity Distribution

FIGURE 14. Locations and Values of Measured Hydraulic Conductivities for the Hanford Unconfined Aquifer

The storage coefficient distribution was assumed constant at 0.1, as described previously.

CALCULATION OF CONDUCTIVITY REFERENCE LINES

The boundary condition required to solve the inverse problem (Equation 8) stipulates that the vertically averaged conductivity must be specified at some point in every streamtube; i.e., the conductivity must be known along a line or lines (conductivity reference lines) that intersect all streamtubes in the groundwater system. These lines generally cannot be constructed from point measurement alone because the measurements rarely span all streamtubes in the flow region and the distance between them is usually too great to obtain a curve by interpolation. In addition, the reference line cannot usually be drawn as one continuous line because of data sparseness and complexities of the flow paths. Locating the reference lines and determining K along them represents the most difficult task in generating the conductivity distribution.

The reference lines are constructed using the TIR and available conductivity data. They are usually drawn in areas where the streamtubes converge, such as infiltration sites and channels of high hydraulic conductivity, to take advantage of the large point density and the smoothness assumption. Figure 15 shows a reference line and associated streamtube centerline in the southeastern portion of the Hanford unconfined aquifer. The conductivity values along the reference lines are obtained by generating streamtubes from the measurement site reference lines. Thus data which are sparsely scattered over a large area can be projected to a common reference for inspection and evaluation.

FIGURE 15. Reference Line and Streamtube Centerlines Used for the Southeastern Portion of the Aquifer

A curve, which the hydrologist feels is most representative of the variation of the hydraulic conductivity, is drawn through the data points to establish the conductivity boundary curve for the reference line involved. Figure 16 is the conductivity curve for the reference line shown in Figure 15.

The scatter of the calculated conductivities at a reference line can be caused by many factors, including both numerical and data errors. As previously mentioned, the numerical errors can be minimized by judicious selection of control parameters. Data errors can occur in:

- interpretation of the groundwater contours;
- hydraulic conductivity measurements;
- interpretation of the lithology (aquifer thickness) and assumption of no flow through the aquifer bottom;
- the temporal rate-of-change distribution.

FIGURE 16. Calculated Conductivity Points and Best-Fit Curve of Conductivity Along Reference Line Shown in Figure 15

Two advantages of the TIR are (1) some of the small data errors may be filtered out when the boundary curve is drawn, and (2) it provides a systematic procedure for investigating the sources of error listed above. For example, three data points on the conductivity reference line (well numbers 8-17, 15-26, and 17-5) shown in Figure 16 fall appreciably below the best-fit curve. On the basis of the lithology and other geohydrological data in the area, little interchange with the underlying confined aquifers would be expected. Thus, the assumption of no interchange would not be expected to contribute significantly to the discrepancies.

The TIR sensitivity tests conducted on the Hanford unconfined aquifer (Appendix B) showed that in this portion of the aquifer a 100 percent variation in the assumed storage coefficient resulted in a variation in calculated conductivity of approximately 20 percent. Thus, assuming a constant storage coefficient of 0.1 would not be expected to cause discrepancies of the magnitude observed. Likewise, errors in the temporal rate-of-change distribution would not be expected to cause such discrepancies since it has the same relative importance as the storage coefficient (the two multiplied together form the transient contribution to Equation 9).

Therefore, the two most likely sources of error are the starting hydraulic conductivities and/or interpretation of the hydraulic potential contours. By examining the pump test records, the physical characteristics of the well and aquifer, and the models used to evaluate the data, confidence limits for the accuracy of the measurements can be estimated. By putting these limits on the calculated values, the analyst can assess how much of the disagreement is attributable to measurement error.

Interpretation of groundwater contours can have an appreciable effect on both the location at which the

streamtube intersects the reference line and the magnitude of the calculated conductivity. To evaluate this type of error, the analyst can reinterpret the groundwater contours in the vicinity of the streamtube in question.

If these procedures do not bring the data point into line, additional field tests may be required. The actual design of the field program depends on the results of the evaluations and varies for different regions of the aquifer. As an illustration, the two data points originating from wells 8-17 and 17-5 were found to be the most sensitive to variations in storage coefficient for this reference line. In fact, when reasonable storage coefficient values were used (0.2) negative conductivities were calculated for these points, suggesting that the measured starting conductivities were too low. Reanalysis of the pump test data conducted at these wells support this observation (see Appendix B). These two wells therefore become candidates for future pump tests.

In theory, knowing the quantity of flow discharged at a source and the surrounding gradients, an average conductivity could be calculated at that node and its boundary used as a reference line for generating conductivities down-gradient. However, for the hydraulic gradients to be sufficiently accurate, the contour of integration around the source must be at least two nodes distant from the source. Since the aquifer is very heterogenous, an average value of conductivity enclosing the source at this distance would not provide accurate starting conductivities for the streamtube calculations. Thus, a reference line near a source must be constructed by generating streamtubes to it and drawing a "best-fit" curve through the available data. Using the reference curve, the seepage from the source can be calculated and compared to the known average discharge to the disposal site. This provides another estimate of the accuracy of the calculations.

In special situations, the TIR can be used as an aid to understanding the aquifer flow systems and constructing reference lines. For example, in the low conductivity area north of B-pond, hydrograph records indicate that the flow moving toward Gable Mountain is going into storage. Therefore, even though the mountain is assumed to be a barrier to flow, the hydraulic potential contours do not have to intersect it at right angles (see Figure 17). A streamtube could be started at the mountain boundary (streamtube #1, Figure 17). The starting flow would be zero since it is assumed that all the flow originating from the source has gone into storage. Thus, the streamtube could be generated to the reference line and the computed conductivity compared with the reference line value. The degree of consistency would indicate the need for supportive field data.

