Adjoint Simulation of Stream Depletion Due to Aquifer Pumping

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Abstract

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If an aquifer is hydraulically connected to an adjacent stream, a pumping well operating in the aquifer will draw some water from aquifer storage and some water from the stream, causing stream depletion. Several analytical, semi-analytical, and numerical approaches have been developed to estimate stream depletion due to pumping. These approaches are effective if the well location is known. If a new well is to be installed, it may be desirable to install the well at a location where stream depletion is minimal. If several possible locations are considered for the location of a new well, stream depletion would have to be estimated for all possible well locations, which can be computationally inefficient. The adjoint approach for estimating stream depletion is a more efficient alternative because with one simulation of the adjoint model, stream depletion can be estimated for pumping at a well at any location. We derive the adjoint equations for a coupled system with a confined aquifer, an overlying unconfined aquifer, and a river that is hydraulically connected to the unconfined aquifer. We assume that the stage in the river is known, and is independent of the stream depletion, consistent with the assumptions of the MODFLOW river package. We describe how the adjoint equations can be solved using MODFLOW. In an illustrative example, we show that for this scenario, the adjoint approach is as accurate as standard forward numerical simulation methods, and requires substantially less computational effort.

Introduction

A stream in the vicinity of a pumping well acts as a source of water to the well; thus pumping can cause a change in the stream flow rate. During well pumping, a gaining stream will gain at a lower rate and perhaps even become a losing stream, while a losing stream will lose water at an even greater rate. This decrease in the natural flow rate is called stream depletion.

Analytical and semi-analytical expressions have been developed to quantify stream depletion for simple systems (e.g., Theis 1941; Glover and Balmer 1954; Hantush 1965; Jenkins 1968; Wallace et al. 1990; Hunt 1999; Butler

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et al. 2001; and others). Numerical models have been used to simulate stream depletion in more complicated systems (e.g., Sophocleous et al. 1995; Chen and Yin 1999; Chen and Shu 2002; Kollet and Zlotnik 2003; Zlotnik 2004; and others). In these prior studies, stream depletion due to pumping was calculated for an existing well. If the location of a new well is to be chosen, it may be necessary to choose a location that limits depletion in a nearby stream. In Colorado, for example, groundwater extracted from a pumping well is subject to water rights unless it can be shown to be nontributary groundwater, which is defined as groundwater that can be withdrawn without depleting flow of a natural stream at an annual rate greater than 1/10 of 1% of the annual rate of withdrawal within 100 years of continuous pumping (Colorado Revised Statutes 37-90-103). Thus, it may be desirable to choose a location for the new well such that the well is extracting nontributary groundwater. To determine the feasible locations, stream depletion must be calculated for all possible well locations, and the computational burden for repeatedly running simulations with different well locations would be excessive.

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In this article, we present an adjoint-based methodology for calculating stream depletion. The adjoint method is a type of sensitivity analysis. Sensitivity analysis calculates the change in a performance measure of the system due to a change in the value of a system parameter. In our application, the performance measure is stream depletion and the system parameter is the pumping rate at a particular pumping well. With only one simulation, the adjoint model calculates stream depletion due to pumping at any location.

The adjoint method has been used in a variety of applications in groundwater modeling including sensitivity analysis (Sykes et al. 1985; Wilson and Metcalfe 1985; Skaggs and Barry 1996; Li and Yeh 1998; Cirpka and Kitanidis 2000; Jyrkama and Sykes 2006), parameter estimation (Neuman 1980; Sun and Yeh 1985, 1990; Townley and Wilson 1985; Lu et al. 1988; Yeh and Sun 1990; Yeh and Zhang 1996; Cardiff and Kitanidis 2008; Fienen et al. 2008; Wu et al. 2008), optimization (Ahlfeld et al. 1988; Tan et al. 2008), source identification (Neupauer and Wilson 1999, 2001; Michalak and Kitanidis 2004), model calibration (Lavenue and Pickens 1992), and others (see Sun 1994).

