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VELOCITY PREDICTION ERRORS RELATED TO FLOW MODEL CALIBRATION UNCERTAINTY (U)

by

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Velocity Prediction Errors Related to Flow Model Calibration Uncertainty

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ABSTRACT At the Savannah River Site (SRS), a United States Department of Energy facility in South Carolina, a three-dimensional, steady-state numerical model has been developed for a four aquifer, three aquitard groundwater flow system. This model has been used for numerous predictive simulation applications at SRS, and since the initial calibration, the model has been refined several times. Originally, calibration of the model was accomplished using a nonlinear least-squares inverse technique for a set of 50 water-level "calibration targets" non-uniformly distributed in the four aquifers. The estimated hydraulic properties from this calibration generally showed reasonable agreement with values estimated from field tests. Subsequent model refinements and application of this model to field problems have shown that uncertainties in the model parameterization become much more apparent in the prediction of the velocity field than in the simulation of the distribution of hydraulic heads.

Further applications of this three-dimensional flow model to simulate the effects of geologic uncertainties on model calibration and velocity field prediction have included: (1) multiple hydraulic conductivity field realizations based on interpretations of the geologic depositional environment, and (2) localized geologic heterogeneities and discontinuities in the aquitards. The results of these simulations have produced only minor differences in the calibration of the model as measured by the set of calibration targets. Furthermore, detecting these simulated variations in the geologic framework and distribution of hydraulic properties by water-level measurements requires very accurately (or fortuitously) placed monitoring wells. Yet, including these uncertainties in the model parameterization strongly influence predictions of advective transport by altering local rates and directions of groundwater flow. Thus, while geologic uncertainties may not severely diminish the ability of a groundwater flow model to predict hydraulic head distributions, transport prediction error can be magnified by these uncertainties when groundwater flow conditions at a specific waste facility are simulated.

The combined use of these three types of information (hydraulic head distributions, geologic framework models, and velocity field monitoring) provide valuable calibration data for flow modeling investigations; however, calibration of a flow model typically relies upon measured water levels. For a given set of water-level calibration targets, the uncertainties associated with imperfect knowledge of physical system parameters or groundwater velocities may not be discernable in the calibrated hydraulic head distribution. In this paper, modeling results from studies at SRS illustrate examples of model inadequacy resulting from calibrating only on observed water levels, and the effects of these inadequacies on velocity field prediction are discussed.

BACKGROUND

At SRS, waste products generated during the past 35 years of operation were stored, buried, or discharged to basins to retain or delay the waste to ensure that concentrations are extremely small at the site boundary. Waste management practices have been systematically improved since operations began in 1953, and as a result of recent studies, further improvements are being made such as removing basins from service and conducting research programs to ensure protection of groundwater resources at SRS.

To the present, hydrogeologic investigations of groundwater flow and solute transport at waste management facilities in the Separations Areas at SRS have included field characterization, groundwater monitoring, and remedial action engineering design studies. In many of these investigations, computer modeling has played an integral role in hydraulic parameter estimation, alternative design evaluation, and performance assessment/risk analysis. In many cases, the results of predictive modeling have supported management decisions. Previous modeling studies, which provide the framework for this paper, are described in Buss *et al.* (1985), Duffield *et al.* (1986), Duffield *et al.* (1987), Root (1987), Stephenson *et al.* (1987a and 1987b), Duffield *et al.* (1989), Pepper & Stephenson (1989), Stephenson *et al.* (1989), and Geraghty & Miller (1989).

SITE DESCRIPTION

The SRS, located in South Carolina, is bordered along its southwest margin by the Savannah River, which is also the geographic border between Georgia and South Carolina (Fig. 1). The site is situated in the Atlantic Coastal Plain physiographic province. In southwest central South Carolina, unconsolidated sediments of the Coastal Plain consist mainly of Cretaceous and Tertiary sands, silts, and clays with some calcareous sediments. These unconsolidated sediments dip gently and increase in thickness toward the coast to the southeast (Fig. 2). Beneath the central portion of SRS, approximately 305 m of Coastal Plain sediments lie above a basement complex of crystalline metamorphic rock and consolidated red beds in a Triassic basin.

The sediments of the Coastal Plain at SRS form a multilayered system of aquifers and aquitards. In general, the Cretaceous sediments overlying the basement rock form the most productive aquifer, while the aquifers comprised by the Tertiary sediments are less productive. Aquitard units in these sediments usually consist of clay and silt strata that frequently have limited areal extent. For this reason, the vertical sequence of hydrostratigraphic units varies across the site.

Onsite SRS streams have cut channels in the surface of the Coastal Plain sediments to produce a topography marked by interstream uplands. This sometimes exposes several aquifer zones along the walls of the stream valleys. As a result, the water table may exist in several aquifer zones in these areas. Furthermore, these incised streams can produce significant downward vertical gradients in the shallow aquifer zones. Therefore, complex three-dimensional groundwater flow paths typically characterize the flow system in the interstream areas.

One of these interstream areas located near the center of SRS has been studied in great detail (Fig. 3). Three streams border this area that influence both the horizontal and vertical flow of groundwater. These streams are the principal groundwater sinks for the shallow aquifer zones, and the variable depths of incision by each of the streams is a controlling factor in the development of local groundwater flow patterns.

