ground water

Modeling Effects of Multinode Wells on Solute Transport

by Leonard F. Konikow[1] and George Z. Hornberger

Abstract

Long-screen wells or long open boreholes with intraborehole flow potentially provide pathways for contaminants to move from one location to another in a ground water flow system. Such wells also can perturb a flow field so that the well will not provide water samples that are representative of ground water quality a short distance away from the well. A methodology is presented to accurately and efficiently simulate solute transport in ground water systems that include wells longer than the grid spacing used in a simulation model of the system and hence are connected to multiple nodes of the grid. The methods are implemented in a MODFLOW-compatible solute-transport model and use MODFLOW's Multi-Node Well Package but are generic and can be readily implemented in other solute-transport models. For nonpumping multinode wells (used to simulate open boreholes or observation wells, for example) and for low-rate pumping wells (in which the flow between the well and the ground water system is not unidirectional), a simple routing and local mixing model was developed to calculate nodal concentrations within the borehole. For high-rate pumping multinode wells (either withdrawal or injection, in which flow between the well and the ground water system is in the same direction at all well nodes), complete and instantaneous mixing in the wellbore of all inflows is assumed.

Introduction

The possibility that flow can occur in a nonpumping well with a relatively long open interval or well screen, and perhaps open to multiple aquifers, has long been recognized. Much of the focus on this phenomenon has been directed toward the development and use of (1) geophysical methods to measure the flow in the borehole (for example, see Izbicki et al. 1999; Paillet et al. 2002) and (2) methods to simulate and characterize the flow (for example, Giddings 1987; Kaleris 1989; Reilly et al. 1989; Hanson and Nishikawa, 1996). Neville and Tonkin (2004) recently reviewed several alternative numerical methods to represent multiaquifer wells with the widely used model MODFLOW. They demonstrated that the Multi-Aquifer Well (MAW1) Package (McDonald 1984) closely matched exact analytic solutions for pumping and nonpumping conditions, and noted that the newer Multi-Node Well (MNW) Package (Halford and Hanson 2002) expanded on the capabilities of the earlier MAW1 Package to simulate flow between a long well and the adjacent ground water system. The value and importance of the MNW Package is illustrated by its application and use in simulating ground water flow in the Santa Clara Valley, California (Hanson et al. 2004).

Because intraborehole flow can have a substantial effect on nearby ground water hydraulics, it is logical to infer that it can therefore affect solute (or contaminant) distribution in an aquifer system. This effect has also been previously recognized, primarily with respect to the difficulty of obtaining representative water quality samples from boreholes or monitoring wells with long open intervals or long well screens. Church and Granato (1996) note that borehole flow redistributes water and solutes in the aquifer adjacent to the well, increasing the risk of bias in water quality samples. Reilly et al. (1989) used flow simulations to demonstrate that contaminant monitoring wells with long screens may completely fail to

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fulfill their purpose in many ground water environments because of intraborehole flow. They conclude that significant borehole flow can occur in wells with long screens, even if they are in relatively homogeneous aquifers with very small vertical head differences in the aquifer.

Relatively little has been done, however, to quantitatively assess the effects of intraborehole flow on solute (or contaminant) distribution in an aquifer or to develop general simulation tools to allow this to be done readily or routinely. One noteworthy exception is Lacombe et al. (1995), who noted that abandoned and improperly sealed boreholes may act as conduits for contaminant transport from contaminated zones to previously uncontaminated strata. They developed a numerical simulation approach in which leaky boreholes are represented as highly conductive one-dimensional line elements superimposed onto a mesh of three-dimensional finite elements. They further developed a one-dimensional advective-dispersive transport model for the borehole, which is solved on the basis of computed flows in the borehole and between the borehole and the aquifer. This, in turn, allows the solute flux between the well and the aquifer to be computed at various locations along the length of the borehole.

The objectives of this study are to describe the effects of intraborehole flow in wells with relatively long open intervals or long well screens on solute distribution in an aquifer and its implications for collecting representative water quality samples, and to develop a relatively simple yet viable approach to numerical simulation of solute transport in a long open borehole and the transport of solutes between such a borehole and an adjacent aquifer. For ease of use and availability, we incorporate this simulation approach into a readily available public domain MODFLOW-based solute-transport model. We evaluate the approach through numerical experiments based on an application to a realistic but hypothetical contaminant scenario, which was selected to demonstrate some of the potential effects of intraborehole flow on solute distribution, contaminant spreading, and water quality monitoring. The hypothetical field scenarios described and analyzed by Reilly et al. (1989) are used as the basis for the numerical simulations and experiments.

Flow Simulation—MNW Package

The MNW Package (Halford and Hanson 2002) allows MODFLOW-2000 (Harbaugh et al. 2000) to simulate wells that extend beyond a single model node. That is, individual wells are not restricted to a single cell in the finite-difference grid but can be more realistically associated with a discrete length. This allows the simulated well to penetrate more than one model layer, more than one aquifer, or to represent a horizontal well.

The MNW Package allows the user to specify a group of nodes that are associated with a single well. The net flux in or out of the well can be negative (representing a withdrawal well), positive (representing an injection well), or zero (representing a nonpumping well or a long-screened observation well). The net flux represents the addition or removal of water from the ground water system and corresponds with the flow at the wellhead.

Regardless of the net flux, when a well is linked to multiple nodes of the finite-difference grid, then the flow between the model domain and the well can vary greatly in magnitude (and perhaps in direction) among the various nodes linked to the single well. The MNW Package assumes that the hydraulic head within the well will equilibrate to a single representative value. Because the heads in the aquifer at various model nodes encompassing a multinode well will vary depending on local and regional aquifer properties and boundary conditions, a well can have nonuniform borehole flow (or intraborehole flow), and the maximum borehole flow rate can exceed the net withdrawal or injection rate specified for the well. The MNW Package partitions the flux among the various nodes connected to a multinode pumping well on the basis of relative heads and hydraulic conductances (the product of hydraulic conductivity and cross-sectional area of flow divided by the length of the flowpath).

For the case of a nonpumping well, differing aquifer heads at the multiple well nodes will produce intraborehole flow, with ground water entering the well at one or more nodes and exiting from the well at other nodes (Figure 1). (Note that in the convention used in Figure 1, the subscripts "SNK" and "SRC" are defined and used in relation to the aquifer, so that flow into the well, for example, would correspond with outflow from the aquifer—a fluid sink with respect to the aquifer.) Solute will be transferred by advection through the well from the aquifer cells having higher heads to aquifer cells having lower heads at rates proportional to the fluid fluxes.

For multinode pumping wells, the MNW Package inherently assumes that the pump intake is located above the first node of the multinode well (R.T. Hanson, written communication, 2005). If the withdrawal or injection rate is sufficiently high so that the flux between the aquifer and the well is in the same direction at every node of the well, then intraborehole flow will have no effect on the

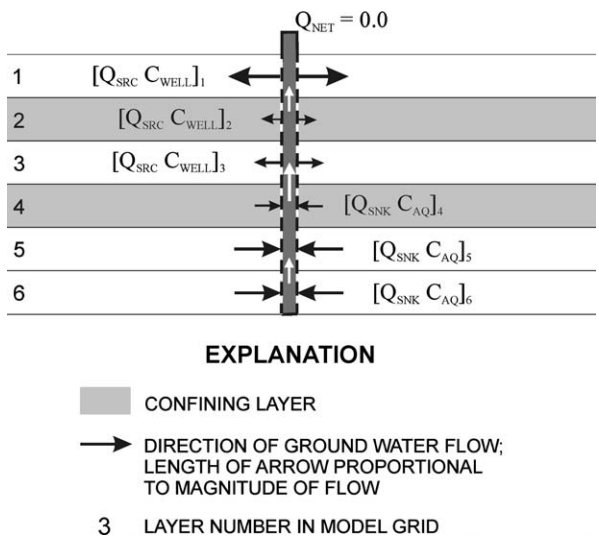

Figure 1. Conceptual cross-sectional view of a nonpumping vertical well that is connected to multiple layers in the model grid for a case where ground water head increases with depth and intraborehole flow is consequently upward.

solute concentration in the wellhead discharge for a withdrawal well or on the solute concentration in the recharge from an injection well. For such a unidirectional borehole flow case with a multinode injection well, the borehole concentration is always equal to the concentration in the fluid being injected. For such a unidirectional flow case with a multinode withdrawal well, any potential concentration difference within the borehole would have no effect on the concentration distribution in the ground water system because flow at all nodes is from the aquifer into the well. If the pumping rate is sufficiently small, however, a multinode pumping well can behave similarly to a nonpumping one in that substantial head differences in the ground water system along the length of the borehole can result in a withdrawal well that has one or more nodes in which water enters the aquifer, or an injection well that has one or more nodes in which water flows into the well from areas of relatively high head in the aquifer.

