XIX International Conference on Water Resources
CMWR 2012
University of Illinois at Urbana-Champaign
June 17-22,2012

ADJOINT METHOD TO SIMULATE STREAM DEPLETION DUE TO PUMPING IN A NON-LINEAR COUPLED GROUNDWATER AND SURFACE WATER SYSTEM

Scott A. Griebling* **and Roseanna M. Neupauer***

*University of Colorado Boulder
Department of Civil, Environmental, and Architectural Engineering
1111 Engineering Dr., ECOT 441, UCB 428
Boulder, CO 80309 USA
e-mail: scott.griebling@colorado.edu, neupauer@colorado.edu

Key words: Stream depletion, adjoint method, groundwater modeling

Summary. The goal of this paper is to introduce an adjoint approach for calculating stream depletion in a river that is hydraulically connected to an aquifer. This paper presents the coupled forward and adjoint equations of flow in an unconfined aquifer, a confined aquifer, and in a river. Flow in the river is assumed to follow Manning's equation, and the river is assumed to have a wide, rectangular cross section. With these assumptions, the governing equation of flow in the river is non-linear; thus its adjoint is linear in the adjoint state, but still depends on the state variable of the forward equation, i.e., on the river head. This paper outlines an approach for solving the adjoint equations, which requires some approximations and some modification of a code that solves the forward equations.

1 INTRODUCTION

If a pumping well is extracting water from an aquifer that is hydraulically connected to a river, some of the pumped water will be drawn from the aquifer, while some of the water may be drawn from the river (e.g., Theis, 1941; Glover and Balmer, 1954). Thus, pumping can lead to a decrease in the flow rate of the river, which is called stream depletion. Stream depletion is often estimated through numerical simulation of flow in a coupled groundwater and surface water system. First, a flow simulation is performed to determine the flow rate in the stream in the absence of pumping; then another simulation is performed to determine the flow rate in the stream during pumping; finally, stream depletion is calculated as the difference between these two flow rates (e.g., Sophocleous et al., 1995; Kollet and Zlotnik, 2003). This standard approach is efficient if the locations of the pumping wells are known. It requires one base case simulation without pumping and one additional simulation for each pumping well.

In some cases, stream depletion may be used as a design criterion for siting a new well location. For example, a location for a new well can be chosen so that stream depletion remains below a specified threshold. In this situation, there may be many possible locations for the new well. If the standard approach is used to calculate stream depletion, one additional simulation must be run, in addition to the base case simulation, for each possible well location, which can be computationally infeasible if the number of possible well locations is high.

As an alternative to the standard forward modeling approach, we develop and present an adjoint approach to calculate stream depletion. With just one simulation of the adjoint model, stream depletion is obtained for a well at any location in the aquifer. Although the development of the adjoint equations is straightforward, solving the equations has some challenges. In this paper, we present the forward and adjoint equations for the coupled groundwater and surface water system. Since the forward equations are non-linear, the adjoint equations do not have the same form as the forward equations, and therefore cannot be solved directly using the same method as the forward equations. We discuss the approach for solving the adjoint equations.

2 FORWARD EQUATIONS OF FLOW AND STREAM DEPLETION

We consider a system with an unconfined aquifer that overlies a confined aquifer, with a confining layer between them. A river partially penetrates the unconfined aquifer and is hydraulically connected to it. We assume the river has a wide, rectangular cross-section. For simplicity, we assume that exchange between the river and aquifer is the only internal source or sink of water to the river. The governing equations of flow in the unconfined aquifer, confined aquifer, and river, respectively, are given by

$$\begin{aligned} S_y\frac{\partial h_u}{\partial t} &= \nabla\cdot[\mathbf{K}(h_u-\zeta)\nabla h_u] - Q_{pu}\delta(x-x_w)\delta(y-y_w) + N(x,y) - E(x,y) \\ &\quad -\frac{K_a}{b_a}(h_u-h_c) + \frac{K_r}{b_r}(h_r-h_u)B(\mathbf{x}), \end{aligned} \tag{1}$$

$$S\frac{\partial h_c}{\partial t} = \nabla\cdot\mathbf{T}\nabla h_c - Q_{pc}\delta(x-x_w)\delta(y-y_w) + \frac{K_a}{b_a}(h_u-h_c), \tag{2}$$

