Three-Dimensional Flow in the Storative Semiconfining Layers of a Leaky Aquifer

by Nicasio Sepúlveda

Abstract

An analytical solution for three-dimensional (3D) flow in the storative semiconfining layers of a leaky aquifer fully penetrated by a production well is developed in this article to provide a method from which accurate hydraulic parameters in the semiconfining layers can be derived from aquifer test data. The analysis of synthetic aquifer test data with the 3D analytical solution in the semiconfining layers provided more accurate optimal hydraulic parameters than those derived using the available quasi-two-dimensional (2D) solution. Differences between the 3D and 2D flow solutions in the semiconfining layers become larger when a no flow boundary condition is imposed at either at the top of the upper semiconfining layer or at the bottom of the lower semiconfining layer or when the hydraulic conductivity ratio of the semiconfining layer to the aquifer is larger than 0.001. In addition, differences between the 3D and 2D flow solutions in the semiconfining layers are illustrated when the thickness ratio of the semiconfining layer to the aquifer is changed. Analysis of water level data from two hypothetical and one real aquifer test showed that the 3D solution in the semiconfining layers provides lower correlation coefficients among hydraulic parameters than the 2D solution.

Introduction

The leaky aquifer theory that considers the effects of storativity and transmissivity of the semiconfining layers and aquifers on water levels was presented by Neuman and Witherspoon (1969a, 1969b) and by Herrera and Figueroa (1969). The main assumptions of this leaky aquifer theory are that the hydraulic conductivity and thickness ratios of the semiconfining layers to the aquifer are significantly small. These assumptions allow the reduction of the ground water flow equations to two-dimensional (2D) in the semiconfining layers when axial symmetry implications are considered. Moench (1985) derived the quasi-2D flow solution in the aquifer and semiconfining layers for an aquifer-well configuration where the well fully penetrates an aquifer with leaky overlying and underlying storative semiconfining layers. The solution by Moench used the numerical inversion of the Laplace transforms using the algorithm presented by Stehfest (1970). The analytical quasi-2D flow solution by Moench (1985) is referred to here as the A-2D solution. Several methods have been used to derive the 2D flow in the semiconfining layers, considering the residual horizontal flow, in a multilayered leaky aquifer system (Neuman 1968; Hemker 1985; Cheng and Morohunfola 1993).

The accuracy of the hydraulic parameters of the semiconfining layers derived from aquifer test data becomes particularly important in aquifer storage and recovery studies. Errors in hydraulic parameters of the semiconfining layers derived from aquifer test data could have large implications in assessing flow exchanges between the aquifer and the semiconfining layers. In cases of ground water contamination, the accurate measurement of hydraulic properties of the semiconfining layers is important for the optimal management of water supply resources. In parts of Florida, the hydraulic conductivity of the semiconfining layer underlying the Upper Floridan aquifer may be large enough (Tibbals 1990) to invalidate the assumptions of the leaky aquifer theory.
The need to investigate the three-dimensional (3D) flow characteristics in the semiconfining layers is illustrated with the aquifer-well configuration of a well of infinitesimal radius that fully penetrates an aquifer overlain and underlain by leaky semiconfining layers with the capacity to store water (Figure 1). A radial numerical model, with axial symmetry, of such aquifer-well configuration was used to test the 2D flow solution in the semiconfining layers. The boundary condition cases treated herein were modified from those previously presented (Hantush 1964; Moench 1985) to exclude the case of no flow boundary conditions above and below the semiconfining layers because of the lack of physical significance of such case.

The drawdown in the aquifer and semiconfining layers was computed using MODFLOW-96 (Harbaugh and McDonald 1996) for the parameter values shown in Table 1. The column lengths of the grid used to develop the numerical (N) solution increased geometrically away from the well from 0.25 m for the first column near the well to 2.1 km for the last column at the lateral boundary of the grid. The 150 columns used in the grid spanned a total distance of 40.2 km. The aquifer and semiconfining layers were discretized with rows of the same thickness within each unit. The N solution obtained from MODFLOW using this high-resolution grid and the computer code MODOPTIM (Halford 2006) is referred to in this article as the N solution.

The drawdown computed in the semiconfining layers from the N solution, for case 1 boundary condition in Figure 1, was close to the drawdown computed from the A-2D solution (Figure 2). A larger root mean square error (RMSE) between the N and the A-2D solutions was calculated in the semiconfining layers for boundary condition cases 2 and 3, where the only difference from case 1 is that a no flow boundary condition is imposed either above or below a semiconfining layer (Figure 2).

The numerical simulations presented in Figure 2 are the preamble of the problem addressed in this article. These simulations suggest that, under some hydraulic conductivity ratios and boundary conditions, the calculated hydraulic parameters of the semiconfining layers may be inaccurate if the quasi-2D drawdown solution is used to analyze the aquifer test data. The question that needs to be answered is whether or not the large RMSE values in Figure 2 are caused by the deletion of the radial-flow component in the semiconfining layers, which reduces the ground water flow equation for these layers to one dimensional or 2D if the axial symmetry is considered.

An analytical solution for 3D flow in the semiconfining layers underlying and overlying a leaky aquifer is...
derived herein to provide a method to calculate the hydraulic parameters of the semiconfining layers from aquifer test data under any hydraulic conductivity and thickness ratios of the semiconfining layers to the aquifer. Such solution also could be used to analyze the flow characteristics in the semiconfining layers under the possibility of no significant hydraulic conductivity contrast between the semiconfining layers and the aquifer.