Solute-Transport Model

Calculating the effects of intraborehole flow in a multinode well on water quality patterns in a ground water system or temporal changes in the average concentration in the borehole requires that solute-transport processes in the aquifer be simulated. The capability to represent multinode wells has been added to the Ground Water Transport (GWT) Process of MODFLOW-2000 (the MODFLOW-GWT model) (Konikow et al. 1996; Kipp et al. 1998; Heberton et al. 2000). The MODFLOW-GWT model is a three-dimensional solute-transport code that is fully integrated with MODFLOW-2000. The solution algorithm used in this study is based on the method of characteristics, which tracks particles moving through the active flow field. Each particle has a location, concentration, and volume-based weight associated with it, so each particle inherently tracks a solute mass. The average concentration in each cell is computed using a volume-weighted average, assuring a global mass balance for the solute. The model computes the concentration of a solute at every node within the transport domain (which can encompass all, or only part, of the MODFLOW grid).

A general form of an equation describing the advection and dispersion of a dissolved chemical in flowing ground water may be written as (Konikow and Grove 1977; Konikow et al. 1996):

$$\frac{\partial C}{\partial t} + \frac{V_i}{R_f}\frac{\partial C}{\partial x_i} - \frac{1}{\varepsilon R_f}\frac{\partial}{\partial x_i}\left(\varepsilon D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\sum [W(C' - C)]}{\varepsilon R_f} + \lambda C = 0 \qquad (1)$$

where C is the volumetric concentration [ML^{-3}], D_{ij} is the coefficient of hydrodynamic dispersion (a second-order tensor) [L^2T^{-1}], V_i is the average interstitial velocity [LT^{-1}], ε is the effective porosity of the porous medium, R_f is the retardation factor for linear, reversible, instantaneous, equilibrium sorption, C' is the concentration of the solute in the source or sink fluid, W is the volumetric flux per unit volume (positive for outflow and negative for inflow) [T^{-1}], λ is the decay rate (assumed identical in the dissolved and sorbed phases) [T^{-1}], and x_i are the Cartesian coordinates, L. The summation convention of Cartesian tensor analysis is implied in Equation 1.

Equation 1 describes solute transport in a porous medium—not in a borehole. The exchange of fluid and solute between a borehole and the aquifer is represented by the fourth term of the equation. The fluid leaving the aquifer in cells (nodes) where there is inflow into a borehole has the same concentration as the fluid in the aquifer (that is, $C' = C$ for $W < 0$, and this term drops out for a fluid sink). Where flow is outward from a borehole into the aquifer (a fluid source with respect to the aquifer), C' depends on the concentration in the borehole in the interval corresponding with that particular cell of the model grid.

Well Concentrations and Solute Budgets

High-Rate Pumping Well

If the pumping rate in a multinode injection well is sufficiently high, flow will leave the borehole along its entire open or screened length. Because the external fluid is the only source of solute to the borehole, there should be no changes or differences in solute concentration within the borehole and the specified external source concentration (C'_{INJ}) would be the concentration in the fluid recharging the aquifer at all nodes of the well.

If the pumping rate in a withdrawal well is sufficiently high so that flow enters the borehole along its entire open or screened length, and the pump intake is located above the uppermost well node that interacts with the ground water system, then the solute concentration in the well discharge will be a function of the flux-weighted mean concentration of the inflows at all nodes of the well. This is consistent with an assumption of complete mixing within the borehole, allowing for differences in solute concentration entering the borehole because of variations in solute concentration in the ground water system from node to node. By assuming (1) complete and instantaneous local mixing in the well; (2) that no reactions affect solute concentration; (3) that wellbore storage is negligible; and (4) that the pump intakes are located above the screened or open intervals of the well, the concentration in water discharging from a high-rate multinode withdrawal well (C_{well}) during time increment t can be computed using a simple mixing formula that computes a flux-weighted average concentration on the basis of fluid inflows as

$$C^t_{well} = \frac{\sum_{i=1}^{n}\left[Q_{snk}C^t_{aq}\right]_i}{\sum_{i=1}^{n}\left[Q_{snk}\right]_i} \qquad (2)$$

where Q_{snk} is the volumetric flow rate [L^3T^{-1}] at a node (or finite-difference cell) from the aquifer into the well (negative in sign according to MODFLOW convention because it represents a withdrawal from the aquifer), C_{aq} is the concentration in the aquifer cell at the start of the time increment, and n is the number of nodes in a well.

Nonpumping Well

Flow will occur in a nonpumping multinode well if aquifer heads differ between well nodes because a long-screened well is equivalent to a high–hydraulic conductivity inclusion. This intraborehole flow can also transport dissolved chemical constituents and affect the solute concentrations in the ground water system. In a nonpumping borehole with intraborehole flow, however, it is observed that water quality differences can be present within the borehole (Church and Granato 1996; Paillet et al. 2002). These water quality differences may occur because the intraborehole flow likely represents a slow laminar flow regime, and we therefore cannot assume that complete mixing occurs within the fluid volume contained in the borehole (as we do for a withdrawal or injection well). Rather, it may be more reasonable to assume that fluid entering the borehole at one location only mixes with the borehole fluid at that location and that the blended water then slowly displaces the fluid in the direction of the intraborehole flow. For example, in Figure 1, the concentration in the well in layer 6 would be equal to the concentration in the aquifer in layer 6. The fluid and solute in the well in layer 6 then flows upward to layer 5, where it mixes with more ground water entering the well at a possibly different concentration. Similar flow and mixing occurs in layer 4. However, because there is only outflow from the well above layer 4, the concentration in the well in layers 1, 2, and 3 will equal the concentration leaving layer 4 by upward flow. Therefore, for cases of nonpumping multinode wells, solute concentration in the water in the well is allowed to vary from node to node, and the nodal concentrations within a nonpumping multinode well are calculated using a simple routing and local mixing model (similar to that used in the StreamFlow-Routing (SFR1) Package of Prudic et al. 2004). These nodal concentrations can then be compared to data collected using a downhole depth-dependent water sampler, such as described by Izbicki et al. (1999).

Head variations with depth may be complex in a multiaquifer system, and intraborehole flow can change direction, perhaps multiple times (e.g., see Figure 2). In this example, the node in layer 8 is considered a "strong source" with respect to the borehole (it is a "sink" for the aquifer) because the direction of intraborehole flow is away from this node toward both the upper and lower adjacent nodes. The concentration at this well node can be set equal to the concentration in the adjacent model layer 8 node because that is the only source of inflow to this node of the multinode well. The node in layer 3 is considered a "strong sink" for the borehole because the direction of intraborehole flow is into this node from both adjacent nodes. The concentration at this node cannot be calculated until after the concentrations in both adjacent nodes are defined by the routing algorithm. The node in layer 7 represents the intermediate case because the direction of intraborehole flow is into this node from only one (in this case underlying) node.