In this study, the unconsolidated sediments at the site are divided into five aquifers separated by four aquitards (Fig. 4). The three uppermost aquifers (Aquifers 3 through 5) consist of Tertiary sands, silts, and some clay. Of the these units, Aquifer 3 is the most productive. Lower permeability sediments of Aquitards 3 and 4 regulate the rate of the vertical groundwater seepage between the three Tertiary aquifers. In most of the study area, the dominant factor controlling the vertical movement of groundwater between these aquifers is Upper Three Runs Creek.

Cretaceous sediments comprising Aquifers 1 and 2 provide a plentiful source of water for production facilities in the study area. Aquitard 2 is an effective barrier to the vertical flow of groundwater between the Cretaceous and Tertiary aquifers.

COMPARISON OF THREE REGIONAL FLOW MODEL CALIBRATIONS

Method of Investigation

Calibration of a mathematical model refers to the process of obtaining a reasonable match between observed data and results computed by the model. For groundwater flow models, the calibration procedure is generally carried out by varying estimates of hydraulic properties from a set of initial values until the best fit of calculated results to observed water-level calibration targets is achieved. Examples of hydraulic properties that may be varies from a set of initial estimates include hydraulic conductivities, leakance coefficients, and precipitation recharge. Calibration targets are used to evaluate the results generated by the model for a given set of input parameters. Observed hydraulic data and stream baseflow measurements are examples of calibration targets.

Parameter estimation during the calibration of a numerical flow model is most frequently achieved by a trial-and-error procedure. Trial-and-error calibration of models requiring the adjustment of a large number of hydraulic parameters can consume much time and demand a large number of simulations. Alternatively, automatic procedures for hydraulic parameter estimation can be devised that significantly reduce the time and effort required for model calibration. Automatic parameter estimation algorithms systematically solve for parameter estimate improvements that minimize the difference between calculated results and calibration targets. Calibration of flow models described in this study were accomplished with a procedure known as the Marquardt (1963) method.

For many groundwater flow problems, the Marquardt procedure converges to the optimum set of parameters required to minimize a residual sum of squares objective function. Calibrations involving a large number of hydraulic parameter variations are more efficiently performed by this method than by a trial-and-error procedure. In addition, the sensitivities of the calculated hydraulic heads to changes individual hydraulic parameters are directly available from this procedure.

Examination of model residuals or model errors provides a check on the adequacy of a calibrated model. Convergence of the estimation procedure should be accompanied by minimization of the residual sum of squares (RSS) and a mean residual equal to zero. The residual standard deviation (RSD) provides a convenient means of comparing the results of separate model calibrations having a different number of calibration targets and hydraulic parameters. Also desireable is a random distribution of model residuals. Methods of detecting departures from randomness include constructing normal probability plots and the examining the spatial distribution of residuals.

Initial Calibration of Regional Flow Model

Numerical simulations were performed with a three-dimensional, steady-state groundwater flow model. This regional model, covering a 45 km^2 area used a finite-difference grid consisting of 39 rows, 39 columns, and 4 layers to simulate flow in Aquifers 2 through 5 and Aquitards 2 through 4. The boundaries of the model, coinciding with major stream and groundwater divide locations, were represented by appropriate combinations of specified head and flux conditions. A constant rate of effective precipitation flux recharged the water table in Aquifer 5, and groundwater extraction from Aquifer 2 occurred at two pumping centers. Hydraulic parameters were estimated with the modified Gauss-Newton automatic calibration procedure using 50 calibration targets (average water levels measured between 1977 and 1979).

Initial hydraulic parameter estimates for the model were selected from values obtained from field and laboratory tests. In general, the values of the initial estimates are not crucial to the convergence of the Gauss-Newton procedure, although convergence is sometimes more quickly obtained if the initial estimates are close to the values which minimize the residual sum of squares objective function. Initially, the distribution of the model parameters was assumed to be homogeneous and isotropic within each aquifer or aquitard in the model. Heterogeneity was introduced during the calibration of the model through the definition of discrete hydraulic parameter zones. Additional zones were added to Aquifer 5 (hydraulic conductivity) and Aquitards 3 and 4 (leakance coefficients). Final estimates of hydraulic conductivities and leakance coefficients in the calibrated model compared well with field and laboratory tests.

A measure of the fit of the flow model to the calibration target data is the RSS objective function. In this initial calibration of the regional flow model, the RSS was 37.4 m^2, and the RSD was 0.97 m. Inspection of normal probability and spatial distribution plots of the model residuals did not reveal nonrandomness.

Particle-tracking simulations with this model predicted groundwater travel time estimates from two seepage basin facilities in the study area. Simulated travel times for four particles originating at the H-Area Seepage Basins to Four Mile Creek ranged from 12 to 30 years (Fig. 5).

Calibration of Regional Flow Model with Nonuniform Geology

Sediments in the study area often display textural and compositional heterogeneity that may influence their hydraulic properties. Geostatistical modeling by Root (1987) showed distinct zones of higher hydraulic conductivity in these aquifers with patterns resembling old stream channels. A later sedimentological study supported this finding (Everest Geotech, 1987). Using these two studies as a basis for defining patterns of large-scale heterogeneity in the uppermost two aquifers (Aquifers 4 and 5), a new calibration of the three-dimensional flow model described in the previous section was attempted.