Table 1: Parameter Values Used to Compare the N and A-2D Solutions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K$</td>
<td>15.0 m/d</td>
</tr>
<tr>
<td>$K'$</td>
<td>0.05 m/d</td>
</tr>
<tr>
<td>$K''$</td>
<td>0.05 m/d</td>
</tr>
<tr>
<td>$K''/K'$</td>
<td>1.0</td>
</tr>
<tr>
<td>$b$</td>
<td>76.0 m</td>
</tr>
<tr>
<td>$b'$</td>
<td>50.0 m</td>
</tr>
<tr>
<td>$b''$</td>
<td>50.0 m</td>
</tr>
<tr>
<td>$Q$</td>
<td>0.15 m$^3$/s</td>
</tr>
<tr>
<td>$r$</td>
<td>10.0 m</td>
</tr>
<tr>
<td>$r'$</td>
<td>30.0 m</td>
</tr>
<tr>
<td>$r''$</td>
<td>20.0 m</td>
</tr>
<tr>
<td>$z$</td>
<td>88.0 m</td>
</tr>
<tr>
<td>$z'$</td>
<td>156.0 m</td>
</tr>
<tr>
<td>$z''$</td>
<td>22.0 m</td>
</tr>
<tr>
<td>$S_N$</td>
<td>$3.0 \times 10^{-5}$/m</td>
</tr>
<tr>
<td>$S'_N$</td>
<td>$9.8 \times 10^{-6}$/m</td>
</tr>
<tr>
<td>$S''_N$</td>
<td>$9.8 \times 10^{-6}$/m</td>
</tr>
</tbody>
</table>

The initial and boundary conditions are:

$$s(r, z, 0) = 0, \quad s(r, 0) = 0, \quad s''(r, z, 0) = 0$$

(4)

$$s(r, b + b' + b'', t) = 0, \quad t \geq 0 \text{ (cases 1 and 3)}$$

(5a)

$$\frac{\partial s'}{\partial z}(r, b + b' + b'', t) = 0, \quad t \geq 0 \text{ (case 2)}$$

(5b)

$$\lim_{r \to 0} s'(r, z, t) = 0, \quad t \geq 0$$

(6)

$$\lim_{r \to 0} \left( r \frac{\partial s'(r, z, t)}{\partial r} \right) = 0, \quad t \geq 0$$

(7)

$$s'(r, b + b'', t) = s(r, t), \quad t \geq 0$$

(8)

$$s''(r, 0, t) = 0, \quad t \geq 0 \text{ (cases 1 and 2)}$$

(10a)

$$\frac{\partial s''}{\partial z}(r, 0, t) = 0, \quad t \geq 0 \text{ (case 3)}$$

(10b)

$$\lim_{r \to 0} s''(r, z, t) = 0, \quad t \geq 0$$

(11)

$$\lim_{r \to 0} \left( r \frac{\partial s''(r, z, t)}{\partial r} \right) = 0, \quad t \geq 0$$

(12)

$$\lim_{r \to 0} s(r, t) = 0, \quad t \geq 0$$

(13)

$$\lim_{r \to 0} \left( r \frac{\partial s(r, z, t)}{\partial r} \right) = - \frac{Q}{2\pi K b}, \quad t \geq 0$$

(14)

The difference between the boundary value problem posed by Equations 1 through 14 and the previous problems solved in the literature consists of the inclusion of the first two terms of Equations 1 and 2, which are the radial-flow components in the semiconfining layers. Li and Neuman (2007) presented the solution to a five-layer system where flow is assumed to be vertical in the semiconfining layers and radial in the aquifer, namely the quasi-2D flow solution. Under such quasi-2D flow assumptions, the first two terms of Equations 1 and 2 are deleted. The purpose of including the first two terms in Equations 1 and 2 for the semiconfining layers is to consider the 3D flow characteristics in these layers.

Formulation

The basic assumptions for the aquifer-well configuration and hydraulic parameters shown in Figure 1 are (1) the well is of infinitesimal radius; (2) the well fully penetrates the aquifer; (3) the aquifer is overlain and underlain by leaky semiconfining layers; (4) the flow in the aquifer is radial; and (5) the flow in the semiconfining layers is 3D, explained by the radial and vertical components and the axial symmetry. A modification to the ground water flow equations in the semiconfining layers presented by Neuman and Witherspoon (1969a) was made to allow 3D flow in these layers. The drawdown equations in the aquifer and semiconfining layers for boundary condition cases 1, 2, and 3 shown in Figure 1 are:

$$\frac{\partial^2 s'}{\partial r^2} + \frac{1}{r} \frac{\partial s'}{\partial r} + \frac{K'_s}{K'} \frac{\partial^2 s'}{\partial z^2} = \frac{S'_N}{K'} \frac{\partial s'}{\partial t}, \quad t \geq 0, \quad b + b'' \leq z \leq b + b' + b''$$

(1)

$$\frac{\partial^2 s''}{\partial r^2} + \frac{1}{r} \frac{\partial s''}{\partial r} + \frac{K''_s}{K''} \frac{\partial^2 s''}{\partial z^2} = \frac{S''_N}{K''} \frac{\partial s''}{\partial t}, \quad t \geq 0, \quad 0 \leq z \leq b'', \quad \text{and}$$

(2)
Derivation of Analytical Solution

Solutions to boundary condition cases 1 and 2, derived using the inverse Laplace and order zero Hankel transforms in Appendix 1, are presented in Appendix 2. To derive the analytical solution for case 3, Equations 1 through 3 were transformed into Laplace domain $s$ and Hankel domain $a$ using initial condition 4 and boundary conditions 5 through 14 to obtain:

$$s(a; p) = Q^2 p K_b p (a^2 - k^2(p))^{15}$$

$$s_9(a; z; p) = \sinh(l(a; p) b_9^1 a_9)$$

$$s_9(r; p)$$

Figure 2. Drawdown at observation wells computed from the N and A-2D solutions, and equal drawdown contours computed numerically at the end of a 1-day period of simulated pumping for the three boundary condition cases and the parameters in Table 1.
\[
\bar{r}(x, z, p) = \frac{\cosh(v(x, p) \frac{z}{a})}{\cosh(v(x, p) \frac{b}{a})} \tilde{s}(r, p) \tag{17}
\]

where
\[
\lambda^2(p) = \frac{S_z}{K} p + \lambda' \mu(x, p) \coth\left(\frac{\mu(x, p) b'}{a}\right) + \lambda'' v(x, p) \tanh\left(\frac{v(x, p) b''}{a''}\right) \tag{18}
\]

\[
u^2(x, p) = x^2 + \frac{S_z}{K'} p, \quad \mu^2(x, p) = x^2 + \frac{S_z}{K''} p \tag{19}
\]

\[
\lambda' = \frac{K'_{\lambda}}{K a'}, \quad \lambda'' = \frac{K''_{\lambda}}{K a''} \tag{20}
\]

\[
a' = \sqrt{\frac{K'_{\lambda}}{K'}}, \quad a'' = \sqrt{\frac{K''_{\lambda}}{K''}} \tag{21}
\]

