Effects of model discretization on zones of contribution to low pumping-rate wells in a hypothetical river-valley aquifer

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ABSTRACT

The selection of an appropriate level of discretization in numerical models is important to accurately delineate zones of contribution (ZOC) to pumped wells. It is particularly important to select proper grid sizes when simulating flow to low-pumping-rate wells (25 gallons per minute or less) in high-permeability aquifers because of problems related to (1) weak sinks, (2) sensitivity of ZOC to different sources of recharge, and (3) sensitivity of ZOC to vertical placement of partially penetrating wells. Solutions to the latter two problems depend on proximity of the wells to recharge boundaries. In urban environments, other factors in discretization should be considered including distribution of cultural features such as buildings, drains, impermeable surfaces, and other engineered structures.

Twenty-four finite-difference ground-water-flow models of the same hypothetical 1.3-square-mile, sand and gravel, river-valley aquifer were constructed to evaluate the effects of model discretization on delineation of ZOC's to four low-pumping-rate wells. The four wells are partially penetrating in an upgradient and downgradient well cluster; each cluster includes one shallow and one deep well. The upgradient wells were positioned 500 feet from a river recharge boundary, and the downgradient wells were positioned 2,000 feet from a discharge boundary.

The size of ZOC's were overestimated in 10 of the 24 models when intercell aquifer fluxes exceeded the rate of withdrawals in the cell---a condition called a weak sink. Weak sinks were a problem for simulations with horizontal cell sizes greater than 5 percent of the aquifer width and vertical thickness greater than 33 percent of total aquifer thickness.

The locations and sizes of ZOC's were affected by changes in sources of

recharge to upgradient wells. Changes in horizontal discretization caused variations in proportions of recharge from river leakage and precipitation recharge. For the coarsest horizontal cell size (5 percent of the aquifer width), upgradient wells derived most of their recharge from the river. ZOC's were smallest for those simulations. Horizontal discretization had little effect on ZOC's of downgradient wells.

The locations of ZOC's were affected by vertical placement of downgradient wells. Changes in vertical discretization caused partially penetrating wells to intercept different flowpaths. For the coarsest vertical cell size (100 percent of aquifer thickness), the shallowest flowpaths were intercepted, and the ZOC's were nearest to the well. Vertical discretization had little effect on the ZOC's to upgradient wells.

INTRODUCTION

Adequate discretization of a ground-water flow model is necessary to accurately represent any hydrogeologic system. In urban environments, consideration must also be given to the spatial distribution of cultural features such as buildings, drains, impermeable surfaces, and other engineered structures.

Simulations of ground-water flow are generally less sensitive to grid cell size than simulations of particle tracking (flowpath analysis) or solute transport (Zheng, 1994). To obtain accurate flowpaths, the ground-water flow simulation must first accurately reflect the hydrogeologic system and urban setting.

Errors in flowpath analysis result from (1) errors in the finite-difference solution of flow, (2) tracking procedures, and (3) the representation of internal sinks (weak sinks). In many cases, the principal error in particle tracking is typically the inability to accurately and unambiguously represent internal sinks.

Weak sinks occur if the total inflow to a cell exceeds the flow to an internal sink such as a withdrawal well. This is a problem in particle tracking simulations because with a weak sink it cannot be determined whether a specific particle should discharge to the sink or pass through the cell (Pollock, 1994). Confidence in a particle tracking simulation is greatly reduced when weak sinks are present. Weak sinks can be avoided by refining a grid to reduce the rate of total inflow to a cell relative to withdrawal out of the cell.

This paper describes a series of finite-difference numerical models of a hypothetical river valley aquifer system that were constructed to evaluate the sensitivity of ground-water flow simulations to cell size. Twenty-four models with different horizontal and vertical cells sizes were constructed of the same hypothetical aquifer. Results reported include analysis of fluxes, [1]flowpaths, and ZOC's to four partially-penetrating wells, two near and two distant to a river

[1]The term flowpaths is used in this paper to describe the patterns of particle pathlines.

boundary. Although the results of the test are dependent on the model parameter selection, the results can be transferred, in a general sense, to ground-water-flow model simulations of similar hydrologic settings.

CONCEPTUAL-FLOW SYSTEM

The hypothetical aquifer is a simple block shape, 100 feet (ft) thick, 4200 ft wide, and 12,000 ft long that is designed to represent one-half, symmetrical with respect to the river, of a typical alluvial river-valley aquifer of the glaciated northeastern United States. River-valley aquifers underlie many highly developed land areas because of past and present cultural demands. The hypothetical aquifer extends from the contact of the river valley aquifer with till and bedrock uplands at the valley edge to a partially incised river in the middle of the river valley. The aquifer consists of sands and gravels. This example is based on a glacial-drift river-valley aquifer in Milford, New Hampshire, described by Harte and Mack (1992).