The routing algorithm is always implemented after the flow equation is solved. Because complex intraborehole flow includes a fluid source term for the ground water system, the concentration associated with that fluid source must be defined before the solute-transport equation for the ground water system can be solved for that time increment. Therefore, the routing algorithm is implemented before the transport equation is solved, and it uses aquifer concentrations from the end of the previous time increment (or from the specified initial concentrations for the first time increment).

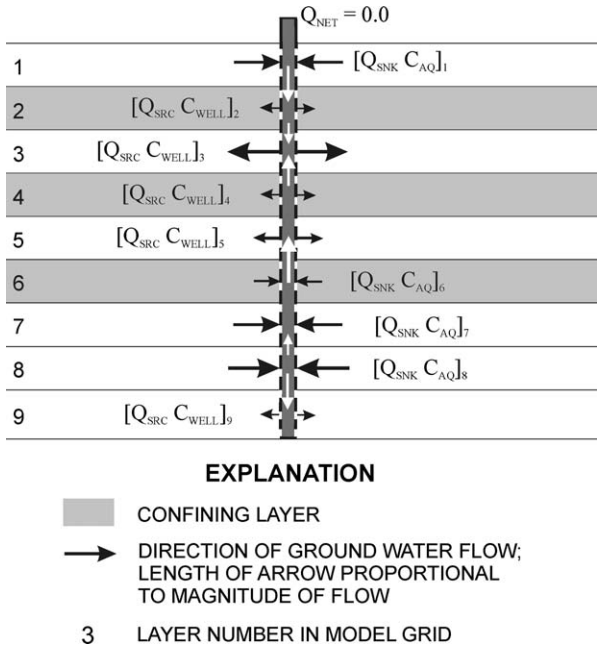

Figure 2. Conceptual cross-sectional view of a nonpumping multinode well showing complex (multidirectional) intraborehole flow.

The first step in the routing algorithm is to compute the flow directions within the borehole on the basis of known fluxes between the aquifer and the well at all nodes of the multinode well. All nodes in a nonpumping multinode well are scanned, and fluxes between nodes are tallied. Next, end nodes (the first and last nodes of the multinode well) are checked to see if the direction of flow is into the well from the aquifer; if it is, as represented by node 1 in Figure 2, the concentration in the well at that location is set equal to the concentration in the aquifer at that node. Otherwise, if there is flow from the well into the aquifer, as in layer 9 in Figure 2, the concentration in the well will be set equal to the concentration in the adjacent well node (node 8 in Figure 2), which by necessity is the only possible source of water to the end node in the well, after that concentration is defined. After the end nodes are checked, the concentration at well nodes representing "strong sources" to the well are defined (for example, node 8 in Figure 2, where because the flow is away from this node in both directions in the borehole, the concentration at the well node must be equal to the concentration at the corresponding aquifer node). From the concentrations initially defined at end nodes and at strong sources, the solute fluxes can be routed to all adjacent nodes and the concentration in those adjacent nodes defined on the basis of a simple mixing

formula. For example, when the routing is in the direction of increasing layer number, as would occur when starting at the top (end) node of the well represented in Figure 2, the routing equation can be written as

$$C_i^t = \frac{Q_{i-1}C_{i-1}^t - \left[Q_{\text{snk}}C_{\text{aq}}^{t-1}\right]_i}{Q_{i-1} - [Q_{\text{snk}}]_i} \quad (3)$$

where C_i is the concentration at well node i (corresponding to layer i in the example vertical well shown in Figure 2, but this one-to-one correspondence between layer number and well node number is not a requirement), Q_{i-1} is the intraborehole flow between well node $i - 1$ and node i (positive for flow toward higher values of i), $[Q_{\text{snk}}C_{\text{aq}}]_i$ is the solute mass inflow from node i in the aquifer, and the superscript $t - 1$ represents the previous time increment. The bracketed terms on the right side of Equation 3 are subtracted because the sign convention for the flow term is that Q_{snk} is negative in sign for inflow to the well (discharge from the ground water system). This routing process is repeated in the direction of flow until all nodes in the sequence have defined concentrations or until a borehole node is reached where flow is in the opposite direction (for example, in layer 3 in Figure 2). From a nonend "strong source" node, such as node 8 in Figure 2, routing must be done in both directions away from that node and the indexes in Equation 3 would be modified according to the direction of routing. Then nodes that are strong sinks for the wellbore (flow into the node from both directions, such as node 3 in Figure 2) can now be defined on the basis of a simple flux-weighted mean concentration.

It is also possible that the head in the aquifer adjacent to several nodes of a multinode well would be exactly identical. With such a condition, we would expect that there would be no intraborehole flow over that segment of the multinode well. However, at the location of such well nodes, there could still be a lateral flow in that model layer because of a regional hydraulic gradient within the aquifer. Thus, for any node of a multinode well for which there is no flow to or from both adjacent well nodes, we assume that there is no intraborehole mixing with fluid in adjacent nodes of the well and that the concentration at such a node in the well is equal to the concentration in the aquifer adjacent to this node.

After the concentration has been defined at all nodes, the average concentration in the well can be defined. However, because there is no complete mixing in a nonpumping well, the average concentration must be defined on a basis other than flux-weighted mixing. For a nonpumping multinode well, we define the average concentration as one that would be measured using a depth-integrating sampling device that continuously obtains samples at every location as it is lowered (or raised) through the entire length of the borehole at a constant rate. This result would represent a depth-averaged concentration in a vertical well (or length-averaged concentration in a nonvertical well). This average concentration is not used in any calculations but is reported for information purposes in the output files.

Low-Rate Pumping Well

If the pumping rate is viewed as transitional between zero and some arbitrarily high rate, the intraborehole flow pattern can then be viewed as representing a continuum between a complex multidirectional intraborehole flow pattern possible with a nonpumping mutinode well (Figure 2) and a simple unidirectional flow pattern for a high-rate pumping well. Increasing the pumping rate causes the flow pattern to shift toward a simple unidirectional mode. However, at sufficiently low pumping rates, the flow pattern may still be as complex as for a nonpumping case. If the withdrawal (or injection) rate specified for a pumping well is insufficient to induce unidirectional flow between all well nodes and the corresponding aquifer cells, the resulting complex intraborehole flow pattern can generate a nonuniform distribution of solute concentrations in the borehole, similar to that in a nonpumping multinode well. For example, Izbicki et al. (2005) collected depth-dependent water quality samples in a well under pumping conditions and demonstrated large changes in chloride concentration with depth. Therefore, the assumption of complete mixing in a pumped borehole may not be valid, and water entering the ground water system from a node in a withdrawal well may not have the same solute concentration as water discharging through a pump at the wellhead. Similarly, water entering the ground water system from one node in a multinode injection well may not have the same solute concentration as water entering the ground water system from another node.

If a pumping multinode well has a complex multidirectional flow pattern between the borehole and the ground water system, the model will calculate the concentration distribution in the wellbore using the same routing routine described previously for nonpumping wells. This will assure that water leaving the well, whether to the ground water system or to the land surface, will have a concentration consistent with a local (single node) mixing assumption rather than a less rigorous assumption of total instantaneous mixing within the entire borehole. To calculate the solute distribution within the borehole using the routing routine, the additional flux between the well and the land surface (Q_{net}) is assigned to the upper bound of the first well node (consistent with the MNW Package assumption that a pump is always located above the screened or open interval of the well). In effect, the pump can be considered to represent node "zero" in the string of well nodes.