Figure 3. Drawdown at observation wells computed from the N and A-3D solutions assuming isotropic conditions for the three boundary condition cases and the parameters in Table 1.

Figure 4. Drawdown at observation wells computed from the N and A-3D solutions assuming anisotropic conditions for the three boundary condition cases and applicable parameters in Table 1.
The drawdown \( s(r, t) \) in the aquifer was obtained by computing the inverse Hankel transform first and then computing the inverse Laplace transform using a Bromwich contour that excludes the origin (Carslaw and Jaeger 1986). The drawdown \( s(r, t) \) in the aquifer can be written as:

\[
s(r, t) = \frac{Q}{2\pi K b} \int_{0}^{\infty} \left( 1 - e^{-ur} \right) J_{0}(f(u)r) du
\]

(22)

where

\[
f^2(u) = \frac{S_{u}^2}{K} - \nu'(u_{i}, -u^2) \coth \left( \frac{(u_{i}, -u^2)b'}{a'} \right)
- \nu''(u_{i}, -u^2) \tanh \left( \frac{(u_{i}, -u^2)b''}{a''} \right) = -\nu^2(u)
\]

(23)

and \( J_{0} \) is the Bessel function of the first kind and order zero. Equation 23 is nonlinear in terms of \( f^2(u) \) or \( \nu^2(u) \). The integrand in Equation 22 vanishes when the root \( u \) of Equation 23 makes \( \nu^2(u) \) positive. Only values of \( u \) for which \( \nu^2(u) \) is negative make the integrand of Equation 22 nonzero. The computation of these roots was based on all four possible combinations of the signs of \( \nu^2(u_{i}, -u^2) \) and \( \nu^2(u_{i}, -u^2) \).

The drawdown \( s'(r, z, t) \) in the upper semiconfining layer was obtained by using the convolution theorem of Laplace transforms and Equations A1 through A3 in that order. The drawdown \( s'(r, z, t) \) in the lower semiconfining layer was obtained by using the convolution theorem of Laplace transforms and Equations A4, A2, and A3 in that order. The drawdown in the semiconfining layers can be written as:

\[
s'(r, z, t) = \frac{QK_{p}}{K b S_{u}^2 (b')^2} \sum_{n=1}^{\infty} \frac{a}{\pi} \sin \left[ \pi \left( \frac{z - b - b'}{b'} \right) \right] \times \int_{0}^{\infty} \Omega \left( u, \frac{\pi a'}{b'} \right)^2 + f^2(u), \frac{K_{p}}{S_{u}} \right) du
\]

(24)

The integrands in Equations 24 and 25 vanish for values of \( u \) that satisfy \( f^2(u) < 0 \) as a result of computing the inverse Laplace transform of a Bessel function of the second kind and order zero shown in Equation A2. The integrals in Equations 22, 24, and 25 were computed using a trapezoid formula with small increments in the integration variable. The analytical solution computed using drawdown Equations 22, 24, and 25 is referred to in this article as A-3D.

The numerical inverse Laplace transform of the analytical inverse Hankel transform of Equation 15 could be calculated numerically using Stehfest (1970) algorithm. However, Equations 24 and 25 could not be derived using the numerical inverse Laplace transform as performed by Moench (1985) and by Li and Neuman (2007) because the inverse Hankel transform had to be computed between Laplace transforms A1 and A3 for Equation 24 and between Laplace transforms A4 and A3 for Equation 25. The solution presented by Li and Neuman (2007) showed that the double transforms for the quasi-2D flow problem could be inverted first by using the analytical inverse Hankel transform and then using the numerical inverse Laplace transform, a procedure that could not be used to

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### Table 2

**Optimal Hydraulic Parameters Computed from the A-2D, N, and A-3D Solutions for the Aquifer Configuration Shown in Figure 1 and the Parameters in Table 1**

