

**Quantification of Stream Depletion Due to Aquifer
Pumping Using Adjoint Methodology**

by

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Thesis directed by Professor Roseanna M. Neupauer

Water availability for humans and the environment faces increasing threats from expanding populations and potential reduction in supply due to changes in climactic patterns. In light of these threats, the need to minimize stream depletion, defined as the depletion of flows in streams and rivers caused by groundwater pumping, becomes paramount. Stream depletion associated with pumping wells has been quantified by both analytical and numerical approaches; however, methods for identifying the stream depletion caused by new wells remain inefficient and require separate simulations for each potential well location. In this work, we develop adjoint equations of a coupled groundwater and surface water system that can be solved to calculate stream depletion. We use MODFLOW with the stream package to solve the adjoint equations, and, unlike previous work, we allow the head and resulting flow in the river to change as a result of depletion. With only one simulation of the adjoint equations, stream depletions can be calculated for a well at any location in the aquifer, making it an efficient method for siting future wells.

To

My lovely wife and son who walked this road with me.

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Contents

Chapter

1	Introduction	1
1.1	Problem Statement	1
1.2	Motivation	2
1.3	Background	3
1.3.1	Coupled stream and groundwater flow	3
1.3.2	Stream depletion	4
1.3.3	Analytical Approaches for Quantifying Stream Depletion	4
1.3.4	Numerical Solutions	7
1.3.5	Groundwater law	8
1.4	Adjoint Methodology	9
1.5	Overview	10
2	One-Dimensional Approach	11
2.1	Forward equations for calculating stream depletion	13
2.2	Adjoint equations for stream depletion	15
2.3	Examples	17
3	Multi-Dimensional Approach	23
3.1	Introduction	23
3.2	Previous work	23

3.3	STR package	25
3.4	Forward equations for stream depletion	26
3.5	Adjoint equations for stream depletion	29
3.6	MODFLOW Modifications	34
3.6.1	Input Modifications	34
3.6.2	STR Code Modifications and Input Modifications	37
4	Test Case	42
4.1	Conceptual Model	42
4.2	Forward Simulations	43
4.3	Adjoint Simulation	45
5	Discussion	50
5.1	Assumptions	50
5.2	Limitations	54
6	Conclusion & Future Work	56
6.1	Conclusions	56
6.2	Future Work	57
	Références	59
	Bibliography	59
	Appendix	
A	Adjoint Version of STR Code	63

Tables

Table

2.1	Parameters for one-dimensional model.	19
3.1	Variables used in the STR and STRADJ code	41
4.1	Forward aquifer and model parameters.	44
4.2	Adjoint aquifer and model parameters.	47

Figures

Figure

2.1	Cross section of one-dimensional aquifer	12
2.2	Finite difference cells on an aquifer cross section.	18
2.3	Aquifer head for pumping wells at (a) 190 m and (b) 590 m	20
2.4	Numerical results of 1-D stream depletion.	21
2.5	1-D Volumetric stream depletion for forward and adjoint approaches	22
3.1	Schematic of the multi-dimensional hypothetical aquifer	24
4.1	Stream depletion from forward and adjoint simulations.	46
4.2	Absolute error between the adjoint and forward simulations.	49
4.3	Relative error between the adjoint and forward simulations.	49
5.1	Head in the model domain.	51
5.2	Linear scaling of forward stream depletion with puming rate.	53
5.3	Example of a model domain where a single value of β cannot be met.	54

Chapter 1

Introduction

1.1 Problem Statement

Stream depletion is the reduction in flow rate that results from groundwater pumping in an aquifer that is hydraulically connected to a stream or river. Extracting water from the pumping well lowers the hydraulic head in the aquifer and results in a depletion of flow in the stream or river. The current method used to determine stream depletion from a well is straightforward if the location of the well is known: a simulation of aquifer-river system is run without pumping, then a second simulation is run with pumping, and the difference in flow from the river to the aquifer between the two simulations is the stream depletion. For instances where a new well is to be drilled in a region, it may be desirable to identify locations where stream depletion is below some minimum value. In this case, separate model simulations are needed for each potential well location to identify the stream depletion corresponding to pumping at each location. For finite difference groundwater models, the number of potential well locations can be as large as the number of grid cells in the model domain. If a large domain is to be modeled, the number of potential well locations is large and the resulting number of model simulations required becomes infeasible. Our work provides a method for calculating stream depletion for any well location in the model domain with only one simulation.

1.2 Motivation

The reality of increasing population directly corresponds to an increased demand for water. In the United States, the western states are currently experiencing some of the highest rates of population growth. Based on 2000 to 2030 census projections, the states of Nevada, Arizona, Texas, Utah, Idaho, Washington, Oregon, California, and Colorado ranked as the first, second, fourth, fifth, sixth, ninth, tenth, thirteenth, and fourteenth fastest growing states in the nation, respectively, and the region is projected to grow by 45.8 percent (www.census.gov). Nationally, groundwater currently comprises 33% of public water use and 99% of domestic water use, with several western states using higher percentages of groundwater to meet public use demands (Kenny et al. 2009). As the population increases, so will the need for new groundwater sources.

Climate change also poses a threat to meeting water needs. The western United States is generally characterized by an arid climate and current water managers struggle to meet the existing demand (Brookshire et al. 2002). Climate predictions indicate this area will experience higher temperatures and less rainfall over the next century (Bernstien et al. 2008). A reduction in rainfall will lead to a reduction in available surface water, while higher temperatures will likely lead to higher demand for water. Climate predictions pose a threat to municipal and agricultural water supplies while at the same time increasing demand, both of which stress the already scarce water resources. Groundwater comprises 42% of irrigation water uses, and as agricultural production increases alongside increased water demand from crops due to climate change, new groundwater sources will be developed to satisfy this increase in demand (Kenny et al. 2009).

As new wells are developed in aquifers that are hydraulically connected to surface water, an increase in groundwater pumping will likely lead to depletion of the surface water. A few of the impacts of stream depletion include a reduction in water supply for municipal, agricultural, and domestic uses, a failure to satisfy existing water rights, and destruction of the ecosystems that depend on streams and rivers. The cost of such impacts is high, as seen by the \$30 million in damages the State of Colorado had to pay to the State of Kansas as a result of Colorado groundwater

wells depleting the Arkansas River along the Colorado-Kansas border (**Kansas v. Colorado**, US Supreme Court, 1995). Quantifying this stream depletion is crucial to protecting surface water rights and municipal water supplies as well as protecting the environments that depend on the streams and rivers.

This work develops a method of quantifying stream depletion for a new well that could be placed anywhere in an entire region using the highly efficient adjoint methodology. Information on the amount of depletion in the stream due to pumping anywhere in a model domain can be used to identify preferred well locations that minimize stream depletion. Stream depletion information can also be used to identify river reaches in a model domain that are more sensitive to pumping, thus guiding environmental protection efforts.