Solute Budget Calculations

For the solute mass balance computed by MODFLOW-GWT, fluid and solute in the borehole of a multinode well is considered to be external to the model domain. This mass-balance approach is consistent with the way that MODFLOW computes the fluid mass balance for a multinode well. The solute mass removed from the transport domain in a multinode well is based on the computed nodal values of Q_{snk} times the appropriate aquifer concentration (C_{aq}^*) summed over all nodes as

$$M_{out} = \sum_{i=1}^{n} \left[Q_{snk} C^{*}_{aq} \right]_i \Delta t \quad (4)$$

where M_{out} is the solute mass discharged from the aquifer into the well during a transport time increment and Δt is the length of the time increment. The time level for the appropriate aquifer concentration in Equation 4 depends on whether the concentration at the sink node of the multinode well was computed using Equation 2 (for a high-rate pumping well) or Equation 3 (for a nonpumping or low-rate pumping well). In the former case, $\left[C^{*}_{aq}\right]_i = \left[C^{t}_{aq} + C^{t-1}_{aq}\right]_i / 2$, whereas in the latter case $\left[C^{*}_{aq}\right]_i = \left[C^{t-1}_{aq}\right]_i$.

The solute mass added to the transport domain from a multinode well is calculated as a summation over all nodes as

$$M_{in} = \sum_{i=1}^{n} \left[Q_{src} C^{t}_{well} \right]_i \Delta t \quad (5)$$

where M_{in} is the solute mass entering the aquifer by flow out of the well during a transport time increment and $[C_{well}]_i$ is the concentration in the well at the ith well node, where fluid is entering the aquifer from the well. The value of $[C_{well}]_i$ equals C'_{INJ} for a high-rate injection well and would be computed by routing for a nonpumping or low-rate pumping well.

The sum of all nodal flows into or out of one multinode well (Q_{snk} or Q_{src}) does not necessarily represent the fluid flux out of or into the ground water system, respectively, because in the low-rate case some of the flux between the well and the model domain can represent internal circulation through the well between different layers or cells of the model rather than flow between the model domain and an external fluid source or sink. Therefore, the solute added or removed from the ground water system must be calculated on the basis of Q_{net} and the appropriate concentration. For a multinode withdrawal well, the appropriate concentration is C_{well}, and for a multinode injection well the appropriate concentration is C'_{INJ}.

Test Problem

Problem Description

A test problem was developed to evaluate the model, to demonstrate its value, and to elucidate problematic field situations in the presence of long open wells. This test problem is a slightly modified version of the one documented by Reilly et al. (1989). Their numerical experiments demonstrated that substantial wellbore flow can occur in observation wells screened through multiple layers, even in homogeneous aquifers having small vertical head differences (<0.01 feet between the top and bottom of the screen).

The hypothetical unconfined ground water system represents regional flow that is predominantly lateral but includes some vertical components because of diffuse areal recharge (at a rate of 0.004566 ft/d) and a constant-head boundary condition at the surface of the right side of the regional ground water system that controls discharge (Figure 3). No-flow boundaries are on all other external boundaries. The system is substantially longer (10,000 ft) than it is thick (205 feet) or wide (200 feet); the width was selected to eliminate any important effect of the position of the lateral no-flow boundary on the solution in the area of the well. A nonpumping borehole with a 60-foot screen is located close to the left side of the system (252 feet from that boundary). Other properties of the system and the model are listed in Table 1. Reilly et al. (1989) simulated the regional system with a two-dimensional cross-sectional model, arguing that the width of the cross section was irrelevant for their analysis, and applied a local (approximately a 100- by 100-foot area) three-dimensional flow model in the vicinity of the wellbore. Their local model was discretized vertically into 5-foot layers and used a variably spaced areal grid with a minimum spacing of ~0.33 by 0.33 feet around the borehole. They represented the borehole using a relatively high vertical hydraulic conductivity, the value of which was based on equivalence of Darcy's law to the equation for laminar pipe flow (Reilly et al. 1989, 272).

Our approach was to simulate the regional flow system with a three-dimensional model with a width

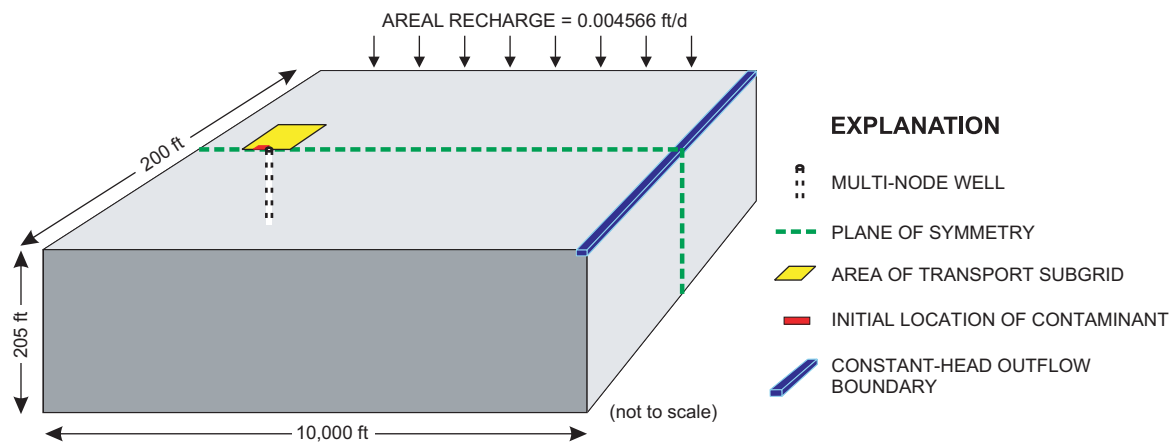

Figure 3. Conceptual diagram showing geometry and boundaries for three-dimensional test problems with a nonpumping multinode well.

Table 1
Selected Physical and Numerical Parameters Used in MODFLOW-GWT Simulation of Ground Water Flow and Transport in a Three-Dimensional, Steady-State Flow System Containing a Multinode Well

Parameter	Value
Horizontal hydraulic conductivity (ft/d)	250
Vertical hydraulic conductivity (ft/d)	50
Well radius (ft)	0.133
Well "skin"	2.6
Effective porosity	0.20
Longitudinal dispersivity (ft)	0.0
Horizontal transverse dispersivity (ft)	0.0
Vertical transverse dispersivity (ft)	0.0
Diffusion coefficient (ft^2/d)	0.0
Recharge rate (ft/d)	0.004566
CELDIS (Courant number for transport)	1.0
NPTPND (initial number of particles per node)	8 or more[1]

[1]The value of NPTPND was increased to 275 in a block of cells surrounding the well.

sufficient to minimize any effects of that dimension on the flow field close to the borehole. Because a vertical plane of symmetry is present and passes through the well, we only simulated one-half of the domain outlined by Reilly et al. (1989) (with our model dimensions being 10,000 feet long by 100 feet wide by 205 feet deep). We applied the solute-transport model to a local area around the well using a transport subgrid. Within the transport subgrid, which included 20 rows, 40 columns, and 41 layers of cells, a uniform areal cell spacing of 2.5 feet was used. Outside of the uniformly spaced subgrid, the lateral grid spacing was increased geometrically to a maximum spacing of 50.25 feet in the row (x) direction and 9.55 feet in the column (y) direction (Figure 4). The vertical discretization (Δz) was 5 feet everywhere in the model domain.

The well was assumed to have a 60-foot well screen that was open to layers 2 through 13 (that is, connected to 12 vertically aligned nodes of the grid) in the bounding row of cells. Reilly et al. (1989) reported that their well was represented by a cell having areal dimensions of 0.333 by 0.333 feet, which yields a cross-sectional area of 0.111 $feet^2$. Because we assume the well lies on the plane of symmetry in our grid, we assign a well radius in our model that yields an equivalent cross-sectional area to one-half of the cross-sectional area of the well in the simulation of Reilly et al. (0.0555 $feet^2$). For a well with a circular casing, this equivalent cross-sectional area would require a well radius of 0.133 feet. We also assumed that there would be a linear well loss coefficient represented by a nondimensional skin coefficient (see Halford and Hanson 2002). The value of the "skin" was adjusted during model calibration to achieve a vertical profile of flows between the aquifer and the well that closely matched that of Reilly et al. (1989; Figure 2).