FIGURE 17. Example of Flow Tubes Converging on a Source (B-Pond Mound)

Thus, one of the most useful aspects of the TIR is that it can be used to systematically evaluate the adequacy of the available data and aid in the specification of the type, quantity and location of additional data required to achieve additional confidence in the understanding of a groundwater flow system. This important capability of the method has yet to be fully utilized on the Hanford unconfined aquifer.

CALCULATION OF THE HYDRAULIC CONDUCTIVITY DISTRIBUTION

Once the conductivity reference lines, which intersect every streamtube at least once, have been constructed the conductivity distribution can be determined for any size grid by generating streamtubes from the reference lines to each of the grid points. The procedure described in connection with Equation 14 is used to calculate the hydraulic conductivity at each grid point.

Both the steady-state and transient versions of the TIR have been applied to the Hanford unconfined aquifer. The initial version of the TIR solved the steady-state equation (Equation 10) and was implemented on a small, man-machine interactive computer to efficiently utilize the method. Since the computer lacked fast access mass storage devices, it was necessary to divide the aquifer into small regions so that all the required input data for the region could be stored within the computer core memory. This artificial division of the aquifer was, however, not conducive to construction of good reference curves when the streamtubes containing known transmissivity data points extended beyond a region. It was also difficult to match the streamtubes between the regions. In spite of these obstacles, the need for a hydraulic conductivity distribution provided the impetus to calculate a distribution. The transmissivity map calculated in 1969 appears in Figure 18.

FIGURE 18. Calculated Transmissivity Distribution
 of the Hanford Groundwater Flow System

The verification results of the transmissivity distribution, although far from perfect, were encouraging and the distribution represented a substantial improvement over that previously available. It was observed that the interpretation of the groundwater contours (yielding the gradients) and the starting transmissivity measurements represented the largest sources of error in the procedure. It also appeared that the transient nature of the Hanford unconfined aquifer, unaccounted for in the calculation, and the division of the aquifer into block segments introduced significant errors in the analysis.

A modified program to solve the transient equations (Equation 9) was written for another interactive computer system which incorporated a light-pen interactive CRT display, adequate disk storage for handling the input data, and a digitizer for rapid reinterpretation and evaluation of groundwater contours. The present hydraulic conductivity distribution was calculated using this version. The conductivity could not be calculated in some areas because there were no data for constructing reference lines. These areas were hand contoured by visual extrapolation.

It was recognized that the computer calculated hydraulic conductivity distribution possessed a scale of detail that could not be supported by the estimated accuracy of the calculation routine and the input data base. Furthermore, early verification simulations using the VTT model indicated that some areas of extrapolated conductivity were very inaccurate. Therefore, the extreme peaks and valleys of the conductivity surface were smoothed by manual editing and use of a numerical algorithm. Figure 19 is a plot of the smoothed hydraulic conductivity map used for the verification simulation runs described below. For comparison with the previous distribution, the associated transmissivity map appears in Figure 20.

EVALUATION OF THE RESULTS

Rigorous analytical techniques for evaluating the accuracy of the calculated conductivity distribution have not yet been developed. The best way to determine its accuracy is to obtain enough additional measurements to be of statistical significance and compare these data to the calculated hydraulic conductivities. However, time and funding limitations have restricted the collection of such data to date, so other indirect procedures must be used to indicate whether the calculated hydraulic conductivity distribution is indeed representative of the actual distribution, at least for model simulation.

Some appreciation of the accuracy of the distribution can be gained by reviewing the quality of the input data. Error estimates are presented below; some are very crude, however, and can only serve to indicate the relative uncertainties associated with the different input data. Two indirect approaches were also used to provide a quantitative evaluation of the quality of the distribution.

In the first, the VTT-predicted water table response was compared with the observed water table response over a test simulation period. This approach is inherently limited because discrepancies between observed and calculated data can result from errors in input data which are unrelated to the TIR. For example, the calculated water table response is a function of the time-dependent quantities of liquid injected to the ground, the storage coefficient distribution, the aquifer bottom map, and the boundary conditions, each of which has an associated error. Thus, the comparison between observed and computed data is really a measure of the model accuracy, of which the hydraulic conductivity is a major input parameter distribution. Furthermore, sensitivity studies on the VTT model¹ have shown that the calculated hydraulic potential has an attenuated sensitivity to errors in the hydraulic conductivity distribution.

The second approach involves computing travel time using the calculated hydraulic conductivity distribution and its potential surface and subsequently comparing these travel times with the observed movement of contaminated groundwater.

ESTIMATED ERRORS IN THE INPUT DATA

It is difficult to quantify the accuracy of the pump test hydraulic conductivity data because the test structures and conditions often departed significantly from the ideal assumptions used to analyze the data. For example, observation wells were available for only three of the tests and fewer than 65 percent of the test wells penetrated the entire estimated thickness of the aquifer. Most of the wells were casing-perforated, rather than screened, and delayed yield effects were not considered because these effects cannot be distinguished in single well tests. The analytical model used to evaluate the data obtained in these wells accounted for the partial penetration but the model was not very sensitive in determining a precise transmissivity. Step drawdown test data were used when available (for approximately 20 percent of the wells) to eliminate the effects of casing resistance. Most of the pump tests were conducted over only an 8 hour period, which is generally regarded as too short for unconfined aquifer pump tests. Often the drawdown quickly approached a quasi-steady value in the pumped well. Erratic pump flow rates were also a problem in many of the tests.

The net results of these deficiencies in the pump test data is difficult to evaluate quantitatively. At one well (699-43-89) where repeated tests were run, the variance in the hydraulic conductivity was nearly 50 percent of the average value. Evaluations using alternate theoretical models gave differences of up to an order of magnitude.¹⁹ In consideration of all these factors, a reasonable estimate of the typical error in the majority of available pump test conductivity values is probably a factor of 5. If established procedures for conducting high quality pump

tests were followed, we feel that conductivity values accurate to a factor of 1.1 to 2 could be obtained. (A factor of uncertainty of 1.5 means that the range of uncertainty about a given conductivity value would extend from 0.67 of that value to 1.5 times that value.)