To simulate these large-scale heterogeneous features, the pattern of hydraulic conductivity zonation in Aquifer 5 was modified, a new hydraulic conductivity zone was added to Aquifer 4, and an additional leakance coefficient zone was added to Aquitard 4. Only minor variations in simulated hydraulic heads and flow balance calculations resulted from the new calibration. For the same 50 calibration targets used in the initial calibration, the new RSS improved slightly to 34.8 m^2; however, with the two new hydraulic parameters in the model, the RSD remained essentially unchanged at 0.96 m.

Compared to the initial calibration, simulated ground-water travel times from the H-Area Seepage Basins did not change significantly.

Recalibration of Regional Flow Model with Additional Water Levels

More recent water-level data measured between 1984 and 1987 were used to recalibrate the ground-water flow model for the study area. In this calibration, the set of calibration targets included of a total of 79 water levels. The four layers of the new model simulated the same four aquifer, three aquitard system, but the areal discretization was modified by adding four new rows and four new columns to represent more accurately the distribution of the calibration targets.

As in the initial calibration, hydraulic property zones were added to the model to reduce the magnitude and spatial correlation of calibration target residuals. The final calibration consisted of a total of 13 zones. Aquifers 4 and 5 each contained two hydraulic conductivity zones, while aquitards 3 and 4 each consisted of three leakance coefficient zones. The distribution of hydraulic properties was uniform in Aquifers 1 and 2, and also Aquitard 2.

This recalibration of the regional model resulted in a RSS of 41.2 m^2; the RSD of 0.79 m shows improvement over the two previous calibration attempts. In addition, flow balance calculations for the model showed a 50 percent increase in ground-water flux from Aquifer 5 to surface streams. As a result, ground-water travel times from the seepage basins decreased. Travel times from the H-Area Seepage Basins to Four Mile Creek ranged from 2 to 15 years (Fig. 6). Compared to the previous calibrations, horizontal travel from this facilities within Aquifer 5 was greatly increased.

COMPARISON OF MODEL RESULTS WITH FIELD TRACER MEASUREMENTS

Observed Tritium Travel Times from H-Area Seepage Basins to Four Mile Creek

Various studies at the H-Area Seepage Basins provide estimates of ground-water velocities near the H-Area Seepage Basins. In 1958, detection of tritium in Four Mile Creek placed an estimate of travel time from seepage basin 1 at approximately three years. From ground-water monitoring well measurements made in 1966, Stone & Christensen (1983) estimated about a four-year travel time from seepage basin 4. This second estimate could be extended to as long as 11 years if the tritium detected in the ground water were the result of tritium disposal prior to the use of basin 4 in 1962.

These estimates of ground-water velocities using a conservative species provide an additional method of checking the calibration of the regional flow model. Both the initial calibration and the its subsequent recalibration employing concepts of large-scale heterogeneity, each displaying comparable calibration statistics, failed to reproduce observed tritium travel times near the H-Area Seepage Basins. The most recent recalibration, which used a larger number of calibration targets with greater spatial coverage, produced the lowest RSD and also provided the most realistic estimates of ground-water travel times from the seepage basins.

Observed Patterns of Contaminant Migration from H-Area Seepage Basins

Ground-water quality monitoring and surface geophysical surveys indicate the existence of several narrow, finger-like plumes extending from H-Area Seepage Basin 4 toward Four Mile Creek (Fig. 7) that suggest preferred zones of ground-water flow (Killian *et al.*, 1987). Plausible mechanisms for this phenomenon may include the following: (1) nonuniform leakage from the basins, (2) influence of the ground-water seep line along Four Mile Creek that forms a cuspate pattern with deep reentrants (Fig. 7), and (3) heterogeneous distribution of hydraulic conductivity in Aquifer 5.

Further complexity in the ground-water flow regime near these basins is indicated by ground-water quality data from wells located to the south of seepage basin 4. In general, contaminants migrate horizontally in Aquifer 5 and in the upper part of Aquifer 4 toward Four Mile Creek; however, localized vertical contaminant migration was detected at monitoring well HSB84A (Fig. 7), where elevated tritium concentrations were found in Aquifer 3 (Killian *et al.*, 1987). A postulated mechanism for contaminant transport into this aquifer is heterogeneous aquitard properties (e.g., thickness or hydraulic conductivity) or a discontinuity in Aquitard 3.

The three previously described calibrations of the three-dimensional model were designed to match the regional characteristics of the ground-water flow system in the study area; no attempt was made in these calibrations to reproduce the detailed features of the flow system near the H-Area Seepage Basins. In an effort to better understand the some of the mechanisms behind the observed patterns of solute migration near these basins, predictive simulations were performed with the model configuration described for the initial calibration. Small-scale geologic heterogeneity and discontinuity features were simulated by refining the finite-difference grid in an area to the south of seepage basin 4. Simulations were performed to investigate the effects of hypothetical "holes" and faults in Aquitard 3 on ground-water flow directions and rates in the vicinity of the seepage basins.

Simulations performed for several different sizes of "holes" and faults showed that a 18.6 m^2 "hole" and a 244-m long fault with a 4.6-m offset are sufficient to produce a gathering effect on ground-water flow patterns similar to the narrow, finger-like plumes shown in Fig. 7. Fig. 8 shows the ground-water flow patterns simulated with the 18.6 m^2 "hole" feature. This example also suggests that these features can actually reverse the flow of ground water in Aquifer 5. In addition, these features also provide a mechanism for increasing the vertical movement of ground water from Aquifer 5 to Aquifer 3.