The hypothetical aquifer is recharged primarily from precipitation onto the land surface and from the upstream reaches of a river. Ground-water discharges to the downstream reach of the river and to withdrawal wells. Two low-pumping rate withdrawal well pairs are simulated, a shallow and deep well pair at an upgradient and downgradient location. The upgradient well pair is close to a river recharge boundary while the downgradient pair is further away from the river boundary. Low-pumping rate wells are sometimes used to remediate contaminants from ground-water flow systems. The edges of the aquifer are no-flow boundaries except where it is in contact with the river.

MODEL CONSTRUCTION

Twenty four finite-difference ground-water-flow models were constructed with identical hydraulic properties and overall dimensions, and nearly identical boundaries. The U.S. Geological Survey finite-difference model, MODFLOW, was used to simulate ground-water flow (McDonald and Harbaugh, 1988). Boundary conditions and aquifer properties were simplified or idealized to isolate the effect of cell sizes on simulated flow. Horizontal grid cell size and vertical layering were changed an order of magnitude while keeping all other model parameters constant.

Although many river-valley aquifers are unconfined, the models were designed as confined systems to eliminate the effects of variable saturated thickness on the analysis. Varying saturated thickness is a result of the hydraulic gradient applied on the system. With horizontal layering and an unconfined simulation, the uppermost layer would become increasingly more wedge shaped, which would accentuate the relative change in saturated thickness from upgradient to downgradient.

Discretization

Each model constructed consists of uniform, square horizontal cell dimensions and uniform vertical cell thickness as listed in table 1. Models are designated by horizontal cell size and number of model layers. For example, model 200H1L designates a model with a 200 by 200 ft horizontal cell size and one layer; model 20H20L designates a model with a 20 by 20 ft horizontal cell size and 20 layers. Models were constructed with horizontal cell sizes of 200, 100, 50, and 20 ft. For each horizontal cell size, seven models with vertical cell thicknesses of 100, 50, 33.3, 20, 16.6, 10, and 5 ft were constructed. The coarsest discretized model had cells 200 ft horizontally and 100 ft thick, resulting in a model of 21 rows, 60 columns, and one layer for a total of 1,260 cells. The finest discretized model had cells 20 ft horizontally and 5 ft thick, resulting in a model of 210 rows, 600 columns, and 20 layers for a total of 2,520,000 cells.

Some small differences exist in the location of wells and boundaries, usually less than 10 percent of length or depth, because of the discretization process. For example, variations in penetration of river and well boundaries occur due to differences in layer thicknesses between models and variations in well location of up to 50 ft occur due to differences in horizontal cell sizes between models.

Boundary conditions

The ground-water flow system is simulated by the following boundaries: a river along the length of the northern side of the modeled area, constant recharge to the uppermost model layer, and no-flow boundaries along three sides and the base of the model. The river is partially penetrating with the exception of the one layer models, in which case the river is fully penetrating.

The river is simulated by a general-head boundary along the outer edge of the aquifer, in MODPATH the general-head boundary was applied to IFACE 4 (Pollock, p. 3-9, 1994), with an external head which slopes from 25 to 0 ft. The general-head boundary conductance was calculated according to the equation for streambed conductance (C) (McDonald and Harbaugh, 1984, p. 6-4) with the following properties:

$$C = \frac{KLW}{M} \tag{1}$$

where:

L = the cell length of the stream reach (cell length),

W = a stream width of 50 ft,

K = a streambed hydraulic conductivity of 5 feet/day (ft/d), and

M = a streambed thickness of 5 ft.

Although the general-head boundary is applied over the thickness of the uppermost model layer, the boundary conductance remains constant with model layer thickness. A single-layer model effectively simulates a fully penetrating river while the models with finer layer discretizations more closely simulate a partially penetrating boundary.

Areal recharge was applied to the uppermost model cells as a specified-flux boundary to simulate infiltration of direct precipitation onto the aquifer. The flux was applied at a rate of 197,125 ft^3/d (18 in/year). Areal recharge and the general-head boundary (river) respectively contribute 80 and 20 percent of the total recharge in the models.

Withdrawal wells

Withdrawal wells were placed at four locations in the aquifer, a shallow and deep well pair upgradient in the aquifer and a second pair downgradient. One well pair was 550 ft (13 percent of the aquifer width) from the upstream reach of the river in the ground-water recharge area. The other well pair, is 6000 ft (50 percent of the aquifer length) downgradient from the upgradient wells, and is 1900 ft (45 percent of the aquifer width) from the river, near the ground-water discharge area. The withdrawals are intended to represent partially penetrating wells with screen intervals 10 to 15 ft below the water surface for the shallow wells, and the bottom 5 ft of the aquifer, for the deep wells. The ability to realistically simulate the true vertical position of a well is a function of the vertical discretization. With more model layers and thinner vertical thicknesses, the vertical positioning of the wells can be simulated with greater precision than with fewer model layers and thicker vertical thicknesses. The 20-layer models are the only designs that explicitly simulate a 5-ft well screen. In the cases with only one model layer, the shallow and deep wells are simulated as one fully penetrating well.