1.3 Background

1.3.1 Coupled stream and groundwater flow

Stream depletion from groundwater pumping can only occur when a river is hydraulically connected with an underlying aquifer. Hydraulic connection results in flow between the aquifer and the river; if the head in the river is higher than that of the aquifer, water flows from the river to the aquifer and the system is called a losing river, and if the head in the river is lower than that of the aquifer, water flows from the aquifer to the river and the system is called a gaining river. Water flows faster through river channels than it does through underground aquifers, usually with a difference of an order of magnitude or more. This is due to the fact that groundwater must travel through the pore space of an aquifer and the rate of flow depends on the hydraulic conductivity, with aquifers comprised of sand and gravel having higher hydraulic conductivities and aquifers comprised of clay, shale, and fractured rock having lower hydraulic conductivities. Aquifers may be comprised of layers or regions of different material with different permeability, and two aquifers may be separated by layers of relatively lower porosity called aquitards or confining layers. Most rivers penetrate unconfined aquifers, but in the case of deep rivers or shallow confining layers, a

river may penetrate into a confined aquifer. Flow between a river and an aquifer occurs across the riverbed. The riverbed often has a different permeability than the underlying aquifer as a result of sand and gravel deposits from river sediment or buildups of silt and clay in muddy rivers.

1.3.2 Stream depletion

When a pumping well is drilled in an aquifer and groundwater is extracted, the aquifer head decreases. When the aquifer is hydraulically connected to a river, the lowered head in the aquifer changes the flow pattern between the river and the aquifer. For a losing river, the flow from the river into the aquifer increases. For a gaining river, the flow from the aquifer into the river decreases, and if the aquifer head drops below the river head, the gaining river system becomes a losing river system. Stream depletion refers to the portion of river flow captured by the pumping well that would otherwise remain in the river.

1.3.3 Analytical Approaches for Quantifying Stream Depletion

The development of methods to quantify stream depletion quickly followed the development of equations to calculate non-equilibrium drawdown of aquifer heads by Theis in his seminal 1935 paper (Theis 1935). A number of analytical and semi-analytical approaches have been developed to determine stream depletion for a variety of hypothetical aquifers, and numerical solutions and models have been developed to solve for stream depletion in hypothetical and real aquifers.

A gradual relaxation of physically unrealistic assumptions has marked the development of analytical techniques to quantify stream depletion. Theis (1941) was the first to calculate unsteady stream depletion analytically, using a hypothetical unconfined, homogeneous, isotropic aquifer that has an infinite extent, a constant thickness, a uniform transmissivity, and no evapotranspiration or precipitation. He assumed a pumping well that fully penetrates the aquifer and approximated it as a point. He used an idealized fully-penetrating river represented as a straight line extending beyond the influence of the pumping well with river heads that remain unaffected by pumping and a riverbed that is in free communication with the groundwater. Theis (1941) simulated flow from

the river by placing an image recharge well on the opposite side of the river from the pumping well. He concluded that, for his hypothetical case, depletion depends primarily on transmissivity and the distance between the pumping well and the river. Theis based his analytical solution for stream depletion from the equation for aquifer head drawdown developed in Theis (1935).

Glover and Balmer (1954) developed an analytical solution based on similar assumptions, expressing stream depletion in dimensionless terms as a fraction of total flow from the well. Hantush (1965) relaxed the assumption of direct connection between the riverbed and aquifer by simulating a riverbed with a lower conductivity than the surrounding aquifer.

The effects of a few of the underlying assumptions for the analytical approaches mentioned above were investigated by Spalding and Khaleel (1991) by comparing results of depletion found using numerical models with those found using the earlier analytical methods. They explored the effect on stream depletion of assuming a fully penetrating river, assuming the hydraulic conductivity of the riverbed was the same as that of the surrounding aquifer, and assuming no aquifer storage was available beyond the hypothetical stream. For stream depletion, the assumption that caused the largest difference between the numerical model and the analytical method was the assumption made by Theis (1941) and Glover and Balmer (1954) of the riverbed and the aquifer having the same hydraulic conductivity. Assuming no storage is available beyond the stream also caused significant differences between the numerically calculated stream depletion and the depletion calculated using the analytical methods.

The development of analytical solutions that addressed the inadequacies of the earlier methods began with Hunt (1999) and his analytical approach to stream depletion that accounted for a partially penetrating river and a clogged (semi-pervious) riverbed. Hunt (2003) further developed his analytical solution to apply to scenarios where a stream partially penetrates a leaky aquitard overlying a confined aquifer from which groundwater is extracted. Zlotnik and Huang (1999) also developed an analytical solution for stream depletion that accounts for partial penetration of the river and a riverbed clogging layer.

Butler et al. (2001) developed another analytical solution that accounts for a partially pene-

trating river of finite width in a finite-sized aquifer. Assuming a confined and isotropic aquifer and a fully penetrating well that is screened for the entire length of the confined aquifer, Butler et al. (2001) demonstrated how the assumption of a fully penetrating stream can lead to overestimations of stream depletion ranging from 100% to 1000% for most realistic scenarios. Their analytical solution assumed only a small degree of river penetration relative to the aquifer thickness and river levels that do not change as a result of pumping.

Zlotnik (2004) built on previous analytical solutions to develop a method of determining the maximum stream depletion rate (MSDR), which he defined as the fraction of the pumping rate supplied by stream depletion achieved once the system has reached steady state after pumping. Previous analytical solutions predicted the MSDR eventually reaching 100%, however this is unrealistic as most aquifers receive some degree of recharge from leaky aquitards that bound them. Zlotnik (2004) showed a range of MSDR for various aquifer and stream configurations and found the MSDR depends on the distance of the pumping well from the stream and from sources of recharge and discharge as well as the hydraulic conductivity of the aquitard.

Butler et al. (2007) extended Zlotnik's (2004) work to provide a semi-analytical method of determining stream depletion and drawdown when pumping occurs in an unconfined aquifer where recharge can come both from the stream and from the underlying confined aquifer separated from it by a leaky aquitard. As the location of the pumping well from the stream increases, the amount of recharge that originated at the stream decreases while the recharge from the underlying aquifer increases. The location at which stream depletion becomes negligible compared to recharge across the leaky aquitard depends on the properties of the riverbed, unconfined aquifer, and aquitard. Zlotnik and Tartakovsky (2008) furthered the scope of this analytical method by accounting for an aquifer with a finite width.

Hunt (2009) also developed an analytical solution for stream depletion in a two layered leaky aquifer system and used it to compare stream depletion found using the assumption of infinite storage in the underlying aquifer with those found under conditions of finite storage in the underlying aquifer. This comparison indicated that Zlotnik's (2004) maximum stream depletion

rate underestimated stream depletion.