SUMMARY AND CONCLUSIONS

At the SRS, three-dimensional models have been used to simulate several hydraulic conductivity realizations in a multiaquifer ground-water flow system. Each of these realizations represented a different interpretation of the hydrogeologic framework, and for each realization, the model was calibrated to a set of observed water levels using a nonlinear least-squares parameter estimation technique. Throughout the evolution of the model, ground-water velocity prediction was recognized as an important calibration parameter.

Two separate calibrations of the regional model of the study site for different realizations of the hydraulic conductivity field using the same set of water-level calibration targets produced nearly identical results in terms of RSD and flow balances. For these calibrations, prediction of ground-water velocities near a seepage basin facility did not adequately reproduce observed ground-water travel times to a nearby surface stream. With a different set of water levels exhibiting better spatial coverage and density, a new representation of the geologic framework was developed during the calibration of the model. This calibration produced an improved RSD and better estimates of ground-water travel times in the vicinity of the seepage basins. Thus, the combined use of geologic information and water levels alone were insufficient to produce a calibrated model suitable for analyzing ground-water flow directions and rates in this aquifer system. The use of observed ground-water velocities played a decisive role in the understanding of hydraulic property variation and the development of a model suitable for making predictive simulations of the velocity field near the seepage basins.

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COMPILED BY	FILE INDEX:	SCALE:	Figure 1.1 Location map of Savannah River Site, Aiken, South Carolina
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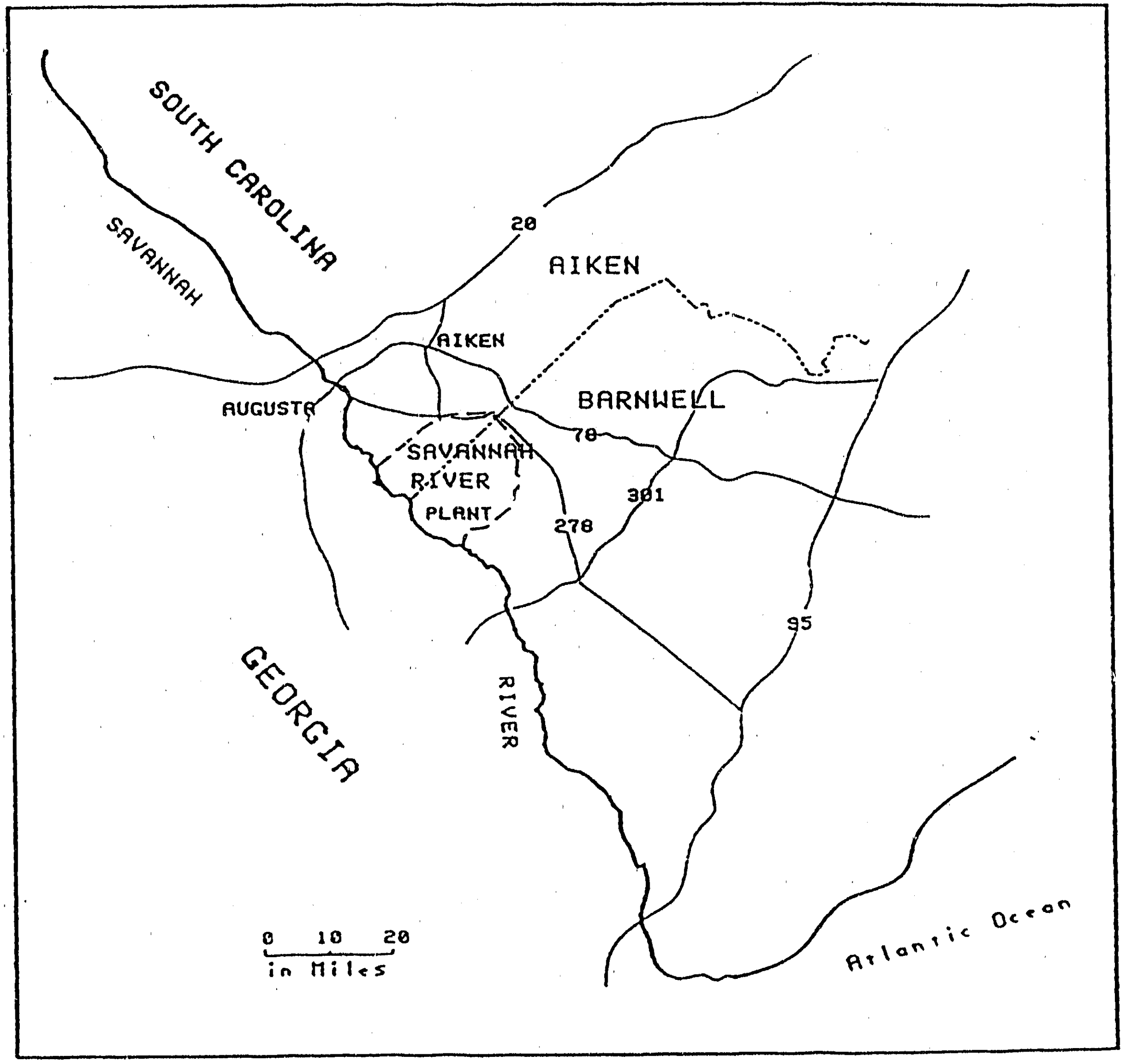

Fig. 1

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COMPILED BY:	FILE INDEX:	SCALE:	Figure 1.2 Location map of General Separations Area, Savannah River Site.
PREPARED BY:	C.F. NAME:	DATE	
PROJECT MGR:			