A low rate of withdrawal, 25 gallons per minute (gal/min) per well, equal to two percent of the total flux through the aquifer, was used to enhance the effects of cell size on weak sinks. For single layer models, a withdrawal rate of 50 gal/min was simulated.

Aquifer properties

The aquifer properties--horizontal hydraulic conductivity, vertical hydraulic conductivity, and streambed conductance--were spatially uniform in each model and were constant between models. A horizontal and vertical hydraulic conductivity of 100 feet/day (ft/d) was used.

Solution algorithms and criteria

The U.S. Geological Survey finite-difference numerical ground-water flow model (MODFLOW) computes hydraulic heads based on mass balance calculations of ground-water for individual cells by use of iterative solvers. A preconditioned, conjugate-gradient solution technique (Hill, 1990) was used to solve the finite difference equations. A head closure criteria of 0.01 ft between successive iterations was used to determine solution convergence. Simulations had mass balance errors of less than 0.1 percent of the total flux and withdrawal cells had mass balance errors of less than 0.003 percent of the total cell flux.

GROUND-WATER-FLOW SIMULATIONS

The ground-water-flow simulations were assessed with respect to cell fluxes (weak sinks), size and shape of ZOC's, and patterns of ground-water flowpaths. Ground-water flowpaths were computed by use of MODFLOW model output and a semianalytical particle tracking procedure, MODPATH, developed by Pollock (1994).

Flux to wells

The flux to each well (or withdrawal) is shown in FIGURE 1 as a percentage of the total flux in the cell in which the well is located. Where cell discretization horizontally was 2 percent of the shortest model axis length, or finer (100H or less), and vertically was 33 percent of the aquifer thickness or finer (3 or more layers), weak sinks are nonexistent or insignificant. All simulations with 200 ft horizontal cells (200H) had weak sinks. This was also true for the 200H simulations with the finest vertical discretization--cells 5-ft thick or 5 percent of the aquifer thickness. Some of the simulations with 100 ft horizontal cells (100H), and all of the 2 layer models, had weak sinks. Withdrawal wells in the one layer models with 100 ft or finer, horizontal cells were strong sinks because with only one layer, withdrawal rates from the shallow and deep wells were combined, increasing the total withdrawal to 50 gal/min. When there were at least 3 layers (each layer one third the aquifer thickness or less) the amount of flow into the withdrawal cell was reduced enough such that withdrawal wells were strong sinks.