In the next section, we present the groundwater flow equations for an aquifer/river system. Next, we present the adjoint equations that are used to calculate stream depletion for this system. We discuss the numerical solution of the adjoint equation using MODFLOW-2000 (Harbaugh et al. 2000). Finally, we present an example of using the adjoint method to calculate stream depletion due to aquifer pumping, and we verify the results by comparing them with stream depletion calculated through forward simulations.

Forward Equations of Groundwater Flow and Stream Depletion

We consider a surface water/groundwater system that contains an unconfined aquifer, an aquitard, and a confined aquifer, as shown in Figure 1. A river is hydraulically connected to the unconfined aquifer, and a pumping well is extracting water from either the confined or unconfined aquifer. For simplicity, we assume that flow is essentially horizontal in the confined aquifer, and we use the Dupuit



Figure 1. Cross section of river/aquifer system that includes an unconfined aquifer, leaky aquitard, and a confined aquifer. The river is hydraulically connected to the unconfined aquifer. A pumping well can be installed in either the unconfined or the confined aquifer.

assumptions in the unconfined aquifer. We also assume the aquifers are isotropic, and that the aquifers are bounded to the north and south by constant head boundaries and to the east and west by no-flow boundaries (Figure 2). Some of these assumptions are relaxed in the Supporting Information. The groundwater flow equations for this system are given by

$$S_{y}\frac{\partial h_{u}}{\partial t} = \nabla \cdot [K(h_{u} - \zeta)\nabla h_{u}] + N(x, y) - Q_{wu}\delta(x - x_{wu}) \cdot \delta(y - y_{wu}) - \frac{K_{a}}{b_{a}}(h_{u} - h_{c}) + \frac{K_{r}}{b_{r}}(h_{r} - h_{u})A(x, y)$$
(1a)

$$S\frac{\partial h_{\rm c}}{\partial t} = \nabla \cdot T \nabla h_{\rm c} - Q_{\rm wc} \delta(x - x_{\rm wc}) \delta(y - y_{\rm wc}) + \frac{K_{\rm a}}{b_{\rm a}} (h_{\rm u} - h_{\rm c})$$
(1b)

with boundary and initial conditions given by

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$$h_{\rm u}(\mathbf{x}, t) = h_{\rm c}(\mathbf{x}, t) = 16 \text{ m at } y = 0 \text{ m and}$$

 $h_{\rm u}(\mathbf{x}, t) = h_{\rm c}(\mathbf{x}, t) = 20 \text{ m at } y = 2000 \text{ m}$ (2a)

$$\nabla h_{\mathbf{u}}(\mathbf{x}, t) \cdot \mathbf{n} = \nabla h_{\mathbf{c}}(\mathbf{x}, t) \cdot \mathbf{n} = 0$$
 at $x = 0$ m and

$$x = 1600 \text{ m}$$
 (2b)

$$h_{\mathrm{u}}(\mathbf{x}, 0) = h_{\mathrm{uo}}(\mathbf{x}) \text{ and } h_{\mathrm{c}}(\mathbf{x}, 0) = h_{\mathrm{co}}(\mathbf{x}),$$
 (2c)

where $h_{\rm u}$ and $h_{\rm c}$ are head in the unconfined and confined aquifers, respectively, t is time, $\mathbf{x} = (x, y)$ are the spatial coordinates, S is the storage coefficient, S_v is the specific yield, K is hydraulic conductivity, T is transmissivity, ζ is the elevation of the bottom of the unconfined aquifer, $h_{\rm u} - \zeta$ is the saturated thickness of the unconfined aquifer, N(x, y) is the spatially varying natural recharge rate, Q_{wu} and $Q_{\rm wc}$ are the pumping rates for a well in the unconfined and confined aquifers, respectively, (x_{wu}, y_{wu}) and (x_{wc}, y_{wc}) are the pumping well locations in the unconfined and confined aquifers, respectively, K_r and b_r are the hydraulic conductivity and thickness, respectively, of the river sediment, h_r is head in the river, K_a and b_a are the hydraulic conductivity and thickness, respectively, of the aquitard, A(x, y) is a dimensionless function that has a value of unity at all points along the river and a value of zero elsewhere, and h_{uo} and h_{co} are the initial heads in the unconfined and confined aquifers, respectively.