<table>
<thead>
<tr>
<th>BC</th>
<th>K (m/d)</th>
<th>S (l/m)</th>
<th>K* (m/d)</th>
<th>S* (l/m)</th>
<th>K** (m/d)</th>
<th>S** (l/m)</th>
<th>RMSE (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>True value</td>
<td>15.0</td>
<td>3.0 × 10^{-5}</td>
<td>5.0 × 10^{-2}</td>
<td>9.8 × 10^{-6}</td>
<td>5.0 × 10^{-2}</td>
<td>9.8 × 10^{-6}</td>
<td>0.0 × 10^{0}</td>
</tr>
<tr>
<td>1 (A-2D)</td>
<td>a,b,12.9</td>
<td>3.2 × 10^{-5}</td>
<td>&lt;0.9 × 10^{-5}</td>
<td>&lt;1.2 × 10^{-8}</td>
<td>b,6,4.6 × 10^{-1}</td>
<td>a,b,1.5 × 10^{-4}</td>
<td>1.3 × 10^{-1}</td>
</tr>
<tr>
<td>1 (N)</td>
<td>16.1</td>
<td>2.1 × 10^{-5}</td>
<td>2.6 × 10^{-2}</td>
<td>15.8 × 10^{-6}</td>
<td>b,2.7 × 10^{-2}</td>
<td>b,5.4 × 10^{-5}</td>
<td>4.8 × 10^{-2}</td>
</tr>
<tr>
<td>1 (A-3D)</td>
<td>15.0</td>
<td>3.0 × 10^{-5}</td>
<td>4.9 × 10^{-2}</td>
<td>9.9 × 10^{-6}</td>
<td>4.9 × 10^{-2}</td>
<td>9.9 × 10^{-6}</td>
<td>1.3 × 10^{-2}</td>
</tr>
<tr>
<td>2 (A-2D)</td>
<td>9.8</td>
<td>*1.5 × 10^{-5}</td>
<td>2.5 × 10^{0}</td>
<td>3.9 × 10^{-4}</td>
<td>b,2.4 × 10^{-4}</td>
<td>b,2.4 × 10^{-4}</td>
<td>6.0 × 10^{-2}</td>
</tr>
<tr>
<td>2 (N)</td>
<td>16.1</td>
<td>2.1 × 10^{-5}</td>
<td>2.4 × 10^{-2}</td>
<td>5.2 × 10^{-6}</td>
<td>b,2.3 × 10^{-2}</td>
<td>b,4.7 × 10^{-5}</td>
<td>4.8 × 10^{-2}</td>
</tr>
<tr>
<td>2 (A-3D)</td>
<td>15.0</td>
<td>3.0 × 10^{-5}</td>
<td>4.9 × 10^{-2}</td>
<td>1.0 × 10^{-5}</td>
<td>b,4.9 × 10^{-2}</td>
<td>b,1.0 × 10^{-5}</td>
<td>3.2 × 10^{-2}</td>
</tr>
<tr>
<td>3 (A-2D)</td>
<td>11.0</td>
<td>2.5 × 10^{-5}</td>
<td>6.4 × 10^{-1}</td>
<td>9.9 × 10^{-5}</td>
<td>b,9.3 × 10^{-1}</td>
<td>b,2.9 × 10^{-4}</td>
<td>1.9 × 10^{-1}</td>
</tr>
<tr>
<td>3 (N)</td>
<td>16.1</td>
<td>2.1 × 10^{-5}</td>
<td>2.3 × 10^{-2}</td>
<td>5.2 × 10^{-6}</td>
<td>b,2.5 × 10^{-2}</td>
<td>b,5.2 × 10^{-6}</td>
<td>5.0 × 10^{-2}</td>
</tr>
<tr>
<td>3 (A-3D)</td>
<td>15.0</td>
<td>3.0 × 10^{-5}</td>
<td>4.9 × 10^{-2}</td>
<td>1.0 × 10^{-5}</td>
<td>b,4.9 × 10^{-2}</td>
<td>b,1.0 × 10^{-5}</td>
<td>3.0 × 10^{-2}</td>
</tr>
</tbody>
</table>

Notes: Values with different superscript letters indicate parameter pairs with a correlation coefficient of 0.95 or higher. BC, boundary condition case number and solution used; true value, hydraulic parameters used to generate the observed drawdown.

N. Sepúlveda  GROUND WATER 46, no. 1: 144–155 149
derive the A-3D solution due to the occurrence of the Hankel domain variable \( z \) in Equations A1 and A5.

The A-3D solution was compared to the N solution obtained from MODFLOW-96 (Harbaugh and McDonald 1996) for isotropic (Figure 3) and anisotropic (Figure 4) conditions in the semiconfining layers. The small drawdown differences between the A-3D and the N solutions shown in Figure 3 shows that the drawdown differences between the A-2D and the A-3D solutions would be similar to those shown between the N and the A-2D solutions in Figure 2. Thus, compared to a constant-head boundary condition, larger RMSE values between the A-2D and the A-3D solutions are observed in the semiconfining layers when a no flow boundary condition is imposed either above or below a semiconfining layer.

Optimization Algorithm

The analytically computed drawdown was linked to an optimization algorithm to determine, from aquifer test data, the optimal set of hydraulic parameters that characterize the aquifer system shown in Figure 1. The optimal hydraulic parameter values were computed by minimizing the RMSE between analytically derived drawdown and either numerically derived or measured drawdown for two hypothetical and one real aquifer test. A modified Levenberg-Marquardt method was used to minimize the RMSE values. The numerically computed drawdown was obtained using MODFLOW-96 (Harbaugh and McDonald 1996), and the optimal set of hydraulic parameters that minimizes the RMSE was computed using MODOPTIM (Halford 2006). Correlation coefficients were calculated for each pair of hydraulic parameters in each optimization simulation to determine if any two hydraulic parameters could be computed independently. Highly correlated parameters indicate that only the ratio of these two can be computed independently.

Applications of Analytical Solutions and Optimization Algorithm

The analytical solution represented by Equations 22, 24, and 25 was used to generate the “observed” or true drawdown at the aquifer and semiconfining layers for two hypothetical aquifer tests for the aquifer-well configuration shown in Figure 1. The first hypothetical test consisted of using the hydraulic parameters and aquifer-well configuration values for isotropic conditions listed in Table 1, and the second one used the same parameters except for the anisotropic conditions given by \( a' = \sqrt{0.2} \) and \( a'' = \sqrt{0.4} \) (Figure 4). The N, A-2D, and A-3D solutions were used to derive optimal hydraulic parameters by applying the optimization algorithm to the observed drawdown data. The same set of arbitrary initial hydraulic parameters was used for all solutions.

Results of optimization simulations for isotropic and anisotropic conditions in the semiconfining layers indicate that more accurate hydraulic parameters can be obtained when the A-3D solution is used (Tables 2 and 3). Differences in all hydraulic parameters in the aquifer and semiconfining layers between the A-3D and the N solutions were smaller than those between the A-3D and the A-2D solutions for all boundary condition cases. The optimization algorithm reduced the RMSE values between the simulated drawdown from the A-2D solution and the observed drawdown from the A-3D solution, but it caused noticeable displacements from the true hydraulic parameters in Table 2. Differences between the drawdown computed from the A-2D solution (for a well with large radius) and that computed from the A-3D solution for a well of infinitesimal radius occur only near the well within a distance of the order of magnitude of the well radius itself (Papadopulos and Cooper 1967), which allows the comparison of the A-2D and the A-3D solutions at such distance away from the well.