Valid storage coefficient data for the Hanford unconfined aquifer are virtually nonexistent. Although storage coefficient values were calculated from some of the pump test data, the absence of observation wells and the resulting error estimates make these values practically worthless. A good estimate of the average storage coefficient, based on sediment types, would be 0.2. However, negative hydraulic conductivities were calculated for some streamtubes when this value was used. Since the sensitivity analysis described in an earlier section had not yet been conducted, the negative values were interpreted to mean that the storage coefficient was too high. However, it now appears that the starting hydraulic conductivity values were unrealistically low.

It is estimated that the highest accuracy to which the storage coefficient could be measured is about a factor of 1.5. The accuracy with which point measurements could be used to construct a storage coefficient distribution would depend on the measurement range, accuracy, and density over the Hanford Reservation. The mean for the expected range in storage coefficient values for the aquifer (0.07-0.3) is 0.15. If the storage coefficient was assumed to be 0.15, then it should be accurate to within a factor of ± 2 and any measurements should improve the accuracy with which a distribution could be constructed.

The values used for the hydraulic potential map (Figure 11) and the temporal rate of change map (Figure 12) were obtained by performing a least-square-linear fit of five bi-weekly

measurements made at each of the observation wells. The temporal rate of change and groundwater potential were then taken from these curves at the midpoint of the measurement period. This procedure minimized the effects of measurement error in the data. Errors in the hydraulic potential measurements can occur from poor communication of the well with the aquifer or from measurement and surveying errors.

If vertical flow is assumed to be negligible, the measurements from both shallow and deep wells which are open to the unconfined aquifer are regarded as equally representative of the hydraulic potential, which is assumed constant with depth. It is possible that vertical potential gradients are reflected in the uppermost tube of piezometer-filled wells where only a sand pack, not cement plugs, separates the various water-bearing zones. It is also possible that errors are due to barometric response transients in some wells. Since not all of the measurements are made within a span of a few hours, these barometric changes (as well as earth tides) affect some of the measurements. Although the present groundwater flow model does not attempt to simulate these effects, it cannot be filtered out of a single set of water level measurements. Use of a series of five measurements increases the probability of filtering out the short term barometric transients. The presence of barometric sensitivity is generally recognized as an indication of a confined zone (at least locally). Much insight into the groundwater hydrology of the Hanford Reservation remains to be gained from further study of barometric and earth-tide water level responses.

If it is assumed that the surveying and measurement errors are normally distributed with variances of 0.05 feet and 0.02 feet, respectively, then the combined variance would be 0.07 feet, provided the two sources of error are uncorrelated. The error introduced by barometric and earth-tide

sensitive wells is assumed to have a normal distribution with a variance of 0.2 feet. However, only about 5 percent of the wells for which water level records have been made indicate a barometric sensitivity. The presence of wells with this sensitivity will reduce the accuracy of the contoured potential data in the affected areas. From a practical standpoint, these errors are negligible (except in the 200 East Area where very flat gradients occur) considering the errors introduced by hand contouring of groundwater potentials using widely and randomly spaced measurements.

The accuracy with which the spatial gradients at a point in time can be obtained is a function of the accuracy of the point measurements of the groundwater potential and the accuracy with which groundwater contours can be constructed from these measurements. To estimate the variance of the gradient distribution, one needs to know the correlation between the neighboring potential measurements used in the linear interpolation for contouring and subsequent differences used to compute the gradients. Insight into the magnitudes of the errors introduced by contouring the potential data may be achieved by adjusting the contours within the uncertainty ranges of the hand contouring procedure. This was done for three local areas of the Hanford Reservation. One contour was held fixed while the neighboring contour was moved as far from it as was reasonable, considering the data points. The percentage of change in the local gradient between the two potential contours involved for three different areas is shown in Table 2. This indicates the general magnitude of error that can be introduced by the contouring process, assuming exact measurements at the wells.

A crude calculation using estimates of maximum errors on the measured potential and the distance between the wells on the contour map indicates that the maximum error in the gradient, assuming no contouring errors, can be 100 percent or more of the gradient value in areas of small gradient (0.00005 ft/ft).

TABLE 2. Sensitivity of Gradients to Contouring

<u>Original Contoured Gradient (ft/ft)</u>	<u>Distance Contour Moved (ft)</u>	<u>Change in Gradient</u>
1.5×10^{-4}	2000	6%
1.5×10^{-3}	2000	25%
1×10^{-2}	500	20%

The estimate of maximum error for regions of medium gradient (0.002 ft/ft) is about 10 percent of the measured value. These data indicate that streamtubes should not be generated through areas of low gradients ($<1 \times 10^{-4}$), such as beneath the 200 East Area, because measurement errors can introduce large discrepancies into the hydraulic conductivity calculations which are then perturbed throughout the remainder of the streamtube.

As would be expected, the error in gradient introduced by measurement error decreases as well spacing increases (i.e., the greater the distance, the less is the effect of the measurement error on accuracy of the gradient). However, the loss in resolution caused by widely spaced measurement points increases the error in the approximation to the local gradient unless the gradient is uniform, which is not the situation for Hanford (Figure 11).

On the positive side, the contouring process can be used to effectively filter out some of the errors in the well measurement data; this effect results from drawing smooth contours with the minimum complexity required to fit the data.