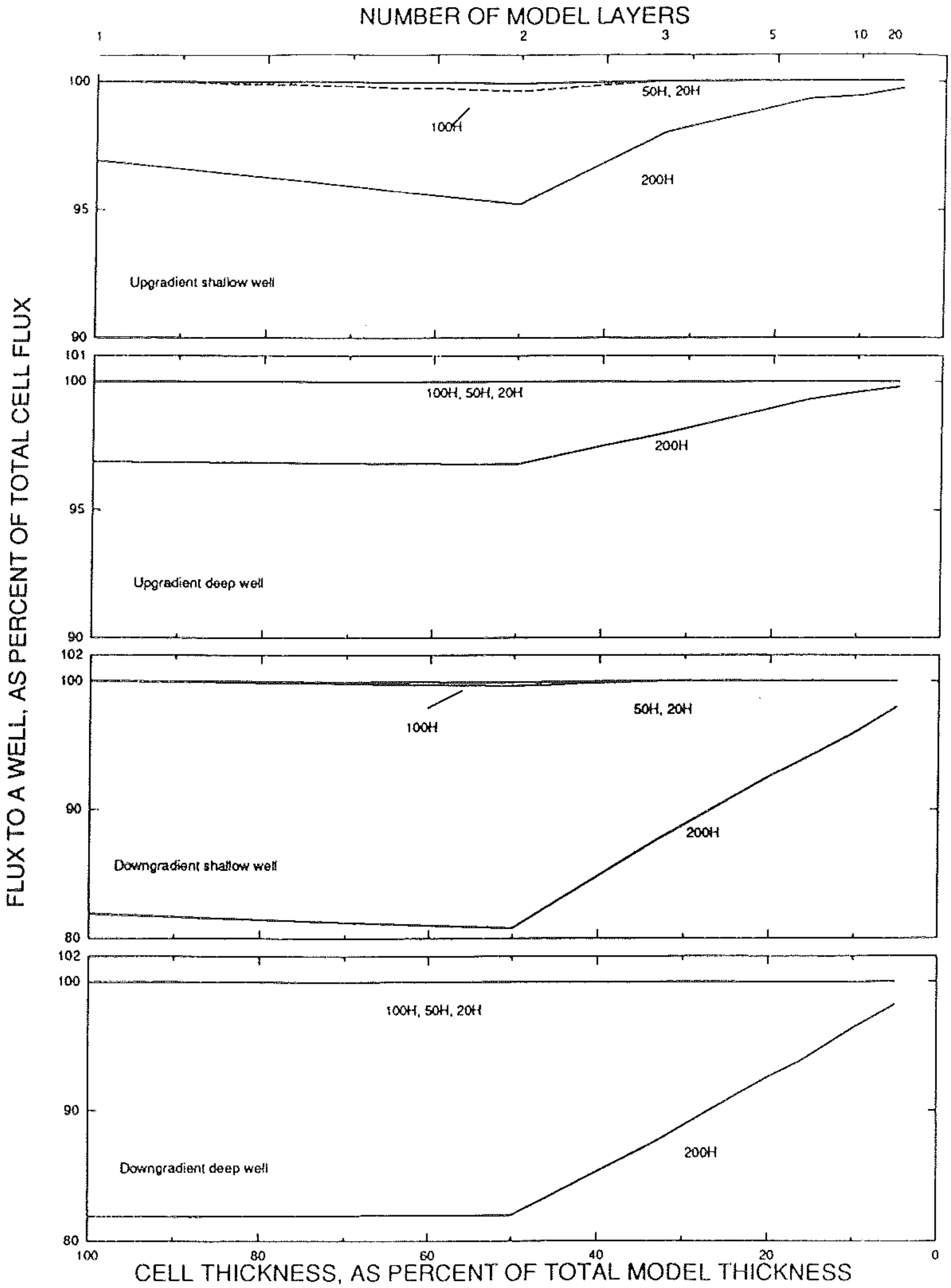

FIGURE 1. Ground-water flux to a well as a percent of the flux to a model cell for various horizontal and vertical cell sizes (200H, 100H, 50H, 20H indicates model and horizontal cell size in feet).

Zones of contribution

The projection of zones of contribution to the water-table surface, called contributing recharge areas (CRA's), are shown in FIGURE 2 for six simulations for models: 200H1L, 200H5L, 200H20L, 20H1L, 20H5L, and 20H20L. The CRAs were produced by showing the particles that when tracked forward in the direction of flow discharge at a withdrawal well. Particles were placed on the top surface of the models at a density of 1 particle per 5 square feet (ft^{2}).

Differences in the shape of CRA's due to horizontal cell size are the largest for the upgradient wells (200H1L and 20H1L). CRA for upgradient wells extend further upgradient for 20H model than 200H model. Recharge to the deep upgradient well is primarily from the river boundary, which is not evident in FIGURE 2. With increasingly finer grid discretization, the upgradient deep well receives more water from areal recharge than from the river boundary. The CRA increases in size as more of its source is areal recharge. Little difference exist in size and shape of CRA's due to horizontal cell size for the downgradient wells.

Differences in the locations of CRA's due to vertical layering are the largest for the downgradient wells in the 200H simulations. The 200H simulations show CRA for the shallow and deep downgradient wells that separate from each other when the model has three or more layers (FIGURE 2).

Analysis of the size of the CRA's produced by different cell sizes shows that models with 100 ft (100H) or finer horizontal cells and three or more model layers have similar sized CRA's (FIGURE 3). Differences in CRA size, for upgradient wells, due to horizontal cell discretization are relatively large due to their close proximity to the river. Horizontal cell size impacts the CRA's to the upgradient wells because it affects the source of water to the wells. With coarser discretization more river water recharges the wells than with finer discretization, in which case the wells receive more water from areal recharge. In contrast, differences in CRA's due to vertical cell discretization are smaller for upgradient wells than downgradient wells. For the 200H simulations the CRA's to the downgradient wells decrease in size with a decrease in vertical cell thickness. This is primarily attributed to a more accurate delineation of the CRA's due to a finer vertical discretization and increasingly stronger sinks.

The size of a CRA to a well will be larger for a weak sink than a strong sink because a weak sink captures some particles that are not captured by a strong sink due to the inability of particle tracking programs to differentiate which particles should be captured. Where the source of water to a well is solely uniform areal recharge, and assuming that all particles that enter a weak sink cell discharge to that sink, the error in the CRA size due to a weak sink is directly proportional to the magnitude of the weak sink. For example, a weak sink well that loses 10 percent of the flux into the cell (captures 90 percent of the total flux into the cell) will overestimate the size of the CRA by 10 percent. A weak sink well that loses 20 percent of the flux into a cell will overestimate the size of the CRA by 20 percent.