Reilly et al. (1989) were concerned with "two situations that represent extreme possibilities for the misrepresentation of aquifer contamination from well samples." They did not, however, actually simulate solute transport in their analysis of these two situations. For their first situation they postulate a contaminant plume in the shallow part of the aquifer that intersects the upper part of the well screen in the monitoring well. To simulate this problem, an initial mass of contaminant was placed in layer 1, immediately upgradient from the borehole, as an initial condition for the solution of the transport equation in the presence of a multinode well. The nonreactive solute was assigned an initial concentration of 100 in the 32 cells of layer 1 located within rows 27 to 30 and columns 33 to 40 (Figures 3 and 4). The simulation was then run for a stress period length of 1.0 year, assuming steady-state flow prevailed. To enable the effects of solute mixing to be seen most clearly, the transport simulations for this situation were run for conditions of no dispersion (Table 1). The method of characteristics is well suited for solving the transport equation for advection-dominated

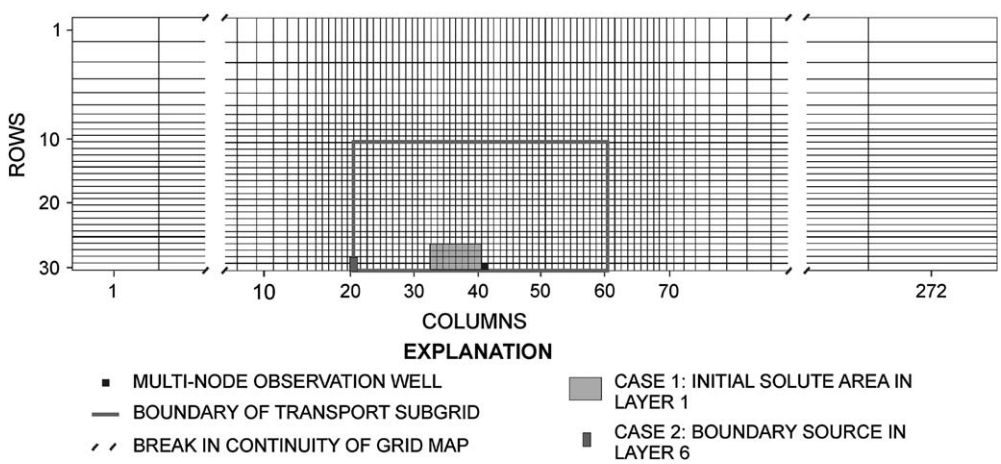

Figure 4. Map view of MODFLOW finite-difference grid showing location of transport subgrid and multinode observation well.

problems and yields accurate numerical solutions with little numerical dispersion.

For the second situation, Reilly et al. (1989) postulate a contaminant plume in the aquifer at the elevation of the lower part of the well screen, where water is discharging from the well. They hypothesize that water samples collected from this monitoring well may fail to detect the contaminants. To test this situation, we introduced solute (at a source concentration of $C' = 100$) in the inflow across the subgrid boundary in two cells (in layer 6, column 21, of rows 29 and 30) upgradient from the well. Except as noted subsequently, system properties are as listed in Table 1. These conditions were simulated for a 10-year stress period with steady-state flow. This produces a plume that interacts with the nodes in the bottom part of the multinode well. To assess the effect of intraborehole flow in the open borehole, two numerical tests were conducted—one without the multinode well to assess baseline conditions and provide a basis of comparison, and one in which the multinode well is represented. In both cases, we assumed nonzero dispersivity values appropriate for the scale of transport distances (longitudinal dispersivity = 2.0 feet, transverse horizontal dispersivity = 0.2 feet, and transverse vertical dispersivity = 0.02 feet). For the baseline case, CELDIS was reduced to 0.25 to minimize oscillations. To test whether water samples obtained from the well could detect the contaminants, an additional 2 day stress period was simulated, in which the well was pumped at a withdrawal rate of 88 ft^3/d (~25 wellbore volumes per day).

Results

Heads were calculated using the PCG2 solver in MODFLOW-2000, and the flow model iteratively converged to a steady-state head distribution with a 0.00% discrepancy. The calculated head in the well was 4.9322 feet. The head distribution in the aquifer near the nonpumping multinode well indicated that water should flow from the aquifer into the upper part of the borehole and discharge back into the aquifer through the lower part of the well (Figure 5), which is consistent with the results of Reilly et al. (1989). The MNW Package calculates the flow between the aquifer and each node along the length

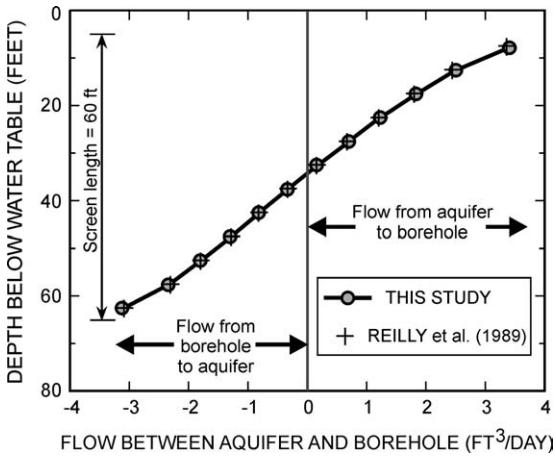

Figure 6. Adjusted flow rates with depth between the aquifer and the borehole calculated with the Multi-Node Well Package in MODFLOW for the test problems.

of the borehole (Figure 6); these calculated flows closely match those published by Reilly et al. (1989; Figure 2). Inflow to the well is greatest near the top of the well screen, and outflow is greatest near the bottom of the well screen. The calculated total flow into the borehole was 9.79 ft^3/d, which compares closely with 9.63 ft^3/d reported by Reilly et al. (1989). (Note that to adjust for using symmetry to simulate half the original domain size, the indicated flow rates were calculated by doubling flows calculated with the reduced domain size.)

The results of simulating the first contamination situation described by Reilly et al. (1989) show that a contaminant plume initially located only in the upper 5 feet of the aquifer rapidly spread through the borehole to depths of 40 to 60 feet in the aquifer because of downward flow in the borehole open to the deeper parts of the aquifer (Figure 7). The initial slug of contaminant in model layer 1 (Figure 7A) is reduced in size and mass in the top part of the aquifer because of capture by the well and because there is no source adding new contaminants at the water table. The reduction in contaminant mass in the shallowest part of the aquifer is matched by the increase in mass in the deeper part of the aquifer—to depths where the contaminant would not have been expected if not for the pathway provided by the open borehole. In 1 year, high

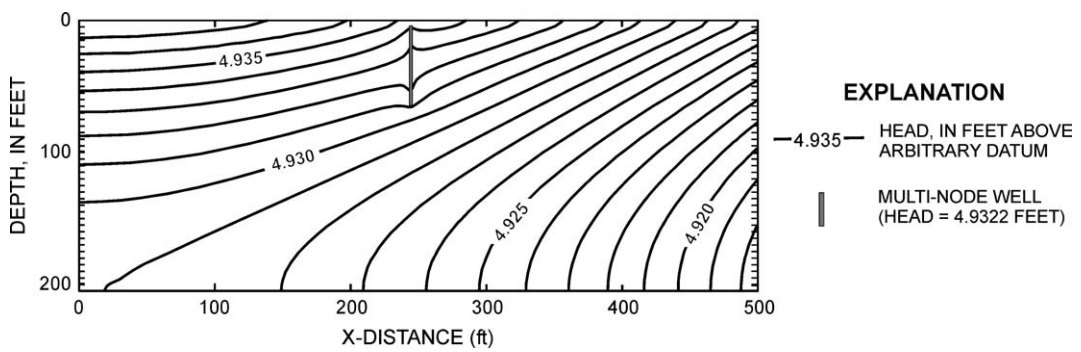

Figure 5. Calculated head distribution in vertical section near well on plane of symmetry. For clarity, only upgradient 5% of domain is shown (flow model domain extends to 10,000 feet in x-direction).