It is extremely difficult to estimate to what extent errors are introduced in the direction of the gradient vectors without conducting numerical experiments. Contamination and other hydrogeologic data are used where available to aid in

verifying these vector directions. The TIR was developed for an interactive computer system so that the groundwater contours could be quickly reinterpreted using all available data to obtain the most consistent gradient distribution and thus the most accurate hydraulic conductivity distribution.

It is also difficult to estimate the accuracy of the hand-contoured distribution of the temporal groundwater rate of change simply from the average accuracy of the values at each well. Using the same reasoning as for groundwater potential contouring, an estimated confidence interval for the temporal rate of change map is about a factor of 2. This indicates that the transient term, which is the product of the storage coefficient and the temporal rate of change, is limited in accuracy equally by the assumption of a constant storage coefficient and errors in the temporal rate of change.

The aquifer bottom is considered in the calculation of the vertically averaged hydraulic conductivity. It does not directly enter into the transmissivity calculation. Errors in the aquifer bottom introduce errors into the hydraulic conductivity, which in turn introduce errors into the calculated groundwater velocities and groundwater changes.

It is difficult to estimate the accuracy of the aquifer bottom map because of the problem of identifying its exact vertical locations. While it is assumed to be continuous to satisfy the requirements of the model, the lack of continuity makes it difficult to extrapolate from point measurements. Where the well penetrates the full depth of the unconfined aquifer, the bottom is probably known within ± 10 feet. Between data points, an estimate would be ± 50 feet. In places where the control is good and the surface is changing in a rather uniform fashion the error would probably be less. A good estimate of its accuracy could be obtained by making enough additional measurements to be of statistical significance and comparing these data with the extrapolated data.

Interchange between the unconfined and underlying confined aquifers is assumed negligible, even though the actual aquifer bottom as defined is not continuous. This assumption is based on the present interpretation of the geology and the measured hydraulic conductivities and hydraulic potentials in the upper two aquifers. The thickness and relatively low conductivity of the silt and clay layers that form the bottom of the unconfined aquifer over much of the Hanford Reservation area sustain a hydraulic potential difference of tens of feet between the aquifers.

According to Brown²⁰ the measured transmissivities in the uppermost confined aquifer range from 3 to 3×10^3 ft²/day, while those in the unconfined aquifer range from 300 to 4×10^6 ft²/day--approximately 100 times greater. Thus, the low conductivities of the uppermost confined aquifer and the confining beds imply little leakage into the unconfined aquifer in these areas. In the remaining areas, where the silt or clay formations are absent, the low conductivity of the basalt suggests an insignificant flux through the unconfined aquifer bottom, except in possible areas of high hydraulic potential difference which have not been identified at this time. Further field measurements are necessary to substantiate these observations.

Table 3 summarizes the estimates of errors in the present data for the unconfined aquifer. It should be re-emphasized that most of these error estimates are crude and subjective and are provided only for comparative purposes. Additional data could change these estimates substantially.

Unfortunately, techniques do not yet exist for combining the effects of all of these error estimates with their associated interactions in the TIR calculation procedure to obtain the final error estimate for the resultant hydraulic conductivity distribution. Preliminary studies indicate only that

TABLE 3. Estimated Errors in Present Data Base
for the Hanford Unconfined Aquifer

<u>Data Type</u>	<u>Estimated Average Error</u>
Hydraulic conductivity measurement	Factor of 5
Storage coefficient	Factor of 2
Temporal rate of change	Factor of 2
Gradient (magnitude)	± 10 to 100%
Computational error	$\pm 5\%$
Aquifer bottom	± 10 to 50 feet

the computational error contributions of the storage coefficient and the temporal rate of change terms (the transient term) are smaller than their respective error estimates, because over most of the unconfined aquifer the ratio of the transient term to the steady flow term is quite small. The computational error contributed by the starting conductivity values is directly proportional to the error in the starting conductivity.

Thus, the possibility exists that the uncertainty of the starting hydraulic conductivity values is the prime limitation on the accuracy of the computed distribution, except for areas where the gradient error estimate is large. However, this hypothesis requires further testing. It should be recalled that when the pump test conductivities are used to prepare the reference line conductivity distributions, some filtering out of inconsistent conductivity values occurs.

It has been estimated that the errors in the starting hydraulic conductivities, storage coefficient, and aquifer bottom might be reduced to factors of 1.5, <2.0 , and ± 10 feet, respectively, by use of the best available techniques for field

data collection and analysis. However, a more thorough sensitivity analysis and a technique to quantify the quality of the resulting hydraulic conductivity distribution should be developed in conjunction with, if not prior to, a field data gathering program.

VERIFICATION OF THE CALCULATED HYDRAULIC CONDUCTIVITY WITH THE VTT MODEL

The smoothed hydraulic conductivity calculated assuming transient conditions (Figure 19) was input to the VTT Model along with the appropriate boundary conditions¹ and the water table response for the period from March 1968 to September 1973 was computed. The liquid discharges to the aquifer as functions of time and location were obtained from facility records. This verification allows the water table to respond to the input data and boundary conditions used without forcing a specified potential at disposal sites, as was the case in earlier verification studies (which will be discussed in the next section). The results should, therefore, be more realistic.