Sun and Zhan (2007) investigated stream depletion using a scenario with two parallel rivers. Using a semi-analytical method, they observe the impact of varying riverbed hydraulic conductivity and well location on stream depletion. The ratio of hydraulic conductivities of the riverbeds proves to be the most important factor impacting stream depletion, with the riverbed thickness ratio playing a lesser role. Yeh et al. (2008) examined stream depletion in wedge-shaped aquifers formed by the confluence of two rivers.

1.3.4 Numerical Solutions

As mentioned in the previous section, the work of Spalding and Khaleel (1991) exposed the shortcomings of the analytical methods. Sophocleous et al. (1995) performed a similar investigation of the assumptions made using the Glover Balmer method by comparing them to the numerical solution found using MODFLOW. Both works highlighted the need for more realistic approaches to quantifying the behavior of stream and aquifer flow in the presence of pumping.

Computer-based numerical models have become the standard approach for investigating stream depletion due to the complex nature of natural aquifer systems. A few examples of these applications include the work of Chen and Yin (1999) involving numerical solutions used in concert with field measurements to show that stream depletion is sensitive to vertical anisotropy and Chen and Yin's (2001) and Chen and Shu's (2002) investigation into the role of baseflow in stream depletion calculations.

Numerical models have been used to aid in siting new wells in the work of Di Matteo and Dragoni (2005) involving a steady state model. Leake (2010) also employed numerical solutions to investigate stream depletion, developing a new method to identify and map stream depletion for an area with a number of possible well locations.

1.3.5 Groundwater law

The evolution of groundwater law in the United States has increased the demand for groundwater modeling. While groundwater and surface water have traditionally been managed as separate entities, many states now recognize the connection between surface and groundwater flows and integrated management approaches are being developed to ensure the protection of both surface and groundwater users' rights.

Colorado was one of the first states to recognize the connection between surface and groundwater and incorporate groundwater into its administration of surface water (Tarlock 2009). Colorado is the only state in the nation with a water rights system based entirely on water courts rather than permits. Colorado's water rights, like many states in the western United States, are based on the doctrine of prior appropriation where the priority of a water right is determined by the date of the right. In the event of a water shortage, those holding old water rights, called "seniors", can require others holding younger water rights, called "juniors", to stop using their water, allowing the seniors to fulfill their full entitlement. Most rivers in Colorado are fully allocated or over allocated, meaning more water rights exist than a river's flow will actually provide in most years. New junior users may only receive water in very wet years while in dry years only the most senior users might receive their entitlement.

In Colorado, water law traditionally focused on disputes over the rights of surface water users until the Ground Water Management Act of 1965 (Colorado Revised Statute Section 37-90-101 to 37-90-143). The Act included groundwater in the priority system for surface water and required that all groundwater be presumed as tributary to surface water unless proven otherwise. Groundwater users must apply for water rights subject to the same priority dates as surface water users and can also have their wells shut off if a senior user is not receiving his or her full entitlement. A new groundwater well will enter the priority system as the most junior user and may not be a dependable source of water during dry years.

Groundwater that is proven to not be connected to surface water is called nontributary

groundwater and is not managed within the priority system of existing water rights. Nontributary groundwater is defined as groundwater that “the withdrawal of which will not, within one hundred years, deplete the flow of a natural stream . . . at an annual rate greater than one-tenth of one percent of the annual rate of withdrawal” (Colorado Revised Statute Section 37-90-103-10.5). A well pumping nontributary groundwater only requires a well permit from the state, not a water right. Colorado relies on groundwater modeling to determine if a given well will extract tributary or nontributary groundwater.

1.4 Adjoint Methodology

In this work we develop adjoint sensitivity equations for coupled groundwater-surface water systems. The adjoint method is a type of sensitivity analysis that efficiently provides information on the sensitivity of a system state to changes in a system parameter.

To find the sensitivity, the performance measure of interest is identified and written as a function of the system parameter of interest and the system state. The general form of this performance measure is

$$P = \int_{\Omega} f(\alpha, h) d\Omega, \quad (1.1)$$

where P is the performance measure, Ω is the system domain, α is the system parameter, and h is the system state. The sensitivity is found by differentiating (1.1) with respect to the system parameter.

$$\frac{dP}{d\alpha} = \int_{\Omega} \left[\frac{\partial f(\alpha, h)}{\partial \alpha} + \frac{\partial f(\alpha, h)}{\partial h} \psi \right] d\Omega, \quad (1.2)$$

where $\psi = \partial h / \partial \alpha$ is the marginal sensitivity of the system state to changes in the system parameter. The resulting expression must be evaluated at every point in the system’s domain where the sensitivity is desired to obtain information on the sensitivity.

To avoid evaluating the sensitivity at every location we manipulate the sensitivity equation and develop adjoint forms of the state sensitivities. Equation (1.2) is modified by eliminating ψ and replacing it with an adjoint state ψ^* that is related to the sensitivity of interest and the governing

equation for ψ^* is defined. This procedure is used in Chapters 2 and 3.

The adjoint method has been applied to solve problems in fields ranging from economics to aerodynamics. Vemuri and Karplus (1969) were some of the first to apply the adjoint approach to solve groundwater problems using hybrid computing, however computing power at the time limited the scope of their application. Since then, others have investigated the usefulness of the adjoint approach for parameter estimation, including Neuman (1980), Sun and Yeh (1985), Townley and Wilson (1985), Lu et. al (1988), Yeh and Sun (1990), Yeh and Zhang (1996), Fienen et. al (2008), Cardiff and Kitanidis (2008), and Wu et. al (2008). The adjoint approach has also been used for sensitivity analysis by Sykes et. al (1985), Wilson and Metcalfe (1985), Skaggs and Barry (1996), Li and Yeh (1998), Cirpka and Kitanidis (2001), and Jyrkama and Sykes (2006). Other uses of the adjoint methodology to solve groundwater problems include the work of Ahlfeld et al. (1988) and Tan et al. (2008) on optimization, Neupauer and Wilson's (1999, 2001) and Michalak and Kitanidis' (2004) work on source identification, and LaVenue and Pickens' (1992) work on model calibration.

In this work we apply the adjoint theory to a coupled groundwater-surface water system to investigate the sensitivities of a system state in the surface water system (the stream flow rate) due to changes in a parameter in the groundwater system (pumping rate).

1.5 Overview

In Chapter 2 we develop the adjoint methodology for a hypothetical one-dimensional aquifer, deriving the adjoint equations from the standard forward equations used to describe stream depletion. We then use numerical simulations to confirm the adjoint approach agrees with the standard approach. In Chapter 3 we develop the adjoint methodology for a multi-dimensional coupled system where stream flowrate is related to stream stage through Manning's equation. In Chapter 4 we use MODFLOW for both forward and adjoint models to calculate stream depletion. We describe how to use MODFLOW to solve the adjoint equations and we modify the code of the stream (STR) package in MODFLOW to handle the adjoint equations. In Chapter 5 we discuss the assumptions and limitations of our method and in Chapter 6 we restate our conclusions and discuss future work.