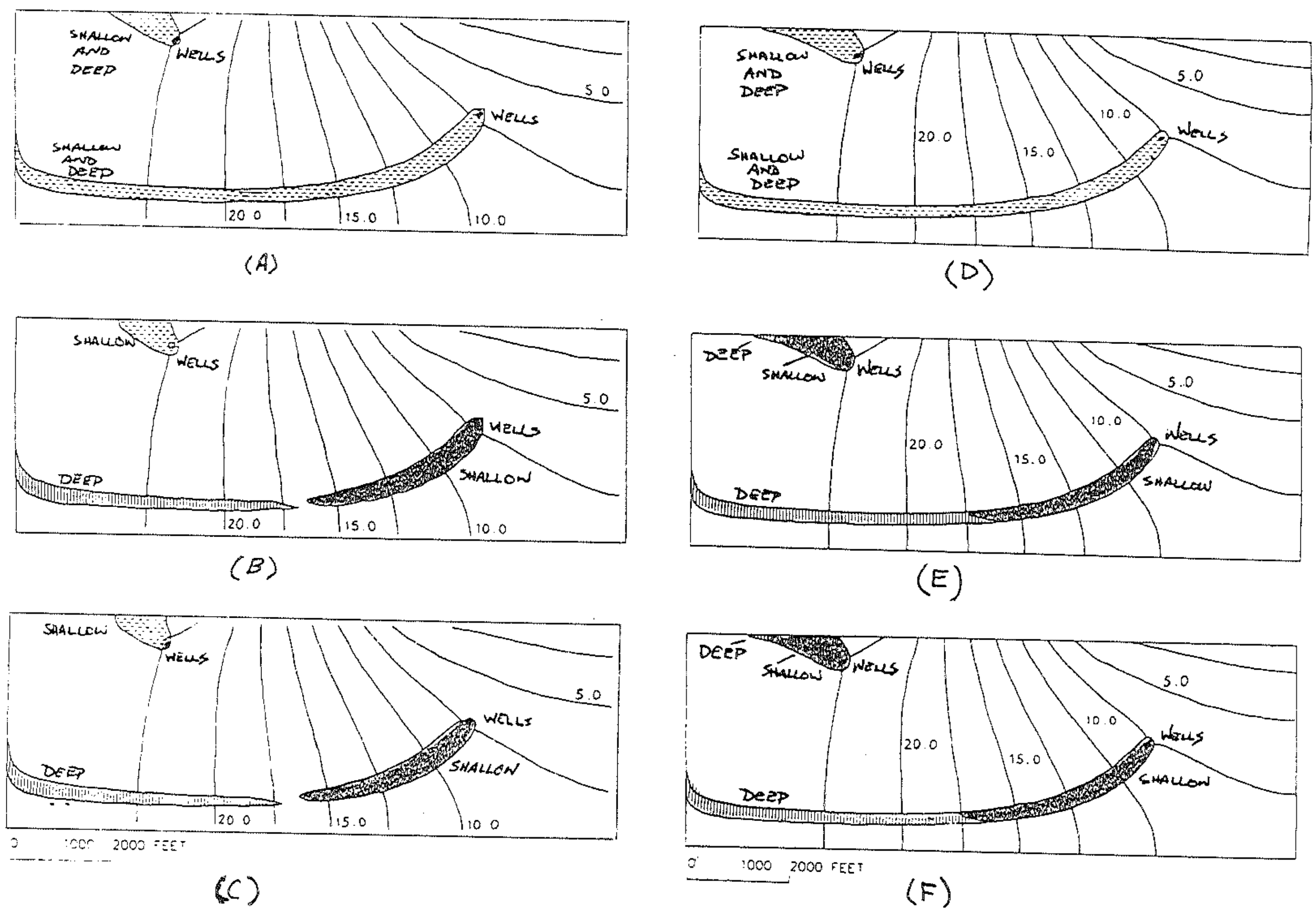

FIGURE 2. Contributing recharge areas for models of 200H1L (A), 200H5L (B), 200H20L (C), 50H1L (D), 50H5L (E), and 50H20L (F).