Figure 21 shows the calculated water table for September 1973, the end of the simulation period; it can be compared with the measured September 1973 water table shown in Figure 11. Figure 22 shows the numerical differences between the two potential surfaces, expressed to the nearest foot. A negative value means that calculated groundwater potentials are below the interpreted potentials. The differences at each node were also tabulated into classes as shown in Table 4. There were 2409 active calculation nodes for this simulation. Other statistics were

- average difference, -4.2 feet
- root mean square difference, 6.3 feet
- maximum difference, 34.2 feet (just east of Umtanum Ridge)

Figure 23 is a map of the difference classes. It can be seen that the two areas of greatest discrepancy are to the

FIGURE 21. Calculated Water Table From VTT Simulation for September 1973

TABLE 4. Differences Between Calculated and Observed Groundwater Potentials at the End of the 5-Year Simulation Period

<u>Class</u>	<u>Range (Ft)</u>	<u>Absolute Difference</u>	<u>% of Nodes</u>	<u>Positive Difference</u>	<u>% of Nodes</u>	<u>Negative Difference</u>	<u>% of Nodes</u>
A	0.000 - 1.000	572	23.744	298	12.370	274	11.374
B	1.000 - 2.000	413	17.144	139	5.770	274	11.374
C	2.000 - 4.000	594	24.658	89	3.694	505	20.963
D	4.000 - 8.000	463	19.220	78	3.238	385	15.982
E	8.000 -15.000	240	9.963	20	0.830	220	9.132
F	15.000 -35.000	<u>127</u>	5.272	<u>3</u>	<u>0.125</u>	<u>124</u>	<u>5.147</u>
		2409		627	26.027	1782	73.973

FIGURE 23. Difference Classes Using September 1973 Measured and Calculated Water Tables

east of Umtanum Ridge and to the east of Rattlesnake Mountain. Hydraulic conductivities were extrapolated into these areas and the recharge flows from the two boundaries are only estimates. It is clear that both the recharge flows and the conductivities need to be field measured in these areas. The other large area of poor model performance is in the high gradient area on the east side of the 200 West Area mound. The hydraulic conductivity appears to be too high in this area. Other minor areas of poor agreement occur near Gable Butte and Gable Mountain, where hand extrapolation of the hydraulic conductivity distribution was necessary because the TIR could not be used in these areas.

Isometric plots of the measured and calculated water table surfaces appear in Figures 24 and 25, respectively. The model performs best in the vicinity of the 200 East Area and down-gradient to the Columbia River. About 2/3 of the nodes over the entire unconfined aquifer agreed within 4 feet at the end of the simulation period.

An alternative method of evaluating the verification simulation is to compare calculated and historically-measured well hydrographs at selected wells over the reservation. This method has the advantage of showing the temporal behavior of the model during the simulation period. Representative hydrographs appear in Figures 26 through 31. In general they illustrate the same quality of model simulation that the September 1973 comparison shows for the respective areas.

VERIFICATION WITH TRAVEL TIME CALCULATIONS

Once the hydraulic conductivity distribution is known, travel times can be calculated which give insight into the validity of the conductivity distribution. For a given potential surface, the travel times of a fluid particle along an instantaneous streamline can be calculated using the following equation:

FIGURE 24. Isometric Plot of the Observed Groundwater Potentials
for the Hanford Unconfined Aquifer, September 1973

FIGURE 25. Isometric Plot of the Calculated Groundwater Potentials
for the Hanford Unconfined Aquifer, September 1973

FIGURE 26. Observed and Calculated Groundwater Hydrographs for Well #299 E29 2

FIGURE 27. Observed and Calculated Groundwater Hydrographs for Well #699 6 32

FIGURE 28. Observed and Calculated Groundwater Hydrographs for Well #699 15 26

FIGURE 29. Observed and Calculated Groundwater Hydrographs for Well #699 83 47

FIGURE 30. Observed and Calculated Groundwater Hydrographs for Well #699 70 68

FIGURE 31. Observed and Calculated Groundwater Hydrographs for Well #699 66 23

$$t = - \int_{s_0}^s \frac{p \, ds}{K \frac{dh}{ds}} \quad (15)$$

where $K = \frac{T}{h-h_0}$ is the hydraulic conductivity

s = distance along the streamline

p = effective porosity over the saturated thickness of the aquifer

$\frac{dh}{ds}$ = hydraulic gradient along the streamline

h = hydraulic potential

A finite difference form of Equation 15 is used for the travel time calculation, as described in BNWL-1707. For a steady flow system, Equation 15 is the integral of the streamline for a fluid particle that starts at s_0 at time zero. Naturally, this calculation reflects convective transport rates valid at the point in time for which the streamlines are generated. Transient boundary conditions or disposal flow rate variations are not taken into account by this calculation.

The instantaneous streamline paths and travel times can be compared with observed contaminant transport patterns to gain insight as to the quality of the computed hydraulic conductivity distribution. Unfortunately, the travel time values are sensitive to the value used for the effective porosity over the saturated aquifer thickness. This value is difficult to determine over the Hanford Reservation. A constant value of 0.067 was assumed for the effective porosity for the travel time calculations in contrast to an assumed storage coefficient of 0.1. This value was chosen because the effective porosity is generally less than the storage coefficient and it gave the best match between observed and calculated travel times. Although lower values of effective porosity would have resulted in better comparisons of travel times, such values would not

be warranted for the sediments typical of the Hanford unconfined aquifer. Table 5 shows the results of calculated and observed travel times for sites where measured contamination data were sufficient to permit interpretation.

The measured travel times are based on observed entry of gross beta emitters to certain wells, entry of tritium into certain wells and the extent of the tritium plume in 1974. Comparable data from the west area were not available due to the limited movement of the contaminated groundwater plumes there. The calculated travel times represent a range that was determined for a number of streamlines from the Purex Plant to the vicinity of the well in question.

Time did not permit a more rigorous examination of the contamination data to establish additional observed travel times and determine them with greater accuracy. An analysis of the

TABLE 5. Calculated and Observed Groundwater Travel Times for Selected Sites in the Hanford Unconfined Aquifer

<u>Well No.</u>	<u>Observed Travel Time (yrs)</u>	<u>Calculated Travel Time (yrs)</u>	<u>Calculated/ Observed</u>
34-39A	2-3	5	2.0
20-20	5.5	22-23	4.0
26-15	6	32-34	5.5
15-26	6	10-12	1.8
S1-7	18	19-33	1.4
2-3	18	19-21	1.1
27-8	18	46-50	2.7
42-12	18	17-32	1.3
35-9	18	49-50	2.7

progress of peaks derived from variations in disposal rates would be more accurate, since these observations are based on a somewhat subjective determination of time of first entry or present plume extent.