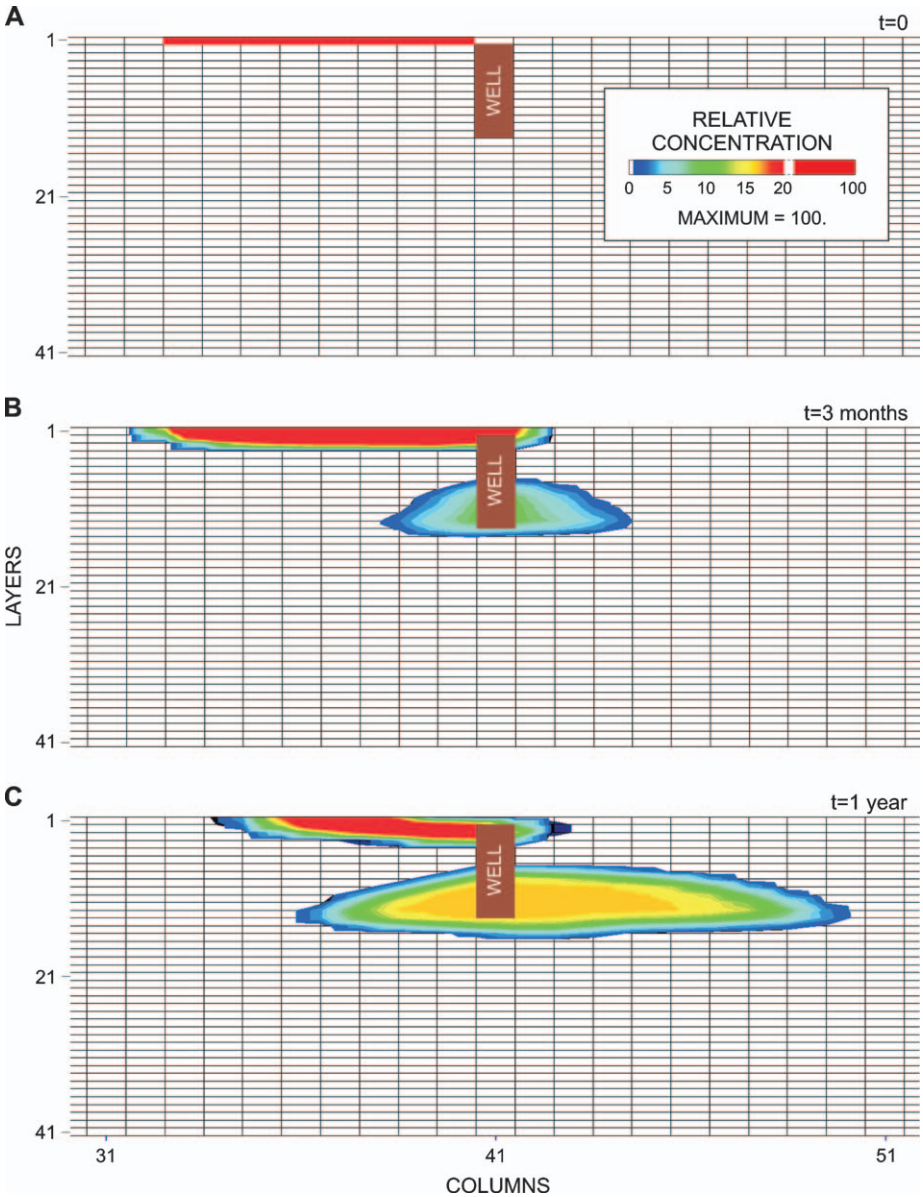

Figure 7. Calculated spreading of contaminant in presence of multinode well showing relative concentrations in vertical section along row 30 of grid (on plane of symmetry) in first test problem: (A) initial conditions, (B) plume at 3 months, and (C) plume after 1 year. Note that only part of grid in column direction is shown; concentrations <1.0 are not shown.

concentrations (>1.0% of the source concentration) had spread ~21 feet downgradient from the borehole, 12 feet upgradient from the borehole, and 15 feet laterally from the borehole at depths of 55 to 60 feet in the aquifer (Figures 7 and 8). If the open borehole did not exist, the plume would simply migrate downgradient within model layers 1 to 3.

The depth-averaged relative concentration in the multinode well changed over time as the solute concentrations in the inflow into the upper nodes of the well changed over time (Figure 9). The minor oscillations in the breakthrough curve are related to the discrete nature of the particles used to track advective transport in the method of characteristics. In this case, particles with both low and high concentrations converged on the uppermost well nodes from all directions. Because a discrete and limited number of particles were used, the particles with high and low relative concentrations entered well cells at different ratios during each time increment, resulting in oscillations over time in the mixed (or averaged) concentrations in the well nodes that represent fluid sinks to the aquifer. The oscillations are greatest when dispersion is zero (as in this example); oscillations can be reduced with higher dispersion and when using a greater density of particles.

Because the well is not pumped, we assume that concentrations can vary with distance along the borehole. The depth-varying concentrations for this example are shown in Figure 10, and the profile reflects the fact that inflow has the highest concentration in the uppermost well node and that the concentration does not change in the deeper part of the borehole where there is outflow from the well to the aquifer. Comparison of Figures 9 and 10 indicates that although the depth-averaged concentration in the well at $t = 1$ year is ~21, water in the deeper well nodes that are discharging into the aquifer has

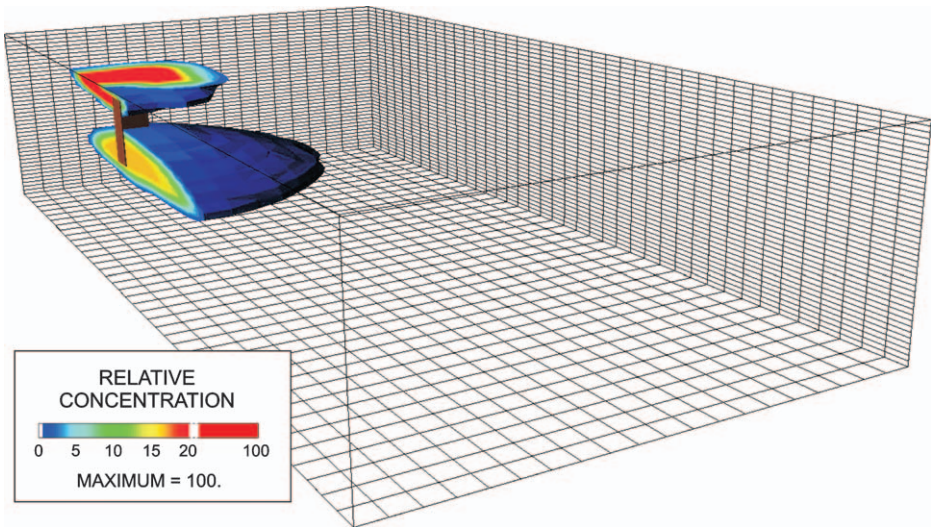

Figure 8. Three-dimensional perspective of model transport domain in first test problem showing calculated solute plume emanating from lower part of well after 1 year (concentrations <1.0, not shown).

a concentration of only ~17, which would represent the source concentration to the aquifer. The concentration in the deeper part of the well is reduced by dilution from water with very low contaminant concentration entering the well in model layers 5 through 7.

Although these results were calculated assuming no dispersion, the presence of concentrations in the solution that are intermediate between 0 and 100 (Figures 7B and 7C) might be taken to reflect a dispersion process (either physical or numerical). In the upper part of the aquifer, this apparent dispersion is largely related to computing an average concentration in a cell that contains some particles with a concentration of 0 and some with a concentration of 100 and is partly induced by the smoothing function inherent in the visualization software. In the deeper part of the aquifer, the intermediate concentrations are primarily a function of the time-varying source concentration in the discharging nodes of the multinode well (Figure 9).