Let $Q_r(t_c)$ be the rate at which river water is recharging the aquifer at some compliance time t_c . Using the notation in Equation 1a, $Q_r(t_c)$ is given by

$$Q_{\rm r}(t_{\rm c}) = \iint_{x,y} \frac{K_{\rm r}}{b_{\rm r}} [h_{\rm r}(x, y, t_{\rm c}) - h_{\rm u}(x, y, t_{\rm c})]$$
$$\times A(x, y) \mathrm{d}y \mathrm{d}x. \tag{3}$$

Stream depletion due to pumping is quantified as the increase in $Q_r(t_c)$. Using standard groundwater flow modeling methods, two simulations are needed to calculate the increase in stream depletion due to pumping at a rate Q_w from a well at (x_w, y_w) . In the first simulation, groundwater flow is simulated over a period from t =0 to $t = t_c$ in the absence of pumping, and $Q_r(t_c)$ is calculated from Equation 3. In the second simulation, the first simulation is repeated with pumping at a rate $Q_{\rm w}$ from a well at (x_w, y_w) , and the new $Q_r(t_c)$ is calculated from Equation 3. The difference between these two values of $Q_{\rm r}(t_{\rm c})$ is the stream depletion due to pumping at rate Q_w at a well at (x_w, y_w) . As an example, consider the aquifer system shown in Figure 2, with parameters identified in Table 1. A meandering river flows from north to south through the domain, and is gaining in the northern part of the domain, and losing in the southern part. Natural recharge is present throughout the domain, with a higher recharge rate $(4.4 \times 10^{-7} \text{ m/d})$ along the eastern and western boundaries, and a lower recharge rate $(3.7 \times 10^{-7} \text{ m/d})$ through the center of the domain. Flow was simulated using MODFLOW-2000, and steadystate head in the aquifer under non-pumping conditions is shown in Figure 2. For this non-pumping scenario, $Q_r =$ 3.4635 m³/d (five digits of accuracy are included here to maintain sufficient precision in the stream depletion calculations). Two additional simulations were run with pumping of 10 m³/d at $(x_w, y_w) = (375 \text{ m}, 1025 \text{ m})$ —one simulation with pumping from the confined aquifer and one with pumping from the unconfined aquifer. The resulting heads after 1825 d of pumping are shown in Figure 3. The resulting Q_r and stream depletion (Q_r - $Q_{\rm r-nopumping}$) is shown in Table 2, and the temporal distribution of stream depletion is shown in Figure 4. Pumping in the confined aquifer produces more stream depletion than pumping in the unconfined aquifer, and stream depletion increases over time.



Figure 2. Steady-state head (in m) in the unconfined (thick line) and confined (dashed line) aquifers without pumping. The pumping well location is shown as a filled circle. Boundary conditions are shown along the boundaries. The thick dashed line is the river. The gray-shaded area represents the high recharge area, and the white area represents the low recharge area.

Table 1					
Aquifer	and	Model	Pro	perties	

Property	Value
Head at north boundary	20 m
Head at south boundary	16 m
Elevation of bottom of confined aquifer	-20 m
Elevation of top of confined aquifer	-10 m
Elevation of bottom of unconfined aquifer, ζ	0 m
Hydraulic conductivity of unconfined aquifer, <i>K</i>	0.2 m/d
Hydraulic conductivity of the aquitard, K_{a}	$2.0 \times 10^{-2} \text{ m/d}$
Transmissivity of confined aquifer, T	$1.0 \text{ m}^2/\text{d}$
Specific yield, $S_{\rm v}$	0.2
Storage coefficient in aquitard	0
Storage coefficient in confined aquifer, S	1×10^{-3}
Recharge rate (high value), N	$4.4 \times 10^{-7} \text{ m/d}$
Recharge rate (low value), N	3.7×10^{-7} m/d
River bottom elevation	15 m
River bed thickness, b_r	0.125 m
Hydraulic conductivity of river bed, $K_{\rm r}$	2.5×10^{-5} m/d
River stage, $h_{\rm r}$	$19 \text{ m} - 0.0005 \text{ s}^1$
River width	25 m
Centerline of river	x = 775 m
	+ 0.8055
	(y - 25m)
Spatial discretization	$50 \times 50 \text{ m}$
Temporal discretization	1 d
Compliance time, t_c	1825 d
Location of well (x_w, y_w)	(375 m, 1025 m)
Pumping rate, $Q_{\rm wc}$	10 m³/d
eta	16/d
γ	0.001