Chapter 2

One-Dimensional Approach

We begin our development of the adjoint methodology with a one-dimensional (1-D) river-aquifer system. The river partially penetrates a confined aquifer separated from an overlying unconfined aquifer by an impermeable confining layer and bounded on the bottom by impermeable bedrock, shown in Figure 2.1. The river and the aquifer are assumed to be of infinite extent in the y -direction and the left and right boundaries of the confined aquifer have a fixed head boundary conditions, while the upper and lower boundaries have no flow boundary conditions. A pumping well extracts water from the confined aquifer, and groundwater flow in the confined aquifer is assumed to be essentially horizontal and toward the well. Lateral flow across the river banks is assumed to be zero, as are losses or gains from precipitation or evaporation. We call the time period for which we are interested in depletion the compliance time period, t_0 to t_c .

We use this one-dimensional aquifer-river system to calculate stream depletion for a pumping well at any position in the confined aquifer, first using the standard approach (which we call the "forward model") in section 2.1 and then using the adjoint approach in section 2.2. Finally, section 2.3 presents results from numerical simulations of both the forward and adjoint method of calculating stream depletion. Due to the constraints of a one-dimensional model, we consider stream depletion in terms of changes in river stage due to pumping rather than changes in stream flow.

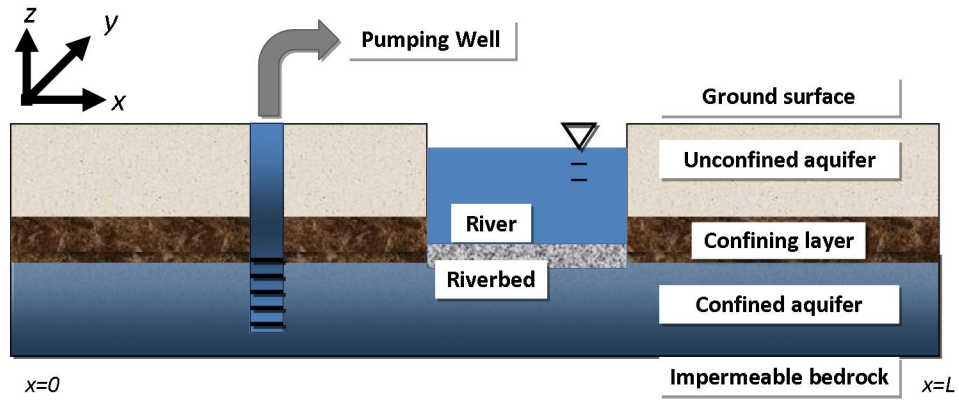


Figure 2.1: Cross section of one-dimensional aquifer

2.1 Forward equations for calculating stream depletion

The governing equation for groundwater flow in this one-dimensional aquifer, which includes terms for aquifer pumping and flow across the riverbed, is

$$S \frac{\partial h}{\partial t} = T \frac{\partial^2 h}{\partial x^2} - Q'_p \delta(x - x_w) + \frac{K_r}{b_r} (h_r - h) B(x), \quad (2.1)$$

with boundary and initial conditions given by

$$h = h_0 \text{ at } x = 0 \text{ and } x = L \quad (2.1a)$$

$$h(x, 0) = h_0 \quad (2.1b)$$

$$h_r(x, 0) = h_{r0} \quad (2.1c)$$

where S is the storage coefficient of the confined aquifer, h is the aquifer head, t is time, T is the transmissivity of the confined aquifer, x is the spatial coordinate, Q'_p the well pumping rate per unit length at x_w , $\delta(x - x_w)$ is the Dirac delta function, x_w is the location of the well, K_r is the riverbed hydraulic conductivity, b_r is the riverbed thickness, h_r is the river head, and $B(x)$ is a dimensionless function that has a value of unity at the river and a value of zero elsewhere.

The mass balance equation for flow in the river is

$$\frac{\partial V_{riv}}{\partial t} = Q_{rb} \quad (2.2)$$

where V_{riv} is the volume of a river segment and Q_{rb} is the flow rate of water from the aquifer to the river across the riverbed, defined using Darcy's law as $Q_{rb} = -A_{rb} \frac{K_r}{b_r} (h_r - h)$, where $A_{rb} = wl$ is the riverbed area per unit length of river, w is the river bed width, and l is unit length. Q_{rb} is positive if flow is entering the river from the aquifer (a gaining river) and negative if flow is leaving the river into the aquifer (a losing river). Assuming a rectangular river channel, the volume of a river segment is defined as $V_{riv} = wl(h_r - z_r)$ where z_r is the riverbed elevation. Using this expression and Darcy's law, (2.2) expands to

$$\frac{\partial V_{riv}}{\partial t} = \frac{\partial}{\partial t} [wl(h_r - z_r)] = -wl \frac{K_r}{b_r} (h_r - h) \quad (2.3)$$

Assuming z_r does not change over time and canceling wl from both sides, (2.3) is expressed in terms of h_r as

$$\frac{\partial h_r}{\partial t} = -\frac{K_r}{b_r}(h_r - h) \quad (2.4)$$

with the same initial conditions as shown in (2.1b) and (2.1c).

As mentioned in 1.3.2, stream depletion is defined as the decrease in stream flow due to aquifer pumping. For this one-dimensional model, the river runs in the y -direction, perpendicularly to the aquifer. The y -direction is not modeled and, consequently, river flow can not be modeled. To model stream depletion we define it as the change in river volume due to pumping and calculate the volume of water leaving or entering the stream from the aquifer.

River volume per unit length, defined as $V'_{riv} = V_{riv}/l$, is found by integrating (2.3) over time to obtain

$$V'_{riv} = V'_{riv_0} - \iint_{x,t} \frac{K_r}{b_r}(h_r - h)B(x) dx dt, \quad (2.5)$$

where $w = \int_x B(x) dx$. The sensitivity of river volume to changes in pumping rate is found by taking the derivative of (2.5) with respect to the pumping rate to obtain

$$\frac{dV'_{riv}}{dQ'_p} = \frac{d}{dQ'_p} \left[V'_{riv_0} - \iint_{x,t} \frac{K_r}{b_r}(h_r - h)B(x) dx dt \right]. \quad (2.6)$$

By employing the definitions $\psi_r = \partial h_r / \partial Q'_p$ and $\psi = \partial h / \partial Q'_p$ and defining stream depletion as positive for flow from the river into the aquifer, (2.6) is rewritten as

$$\frac{dV'_{riv}}{dQ'_p} = \iint_{x,t} \frac{K_r}{b_r}(\psi_r - \psi)B(x) dx dt. \quad (2.7)$$

Once solved, the sensitivity expressed in (2.7) provides the stream depletion values that result from pumping at one location in the aquifer. Equations (2.1) and (2.4) are first solved to find $h(x, t)$ and $h_r(x, t)$ over the compliance time, t_c , which is the time for which depletion information is desired, in the absence of pumping then solved again with a pumping well activated. The values of $h(x, t)$ and $h_r(x, t)$ found with and without pumping are used to calculate $\psi(x, t)$ and $\psi_r(x, t)$ then (2.7) is solved to determine stream depletion. This value of stream depletion depends on the location of the pumping well; calculating stream depletion values at a different well requires solving (2.1) and (2.4)

with a pumping well activated at the new location to find $\psi(x, t)$ and $\psi_r(x, t)$ then solving (2.7) to provide depletion values. To determine stream depletion values for an entire aquifer requires solving (2.1), (2.4), and (2.7) for each potential well location in the aquifer, a process which proves computationally inefficient.