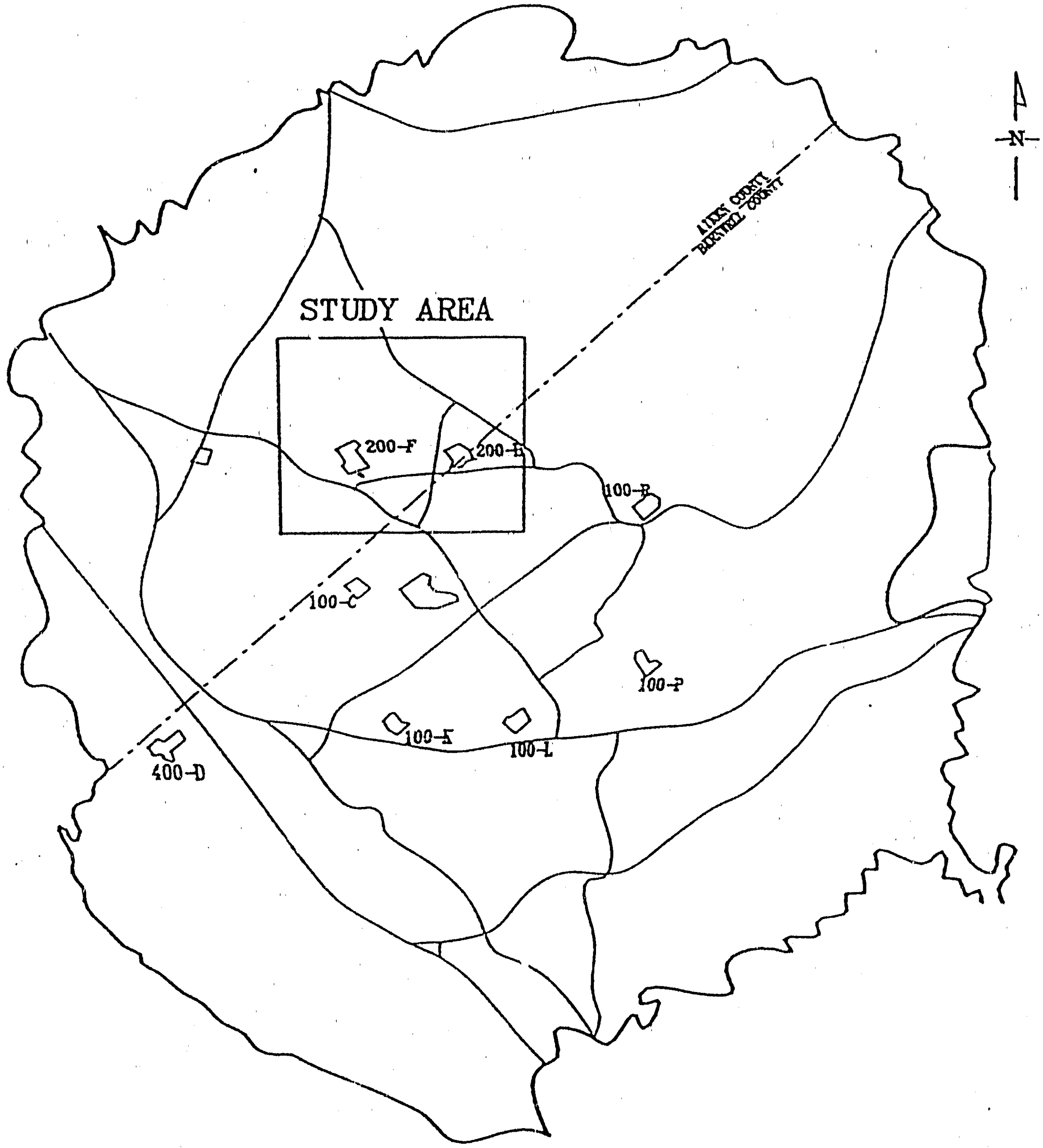

Fig. 3

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Figure 3.1 Hydrostratigraphic nomenclature for General Separations Area, Savannah River Site.

SRP NOMENCLATURE -- VARIOUS WORKERS	PROVISIONAL NOMENCLATURE[1]	HYDRO-STRATIGRAPHIC UNIT
HAWTHORNE BARNWELL	"UPLAND UNIT" TOBACCO ROAD	AQUIFER ~~1~~ 5
TAN CLAY	TWIGGS CLAY	AQUITARD ~~1~~ 4
MCBEAN	DRY BRANCH SANTEE	AQUIFER ~~2~~ 4
GREEN CLAY	CAW CAW SHALE	AQUITARD ~~2~~ 3
CONGAREE	CONGAREE	AQUIFER ~~3~~ 3
ELLENTON	ELLENTON	AQUITARD ~~3~~ 2
UPPER TUSCALOOSA	PEEDEE BLACK CREEK	AQUIFER ~~4~~ 2
MIDDLE TUSCALOOSA	MIDDENDORF	AQUITARD ~~4~~ 1
LOWER TUSCALOOSA	CAPE FEAR	AQUIFER ~~5~~ 1

PIEDMONT CRYSTALLINE BASEMENT ROCKS

[1] After Price et al. (1988)

Fig. 4

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Figure 4.22 Particle traces from the H-Area Seepage Basins under no cap conditions.