 ^{1}s is the distance along the river channel in the flow direction (s = 0 at y = 2000 m).



Figure 3. Head (in m) in the unconfined (thick line) and confined (dashed line) aquifers at t = 1825 d with pumping in the unconfined aquifer (a) and with pumping in the confined aquifer (b). Well location is shown as a filled circle. The thick dashed line is the river.

Table 2Aquifer Recharge from the River and StreamDepletion at $t = 1825$ d							
Pumped	0 _r	Stream De	Error				
Aquifer	$(\widetilde{m^{3}/d})$	Forward	Adjoint	(%)			
None	3.4635	NA	NA	NA			
Unconfined	3.6616	0.1981	0.2045	3.2			
Confined	3.6931	0.2296	0.2361	2.4			



Figure 4. Stream depletion as a function of time.

Adjoint Equations of Groundwater Flow and Stream Depletion

If multiple locations are considered for the pumping well location, a forward simulation must be run for each potential well location, which can be computationally inefficient. Instead, we propose an adjoint-based approach. With one simulation of the adjoint equation, stream depletion can be calculated for pumping at a well at any location in the aquifer. If many possible well locations are being considered, the computational savings of the single adjoint simulation compared to the multiple forward simulations can be enormous.

The development of the adjoint model is based on sensitivity analysis, in which we calculate the sensitivity of $Q_r(t_c)$ to pumping at a specified rate at a well. This sensitivity can be expressed as $dQ_r(t_c)/dQ_{wk}(x_{wk}, y_{wk})$, where the subscript k represents the aquifer in which pumping occurs (k = u for pumping in the unconfined aquifer and k = c for pumping in the confined aquifer).

The sensitivity is obtained by differentiating Equation 3 with respect to Q_{wk} to obtain

$$\frac{\mathrm{d}Q_{\mathrm{r}}(t_{\mathrm{c}})}{\mathrm{d}Q_{\mathrm{wc}}(x_{\mathrm{wk}}, y_{\mathrm{wk}})} = \frac{\mathrm{d}}{\mathrm{d}Q_{\mathrm{wk}}(x_{\mathrm{wk}}, y_{\mathrm{wk}})} \left[\iint_{x,y} \frac{K_{\mathrm{r}}}{b_{\mathrm{r}}} (h_{\mathrm{r}} - h_{\mathrm{u}}) A(x, y) \mathrm{d}y \mathrm{d}x \right] \\
= -\iint_{x,y} \psi_{\mathrm{u}} \frac{K_{\mathrm{r}}}{b_{\mathrm{r}}} A(x, y) \mathrm{d}y \mathrm{d}x,$$
(4)

where $\psi_u(x, y, t) = \partial h_u(x, y, t)/\partial Q_{wk}(x_{wk}, y_{wk})$ is the sensitivity of head in the unconfined aquifer to pumping at rate Q_{wk} at location (x_{wk}, y_{wk}) . In Equation 4, the last line follows from the first line because h_u is the only parameter in the integral in the first line that depends on Q_{wk} . For this work, we assume that the river head, h_r , is known and is independent of the state of the aquifer; thus, h_r is independent of Q_{wk} . This assumption is the same as that used in the MODFLOW river package. Ignoring the change in river head due to stream depletion leads to an overestimation of actual stream depletion (Sophocleous et al. 1995); therefore the assumption produces conservative estimates of stream depletion.