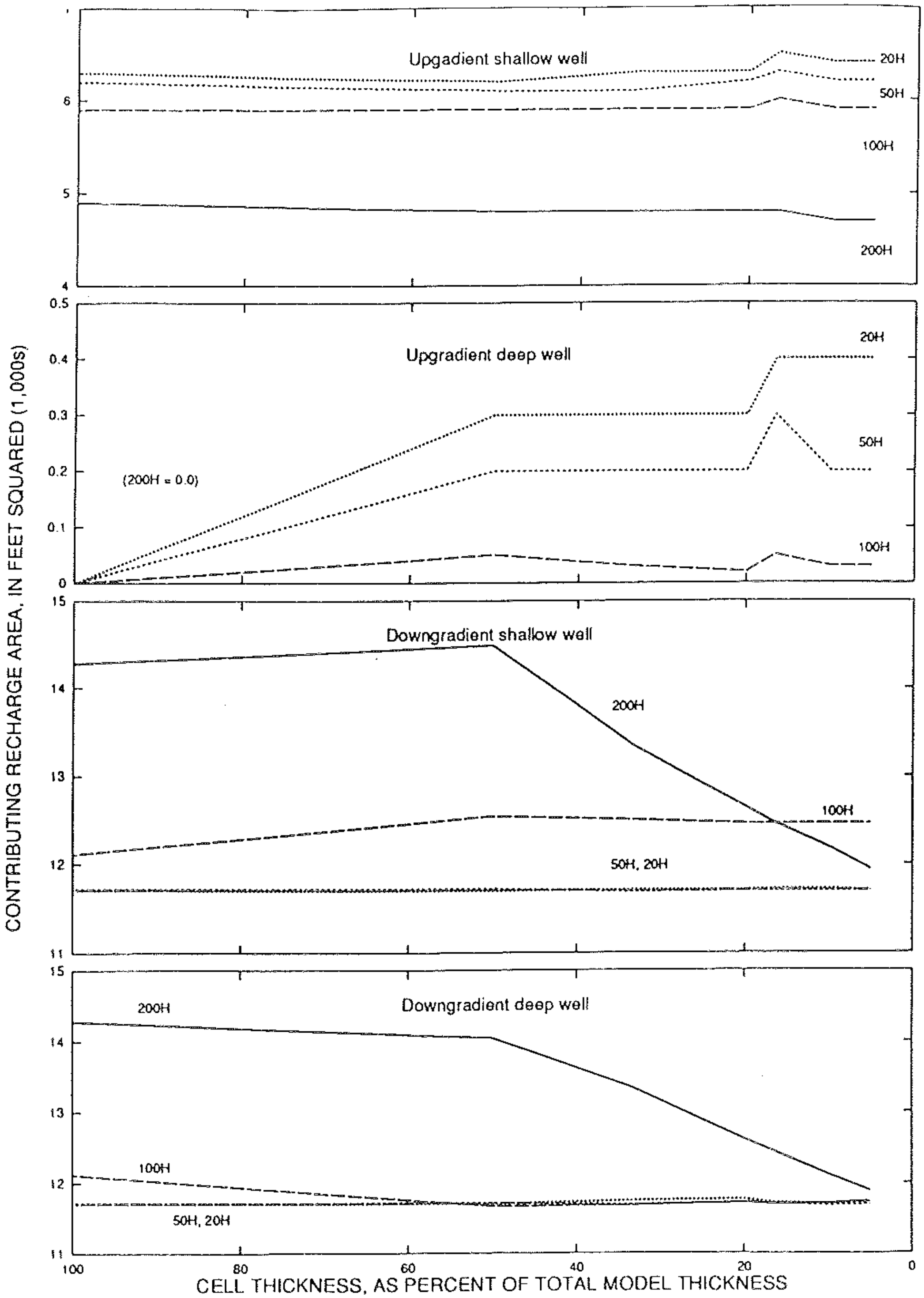

FIGURE 3. Effects of cell area, thickness, and location in a flow system on the contributing recharge area to a pumped well(200H, 100H, 50H, and 20H indicate model and horizontal cell size in feet).

Flowpaths to wells

A primary concern in model construction is what is the number of cells needed for an acceptable solution between boundaries of interest, in this case the river boundary and the upgradient wells. Analysis of the flowpaths to the upgradient wells (FIGURE 4), which are 450 ft from the river boundary (11 percent of the aquifer width), indicates that flowpaths close to a boundary are sensitive to horizontal discretization. Smooth flowpaths were produced by models with a horizontal cell size less than 100 ft (100H models), or 5 model cells or more between the well and the river boundary (a discretization of 20 percent of the distance between boundaries). For the conceptual system presented, at least 5 model cells, a horizontal cell size of 100 ft, are needed between the river boundary and the well to produce a realistic solution.

Horizontal cell sizes also affect the impact that vertical discretization has on flow to wells. For example, flowpaths to the 20-layer model show large differences between the 200H and 20H models. An area of stagnation develops between paths flowing to the shallow and deep wells for the 5 and 20-layer model. This stagnation area decreases in size with a refinement of horizontal cell size. Vertical discretization is also important in that it determines the placement of partially penetrating sources and sinks and how precisely they are represented. With a 1-layer model, the river and well are fully penetrating and the flowpaths are nearly horizontal throughout the aquifer thickness (FIGURE 4). With the 5-layer model, flowpaths are more realistically distributed to the shallow and deep wells. Little difference occurs between 5 and 20-layer models. The flowpaths shown in FIGURE 4 suggest that it may not be necessary to exactly simulate a well screen length, through the use of fine vertical discretization, to produce adequate flowpaths.

Analysis of the cross sectional flowpaths to the downgradient wells indicates that the paths to the downgradient wells are generally similar for the coarse and fine horizontal discretizations (not shown). However, differences in flowpaths to the downgradient wells in the 200H models (FIGURE 5) are noted with respect to vertical discretization. Flowpaths to the shallow and deep wells, for the one and two layer 200H models, are adjoining (FIGURE 5; models 200H1L and 200H2L). Flowpaths to the wells for 200H models with three or more layers are discontinuous (FIGURE 5; model runs 200H5L and 200H20L). The flowpaths to the deep well shifts 1,000 ft farther from the withdrawal well, when increasing from two to three layers. With increased layering the flowpaths shift an additional 600 ft farther from the well (FIGURE 5). With an increase in vertical and horizontal discretization withdrawals can be more precisely positioned in the model and, in the case of the deep downgradient well, deeper flowpaths are intercepted. The deeper flowpaths are recharged further upgradient in the flow system and will result in the CRA being further upgradient.