2.2 Adjoint equations for stream depletion

The adjoint approach greatly reduces this computational burden. The derivation of the adjoint equations for calculating stream depletion builds off the sensitivity of river volume to change in pumping rate developed in the previous section. Similarly to (2.7), we derive an expression for $\frac{dV'_{riv}}{dQ'_p}$, however, we avoid solving for all $\psi(x, t)$ values by focusing only on the head changes at the river. Our related expression for $\frac{dV'_{riv}}{dQ'_p}$ contains new variable in place of ψ and ψ_r . We begin by taking the derivatives of (2.1) and (2.4) with respect to the system parameter, Q_p , resulting in

$$0 = -S \frac{\partial \psi}{\partial t} + T \frac{\partial^2 \psi}{\partial x^2} - \delta(x - x_w) + \frac{K_r}{b_r} (\psi_r - \psi) B(x) \quad (2.8)$$

$$0 = -\frac{\partial \psi_r}{\partial t} B(x) - \frac{K_r}{b_r} (\psi_r - \psi) B(x). \quad (2.9)$$

Next, we introduce two arbitrary functions, ψ^* and ψ_r^* , which will become the adjoint states for aquifer head, h , and river head, h_r , respectively. We take the inner product of each term in (2.8) with ψ^* and of each term in (2.9) with ψ_r^* to obtain

$$0 = \iint_{x,t} \left[-\psi^* S \frac{\partial \psi}{\partial t} + \psi^* T \frac{\partial^2 \psi}{\partial x^2} - \psi^* \delta(x - x_w) + \psi^* \frac{K_r}{b_r} (\psi_r - \psi) B(x) \right] dx dt \quad (2.10)$$

$$0 = \iint_{x,t} \left[-\psi_r^* \frac{\partial \psi_r}{\partial t} B(x) - \psi_r^* \frac{K_r}{b_r} (\psi_r - \psi) B(x) \right] dx dt \quad (2.11)$$

with the inner product defined as

$$\langle f, g \rangle = \iint_{x,t} fg dx dt.$$

Equations (2.10) and (2.11) are added to (2.7). Because the right hand sides of both (2.10) and (2.11) evaluate to zero, adding them to the right hand side of (2.7) is equivalent to adding zero,

yielding

$$\begin{aligned} \frac{dV_{riv}}{dQ'_p} = \iint_{x,t} \left[-\psi^* S \frac{\partial \psi}{\partial t} + \psi^* T \frac{\partial^2 \psi}{\partial x^2} - \psi^* \delta(x - x_w) + \psi^* \frac{K_r}{b_r} (\psi_r - \psi) B(x) \right. \\ \left. - \psi_r^* \frac{\partial \psi_r}{\partial t} B(x) - \psi_r^* \frac{K_r}{b_r} (\psi_r - \psi) B(x) + \frac{K_r}{b_r} (\psi_r - \psi) B(x) \right] dx dt. \end{aligned} \quad (2.12)$$

Now we use the product rule on the terms in (2.12) containing derivatives of ψ and ψ_r to obtain terms containing derivatives of ψ^* and ψ_r^* . This operation results in divergence terms which will be used to define the boundary conditions for our derivation. The product rule expansion for each term is

$$-\psi^* S \frac{\partial \psi}{\partial t} = -S \frac{\partial}{\partial t} (\psi^* \psi) + S \psi \frac{\partial \psi^*}{\partial t} \quad (2.13)$$

$$\psi^* T \frac{\partial^2 \psi}{\partial x^2} = T \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} \right) - T \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} = T \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} \right) - T \frac{\partial}{\partial x} \left(\psi \frac{\partial \psi^*}{\partial x} \right) + T \psi \frac{\partial^2 \psi^*}{\partial x^2} \quad (2.14)$$

$$-\psi_r^* \frac{\partial \psi_r}{\partial t} B(x) = -\frac{\partial}{\partial t} (\psi_r^* \psi_r) B(x) + \psi_r \frac{\partial \psi_r^*}{\partial t} B(x). \quad (2.15)$$

All terms on the right hand side of (2.13) through (2.15) are divergence terms except the last term in each equation. Using (2.13), (2.14), and (2.15), (2.12) is rewritten as

$$\begin{aligned} \frac{dV_{riv}}{dQ'_p} = \iint_{x,t} \left[-S \frac{\partial}{\partial t} (\psi^* \psi) + S \psi \frac{\partial \psi^*}{\partial t} + T \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} \right) - T \frac{\partial}{\partial x} \left(\psi \frac{\partial \psi^*}{\partial x} \right) + T \psi \frac{\partial^2 \psi^*}{\partial x^2} \right. \\ \left. - \psi^* \delta(x - x_w) + \psi^* \frac{K_r}{b_r} (\psi_r - \psi) B(x) - \frac{\partial}{\partial t} (\psi_r^* \psi_r) B(x) + \psi_r \frac{\partial \psi_r^*}{\partial t} B(x) \right. \\ \left. - \psi_r^* \frac{K_r}{b_r} (\psi_r - \psi) B(x) + \frac{K_r}{b_r} (\psi_r - \psi) B(x) \right] dx dt. \end{aligned} \quad (2.16)$$

We rearrange (2.16) to isolate terms with ψ and ψ_r and divergence terms

$$\begin{aligned} \frac{dV_{riv}}{dQ'_p} = \iint_{x,t} \left[\psi \left\{ S \frac{\partial \psi^*}{\partial t} + T \frac{\partial^2 \psi^*}{\partial x^2} + \frac{K_r}{b_r} (\psi_r^* - \psi^* - 1) B(x) \right\} \right. \\ \left. + \psi_r \left\{ \frac{\partial \psi_r^*}{\partial t} B(x) - \frac{K_r}{b_r} (\psi_r^* - \psi^* - 1) B(x) \right\} - \psi^* \delta(x - x_w) \right] dx dt + \text{divergence terms}, \end{aligned} \quad (2.17)$$

where the divergence terms are

$$\iint_{x,t} \left[-S \frac{\partial}{\partial t} (\psi^* \psi) + T \frac{\partial}{\partial x} \left(\psi^* \frac{\partial \psi}{\partial x} \right) - T \frac{\partial}{\partial x} \left(\psi \frac{\partial \psi^*}{\partial x} \right) - \frac{\partial}{\partial t} (\psi_r^* \psi_r) \right] dx dt. \quad (2.18)$$