Equation 4 can be used to directly calculate stream depletion due to pumping at a single well at (x_{wk}, y_{wk}) . However, if the well location has not been chosen and multiple possible well locations are considered, this equation would have to be solved multiple times to obtain stream depletion for all possible well locations. Instead, we solve a similar equation, given by (Supporting Information)

$$\frac{\mathrm{d}Q_{\mathrm{r}}(t_{\mathrm{c}})}{\mathrm{d}Q_{\mathrm{wu}}(x,y)} = \int_{0}^{t_{\mathrm{c}}} \psi_{\mathrm{u}}^{*}(x,y,\tau)\mathrm{d}\tau \qquad (5a)$$

$$\frac{\mathrm{d}Q_{\mathrm{r}}(t_{\mathrm{c}})}{\mathrm{d}Q_{\mathrm{wc}}(x,\,y)} = \int_{0}^{t_{\mathrm{c}}} \psi_{\mathrm{c}}^{*}(x,\,y,\,\tau)\mathrm{d}\tau \tag{5b}$$

for pumping in the unconfined and confined aquifers, respectively, where $\tau = t_c - t$ is backward time (or time prior to the compliance time) and ψ_u^* and ψ_c^* are adjoint states of h_u and h_c , respectively, that are obtained by solving the adjoints of Equations 1a and 1b, which are given by (Supporting Information)

$$S_{y} \frac{\partial \psi_{u}^{*}}{\partial \tau} = \nabla \cdot [\mathbf{K}(\overline{h}_{u} - \zeta) \nabla \psi_{u}^{*}] - \frac{K_{a}}{b_{a}} (\psi_{u}^{*} - \psi_{c}^{*}) - \psi_{u}^{*} \frac{K_{r}}{b_{r}} A(x, y) + \frac{K_{r}}{b_{r}} A(x, y) \delta(\tau)$$
(6a)

$$S\frac{\partial\psi_{\rm c}^*}{\partial\tau} = \nabla \cdot \mathbf{T}\nabla\psi_{\rm c}^* + \frac{K_{\rm a}}{b_{\rm a}}(\psi_{\rm u}^* - \psi_{\rm c}^*) \tag{6b}$$

Here $\overline{h}_u - \zeta$ is the saturated thickness of the unconfined aquifer, \overline{h}_u is the initial head in the unconfined aquifer, and all other parameters are defined earlier. Note that the units on the adjoint states are reciprocal time. The boundary and initial conditions (in backward time) of the adjoint states are given by (Supporting Information)

$$\psi_{u}^{*}(\mathbf{x}, t) = \psi_{c}^{*}(\mathbf{x}, t) = 0 \text{ at } y = 0 \text{ m and } y = 2000 \text{ m}$$
(7a)

$$\nabla \psi_{\mathbf{u}}^*(\mathbf{x}, t) \cdot \mathbf{n} = \nabla \psi_{\mathbf{c}}^*(\mathbf{x}, t) \cdot \mathbf{n} = 0$$
 at $x = 0$ m and

$$x = 1600 \text{ m}$$
 (7b)

$$\psi_{\mathbf{u}}^{*}(\mathbf{x},0) = \psi_{\mathbf{c}}^{*}(\mathbf{x},0) = 0.$$
 (7c)

To summarize, Equations 6a and 6b are solved to obtain the adjoint states that are used in Equation 5a or Equation 5b to calculate $dQ_r(t_c)/dQ_{wk}(x_w, y_w)$, and

stream depletion is calculated as $Q_r(t_c) = -Q_{wk}(x, y)$ [d $Q_r(t_c)/dQ_{wk}(x_w, y_w)$].

Natural recharge does not appear in the adjoint equation because it does not directly affect stream depletion. Suppose that in the absence of pumping, natural recharge flows to the stream; and suppose that with pumping, a portion of the pumped water comes from the stream and a portion comes from natural recharge. The natural recharge that is captured at the well is no longer available to flow to the stream; therefore the total stream depletion is equal to the amount of pumped water that is drawn from the stream and the reduction in the amount of recharge reaching the stream, which is equal to the amount of recharge captured by the well. Thus, natural recharge does not impact stream depletion due to pumping.