$$\frac{\partial Q_{riv}}{\partial s} = -\frac{K_r}{b_r}(h_r-h_u)w\ , \tag{3}$$

where h_u and h_c are the heads in the unconfined and confined aquifers, respectively, $\mathbf{x} = (x,y)$ are spatial coordinates, t is time, S_y is the specific yield, S is the storage coefficient, $\mathbf{K}$ is the hydraulic conductivity tensor, $\mathbf{T}$ is the transmissivity tensor, ζ is the elevation of the bottom of the unconfined aquifer, $(h_u-\zeta)$ is the saturated thickness of the unconfined aquifer, $N(x,y)$ is the natural recharge rate, $E(x,y)$ is the evapotranspiration rate, Q_{pu} and Q_{pc} are the pumping rates for the unconfined and confined aquifers, respectively, (x_w,y_w) is the location of a pumping well, $\delta(\cdot)$ is the Dirac delta function, K_a and b_a are

the hydraulic conductivity and the thickness of the confining layer, respectively, K_r and b_r are the hydraulic conductivity and thickness of the riverbed sediment, respectively, h_r is the head in the river, $B(\mathbf{x})$ is a dimensionless function that has a value of unity at the river and a value of zero elsewhere, Q_{riv} is the flow rate in the river, s is the spatial coordinate along the river channel in the flow direction, and w is the width of the river channel.

Let the boundary and initial conditions be defined as

$$\begin{aligned} h_u(x,y,0) &= h_{u0} \ , & (4)\\ h_u(x,y,t) &= g_{1u}(t) \text{ on } \Gamma_{1u} \ , & (5)\\ \nabla h_u \cdot \mathbf{n} &= g_{2u}(t) \text{ on } \Gamma_{2u} \ , & (6)\\ h_c(x,y,0) &= h_{c0} \ , & (7)\\ h_c(x,y,t) &= g_{1c}(t) \text{ on } \Gamma_{1c} \ , & (8)\\ \nabla h_c \cdot \mathbf{n} &= g_{2c}(t) \text{ on } \Gamma_{2c} \ , & (9)\\ h_r(s,t) &= h_{r0} \ , & (10)\\ Q_{riv}(s,t) &= Q'_{riv}(t) \text{ at } s = 0 \ , & (11) \end{aligned}$$

where g_{ij} are known functions, Γ_{ij} are aquifer boundaries, $i = 1, 2$, $j = u, c$, where u denotes the unconfined aquifer and c denotes the confined aquifer, and h_{u0}, h_{c0}, and h_{r0} are the initial heads in the unconfined aquifer, confined aquifer, and river, respectively.

To relate the river flow rate to the river head, we use Manning's equation, which, for a river with a wide, rectangular cross-section, is given by

$$Q_{riv} \approx \frac{c}{n}(h_r - z_r)^{5/3} S_0^{1/2} w, \tag{12}$$

where c is a constant, n is Manning's coefficient of roughness, z_r is channel bottom elevation, $h_r - z_r$ is the flow depth in the river, and S_0 is channel slope. With this definition, (3) and (11) become

$$\begin{aligned} \frac{\partial}{\partial s}\left[\frac{c}{n}(h_r - z_r)^{5/3} S_0^{1/2}\right] &= -\frac{K_r}{b_r}(h_r - h_u), & (13)\\ h_r(s,t) &= h'_r(t) \text{ at } s = 0 \ . & (14) \end{aligned}$$

Stream depletion, ΔQ_{riv}, is the decrease in river flow rate, Q_{riv}, as a result of pumping, and can be expressed mathematically as

$$\Delta Q_{riv}(x_c, y_c, t_c) = \frac{dQ_{riv}(x_c, y_c, t_c)}{dQ_{pj}} Q_{pj} \ , \tag{15}$$

where t_c is the compliance time (i.e., the time at which stream depletion is desired), (x_c, y_c) is the compliance location (i.e., the location at which stream depletion is desired), and j represents the aquifer in which the pumping occurs ($j = u$ for pumping in the unconfined aquifer, $j = c$ for pumping in the confined aquifer), and $dQ_{riv}(x_c, y_c, t_c)/dQ_{pj}$ is the sensitivity of river flow rate at compliance point to the pumping rate Q_{pj} in aquifer j. The right-hand side of (13) represents the exchange of water between the river and the aquifer; thus, any change in flow rate in the river as a result of pumping is equivalent to a change in the quantity represented by this term. Using this fact, the sensitivity can be calculated as

$$\begin{aligned}\frac{dQ_{riv}(x_c,y_c,t_c)}{dQ_{pj}(x_w,y_w)} &= -\frac{d}{dQ_{pj}(x_w,y_w)}\left[\iiint_{x,y,t}\frac{K_r}{b_r}(h_r-h_u)wB(\mathbf{x})\delta(t-t_c)dx\,dy\,dt\right] \\ &= -\iiint_{x,y,t}\frac{K_r}{b_r}(\psi_r-\psi_u)wB(\mathbf{x})\delta(t-t_c)dx\,dy\,dt\;, \end{aligned} \tag{16}$$

where $\psi_u = \partial h_u/\partial Q_{pj}$ and $\psi_r = \partial h_r/\partial Q_{pj}$. Multiplying this sensitivity by the pumping rate produces the stream depletion, as shown in (15).