However, Table 5 indicates that errors of a factor of 2-3 are typical for the travel time calculations on the basis of the present data and aquifer parameter distributions. Errors as high as a factor of 6 can occur. Considering the reliability of the input data and knowledge of the geohydraulic characteristics of the Hanford unconfined aquifer, the agreement between observed and calculated travel times is good and supports the use of the TIR method.

Probably the most serious assumption of this calculation is that of constant effective porosity; the next most compromising feature is the inherent steady state assumption. Pathline calculations taking into account the transient water table conditions would be more accurate. Finally, although the three-dimensional nature of the contamination plumes is not known, it is suspected to be a source of disagreement between reality and this two-dimensional calculation approach.

It is clear that a procedure for calculating the uncertainty associated with any computed travel time should be developed. At present it is virtually impossible to estimate error associated with travel paths that do not pass through areas of observed contamination plume movement.

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APPENDIX A

TESTING THE TRANSMISSIVITY ITERATIVE
ROUTINE ON SYNTHETIC SURFACES

APPENDIX A

The Transmissivity Iterative Routine was tested on a synthetic surface to determine the best combination of control parameters, within acceptable accuracy and computation time constraints. Accuracy was the prime consideration because when inconsistencies occur in the construction of the hydraulic conductivity reference curves when using the TIR method, the analyst must be able to construe that the inconsistencies are a result of data or data interpretation errors and not computational errors.

The test surface used is shown in Figure A-1. It satisfies the Laplace Equation for steady state groundwater flow, $\nabla^2 h = 0$, where the hydraulic conductivity is assumed equal to 1000 ft/day. The equation for the surface is

$$h_2 = -\frac{m}{2} \ln \left\{ [(y-y_1)(x-x_2) - (y-y_1)(y-y_2)]^2 + [(y-y_1)(x-x_2) + (y-y_2)(x-x_1)]^2 \right\} + C$$

where

x, y = axis

x_1, x_2 = location along the x axis of sources 1 and 2, respectively

y_1, y_2 = location along the y axis of sources 1 and 2, respectively

The sources were scaled to give the same range of gradients as those in the Hanford unconfined aquifer. In addition, the grid spacing was scaled to be representative of the grid spacing used in the analysis of the Hanford unconfined aquifer. Preliminary tests were conducted on simple one-dimensional surfaces to insure that calculations were being performed correctly.

The control parameters evaluated on the above surface were:

FIGURE A-1. Synthetic Groundwater Potential Surface and Streamlines Used in Sensitivity Tests of the TIR Method

- starting width
- minimum width
- maximum width
- width adjustment factor
- starting step
- step adjustment factor
- maximum step size
- angle correction

The effects of these parameters on the computational accuracy and run time were systematically evaluated. A complete description of the function of these control parameters is given in BNWL-1708, "Transmissivity Iterative Program-User's Manual." A very brief description is presented here.

The starting width, W_0 , is the initial width of the streamtube. The purpose of the maximum width control parameter is to limit the area over which the permeability is averaged, since the width of the streamtube can get very large when the flow paths diverge. The minimum width control parameter keeps the width of the streamtube from becoming too small and causing numerical round-off problems. The width of the streamtube is either increased or decreased when it is less than the minimum or greater than the maximum width.

The initial step size taken by the program is Δs (see Figure A-2). It is also the maximum allowable step size, since large step sizes result in poor approximations to the gradients due to the linear interpolation methods used. The minimum step size is $1/2$ the minimum width; this size prevents numerical problems associated with short, wide elements.

The program always tries to use the maximum step size by increasing the step size by the step adjustment factor. The angle correction is the maximum allowable deviation of the gradient from the perpendicular, θ , at the midpoint of the ending streamtube (see Figure A-2). As this angle gets larger, the accuracy of the integration for flow crossing this boundary

FIGURE A-2. Schematic Diagram of a Streamtube Step

decreases. The details of how these factors interact to change the streamtube width, step size, etc., is described in BNWL-1708.

The sensitivity tests were performed for streamline #2 shown in Figure A-1. Previous tests had shown that the largest errors in the calculated hydraulic conductivity occur on those streamlines which pass near stagnation points. Thus streamline #2 was selected as the critical streamline for the test surface.

The first series of tests, in which the minimum and maximum widths and width adjustment factor were varied and the other control parameters were fixed, are summarized in Table A-1 and Figures A-3 through A-7. These figures show that doubling the width adjustment factor has very little effect on the error in the hydraulic conductivity (less than 2 percent) for the lower width controls (Figures A-3 and A-4). At the higher width controls (Figures A-5 and A-6) doubling the width adjustment factor can introduce 3 to 4 percent error over that of the lower factor. On the other hand, the computational time for the largest adjustment factor is appreciably less than for the smallest adjustment factor (see Table A-1).