The RMSE values between the A-3D and the A-2D solutions were small in the aquifer and large in the

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**Table 3**

Optimal Hydraulic Parameters Computed from the N and A-3D Solutions for the Aquifer Configuration Shown in Figure 1, the Parameters in Table 1, and the Specified Anisotropic Conditions

<table>
<thead>
<tr>
<th>BC</th>
<th>( K ) (m/d)</th>
<th>( S_s ) (m)</th>
<th>( K' ) (m/d)</th>
<th>( S_s' ) (m)</th>
<th>( K'' ) (m/d)</th>
<th>( S_s'' ) (m)</th>
<th>( K_z/K ) (—)</th>
<th>( K'/K ) (—)</th>
<th>RMSE (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>True value</td>
<td>15.0</td>
<td>3.0 ( \times 10^{-5} )</td>
<td>5.0 ( \times 10^{-2} )</td>
<td>9.8 ( \times 10^{-6} )</td>
<td>5.0 ( \times 10^{-2} )</td>
<td>9.8 ( \times 10^{-6} )</td>
<td>0.200</td>
<td>0.400</td>
<td>0.0 ( \times 10^0 )</td>
</tr>
<tr>
<td>1 (N)</td>
<td>16.0</td>
<td>2.0 ( \times 10^{-5} )</td>
<td>2.6 ( \times 10^{-2} )</td>
<td>3.4 ( \times 10^{-6} )</td>
<td>2.2 ( \times 10^{-2} )</td>
<td>3.7 ( \times 10^{-6} )</td>
<td>0.140</td>
<td>0.336</td>
<td>3.5 ( \times 10^{-2} )</td>
</tr>
<tr>
<td>1 (A-3D)</td>
<td>15.0</td>
<td>3.0 ( \times 10^{-5} )</td>
<td>5.1 ( \times 10^{-2} )</td>
<td>1.0 ( \times 10^{-5} )</td>
<td>5.1 ( \times 10^{-2} )</td>
<td>1.0 ( \times 10^{-5} )</td>
<td>0.202</td>
<td>0.405</td>
<td>2.3 ( \times 10^{-2} )</td>
</tr>
<tr>
<td>2 (N)</td>
<td>16.0</td>
<td>2.0 ( \times 10^{-5} )</td>
<td>2.8 ( \times 10^{-2} )</td>
<td>3.1 ( \times 10^{-6} )</td>
<td>2.2 ( \times 10^{-2} )</td>
<td>3.7 ( \times 10^{-6} )</td>
<td>0.120</td>
<td>0.337</td>
<td>3.8 ( \times 10^{-2} )</td>
</tr>
<tr>
<td>2 (A-3D)</td>
<td>15.1</td>
<td>3.1 ( \times 10^{-5} )</td>
<td>4.8 ( \times 10^{-2} )</td>
<td>1.1 ( \times 10^{-5} )</td>
<td>4.8 ( \times 10^{-2} )</td>
<td>1.1 ( \times 10^{-5} )</td>
<td>0.205</td>
<td>0.405</td>
<td>2.4 ( \times 10^{-2} )</td>
</tr>
<tr>
<td>3 (N)</td>
<td>16.1</td>
<td>2.0 ( \times 10^{-5} )</td>
<td>2.5 ( \times 10^{-2} )</td>
<td>3.4 ( \times 10^{-6} )</td>
<td>2.1 ( \times 10^{-2} )</td>
<td>3.8 ( \times 10^{-6} )</td>
<td>0.143</td>
<td>0.348</td>
<td>3.4 ( \times 10^{-2} )</td>
</tr>
<tr>
<td>3 (A-3D)</td>
<td>15.1</td>
<td>3.1 ( \times 10^{-5} )</td>
<td>4.9 ( \times 10^{-2} )</td>
<td>1.0 ( \times 10^{-5} )</td>
<td>4.9 ( \times 10^{-2} )</td>
<td>9.9 ( \times 10^{-6} )</td>
<td>0.195</td>
<td>0.395</td>
<td>3.7 ( \times 10^{-2} )</td>
</tr>
</tbody>
</table>

Notes: Values with different superscript letters indicate parameter pairs with a correlation coefficient of 0.95 or higher. BC; boundary condition case number and solution used; true value, hydraulic parameters used to generate the observed drawdown.

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**Table 4**

Parameter Values Used to Analyze the Aquifer Test Data from Jacksonville, Florida

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( b )</td>
<td>77.7 m</td>
</tr>
<tr>
<td>( b' )</td>
<td>129.6 m</td>
</tr>
<tr>
<td>( b'' )</td>
<td>41.2 m</td>
</tr>
<tr>
<td>( Q )</td>
<td>0.156 m³/s</td>
</tr>
<tr>
<td>( r )</td>
<td>740.9 m</td>
</tr>
<tr>
<td>( z )</td>
<td>113.4 m</td>
</tr>
</tbody>
</table>
The residuals between the A-3D and the A-2D solutions in the semiconfining layers caused the optimization algorithm for the A-2D solution to converge to a different set of hydraulic parameters that reduced these residuals, emphasizing the nonuniqueness of the solution to the ground water flow equation. This explains the differences in optimal hydraulic parameters between these two solutions. The relatively small RMSE values shown in Figure 4 caused the N solution to converge to slightly lower vertical hydraulic conductivities in the semiconfining layers indicated by lower anisotropies than those derived using the A-3D solution (Table 3).