To calculate stream depletion for a single, known pumping well location, (1), (2), and (13) are solved to obtain h_u and h_r, which are used in (16) to calculate the sensitivity, which is then used in (15) to calculate the stream depletion.

3 ADJOINT EQUATIONS OF FLOW AND STREAM DEPLETION

While (16) with (15) can be used to calculate stream depletion, it is an inefficient approach if there are many possible pumping well locations because one simulation of (1), (2), and (13) must be run for each possible pumping well location. Instead, the adjoints of (1), (2), and (13) can be solved, with the resulting adjoint states used in an adjoint version of (16) to calculate the sensitivity that leads to stream depletion. With the adjoint approach, only one adjoint simulation is needed to calculate stream depletion for a well at any possible location in the aquifer.

The adjoints of (1), (2), (4) – (9), (13) and (14) are given by (Griebling, 2012)

$$\begin{aligned} S_y\frac{\partial\psi_u^*}{\partial\tau} &= \nabla\cdot[\mathbf{K}(h_u-\zeta)\nabla\psi_u^*] - \frac{K_a}{b_a}(\psi_u^*-\psi_c^*) \\ &\quad + \frac{K_r}{b_r}(\psi_r^*-\psi_u^*)B(\mathbf{x}) \end{aligned} \tag{17}$$

$$S\frac{\partial\psi_c^*}{\partial\tau} = \nabla\cdot\mathbf{T}\nabla\psi_c^* + \frac{K_a}{b_a}(\psi_u^*-\psi_c^*) \tag{18}$$

$$\frac{5c}{3n}S_0^{1/2}(h_r-z_r)^{2/3}\frac{\partial\psi_r^*}{\partial s} = \frac{K_r}{b_r}[\psi_r^*-\psi_u^*] \tag{19}$$

$$\psi_u^*(x,y,0) = \beta + \frac{K_r}{b_r S_y\gamma}B(\mathbf{x})\;, \tag{20}$$

$$\psi_u^*(x,y,t) = \beta \text{ on } \Gamma_{1u} , \tag{21}$$
$$\nabla\psi_u^* \cdot \mathbf{n} = 0 \text{ on } \Gamma_{2u} , \tag{22}$$
$$\psi_c^*(x,y,0) = \beta , \tag{23}$$
$$\psi_c^*(x,y,t) = \beta \text{ on } \Gamma_{1c} , \tag{24}$$
$$\nabla\psi_c^* \cdot \mathbf{n} = 0 \text{ on } \Gamma_{2c} , \tag{25}$$
$$\psi_r^*(s,t) = \beta + \frac{K_r}{b_r\gamma} , \tag{26}$$
$$\psi_r^*(s,t) = \beta \text{ at } s = s_L , \tag{27}$$

where ψ_u^*, ψ_c^*, and ψ_r^* are adjoint states of h_u, h_c, and h_r, respectively, $\tau = t_c - t$ is backward time, s_L is the downstream boundary of the river, β is a constant chosen so that its magnitude is above the magnitude of the aquifer bottom elevation and the river bottom elevation, and γ is a constant defined so that the two terms in (20) and (26) are approximately the same order of magnitude (See Neupauer and Griebling (2011) for more information).

The adjoint equivalent of the sensitivity equation (16) depends on whether a pumping well is in the unconfined or confined aquifer, and is given by (Griebling, 2012)

$$\frac{dQ_{riv}(x_c,y_c,\tau=0)}{dQ_{pu}(x,y)} = -\gamma\int_{\tau=0}^{t_c}\left[\psi_u^*(x,y,\tau)+\beta\right]\,d\tau , \tag{28}$$
$$\frac{dQ_{riv}(x_c,y_c,\tau=0)}{dQ_{pc}(x,y)} = -\gamma\int_{\tau=0}^{t_c}\left[\psi_c^*(x,y,\tau)+\beta\right]\,d\tau , \tag{29}$$

for a pumping well in the unconfined and confined aquifers, respectively.

To solve for stream depletion using the adjoint approach, (17)–(27) are solved to obtain the adjoint states, ψ_u^* and ψ_c^*, which are used in (28) and (29) to obtain the sensitivity, dQ_{riv}/dQ_{pj}, which is then used in (15) to calculate the stream depletion.