TABLE A-1. Width Parameter Analysis - Streamtube #2

Figure	Case No.	Start Width (ft)	Min. Width (ft)	Max. Width (ft)	Width Adj. Factor (%)	Starting Step (ft)	Step Adj. Factor (%)	Angle (Degrees)	Run Time (Seconds)
A-3	A01				0.1	5.0	0.2	5.0	93
	A02	0.5	0.25	1.0	0.2				60
	A03				0.4				52
A-4	A04				0.1				89
	A05	1.25	0.5	2.0	0.2				57
	A06				0.4				43
A-5	A07				0.1				85
	A08	2.5	1.0	4.0	0.2				54
	A09				0.4				36
A-6	A10				0.1				83
	A11	5.0	2.0	8.0	0.2				48
	A12				0.4				33

ERROR ANALYSIS

FIGURE A-3. Computational Errors - Streamtube #2, Cases A01, A02, A03

ERROR ANALYSIS

FIGURE A-4. Calculational Errors - Streamtube #2, Cases A04, A05, A06

ERROR ANALYSIS

FIGURE A-5. Calculational Errors - Streamtube #2, Cases A07, A08, A09

ERROR ANALYSIS

FIGURE A-6. Computational Errors - Streamtube #2, Cases A10, A11, A12

ERROR ANALYSIS

FIGURE A-7. Computational Errors - Streamtube #2, Cases A03, A06, A09, A12

Figure A-7 shows the effect on the error in K of changing the width limits for the 0.4 width adjustment factor. The largest width limits showed a maximum error 5 percent greater than that of the lowest width limits. Considering the calculational error and the computational time, case number A06 was selected as the best. Although case A06 shows a slightly larger error (0.5 percent) than case A03 (which had the minimum control limits), the computational time for A03 was approximately 20 percent greater than that for A06. The maximum error in K for case A06 was 13 percent.

The parameter values selected were:

starting width (ft)	1.25
minimum width	0.5
maximum width	2.0
width adjustment factor	0.4

Table A-2 and Figures A-8 through A-13 summarize the results of the second series of tests in which the starting step and step adjustment factor were varied with the width control parameters fixed at the values determined previously and the angle held constant. Figures A-8 through A-11 show the effects of varying the step adjustment factor for various starting steps. It can be seen from these figures that a step adjustment factor of 0.01 gives the smallest error for all of the starting step sizes except the 1.25 starting step. The difference in calculational error between the 0.01 and 0.05 step adjustment factor is small even at the largest starting step size. Considering accuracy and run time alone, these data indicate that a step adjustment factor of 0.05 would be the best since the computational time when using a 0.05 factor is 30 percent less than when using the 0.01 factor, whereas the error is only 3 percent more when using the 0.05 factor.

TABLE A-2. Step Parameter Analysis - Streamtube #2

<u>Figure</u>	<u>Case No.</u>	<u>Starting Step (ft)</u>	<u>Step Adj. Factor (%)</u>	<u>Angle Degrees</u>	<u>Run Time (Seconds)</u>
A-8	B01	1.25	0.01	5.0 ↓	105
	B02		0.05		80
	B03		0.1		70
	B04		0.2		62
	B05		0.4		58
A-9	B06	2.5	0.01		97
	B07		0.05		68
	B08		0.1		57
	B09		0.2		49
	B10		0.4		44
A-10	B11	5.0	0.01		98
	B12		0.05		63
	B13		0.1		52
	B14		0.2		43
	B15		0.4		36
A-11	B16	10.0	0.01		98
	B17		0.05		60
	B18		0.1		48
	B19		0.2		39
	B20		0.4		33

ERROR ANALYSIS

FIGURE A-8. Computational Errors - Streamtube #2, Cases B01, B02, B03, B04, B05

ERROR ANALYSIS

FIGURE A-9. Calculational Errors - Streamtube #2, Cases B06, B07, B08, B09, B10

ERROR ANALYSIS

FIGURE A-10. Computational Errors - Streamtube #2, Cases B11, B12, B13, B14, B15

FIGURE A-11. Calculational Errors - Streamtube #2, Cases B16, B17, B18, B19, B20

ERROR ANALYSIS

FIGURE A-12. Computational Errors - Streamtube #2, Cases B01, B06, B11, B16

ERROR ANALYSIS

FIGURE A-13. Calculational Errors - Streamtube #2, Cases B02, B07, B12, B17

However, Figures A-12 and A-13, which show the effect of starting step size for step adjustment factors of 0.01 and 0.05, indicate that the least error occurs for the smallest starting step. The largest starting step shows an error approximately 14 percent greater than that for the smallest starting step. Considering the 0.05 step adjustment factor, the computational time when using the smallest step is approximately 30 percent greater than when using the largest step. These data would indicate that the smallest starting step is the best.

However, selection of the best step adjustment factor is more subtle. Based on the results for the smallest starting step (Figure A-8), a step adjustment factor of 0.1 appears most accurate, but the error generated by any of the factors used is small. Therefore, computational time considerations alone would dictate the use of the largest step adjustment factors. Considering the effect of the step adjustment factor when larger starting steps were used (Figure A-11), an adjustment factor of 0.05 was selected as a precaution. The penalty for this selection is an increase of approximately 38 percent in computational time for this streamtube.

The parameter values selected for this series of tests were:

starting step size	1.25
step adjustment	0.05

Table A-3 and Figure A-14 summarize the next series of tests in which angle correction was varied and the other control parameters were fixed at the values determined previously. Figure A-14 graphically shows that the errors increase substantially as the correction angle is increased. Considering both accuracy and computational time, an angle correction of 5 degrees was selected. Using a 30 degree angle correction the computational time is reduced by about 50 percent but the error is increase by approximately 30 percent. The

TABLE A-3. Angle Parameter Analysis - Streamtube #2

<u>Figure</u>	<u>Case No.</u>	<u>Angle (Degrees)</u>	<u>Run Time (Seconds)</u>
A-14	C01	2.5	97
	C02	5.0	80
	C03	10.0	66
	C04	20.0	56
	C05	30.0	53

maximum error in calculated K of ± 2 percent was observed when using the selected control parameters (case C02).

Since the step size appeared to be the most sensitive, it was further analyzed on streamtubes #1 and #3 (shown in Figure A-1). The step adjustment factor was also varied as shown in Table A-4. The data for streamtube #3 (Figures A-15 and A-16) show few differences in the calculational error for the different starting steps and step adjustment factors. Using the smaller step adjustment factor increased the computational time by approximately 30 percent but did not significantly improve the calculational accuracy, which is in contrast to the observations of the previous tests. It is interesting to note that the starting step size did not appreciably affect the computational time.