Now we define the arbitrary functions ψ^* and ψ_r^* so that ψ and ψ_r are removed from (2.17) to obtain

$$S \frac{\partial \psi^*}{\partial \tau} = T \frac{\partial^2 \psi^*}{\partial x^2} + \frac{K_r}{b_r} (\psi_r^* - \psi^* - 1) B(x) \quad (2.19)$$

$$\frac{\partial \psi_r^*}{\partial \tau} B(x) = -\frac{K_r}{b_r} (\psi_r^* - \psi^* - 1) B(x) \quad (2.20)$$

where $\tau = t_c - t$ is backward time and t_c is the compliance time. The divergence terms in (2.18) are set equal to zero by defining the boundary and initial conditions on ψ^* and ψ_r^* as follows,

$$\psi^* = 0 \text{ at } x = 0 \text{ and } x = L, \quad (2.21)$$

$$\psi^*(x, 0) = 0 \text{ and } \psi_r^*(x, 0) = 0. \quad (2.22)$$

Equations (2.19) represents the adjoint of (2.1) and (2.20) represents the adjoint of (2.3). Their state variables, ψ^* and ψ_r^* , are the adjoint states of h and h_r , respectively. Employing the above definitions allows (2.17) to reduce to

$$\frac{dV_{riv}}{dQ'_p(x_w)} = \iint_{x,t} -\psi^*(x, t) \delta(x - x_w) dx dt = \int_t -\psi^*(x_w, t) dt. \quad (2.23)$$

We use a change of variable, replacing x_w with x , to get dV_{riv}/dQ'_p for any x location, resulting in

$$\frac{dV_{riv}}{dQ'_p} = \int_t -\psi^*(x, t) dt. \quad (2.24)$$

Equations (2.24), (2.19), and (2.20) comprise the system of equations used to find stream depletion. Solving (2.19) and (2.20) for ψ^* and then integrating ψ^* over the time domain as indicated in (2.24) yields stream depletion values for any well location in the aquifer.

2.3 Examples

Numerical simulations of both the forward and adjoint method are used to confirm the derivations above. Equations (2.1), (2.4), (2.7), (2.19), (2.20), and (2.24) are evaluated in MATLAB to calculate the volumetric stream depletion (dV'_{riv}/dQ'_p) for the river-aquifer system. The numerical model runs a cell-centered finite difference approximation with uniform discretization. The Euler

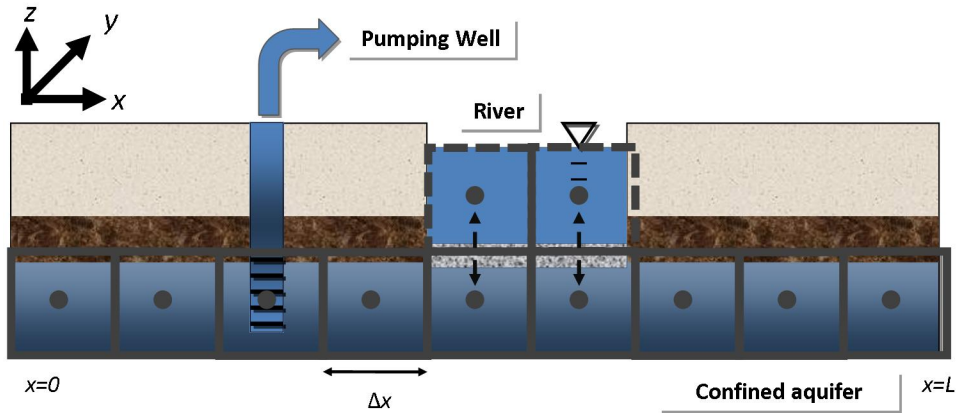


Figure 2.2: Finite difference cells on an aquifer cross section. Boxes represent finite difference cells and circles within the boxes represent where head is approximated. Arrows represent flow across the riverbed.

backward method is used to calculate h and ψ^* and the Euler forward method is used to calculate h_r and ψ_r^* . Figure 2.2 shows an example finite difference grid with a discretization of Δx overlaid on the aquifer cross section from Figure 2.1. The aquifer is divided into cells and the head is calculated at the center of each cell. The river is also divided into cells, shown by dashed boxes, and the river head is connected to the aquifer via flow across the riverbed. The values of the parameters used in the model are shown in Table 2.1.

For the forward model, an initial simulation is run without pumping to establish a baseline change river volume, V_{riv}^l over the model run. For this model, the initial head in the aquifer, h_0 , and the initial head in the river, h_{r0} , are the same so there is no change in river volume when there is no pumping in the aquifer. Once the baseline river volume is established, the model is run with a pumping well activated in one of the model grid cells. We use a unit pumping rate of $1 \text{ m}^3/\text{d}/\text{m}$, noting that depletion will increase linearly as pumping rate increases. Figure 2.3 shows the aquifer head at the end of the model run, $h(x, t_c)$, for two different pumping well locations and the river located at $x = 800 \text{ m}$. Head varies from 10 m at the constant head boundaries ($x = 0 \text{ m}$ and $x = 1600 \text{ m}$) to just above 6 m when the pumping well is at 190 m and to about 4 m when the pumping well is located at 590 m. Figure 2.3 illustrates the effect of pumping well location on

Table 2.1: Parameters for one-dimensional model.

Aquifer length, L	1600 m
Initial aquifer head, h_0	10 m
Storage coefficient, S	0.0001
Transmissivity, T	2 m ² /d
Pumping rate per unit length, Q'_p	0.05 m ³ /d/m
River width, w	50 m
Initial river head, h_r	10 m
Riverbed hydraulic conductivity, K_r	0.0001 m/d
Riverbed thickness, b_r	1 m
Simulation spatial discretization, Δx	20 m
Simulation temporal discretization, Δt	1 d
Compliance time, t_c	20 d
Spatial extent where $B(x) = 1$	775 m to 825 m