Using MODFLOW to Solve the Adjoint Equations

In this section, we describe how to solve the adjoint equations 6 and 7 using MODFLOW-2000 (Harbaugh et al. 2000). The state variables in the adjoint simulation are the adjoint states; in the MODFLOW simulation, "head" is a surrogate for the adjoint states. From Equation 8c, the initial value of the state variable is zero, which is equivalent to setting the initial head to zero in a forward simulation. Depending on the top and bottom elevations of aquifers and the bottom elevation of the river, however, a value of zero for the state variable may be physically unrealistic. For example, if the elevations are measured relative to sea level, the aquifer bottom elevation may be substantially higher than sea level; thus, setting the initial value of the state variable to zero would be equivalent to the initial "head" in the aquifer to be well below the aquifer bottom. To address this issue, we define new state variables, $\Psi_{u}^{*}(\mathbf{x},\tau) = \beta + \psi_{u}^{*}(\mathbf{x},\tau)/\gamma$ and $\Psi_{c}^{*}(\mathbf{x},\tau) = \beta + \psi_{c}^{*}(\mathbf{x},\tau)/\gamma$, where β is chosen such that it is higher than the bottom elevation of any aquifer layer and the river and is less than the land surface elevation, and γ is defined in the subsequent equations. Substituting these expressions into Equations 6 and 7, we obtain a new set of governing equation in terms of $\Psi_{u}^{*}(\mathbf{x},\tau)$ and $\Psi_{c}^{*}(\mathbf{x},\tau)$ that can be solved directly in MODFLOW, given by

$$S_{y} \frac{\partial \Psi_{u}^{*}}{\partial \tau} = \nabla \cdot [\mathbf{K}(\overline{h}_{u} - \zeta) \nabla \Psi_{u}^{*}] - \frac{K_{a}}{b_{a}} (\Psi_{u}^{*} - \Psi_{c}^{*})$$
$$+ (\beta - \Psi_{u}^{*}) \frac{K_{r}}{b_{r}} A(x, y)$$
(8a)

$$S\frac{\partial \Psi_{\rm c}^*}{\partial \tau} = \nabla \cdot \mathbf{T} \nabla \Psi_{\rm c}^* + \frac{K_{\rm a}}{b_{\rm a}} (\Psi_{\rm u}^* - \Psi_{\rm c}^*) \tag{8b}$$

with boundary and initial conditions given by

$$\Psi_{u}^{*}(\mathbf{x}, t) = \Psi_{c}^{*}(\mathbf{x}, t) = \beta$$
 at $y = 0$ m and $y = 2000$ m (9a)

$$\nabla \Psi_{\mathbf{u}}^{*}(\mathbf{x}, t) \cdot \mathbf{n} = \nabla \Psi_{\mathbf{c}}^{*}(\mathbf{x}, t) \cdot \mathbf{n} = 0 \text{ at}$$

 $x = 0 \text{ m and } x = 1600 \text{ m}$ (9b)

$$\Psi_{\rm u}^*(\mathbf{x},0) = \beta + \frac{K_{\rm r}}{S_{\rm y} b_{\rm r} \gamma} A(x,y) \tag{9c}$$

$$\Psi_{\rm c}^*(\mathbf{x},0) = \beta \tag{9d}$$

Note that the last term in Equation 6a is non-zero only at time $\tau = 0$; thus, it is treated as an initial condition in Equation 9c. For certain values of β , K_r , S_y , and b_r , it is possible that the second term in Equation 9c is negligible compared to β ; however, this term is critical in the calculation of stream depletion because it is the source of the adjoint state. The constant γ should be defined such that the second term in Equation 9c is the same order of magnitude of β . With the change of variables used to create the equations given earlier, the stream depletion ΔQ_r is modified from Equations 5a and 5b as

$$\Delta Q_{\rm r} = -Q_{\rm wc}(x, y) \int_0^{t_{\rm c}} \gamma [\Psi_{\rm u}^*(x, y, \tau) - \beta] \mathrm{d}\tau \quad (10a)$$

$$\Delta Q_{\rm r} = -Q_{\rm wc}(x, y) \int_0^{t_{\rm c}} \gamma [\Psi_{\rm c}^*(x, y, \tau) - \beta] \mathrm{d}\tau. \quad (10b)$$