Tables 2 and 3 list a higher number of correlated hydraulic parameter pairs for the A-2D solution than for the A-3D solution. Compared to the correlation results obtained from the A-3D and N solutions, the higher number of pairs of correlated hydraulic parameters for the A-2D solution is explained by the radial-flow component simulated in the semiconfining layers by the A-3D and N solutions, which allows the flow in the semiconfining layers to be better defined and less correlated to other hydraulic properties.

The A-2D, N, and A-3D solutions were used to analyze the aquifer test data from a production well that fully penetrates the Upper Floridan aquifer near Jacksonville, Florida. The set of boundary conditions for case 3 was more appropriate than cases 1 and 2 based on flow logs (Sepúlveda 2006). Aquifer-well configuration parameters for this test are listed in Table 4. Only drawdown data from the Upper Floridan aquifer were available for the analysis of this aquifer test. Optimal hydraulic parameters derived from the aquifer test data and the optimization algorithm showed that differences between the three solutions (Table 5) were negligible. Essentially, there is no difference in using one solution over another when only the drawdown data from the aquifer are available. Differences in optimal hydraulic parameters among the three solutions (A-2D, N, and A-3D) should be minimal if there are drawdown data available for the aquifer but not for the semiconfining layers.

The optimal hydraulic parameters in Table 5 derived from the A-3D solution were used to generate observed drawdown data in the semiconfining layers. These observed data were used together with the drawdown data from the Upper Floridan aquifer to reanalyze the aquifer test. The purpose of this test was to illustrate the effect of the drawdown in the semiconfining layers on the derivation of the optimal hydraulic parameters of the system shown in Figure 1. Results in Table 6 indicate that the optimal hydraulic parameters of the aquifer and semiconfining layers between the A-3D and the N solutions were very similar. However, the A-2D solution distributed the larger RMSE values in the semiconfining layers over the lower RMSE values in the aquifer, departing from the optimal hydraulic parameters that would be obtained with the A-3D or N solutions. If drawdown data from the semiconfining layers are available, then the A-3D or N solutions should be used to analyze the aquifer test data.

The effect of the hydraulic conductivity ratios $K'/K$ and $K''/K$ on the flow in the semiconfining layers was assessed by computing the RMSE values between the A-2D and the A-3D solutions. RMSE values computed for various hydraulic conductivity ratios showed that the 3D flow in the semiconfining layers could be significant, for all boundary condition cases, when the ratio $K'/K$ (or $K''/K$) exceeds 0.001 (Figure 5). Thus, the partial derivatives in

### Table 5

**Optimal Hydraulic Parameters Computed from the N, A-2D, and A-3D Solutions for the Aquifer Test in Jacksonville, Florida, Using Case 3 Boundary Conditions**

<table>
<thead>
<tr>
<th>SOLN</th>
<th>$K$ (m/d)</th>
<th>$S_x$ (l/m)</th>
<th>$K'$ (m/d)</th>
<th>$S'_x$ (l/m)</th>
<th>$K''$ (m/d)</th>
<th>$S''_x$ (l/m)</th>
<th>RMSE (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A-2D</td>
<td>$a^{16.4}$</td>
<td>$a^{3.3 \times 10^{-6}}$</td>
<td>$b^{9.1 \times 10^{-4}}$</td>
<td>$b^{3.3 \times 10^{-6}}$</td>
<td>$b^{1.5 \times 10^{-2}}$</td>
<td>$b^{1.8 \times 10^{-5}}$</td>
<td>$3.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>N</td>
<td>$a^{16.6}$</td>
<td>$a^{3.2 \times 10^{-6}}$</td>
<td>$b^{8.6 \times 10^{-4}}$</td>
<td>$b^{1.5 \times 10^{-5}}$</td>
<td>$b^{1.2 \times 10^{-2}}$</td>
<td>$b^{1.3 \times 10^{-5}}$</td>
<td>$1.8 \times 10^{-2}$</td>
</tr>
<tr>
<td>A-3D</td>
<td>$a^{16.6}$</td>
<td>$a^{3.3 \times 10^{-6}}$</td>
<td>$b^{9.1 \times 10^{-4}}$</td>
<td>$b^{1.6 \times 10^{-5}}$</td>
<td>$b^{1.2 \times 10^{-2}}$</td>
<td>$b^{1.3 \times 10^{-5}}$</td>
<td>$1.8 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Notes: Values with different superscript letters indicate parameter pairs with correlation coefficient of 0.95 or higher. SOLN, solution used.

### Table 6

**Optimal Hydraulic Parameters Computed from the N, A-2D, and A-3D Solutions for the Aquifer Test in Jacksonville, Florida, Using Case 3 Boundary Conditions and Adding the Drawdown in the Semiconfining Layers Generated Using the A-3D Solution**

<table>
<thead>
<tr>
<th>SOLN</th>
<th>$K$ (m/d)</th>
<th>$S_x$ (l/m)</th>
<th>$K'$ (m/d)</th>
<th>$S'_x$ (l/m)</th>
<th>$K''$ (m/d)</th>
<th>$S''_x$ (l/m)</th>
<th>RMSE (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A-2D</td>
<td>20.7</td>
<td>$4.0 \times 10^{-6}$</td>
<td>$a^{2.8 \times 10^{-4}}$</td>
<td>$b^{3.3 \times 10^{-6}}$</td>
<td>$a^{8.92 \times 10^{-3}}$</td>
<td>$c^{d7.7 \times 10^{-6}}$</td>
<td>$2.2 \times 10^{-2}$</td>
</tr>
<tr>
<td>N</td>
<td>16.2</td>
<td>$3.0 \times 10^{-6}$</td>
<td>$9.2 \times 10^{-4}$</td>
<td>$1.6 \times 10^{-5}$</td>
<td>$9.2 \times 10^{-3}$</td>
<td>$b^{5.0 \times 10^{-5}}$</td>
<td>$3.5 \times 10^{-2}$</td>
</tr>
<tr>
<td>A-3D</td>
<td>16.6</td>
<td>$3.2 \times 10^{-6}$</td>
<td>$b^{9.1 \times 10^{-4}}$</td>
<td>$b^{1.6 \times 10^{-5}}$</td>
<td>$1.2 \times 10^{-2}$</td>
<td>$1.3 \times 10^{-5}$</td>
<td>$2.0 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Notes: Values with different superscript letters indicate parameter pairs with correlation coefficient of 0.95 or higher. SOLN, solution used.
the radial direction of the ground water flow equation for the semiconfining layers become significant when either one of these hydraulic conductivity ratios exceeds 0.001, even more so under a no flow boundary condition near a semiconfining layer. Hydraulic parameters shown in Table 1 were used to generate the results shown in Figure 5 except for the values of $K'_9$ and $K''_9$, which were varied to provide several hydraulic conductivity ratios. Figure 5 shows the results when the hydraulic conductivity ratio $K'/K''$ is equal to $K''_9/K$ because no significant changes were obtained when the hydraulic conductivity ratios in the semiconfining layers were different.