4 SOLVING THE ADJOINT EQUATIONS

Comparison of (1) with (17) and of (2) with (18) shows that the adjoint equations of groundwater flow have very similar form as the forward equations of groundwater flow; thus, any code that can solve the forward equations can also be used to solve the adjoint equations. In our work, we use MODFLOW (Harbaugh et al., 2000). A few modification must be made to the MODFLOW input files to use it to solve the adjoint equations of *groundwater* flow:

- The output in MODFLOW is head; however, for the adjoint simulation, we interpret the output as the adjoint states.
- The time variable is interpreted as backward time, τ.

- Recharge, evapotranspiration, and pumping do not appear in the adjoint equation (17), so they are not simulated in the adjoint simulation.
- The first type boundaries on Γ_{u1} and Γ_{c1} have a specified adjoint state value of β.
- Since the second derivative term in (17) contains the state variable of the forward equation, we assume that the change in head is small relative to the saturated thickness, so $h \approx h_{u0}$. To force MODFLOW to use this assumption, we treat the unconfined aquifer as a confined aquifer with $\mathbf{T} = \mathbf{K}(h_{u0} - \zeta)$.
- The initial condition in the adjoint simulation is that the state variable is equal to β everywhere except where $B(\mathbf{x}) = 1$, i.e., at the river, where the state variable in the unconfined aquifer is initially set to $\psi_u^* = \beta + K_r/(b_r S_y \gamma)$.

Comparison of (13) with (19) shows that the forward equation of river flow (13) is nonlinear in the state variable, while its adjoint (19) is linear in the state variable. Because these two equations have different forms, modifications must be made to the code that solves the forward governing equation in order for it to solve the adjoint equation. We use the Stream (STR) package (Prudic, 1989) in MODFLOW to solve the forward equation. The following modifications were made to the STR package:

- The flow direction was reversed so that flow is propagated from the most downstream reach to the most upstream reach.
- The forward code uses the relationship between flow rate and flow depth shown in (12); based on (19), the relationship was modified as

$$\overline{Q}_{riv} = \frac{5c}{3n}(h_{r0} - z_r)^{2/3}\psi_r^* S_o^{1/2} w \ , \tag{30}$$

  where the overbar denotes the adjoint simulation surrogate for the forward model parameter and h_{r0} is the initial head in the river, which is assumed to change slowly.
- The boundary condition is applied at the downstream boundary, and is a specified value of $\overline{Q}_{riv}$ obtained by solving (30) with $\psi_r^* = \beta$.
- The initial value of the state variable is $\psi_r^* = \beta + K_r/(b_r\gamma)$.
- Additional modifications are made to account for spatial variability of S_o, n, w, h_{r0}, and z_r, which are not part of the forward equation, but are necessary in the adjoint solution (see Griebling, 2012).

REFERENCES

[1] R.E. Glover and G.G. Balmer. River depletion resulting from pumping a well near a river, *Transactions of the American Geophysical Union*, **35** 468–470, (1954).

[2] S.A. Griebling. *Quantification of stream depletion due to aquifer pumping using adjoint methodology*, M.S. thesis, University of Colorado Boulder, Boulder, Colorado, in preparation, (2012).

[3] A.W. Harbaugh, E.R. Banta, M.C. Hill, and M.G. McDonald. *MODFLOW-2000, The U.S. Geological Survey modular ground-water model – User guide to modularization concepts and the ground-water flow process*, U.S. Geological Survey Open-File Report 00-92, (2000).

[4] S.J. Kollet and V.A. Zlotnik. Stream depletion preductions using pumping test data from a heterogeneous stream-aquifer system (a case study from the Great Plains, USA), *J. Hydrol.*, **281**, 96–114, (2003).

[5] R.M. Neupauer and S.A. Griebling. Adjoint simulation of stream depletion due to aquifer pumping, *Ground Water*, doi:10.11/j.1745-6584.2011.00901.x, (2011).

[6] D.E. Prudic. *Documentation of a computer program to simulate stream-aquifer relations using a modular, finite difference, ground-water flow model*, U.S. Geological Survey Open-File Report 88-729, (1989).

[7] M. Sophocleous, A. Koussis, J.L. Martin, and S.P. Perkins. Evaluation of simplified stream-aquifer depletion models for water rights administration, *Ground Water*, **33**, 579–588, (1995).

[8] C.V. Theis. The relation between the lowering of the piezometric surface and the rate and duration of discharge of a well using ground-water storage, *Transactions of the American Geophysical Union*, **22**, 734–738, (1941).