To obtain the adjoint states from MODFLOW, a few additional modifications must be made to the forward model input files to account for the differences between the adjoint equations and the forward equations:

- The time variable in the adjoint simulation is interpreted as backward time *τ*.
- The river term in Equation 8a is defined using the MODFLOW river (RIV) package. The same RIV package input file can be used for the adjoint simulation, except that β is used in place of the river stage for the adjoint simulation.
- Recharge is omitted in the adjoint simulation.
- The second derivative term in the forward governing equation for flow in the unconfined aquifer in Equation 1a is nonlinear in the state variable $h_{\rm u}$; however, in the adjoint equation 8a, the second derivative term is linear in the state variable Ψ_{u}^{*} and also depends on the initial head in the aquifer. As the forward and adjoint equations have different structures, this adjoint equation cannot be solved in the same way as the forward equation. Instead, in the adjoint simulation, the unconfined aquifer must be modeled as a confined aquifer with transmissivity defined as $T = K(\bar{h} - \zeta)$. The storage property for this aquifer is the specific yield $S_{\rm v}$. Note that this modification assumes that drawdown in the unconfined aquifer is small relative to the aquifer thickness; this assumption is discussed in the following.
- In Equation 10, the adjoint state at each location is integrated over the backward time domain to obtain stream depletion. This integral can be approximated as a summation. In order for this summation to approximate the integral in Equation 10 accurately, the temporal discretization of the simulation and the reported output must be sufficiently small.

Example

We used MODFLOW with the changes identified earlier to calculate stream depletion for the system shown in Figure 2. For these simulations, we used $\gamma = 0.001$ and $\beta = 16/d$. The value of β was chosen so that its magnitude is higher than the bottom elevation of the unconfined aquifer and river. Although the units of β are different than the unit of elevation, it is necessary to maintain this relationship between the magnitudes. If the magnitude of β were below the bottom elevation of the unconfined aquifer, the unconfined aquifer would be dry in the MODFLOW simulation, resulting in no hydraulic connection between the river and the aquifer. Also, if the magnitude of β were below the bottom elevation of the river, the river would not be hydraulically connected to the aquifer.

With one simulation of the adjoint simulation, we obtain both $\Psi_u^*(\mathbf{x},\tau)$ and $\Psi_c^*(\mathbf{x},\tau)$, and we use them in Equation 10 to obtain stream depletion due to pumping at any location in the unconfined and confined aquifers, respectively. These results are shown in Figure 5a, b. The value at any location in Figure 5a, b represents the stream depletion after 1825 d of pumping at a rate of 10 m³/d from a well at that location. For a well near the river, stream depletion is high because a substantial amount of pumped water is drawn from the river. For a well near the north and south boundaries, stream depletion is low because a substantial amount of the pumped water is supplied by the constant head boundary. Stream depletion



Figure 5. Stream depletion (m^3/d) : (a) ΔQ_r from adjoint simulation with pumping in the unconfined aquifer, (b) ΔQ_r from adjoint simulation with pumping in the confined aquifer, (c) ΔQ_r from forward simulations with pumping in the unconfined aquifer, (d) ΔQ_r from forward simulations with pumping in the confined aquifer.

decreases with distance from the river because more pumped water is coming from aquifer storage or across the boundaries.

To validate the results, we ran forward simulations to calculate stream depletion due to pumping from a well at each model grid block in both the confined and unconfined aquifers, for a total of 2560 simulations (40 rows, 32 columns, 2 aquifers). Stream depletion for each simulation is plotted in Figure 5c, d, respectively. Comparison with Figure 5a, b shows that the calculated stream depletions with the forward and adjoint methods are visually indistinguishable, confirming the reliability of the adjoint approach for calculating stream depletion for this aquifer system.