Similarly, the effect of the thickness ratios $b'/b$ and $b''/b$ on the flow in the semiconfining layers was assessed by computing the RMSE values between the A-2D and the A-3D solutions. Figure 6 shows that 3D flow in the semiconfining layers also could be significant for all boundary condition cases and regardless of the thickness ratio, although the 3D flow effects in the semiconfining layers were stronger for changes in hydraulic conductivity...
ratios than for changes in thickness ratios. Hydraulic parameters shown in Table 1 were used to generate the results shown in Figure 6 except for the values of \( b' \) and \( b'' \), which were varied to provide several thickness ratios. Values of \( K' \) and \( K'' \) were set equal to one thousandth the value of \( K \) listed in Table 1. For illustration purposes, the thickness ratio \( b''/b' \) was chosen to be equal to \( b'/b \).

Summary and Conclusions

The A-3D analytical solution derived herein applies to flow near a fully penetrating well in a leaky aquifer with storative semiconfining layers assuming 3D flow in the semiconfining layers. The A-3D solution allows for a hydraulically based computation of drawdown in the aquifer and semiconfining layers. When used to solve the inverse problem, the A-3D solution could allow for the computation of more accurate hydraulic parameters than those that would be obtained from the A-2D solution if drawdown data from the semiconfining layers were available as part of the aquifer test data. Three-dimensional flow becomes significant in the semiconfining layers when the hydraulic conductivity ratio \( K'/K \) is larger than 0.001. Changes in the thickness ratio \( b'/b \) (or \( b''/b' \)) have a weaker impact toward the onset of 3D flow in the semiconfining layers than changes in the hydraulic conductivity ratios \( K'/K \) and \( K''/K \). The 3D flow in the semiconfining layers becomes even more significant when a no flow boundary condition is imposed either above or below a semiconfining layer. Under these conditions in the semiconfining layers, an accurate computation of the hydraulic parameters of the semiconfining layers from aquifer test data could be derived using the A-3D solution.

Synthetic drawdown data were generated for a hypothetical but realistic aquifer using the A-3D solution. These synthetic data were analyzed using the N solution based on the MODFLOW-based computer code MODOPTIM and the A-2D and A-3D analytical solutions. The main difference in the optimal hydraulic parameters was the higher accuracy shown by the N and A-3D solutions compared to the A-2D solution. The addition of the partial derivatives in the radial direction of the groundwater flow equation for the semiconfining layers characterizes the potential 3D flow properties in these layers.

Another improvement of the N and A-3D solutions over the A-2D solution was the computation of smaller correlation coefficients among the hydraulic parameters. The results presented here indicate that an appropriate coupling of the numerical model (MODFLOW-96) with an optimization algorithm, provided by MODOPTIM, should suffice to derive the optimal hydraulic parameters of the aquifer and semiconfining layers from aquifer test data with approximately the same accuracy as those obtained using the A-3D solution.

Higher accuracy for the optimal hydraulic parameters in the aquifer and semiconfining layers may be obtained by using the A-3D or N solutions instead of the A-2D solution because the former solutions consider the possible 3D flow in the semiconfining layers. Studies requiring the most accurate estimation of hydraulic parameters of the semiconfining layers should record the measured drawdown in the semiconfining layers and could make use of the A-3D solution presented in this article to analyze the aquifer test data given the gain in accuracy over the A-2D solution.

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References


N. Sepulveda GROUND WATER 46, no. 1: 144–155 153
Appendix 1

Selected Inverse Laplace and Hankel Transforms

The derivation of Equation 24 required the following inverse transforms:

\[ L^{-1} \left[ \frac{\sinh \left( \mu(x, p) \frac{b + b' + b'' - z}{a'} \right)}{\sinh \left( \mu(x, p) \frac{b'}{a'} \right)} \right] = \frac{2\pi K'_s}{S'_s(b')^2} \]

\[ \sum_{n=1}^{\infty} n \sin \left[ n\pi \left( \frac{z - b - b''}{b'} \right) \right] e^{-n\pi \frac{a''}{b'}} \left( \frac{n\pi a''}{b''} \right)^2 + x^2 \right] t \]

(A1)

where \( \Psi'' = K''/S'_s \)

\[ H^{-1} \left[ \frac{\alpha J_0(\alpha x) e^{-\alpha x^2}}{\alpha^2 + \alpha^2(x^2)} \right] = K_0(\alpha r)e^{\alpha z^2(r^2)} \] and (A2)

\[ L^{-1} \left[ \frac{K_0(\alpha r)}{p} e^{-\Psi \Phi t} \right] = \int_0^\infty \int_0^\infty \int_0^\infty \left( 1 - e^{-a^2(t - \tau)} \right) J_0(f(u)r)du \]

(A3)