Streamtube #1 comes closer to the stagnation point than did streamtube #2 (Figure A-1). These tests (Figures A-17 and A-18) confirm the results of the tests conducted on streamtube #2; i.e., that the computational accuracy is sensitive to the starting step and step adjustment factors. The data also show that the computational time is significantly reduced by using 0.05 as a step adjustment factor, instead of 0.01.

ERROR ANALYSIS

FIGURE A-14. Calculational Errors - Streamtube #2, Cases C01, C02, C03, C04, C05

ERROR ANALYSIS

FIGURE A-15. Calculational Errors - Streamtube #3, Cases 302, 307, 317

ERROR ANALYSIS

FIGURE A-16. Calculational Errors - Streamtube #3, Cases 303, 308, 313, 318

APPENDIX B

Because of the problems experienced in calculating negative hydraulic conductivities for some streamtubes when a storage coefficient value of 0.2 was used, a limited sensitivity analysis for the storage coefficient was conducted on the Hanford unconfined aquifer. The analysis was limited to the southeastern portion of the aquifer because it was the only region which had sufficient data to make observations meaningful. The optimum control parameter values determined by the synthetic tests were used in these tests. The temporal rate of change in this region nearly covers the range of values observed for the entire aquifer.

Table B-1 shows the variation in hydraulic conductivity for two values of the storage coefficient, 0.1 and 0.2, at the reference line shown in Figure B-1. Figure B-1 also shows the path of the streamtubes from the wells to the reference line. It appears that some meaningful observations can be made when these data are used in conjunction with other data.

Based on the values of porosity observed for the aquifer, the geohydrological characteristics of the aquifer, and the values of storage coefficients observed for similar types of aquifers, it would appear that a good estimate for the storage coefficient would be 0.2. However, using this value results in the calculation of negative hydraulic conductivities for some streamtubes. This could mean either that some of the initial measured hydraulic conductivities are too low (which would make the flow in the streamtube too low to satisfy both the storage and flow requirements for the streamtube) or that the storage coefficient is significantly less than 0.2.

Available data tend to indicate that the starting hydraulic conductivity is too low. First, half the streamtubes contained in Table B-1 show less than 15 percent variation in K

TABLE B-1. Sensitivity of Calculated Hydraulic Conductivity to Storage Coefficient

Well No.	Measured K (ft/day)	Reference Line		Percent Change in K at Reference Line
		Calculated K at Reference Line		
		(ft/day)	(ft/day)	
		(σ=0.1)	(σ=0.2)	
1-18	100	1270	620	105
S1-7B	40	6250	5550	13
2-3	130	27200	27060	<1
8-17	140	3080	-45	6940
15-26	320	4680	4100	14
17-5	11	15170	-34320	144
20-20	300	79700	75200	6
26-15	140	30800	21800	41
35-9	40	25400	12200	108
31-31	1200	10800	10050	7
42-12	750	16750	16000	3
41-23	410	1250	1000	24

FIGURE B-1. Plan View Showing the Wells and Streamtube Paths Used in Generating the Reference Curve

resulting from a 100 percent variation in storage coefficient. Some of these streamtubes have low initial starting hydraulic conductivities and long flow tube lengths (S1-7B and 2-3). Although errors in the temporal rate of change could be the major contributing factor to the calculation of negative hydraulic conductivities, it is felt that this is not the case because the streamtubes which show extreme sensitivity to storage coefficients are randomly spaced rather than systematically grouped; i.e., streamtubes which pass through the same areas do not show the same degree of sensitivity.

Second, if the hydraulic conductivity reference curve (Figure B-2) is examined, it is noted that the two streamtubes, 8-17 and 17-5, for which negative Ks were calculated with an assumed storage coefficient of 0.2 are low compared to the reference curve which was drawn. Analysis of the pump test data indicates that 17-5 is a very poor pump test since the drawdown in the well during the test was below the perforated interval. The recovery data for the pump test conducted at well 8-17 gave a hydraulic conductivity of 640 ft/day as compared to the drawdown value of 140 ft/day used. This would indicate that the value obtained from the recovery data is more reliable.

The other two wells which show strong sensitivity to the storage coefficient, 1-18 and 35-9, could also have low estimates of hydraulic conductivities. Reanalysis of the pump test data at 35-9 indicates that a hydraulic conductivity as high as 740 ft/day, in contrast to the value used of 40 ft/day, could be interpreted. Using larger starting hydraulic conductivities for these streamtubes would decrease their sensitivity to the storage coefficient to levels comparable to the other streamtubes and still be consistent with the interpreted reference curve (Figure B-2) if a storage coefficient of 0.2 was used.

FIGURE B-2. Calculated Conductivity Points and Best-Fit Curve of Conductivity Along Reference Line Shown in Figure B-1

Another inconsistency is that the hydraulic conductivity generated from well 15-26 is low compared to the reference curve (Figure B-2). This could be a streamtube that is relatively insensitive to storage coefficient with a starting K that is too low. Thus, sensitivity to the storage coefficient for the above system is indicative of a bad starting hydraulic conductivity, but the converse is not necessarily true.

The discrepancy shown in 15-26 could also be explained by poor interpretation of the groundwater potential in the local area. A slight change in the shape of the groundwater contours in the region through which that streamtube passes could easily change the location of its intersection with the reference line and cause the streamtube originating at 15-26

to intersect the reference line at the same location as stream-tube S1-7B (see Figure B-1). The calculated value of hydraulic conductivity at the reference line would then agree more closely with the interpreted reference curve.

Preliminary tests indicate that the calculated conductivity may be more sensitive to error in storage coefficient in other regions of the aquifer.

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