To further verify that the adjoint simulation is producing accurate results, we compare the adjointcalculated stream depletion for pumping at (375 m, 1025 m) to the results of the forward simulation (Table 2). The adjoint results are accurate to within 3% of the forward simulation results. The differences between the two sets of results occur because the adjoint model assumed that the change in the saturated thickness of the unconfined aquifer due to pumping was negligible; however, the saturated thickness does change slightly, leading to slight differences between the adjoint and forward simulation results. Nevertheless, the adjoint results are quite accurate and can be obtained with a substantial savings in computational effort (discussed below).

Discussion

For each possible pumping well location that led to appreciable stream depletion (defined as $0.0895 \text{ m}^3/\text{d}$,which is one-tenth of the maximum stream depletion with pumping in the confined aquifer), Figure 6 shows the percent error in streamflow depletion from the adjoint simulation as a function of the maximum percent change in the saturated thickness of the unconfined aquifer. Error is less than 6% for all simulations. Large



Figure 6. Percent error in stream depletion calculations vs. % maximum head change in the unconfined aquifer. Circles and triangles denote results from simulation with pumping in the unconfined aquifer and confined aquifer, respectively.

changes in saturated thickness occur when the pumping well is located far from the river or constant head boundaries, which are both sources of water; however, pumping at these locations lead to low values of stream depletion because these locations are far from the river.

The adjoint simulation is more computationally efficient than the forward approach. The results in Figure 5a, b were obtained with one adjoint simulation that took approximately 19 s to run on a Dell Inspiron 1525 with an Intel[®] Pentium[®] Dual Core CPU T3200 Processor @ 2.00 GHz with 4.00 Gb RAM. Almost identical results were obtained from 2560 forward simulations that took approximately 3 h to run on the same computer. Thus, the adjoint approach produced a speed up of over 500 times for only a small sacrifice in accuracy (<6%).

One potential limitation of the adjoint approach is in the required storage space. To obtain stream depletion, the adjoint state must be saved for a small time increment. Depending on the simulation duration, the storage requirements may become prohibitive. For the example in this article, the output file from the adjoint simulation was 65 Mb for this 1825-d simulation with 1-d time steps, and the output files for the 2560 forward simulations totaled 911 Mb. For this domain size, the size of the adjoint output file could have been approximately 15 times larger before the storage requirements of the adjoint simulation matched the storage requirements of the forward simulation. Equivalently, the duration of the simulation could have been approximately 15 times longer, if 1-d time steps were still used. Thus, the storage requirements are not likely to be a limitation of the adjoint approach. All models are simplifications of reality, and many assumptions must be made in the development of a model (e.g., parameter values, spatial and temporal variability of parameters, boundary conditions, etc.). These assumptions may lead to inaccuracies in the model results. As the adjoint model is based on the choice of the forward mathematical and numerical model, any inaccuracies due to assumptions made in the forward model also occur in the adjoint model.

Conclusions

Pumping in an aquifer that is hydraulically connected to a stream can lead to stream depletion. In this article, we presented an adjoint approach to calculate stream depletion. In the adjoint approach, only one simulation is needed to calculate stream depletion due to a pumping well at any location in the aquifer system. If the installation of a new well is planned, but the location of the new well has not yet been chosen, the adjoint method is an efficient tool for identifying the locations that would lead to minimal stream depletion.

We derived the adjoint equations from the governing equations of groundwater flow. We assumed that the river stage is known and is independent of pumping. We also assumed that the change in the saturated thickness of the unconfined aquifer due to pumping is negligible. The resulting adjoint equations have a similar form as the forward equations of groundwater flow, and therefore can be solved using standard groundwater flow simulators, such as MODFLOW. We described how to use MODFLOW to solve the adjoint equations, and we presented results using a hypothetical example. The results show that the adjoint method calculates stream depletion accurately for a system that satisfies the assumptions made in this study. Also, the adjoint approach is much more efficient because only one simulation is needed to calculate stream depletion due to pumping at a well at any location in the aquifer.

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Supporting Information

Additional Supporting Information may be found in the online version of this article:

Derivation of the adjoint equations and adjoint sensitivities for pumping in either the confined aquifer or the unconfined aquifer. The adjoint equations are defined for heterogeneous, anisotropic aquifers with general boundary conditions.

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