The derivation of Equation 25 required using Equations A2 and A3, and the inverse transform:

\[ L^{-1} \left[ \frac{\cosh \left( \frac{\mu(x, p) b''}{a''} \right)}{\cosh \left( \frac{\mu(x, p) b''}{a''} \right)} \right] = -\frac{2\pi K'_s}{S'_s(b')^2} \sum_{n=1}^{\infty} (-1)^n \frac{2n(2n - 1)}{2} \]

\[ \times \cos \left[ \frac{(2n - 1)}{2} \frac{\pi z}{b''} \right] e^{-n\pi \frac{a''}{b''}} \Phi'' t \]

(A4)

where \( \Psi'' = K''/S'_s \) and \( \Phi'' = \left( ((2n - 1)/2) \frac{\pi a''}{b''} \right)^2 + x^2 \). Additional inverse Laplace transforms needed for boundary condition cases 1 and 2 were:

\[ L^{-1} \left[ \frac{\sinh \left( \frac{\mu(x, p) b''}{a''} \right)}{\sinh \left( \frac{\mu(x, p) b''}{a''} \right)} \right] = -\frac{2\pi K'_s}{S'_s(b')^2} \sum_{n=1}^{\infty} (-1)^n n \sin \left[ \frac{n\pi z}{b''} \right] e^{-n\pi \frac{a''}{b''}} \left( \frac{n\pi a''}{b''} \right)^2 + x^2 \right] t \] and (A5)

\[ L^{-1} \left[ \frac{\cosh \left( \frac{\mu(x, p) (b + b' + b'' - z)}{a'} \right)}{\cosh \left( \frac{\mu(x, p) b'}{a'} \right)} \right] = \frac{2\pi K'_s}{S'_s(b')^2} \sum_{n=1}^{\infty} (2n - 1) \sin \frac{(2n - 1 \pi)}{2} \left( \frac{z - b - b''}{b'} \right) \right] e^{-n\pi \frac{a''}{b''}} \]

(A6)

where \( \Phi' = ((2n - 1)/2)(\pi a''/b'') \) \( \cosh^2 \) terms of Laplace transforms. Equation A2 was derived using Hantush (1964), the contour integration over the upper half of the complex plane, and the definitions of Hankel functions of order zero in terms of Bessel functions of the first and second kinds and order zero (Abramowitz and Stegun 1970).

Appendix 2

Analytical Solutions to Boundary Condition Cases 1 and 2

The solution to the boundary value problem for case 1 boundary conditions in Figure 1 is given by Equations 22, 24, and the drawdown in the lower semiconfining layer, obtained from the double inversion of:

\[ \bar{S}(r, z, p) = \frac{\sinh \left( \frac{\nu(x, p) z}{a''} \right)}{\sinh \left( \frac{\nu(x, p) b''}{a''} \right)} \]

(A7)

The double inversion of Equation A7 is obtained by using the convolution theorem for Laplace transforms and applying Equations A5, A2, and A3 in the specified order and using the convergence properties of the integrands. The drawdown in the lower semiconfining layer can be written as:

\[ s''(r, z, t) = -\frac{QK_r^2}{KbS''(b'')} \sum_{n=1}^{\infty} \frac{(-1)^n n \sin \left[ \frac{n\pi z}{b''} \right]}{\sinh \left( \frac{\nu(x, p) b''}{a''} \right)} \times \int_0^\infty \Omega(u, f^2(u) + \left( \frac{n\pi a''}{b''} \right)^2, K''/S''_s) du \]

(A8)

where \( \Omega(u, \Phi, \Psi) \) is defined by Equation 26 and the expression for \( f^2(u) \) in Equation 23 is replaced by:

\[ f^2(u) = \frac{S_a u^2}{K} - \frac{\mu(i\lambda - u^2) \cosh \left( \frac{\mu(i\lambda - u^2) b''}{a''} \right)}{a''} \]

\[ - \frac{\nu(x, p) z}{a''} \frac{(i\lambda - u^2) \cosh \left( \frac{\mu(i\lambda - u^2) b''}{a''} \right)}{a''} = -\lambda^2(u) \]

(A9)

The solution to the boundary value problem for case 2 boundary conditions in Figure 1 is given by Equation 22, Equation A8, and the drawdown in the upper semiconfining layer obtained from the double inversion of:

\[ \bar{S}(x, z, p) = \frac{\cosh \left( \frac{\mu(x, p) b''}{a''} \right)}{\cosh \left( \frac{\mu(x, p) b' \right)}{a''} \bar{s}(r, p) \]

(A10)

The double inversion of Equation A10 is obtained by using the convolution theorem for Laplace transforms and applying Equations A6, A2, and A3 in the specified order and using the convergence properties of the integrands. The drawdown in the upper semiconfining layer can be written as:
$s'(r, z, t) = \frac{2QK_z}{KbS'_t(b')}^2 \sum_{n=1}^{\infty} \frac{(2n-1)}{2} \sin \left[ \frac{(2n-1)\pi}{2} \left( \frac{z - b - b'}{b'} \right) \right] \int_0^\infty \Omega \left( u, \Phi, \frac{K_z}{S'_t} \right) du$ (A11)

where $\Omega(u, \Phi, \Psi)$ is defined by Equation 26, $\Phi = f^2(u) + \left( \left( (2n-1)/2 \right)(\pi a'/b') \right)^2$ and the expression $f^2(u)$ in Equation 23 is replaced by:

$f^2(u) = \frac{S_u u^2}{K} - z' \mu(i\lambda, -u^2) \tanh \left( \frac{u(i\lambda, -u^2)b^*}{a^*} \right)$

- $z'' v(i\lambda, -u^2) \coth \left( \frac{v(i\lambda, -u^2)b^*}{a^*} \right)$ (A12)

The term $f^2(u)$ in the definition of $\Omega(u, \Phi, \Psi)$ in Equation 26 should be evaluated from the new definition of $f^2(u)$ in Equations A9 or A12.