For the second situation of Reilly et al. (1989), a base case was simulated first with the multinode well absent. This generated a contaminant plume that spread a relatively large distance downgradient (mostly because of advection) and spread relatively small distances laterally in response to hydrodynamic dispersion (Figure 11A). Its linear path and smooth boundaries reflect the uniformity of the flow field under the prevailing symmetrical hydrologic boundary conditions. The position of the inactive multinode well is shown in Figure 11A, and the axis of the plume passes directly through the location of the bottom node of the multinode well. The breakthrough curve for that location shows a sharp increase in concentration after 3 years have elapsed, but by 10 years, the concentration had nearly stabilized at a value of ~18 (Figure 12).

Then a simulation was made under the same external boundary conditions, but with the multinode well activated, which created the same head distribution and flow field (Figure 5) as simulated for the first situation of Reilly et al. (1989). Under this flow regime, discharge occurs from nodes in the bottom half of the well. The flux

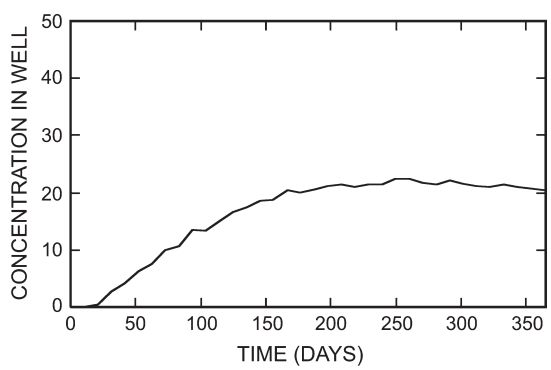

Figure 9. Calculated depth-averaged concentration in non-pumping multinode well in first test problem.

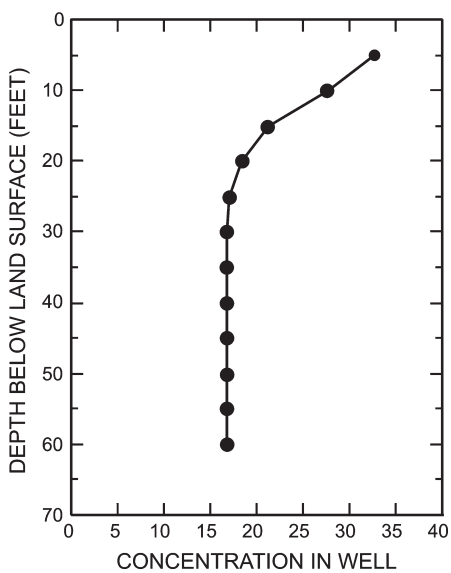

Figure 10. Relative concentration variations within the non-pumping multinode well in first test problem after 1 year.

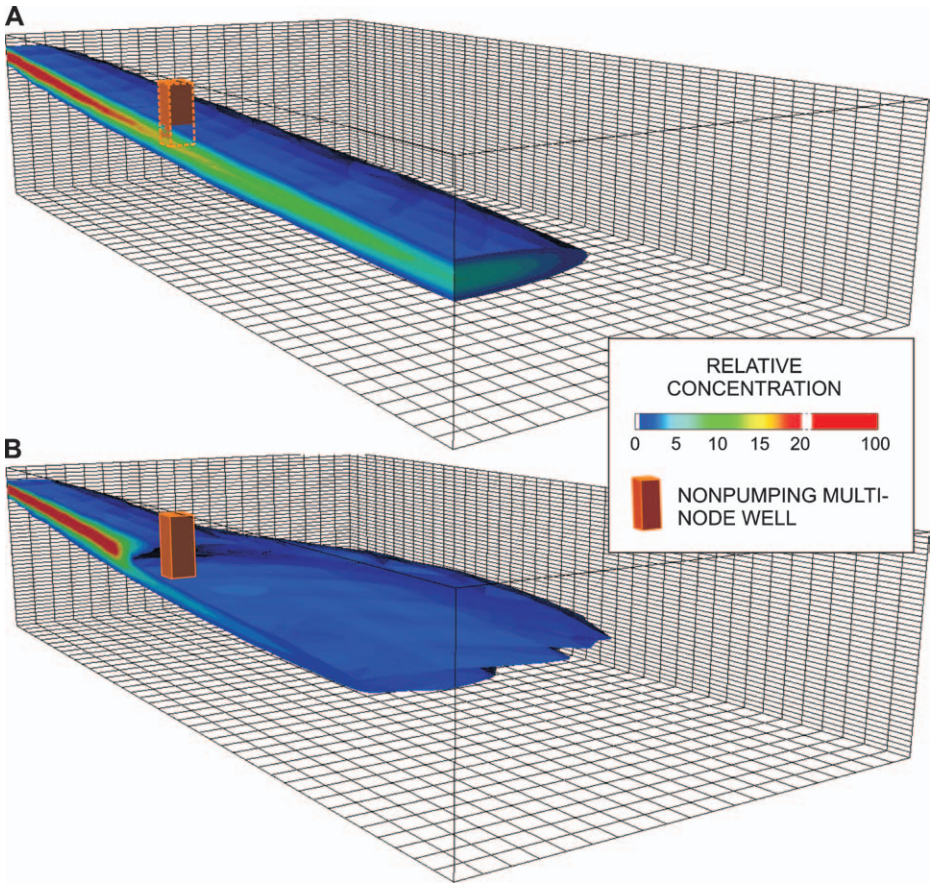

Figure 11. Three-dimensional perspective of model transport domain showing calculated solute plume for second test problem after 10 years: (A) when the multinode well is inactive and (B) with multinode well active (concentrations <1.0, not shown).

is great enough that it induces radially outward flow at that depth in the system, causing some flow to be directed against the regional flow direction. This perturbation of the flow field diverts the advecting solute plume away from and around the location of the discharging well nodes, causing the plume to spread a much greater lateral distance (Figure 11B) than when the well did not exist. (Note that this numerical solution included some small negative concentrations calculated at several cells—typical of a numerical solution to the advective-dispersive transport equation. The negative concentrations are always smaller than −0.05 and do not affect the nature of the plume or its depiction in the illustrations.) A small part of the plume also was forced to depths greater than in the base case as some of the solute was diverted below the bottom of the multinode well. The magnitude of the velocities directed away from each well node increase with depth, in proportion to the flux (Figure 6), so that in the layers closer to the middle of the well, the plume advances closer to the well.

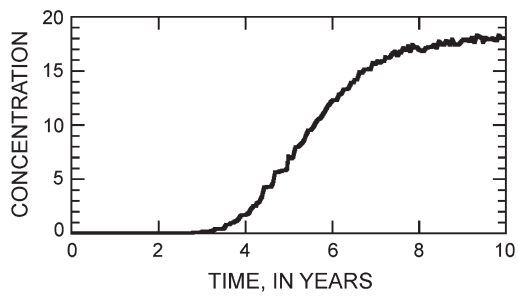

Figure 12. Breakthrough curve in second test problem for cell at bottom of multinode well for case when multinode well is inactive. When multinode well is active, concentrations at this location are always <0.005, which cannot be seen at the scale of this plot.

The net effect of the long-screened well on the proximity of the plume means that if the well were to be used as a monitoring well to assess the presence of contaminants in the aquifer, the water samples would yield a false negative. That is, no contaminants would be detected with normal sampling protocols involving evacuation of several casing volumes or pumping at low rates for even several hours to days. The prior well discharge of shallower ground water into the deeper part of the aquifer caused the plume to move around and away from the monitoring well. Simulation results with the additional 2 day withdrawal period showed that any samples collected would only include recently recharged uncontaminated water derived from the shallow part of the aquifer. At the deepest cell of the well, after "sampling" the concentration after 10 years for the control case was ~18, but when the multinode well was active, the concentration at

that same point after 2 d of pumping was <0.02. This large difference highlights (1) that in some situations long-screen monitoring wells can have a profound influence on the hydraulics of a ground water system and on the composition and reliability of a ground water sample; (2) the potential significance of abandoned wells; (3) the value of multilevel samplers; and (4) the need for the capability to simulate the effects of multinode wells on solute-transport phenomena.