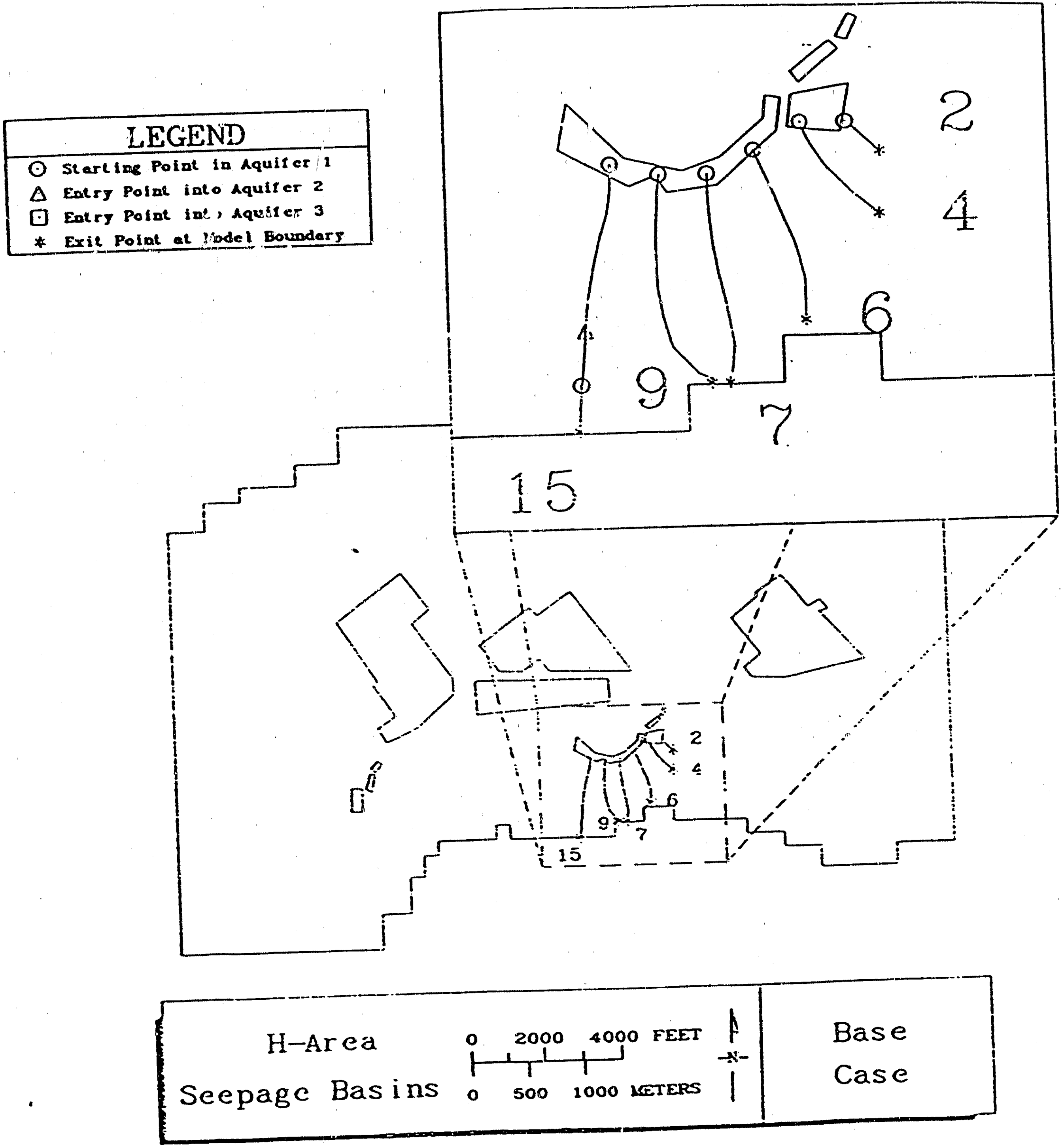
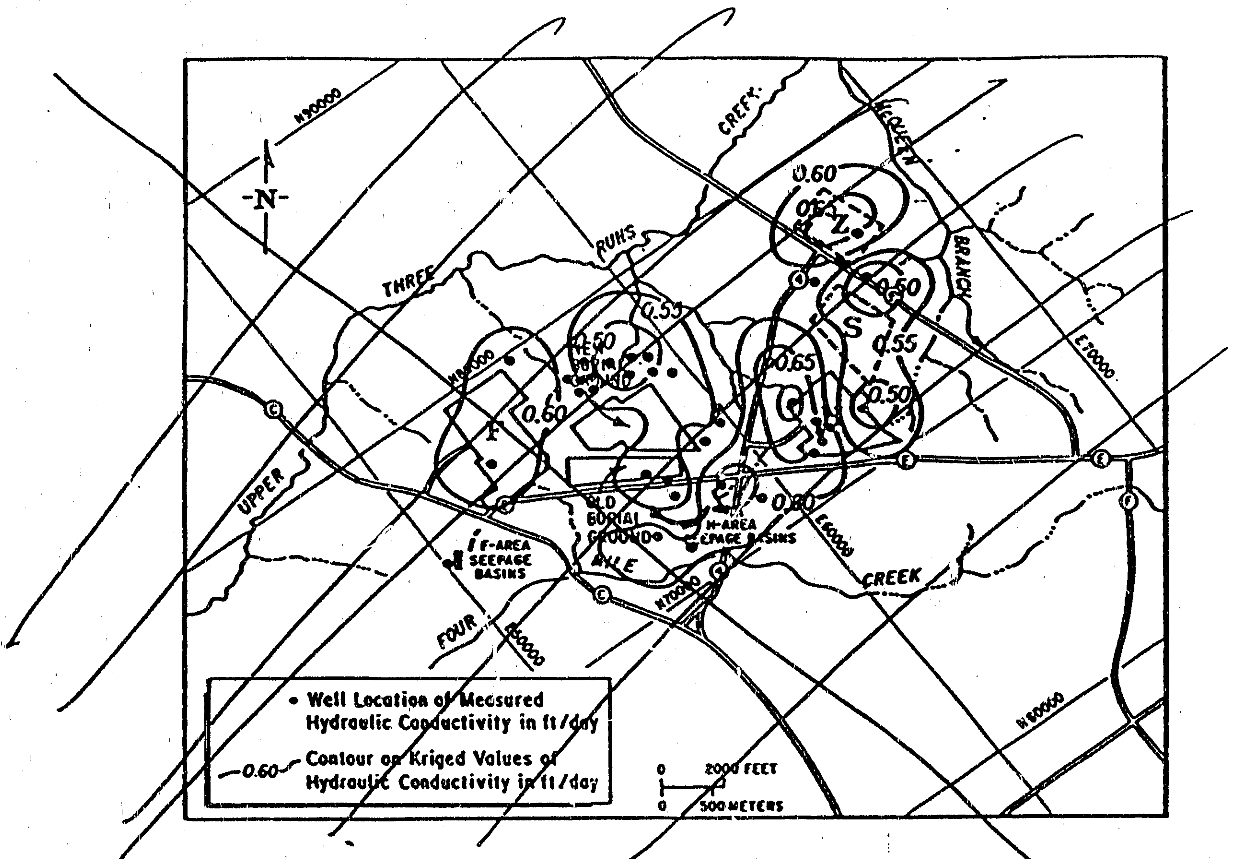