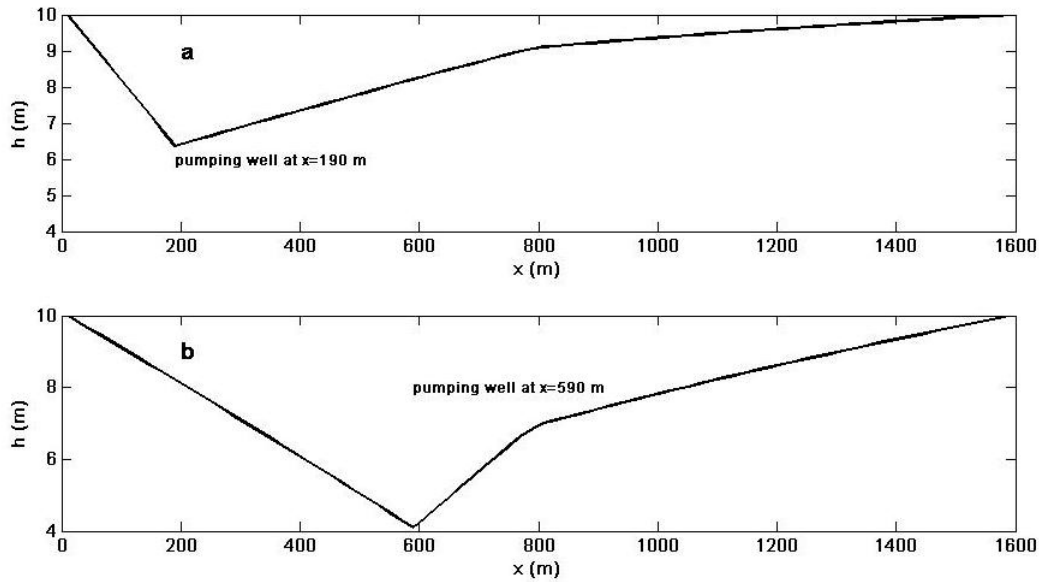


Figure 2.3: Aquifer head for pumping wells at (a) 190 m and (b) 590 m

stream depletion, showing a lower aquifer head when the pumping well is closer to the river at 600 m (subplot b on Figure 2.3) than when the pumping well is farther from the river at 200 m (subplot a on Figure 2.3). When the aquifer head below the riverbed is lower, more water will enter the aquifer from the river and the stream depletion will be larger.

Figure 2.3 only shows the aquifer head at the end of the model run, t_c . To calculate stream depletion, the volume of water that passes from the river to the aquifer during each time step is added to find the total change in river volume. This total change in river volume is then divided by the pumping rate, Q'_p , to obtain stream depletion. Stream depletion from a pumping well at any location across the entire aquifer domain can be found by running separate forward simulations for each potential well location. For this model, a discretization of 20 m resulted in 80 cells for the 1600 m aquifer, so 80 separate forward runs are needed to calculate the depletion across the aquifer. The number of model runs increases as the discretization increases, making this method computationally inefficient for identifying stream depletion for a well anywhere in the aquifer. The adjoint model provides depletion values for a well at any location in the aquifer in a more efficient manner, requiring only one model run to determine stream depletion. The adjoint model solves

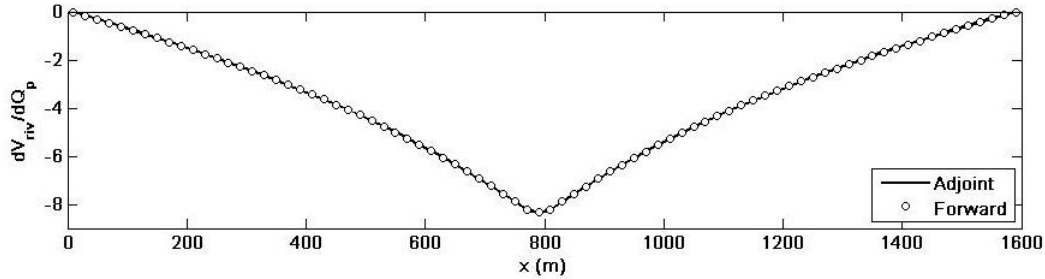


Figure 2.4: Numerical results of 1-D stream depletion for forward and adjoint approaches

(2.19)), (2.20), and (2.24) using a similar model structure as the forward model. The values of ψ^* are calculated at each time step then integrated over time to produce the total depletion for the model run.

The results of the forward and adjoint numerical simulations are shown in Figure 2.4. For each position in the spatial domain, the plot shows the stream depletion that would occur if a well is pumped at that location, with units of days (m^3 per m^3/d). For example, a well pumping at $x = 190$ m produces a depletion of -1.422 days while a well pumping at $x = 590$ m produces a depletion of -5.5201 days. As shown in Figure 2.3, depletion increases as the pumping well location moves towards the river in the center ($x = 800$ m). Stream depletion is equal to zero when the pumping well is located at the boundaries ($x = 0$ m and $x = 1600$ m) due to the constant head boundary condition.

The forward and adjoint simulations agree closely with each other across the aquifer, with the greatest variance occurring at the river. Stream depletion values at the river are -8.3389 days for the forward simulation and -8.3589 days for the adjoint simulation, differing by 0.0135 days. The adjoint solution varies from the forward solution by 0.1276% of the forward solution near the boundaries and 0.1614% of the forward solution below the river, indicating the adjoint solution accurately calculates stream depletion for this one-dimensional case.

Another expression of stream depletion for the one-dimensional simulations is shown in Figure 2.5 as the change in stream volume due to changes in pumping volume. This volumetric stream depletion has units of m^3 per m^3 and represents the fraction of river volume removed from the

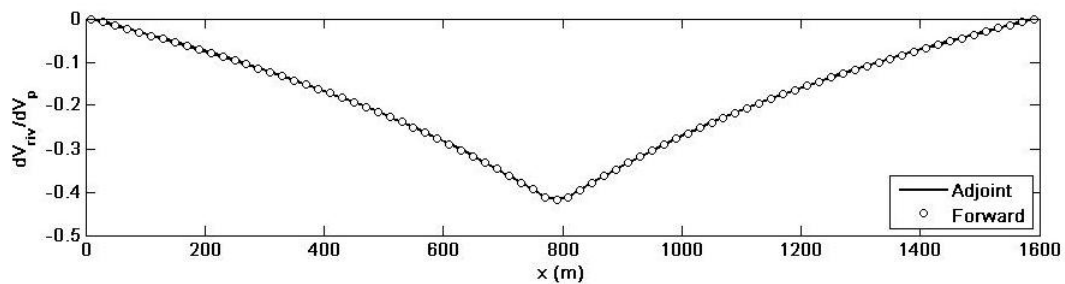


Figure 2.5: 1-D Volumetric stream depletion for forward and adjoint approaches

pumping well, with unity being the upper bound. Figure 2.5 shows stream depletion values varying from zero at the boundaries to -0.4176 at the river, indicating just under half of the water in the river is extracted by the pump if a well pumps adjacent to the river.

Chapter 3

Multi-Dimensional Approach

3.1 Introduction

With the confirmation of the adjoint methodology from the one-dimensional simulation, we proceed to derive the adjoint equations for more complex, multi-dimensional cases. A hypothetical river-aquifer system, shown in Figure 3.1, is used in the development of the forward and adjoint methodology. A river partially penetrates an unconfined aquifer that is separated from an overlying unconfined aquifer by a confining layer. The confined aquifer is bounded below by a layer of impermeable bedrock. The right and left edges of the aquifer system, $x = 0$ and $x = L_x$, respectively, have no flow boundaries and fixed head boundaries exist at $y = 0$ and $y = L_y$. We investigate the depletions associated with wells pumping in either the unconfined aquifer or the confined aquifer.