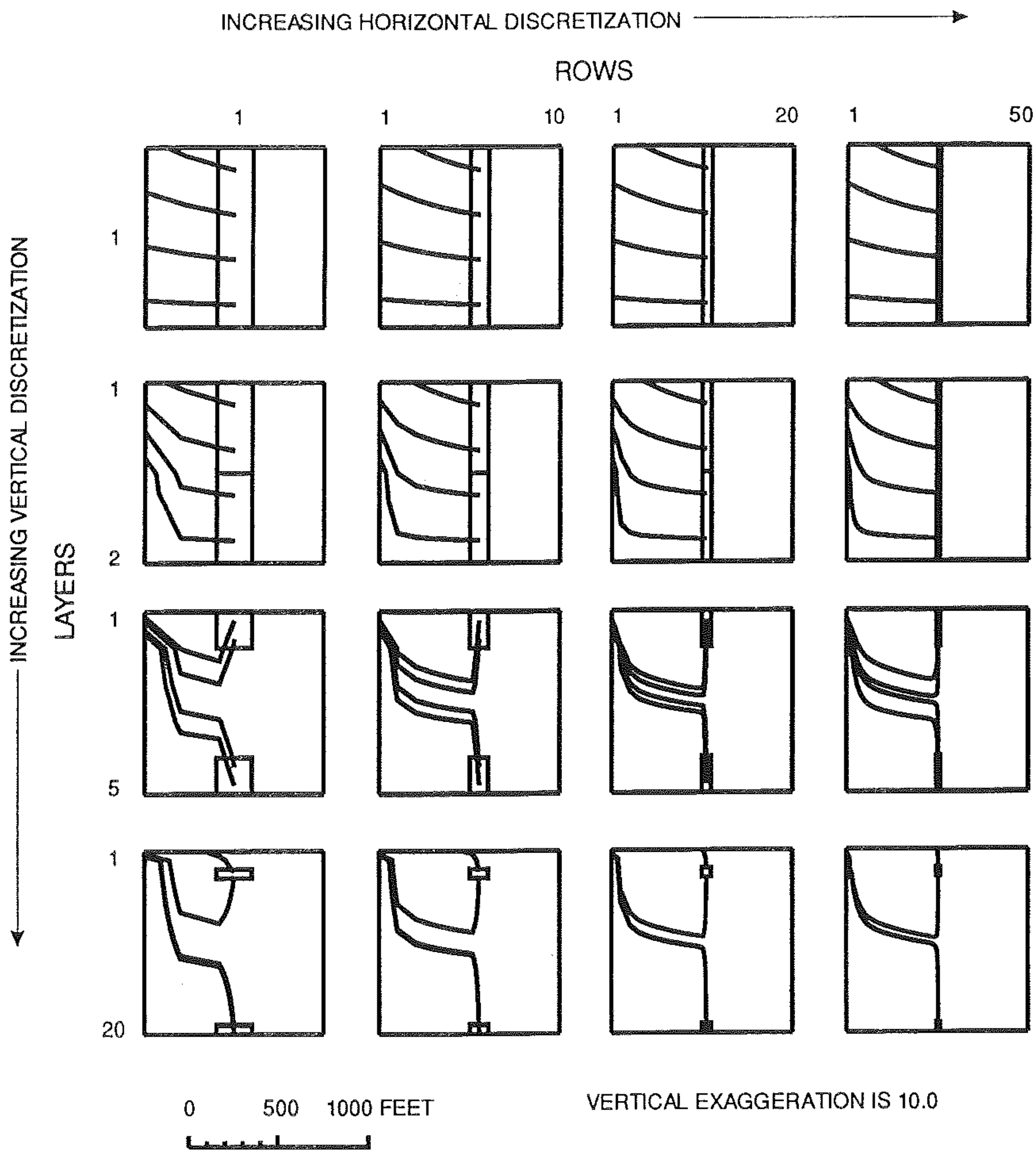

FIGURE 4. Pathlines along columns between the river boundary and the upgradient wells for models with horizontal cell sizes of two-hundred feet (200H), one-hundred feet (100H), fifty feet (50H), and twenty feet (20H) and one (1L), two (2L), five (5L), and twenty (20L) layers.