Fig. 6



~~Figure 4. Kriged values of hydraulic conductivity in Aquifer 1 (modified from Root, 1987).~~

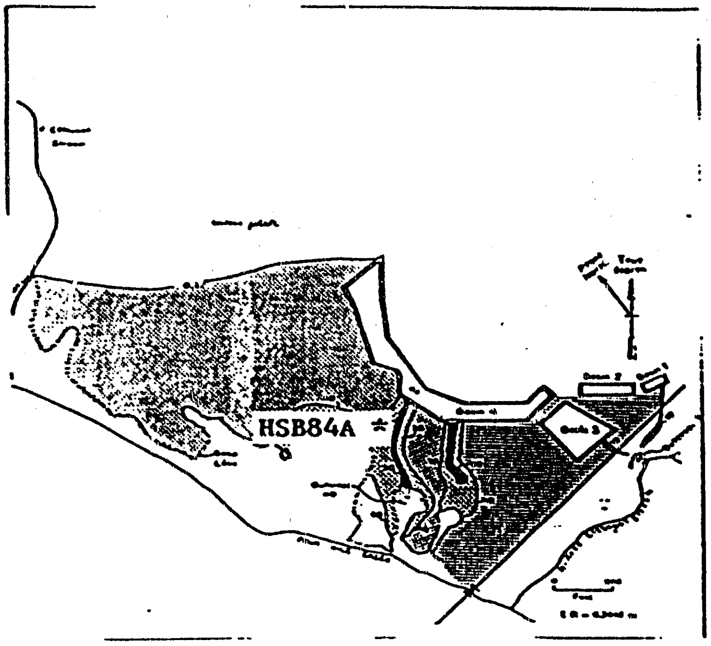


Figure ~~8~~ 7. Isoconcentration contours of tritium in Aquifer 1 at H-Area Seepage Basins (from Stone and Christensen, 1983).