Conclusions

Because wells (or boreholes) with long open intervals or long screens can allow nonuniform flow to occur within a borehole, solute can be transported directly and quickly from one location to another through such a well. Calculating the interaction and effects of intraborehole flow and solute transport on water quality patterns in an aquifer requires a coupled ground water flow and solute-transport simulation capability. We developed an approach to couple MODFLOW's MNW Package (Halford and Hanson 2002), which simulates flow in wells that extend beyond a single model node, with a MODFLOW-compatible solute-transport model (MODFLOW-GWT).

If the flow between a multinode well and the model domain is in the same direction at all well nodes, as would occur with a high-rate injection or withdrawal well, the solute concentration in the borehole is assumed to be uniform—consistent with an assumption of complete mixing within the borehole during a given time increment. The wellbore concentration in such a withdrawal well is computed as a flux-weighted mean. If the flow between a multinode well and the model domain is complex (into the well at some nodes while out of the well at other nodes), the solute concentration in the borehole is computed using a routing algorithm that only assumes local mixing at each node in the well during a given time increment. Flow and solute routing with local mixing enables concentrations to vary with distance in the borehole. The mean concentration in these types of wells is computed as a distance-weighted average. Because concentrations can vary with location within the borehole, the fluid source concentration for well outflow to the aquifer can differ simultaneously among nodes in a single borehole.

In some cases, a long borehole (such as a monitoring well or an abandoned well) can provide a fast pathway that facilitates the movement of contaminants through an aquifer system and therefore needs to be recognized when predicting changes in concentration in the system. This was demonstrated through a test problem designed to simulate ground water flow and solute transport in an aquifer that contains a contaminant plume near its top surface and a borehole extending through multiple model layers (represented as a multinode well) in which local head gradients induced downward flow in the well. Simulation of this test problem (originally proposed by Reilly et al. 1989) clearly showed that downward flow in the borehole caused cross contamination of the deeper part of the aquifer. A secondary contaminant plume developed at a greater depth in the ground water system than would have occurred if the well did not exist or had been effectively plugged or sealed.

A variant of the same test problem also demonstrated that intraborehole flow can cause a sampling bias in detecting the presence of contaminants in a ground water system. For the same flow field, but with an alternative situation where a contaminant plume existed in a deeper part of the aquifer and no contamination was present in the shallower part of the aquifer, the deeper plume was diverted away from and around the multinode "monitoring" well. At the level where water discharges from the long borehole, the history of well discharge creates a buffer of uncontaminated water around the well that may preclude the practical collection of representative water samples from that area of the aquifer. Samples collected from such a monitoring well would fail to indicate the presence of contaminants, even though they are present around and below the location of the well.

The approach documented in this paper is accurate, efficient, and relatively simple. It was implemented and tested in a code to provide compatibility between the MNW Package of MODFLOW and the MODFLOW-GWT solute-transport model. This enhancement improves the capability of MODFLOW-GWT to accurately simulate transport in cases that involve fluxes to or from multinode wells. The methodology, however, can readily be incorporated into other solute-transport models.

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References

Church, P.E., and G.E. Granato. 1996. Bias in ground-water data caused by well-bore flow in long-screen wells. *Ground Water* 34, no. 2: 262–273.

Giddings, T. 1987. What is an adequate screen length for monitoring wells? Opinion I. *Ground Water Monitoring Review* 7, no. 2: 96–97.

Halford, K.J., and R.T. Hanson. 2002. MODFLOW-2000, User guide for the drawdown-limited, Multi-Node Well (MNW) Package for the U.S. Geological Survey's modular three-dimensional ground-water flow model, Versions MODFLOW-96 and MODFLOW-2000. USGS Open-File Report 02-293. Reston, Virginia: USGS.

Hanson, R.T. 2005. U.S. Geological Survey, San Diego, California. Written communication, December 2, 2005.

Hanson, R.T., Z. Li, and C.C. Faunt. 2004. Documentation of the Santa Clara Valley regional ground-water/surface-water flow model, Santa Clara County, California. USGS Scientific Investigation Report 2002-5231. Reston, Virginia: USGS.

Hanson, R.T., and T. Nishikawa. 1996. Combined use of flowmeter and time-drawdown data to estimate hydraulic conductivities in layered aquifer systems. *Ground Water* 34, no. 1: 84–94.

Harbaugh, A.W., E.R. Banta, M.C. Hill, and M.G. McDonald. 2000. MODFLOW-2000, The U.S. Geological Survey modular ground-water model—User guide to modularization concepts and the ground-water flow process. USGS Open-File Report 00-92. Reston, Virginia: USGS.

Heberton, C.I., T.F. Russell, L.F. Konikow, and G.Z. Hornberger. 2000. A three-dimensional finite-volume Eulerian-Lagrangian Localized Adjoint Method (ELLAM) for solute-transport modeling. USGS Water-Resources Investigations Report 00-4087. Reston, Virginia: USGS.

Izbicki, J.A., A.H. Christensen, and R.T. Hanson. 1999. U.S. Geological Survey combined well-bore flow and depth-dependent water sampler. USGS Fact Sheet 196-99. Reston, Virginia: USGS.

Izbicki, J.A., A.H. Christensen, M.W. Newhouse, G.A. Smith, and R.T. Hanson. 2005. Temporal changes in the vertical distribution of flow and chloride in deep wells. *Ground Water* 43, no. 4: 531–544.

Kaleris, V. 1989. Inflow into monitoring wells with long screens. In *Contaminant Transport in Groundwater*, ed. H.E. Kobus and W. Kinzelbach, 41–50. Rotterdam: Balkema Publishers.

Kipp, K.L., Jr., L.F. Konikow, and G.Z. Hornberger. 1998. An implicit dispersive transport algorithm for the U.S. Geological Survey MOC3D solute-transport model. USGS Water-Resources Investigations Report 98-4234. Reston, Virginia: USGS.

Konikow, L.F., D.J. Goode, and G.Z. Hornberger. 1996. A three-dimensional method of characteristics solute-transport model (MOC3D). USGS Water-Resources Investigations Report 96-4267. Reston, Virginia: USGS.

Konikow, L.F., and D.B. Grove. 1977. Derivation of equations describing solute transport in ground water. USGS Water-Resources Investigations Report 77-19. Reston, Virginia: USGS.

Lacombe, S., E.A. Sudicky, S.K. Frape, and A.J.A. Unger. 1995. Influence of leaky boreholes on cross-formational groundwater flow and contaminant transport. *Water Resources Research* 31, no. 8: 1871–1882.

McDonald, M.G. 1984. Development of a multi-aquifer well option for a modular ground-water flow model. In *Proceedings of the National Water Well Association Conference on Practical Applications of Ground Water Models*, 786–796. Columbus, Ohio: National Water Well Association.

Neville, C.J., and M.J. Tonkin. 2004. Modeling multiaquifer wells with MODFLOW. *Ground Water* 42, no. 6: 910–919.

Paillet, F.L., J.H. Williams, D.S. Oki, and K.D. Knutson. 2002. Comparison of formation and fluid-column logs in a heterogeneous basalt aquifer. *Ground Water* 40, no. 6: 577–585.

Prudic, D.E., L.F. Konikow, and E.R. Banta. 2004. A new streamflow-routing (SFR1) package to simulate stream-aquifer interaction with MODFLOW-2000. USGS Open-File Report 2004-1042. Reston, Virginia: USGS.

Reilly, T.E., O.L. Franke, and G.D. Bennett. 1989. Bias in groundwater samples caused by wellbore flow. *Journal of Hydraulic Engineering* 115, no. 2: 270–276.