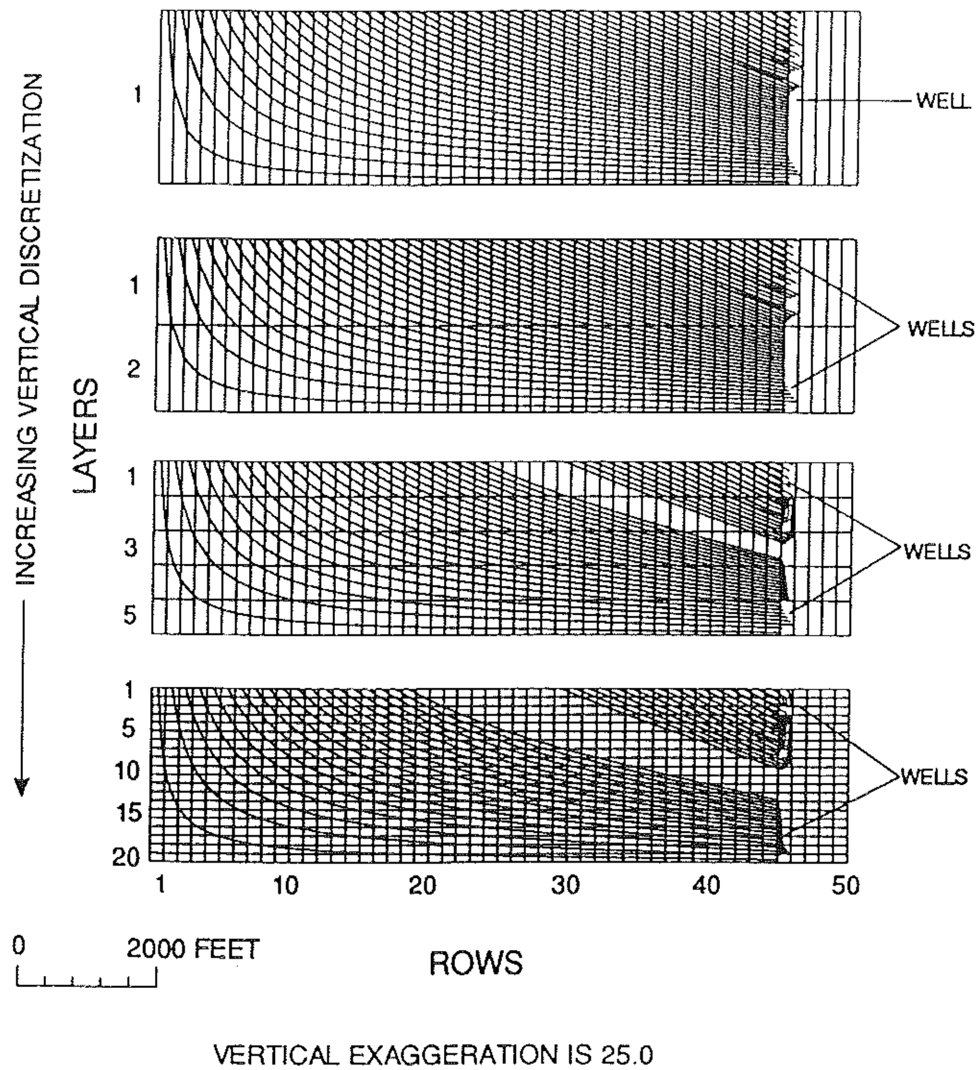

FIGURE 5. Flow pathlines along model row 14 between the no-flow boundary and downgradient wells for models with two-hundred foot horizontal cell sizes and one (200H1L), two (200H2L), six (200H6L), and twenty (200H20L) layers.

CONCLUSIONS

For the problem considered in this study--a hypothetical river valley aquifer, weak sinks are a factor in assessing zones of contribution (ZOC) to wells that withdraw 2 percent of the total model flux or less, for models with horizontal cell discretization greater than 2 percent of the models shortest horizontal dimension and vertical discretization one third the total thickness. This shows that care must be taken in the discretization of numerical models that are used to analyze flow to low withdrawal wells, because weak sink errors can lead to an overestimation of the ZOC size. With recharge only from a spatially uniform, areal source, overestimation of the ZOC is directly related to the weak sink loss (the percent of flux into the cell that is not captured by the sink).

The degree of discretization necessary for analysis of ZOC's or flowpaths is most dependent on the proximity of the withdrawal well to boundaries. For wells close to boundaries, horizontal cell size is more important than vertical cell thicknesses; for wells distant from boundaries, the opposite is true. The ZOC for wells 10 percent of the aquifer width from the river boundary (upgradient wells), were more sensitive to horizontal discretization than for wells 45 percent of the aquifer width from the river boundary (the downgradient wells). Differences in ZOC size and shape near the river boundary were due primarily to the changes in the source of water to the well, areal recharge or river leakage. The ZOC size for wells close to the river changed by 37 percent, with a 1-order of magnitude reduction in horizontal cell size, compared to a ZOC change of 19 percent at wells farther from the river for same reduction in cell size.

The ZOC for the downgradient wells, farther from a boundary, were sensitive to vertical cell thicknesses, as indicated by variations in ZOC patterns, because the downgradient wells are recharged predominantly through vertical flow from areal recharge. The ZOC for downgradient deep wells shifted 1000 feet farther from the withdrawal well as vertical discretization was refined from one model layer (100 percent of aquifer thickness) to three model layers (33 percent of aquifer thickness). Further vertical discretization, from 3 to 20 layers (33 to 5 percent of the aquifer thickness), causes the ZOC for the downgradient deep well to shift an additional 600 feet from the well. With finer vertical discretization the deep well intercepts flowpaths recharged from more distant sources.

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