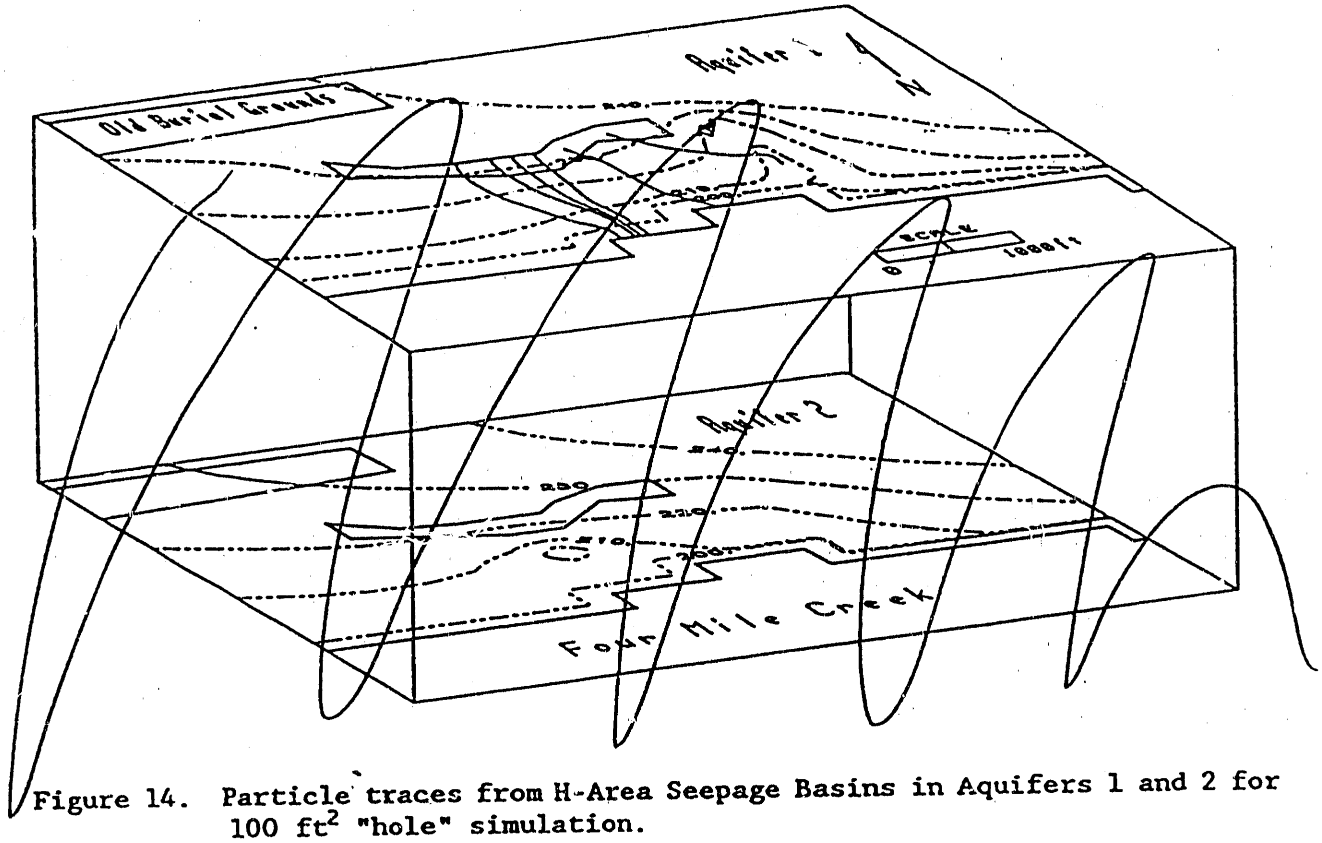


Figure 14. Particle traces from H-Area Seepage Basins in Aquifers 1 and 2 for 100 ft^2 "hole" simulation.

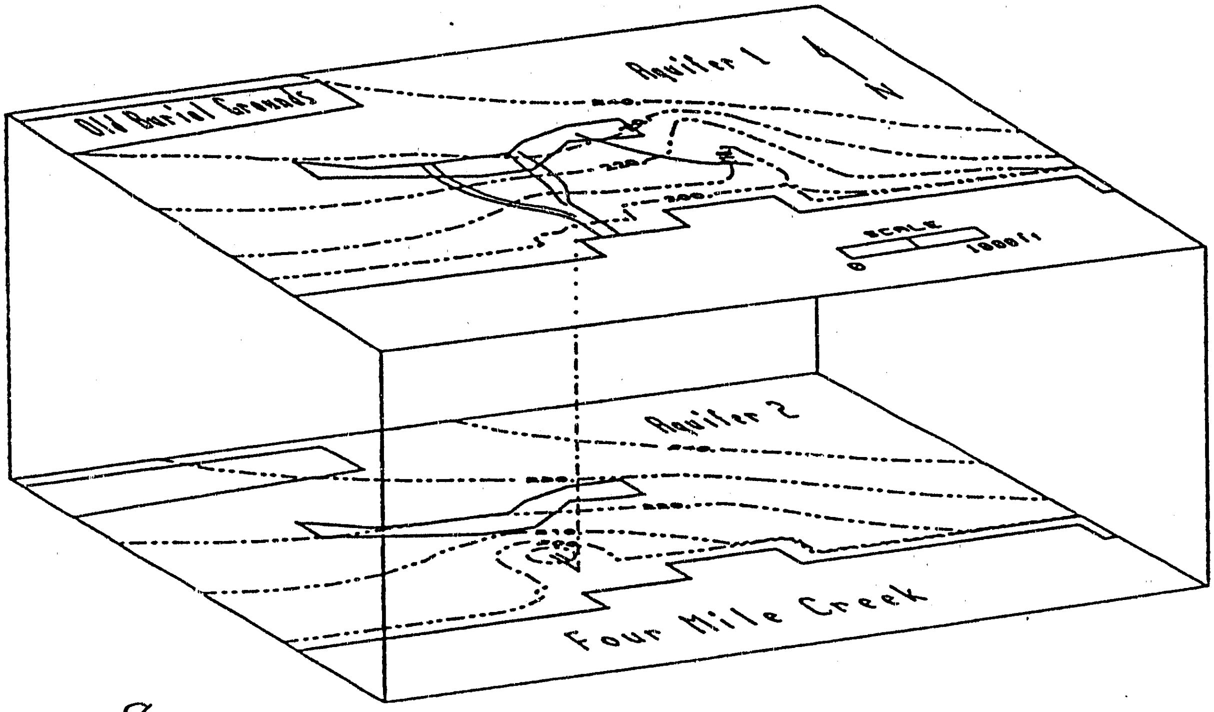


Figure ~~15~~ 8. Particle traces from H-Area Seepage Basins in Aquifers 1 and 2 for 200 ~~ft~~^{2} "hole" simulation.
18.6 m^2

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