We begin by discussing previous work of Neupauer and Griebing (2011) using the adjoint methodology and MODFLOW's River package to calculate stream depletion when the river head is known in section 3.2 and present some background on MODFLOW's STR package in Section 3.3. We then proceed to develop the equations for the forward and adjoint stream depletion calculations in Sections 3.4 and 3.5. Section 3.6 details the modifications to the MODFLOW code that we made in order for it to solve the adjoint equations.

3.2 Previous work

The adjoint methodology was used by Neupauer and Griebing (2011) to evaluate stream depletion in a multi-dimensional aquifer. The aquifer-river system used to develop the methodology

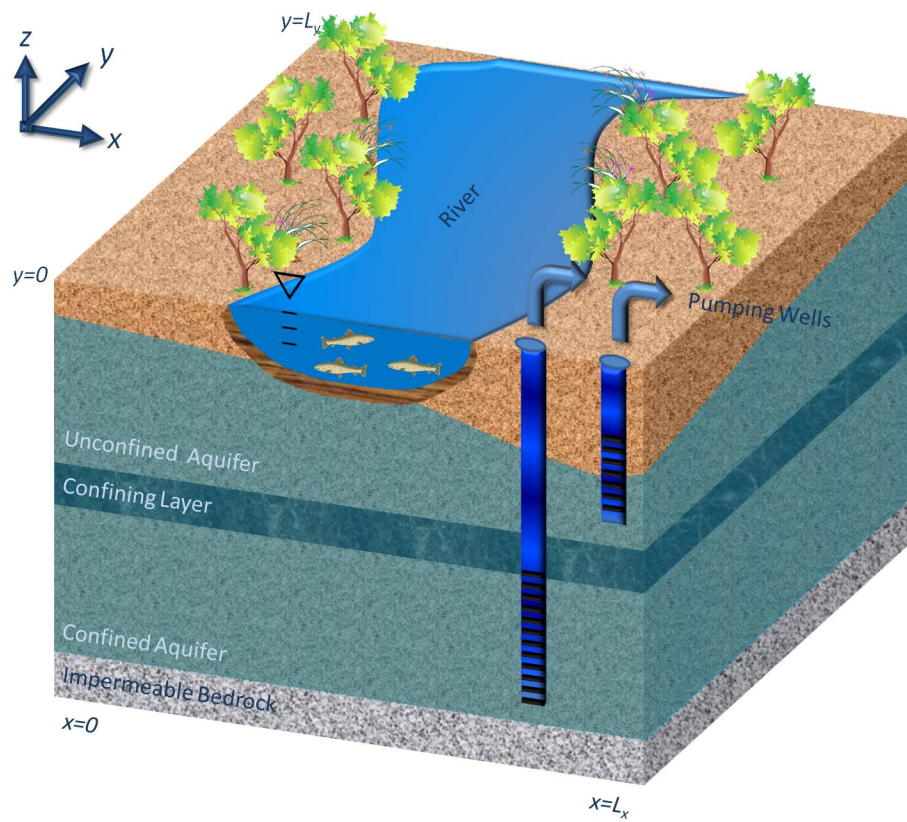


Figure 3.1: Schematic of the multi-dimensional hypothetical aquifer

included an unconfined aquifer separated from a confined aquifer by a leaky confining layer with a river partially penetrating the unconfined aquifer. Groundwater pumping extracted water from either the unconfined or the confined aquifer. The river head was assumed to be independent of the aquifer system, requiring a user-specified head in the river. Stream depletion was evaluated as the decrease in the rate of water flowing from the river into the aquifer due to a change in pumping.

MODFLOW's River (RIV) package was used to simulate the interaction between the aquifer and the river for a hypothetical aquifer with a user-specified head in the river. The adjoint equations developed by Neupauer and Griebing (2011) had similar forms to the forward equations solved in MODFLOW, allowing them to be solved in MODFLOW with some modifications to the forward model input. The adjoint stream depletion was compared to the stream depletions found using forward simulations and they were found to be within six percent of each other.

3.3 STR package

The assumption of river head behaving independently of the aquifer system made by Neupauer and Griebing (2011) is not realistic and the stage in many rivers is connected to the hydraulic head in the underlying aquifer. To better capture the behavior of natural systems, we develop an adjoint approach that couples the behavior of the river stage to the head in the aquifer. The adjoint methodology is developed to be used in the Streamflow Routing (STR) package of MODFLOW (McDonald and Harbaugh 1988). Surface flows were first incorporated into MODFLOW with the River package in the original MODFLOW code. The River (RIV) package connects surface flows with the groundwater flows by adding a term to the groundwater flow equations that accounts for flow across the riverbed. Flow across the riverbed is calculated using a user-defined river head, riverbed thickness, and riverbed hydraulic conductivity to calculate Darcy's law across the riverbed. The River package assumes that model cells underlying river segments remain fully saturated.

The STR package was developed by Prudic (1989) and couples the river and aquifer systems more fully than the RIV package because streamflow, and consequently river head, change as a result of exchange with the groundwater. This is the main improvement in the STR package and it

uses Manning's equation to calculate changes in streamflow and river head with the assumption of a wide rectangular river channel. It calculates flow across the riverbed in a similar manner as the RIV package. River flows entering a reach are assumed to be immediately available to downstream reaches (Prudic 1989). In this thesis, we are improving upon the work of Neupauer and Griebing (2011) by allowing for coupling of the river and the aquifer through the STR package.

Another surface flow package developed for MODFLOW is the Streamflow-Routing (SFR) package, released in 2004 (Prudic 2004). It expands the stream flow capabilities of the STR package by providing additional methods for calculating stream flows and riverbed conductance and by allowing for unsaturated flow beneath the river (Prudic et al. 2004, Niswonger 2010). Adapting the adjoint methodology for this level of river/aquifer coupling will be the subject of future work.

3.4 Forward equations for stream depletion

As is done for the one-dimensional case, the governing equation for groundwater flow is used in conjunction with a mass balance on the river to determine heads in the river and aquifer. The multi-dimensional version of the governing equations for groundwater flow with a river partially penetrating the unconfined aquifer and with pumping in either an unconfined or a confined aquifer are

$$S_y \frac{\partial h_u}{\partial t} = \nabla \cdot [\mathbf{K}(h_u - \zeta) \nabla h_u] - Q_{pu} \delta(x - x_w) \delta(y - y_w) + N(x, y) - \frac{K_a}{b_a} (h_u - h_c) + \frac{K_r}{b_r} (h_r - h_u) B(\mathbf{x}), \quad (3.1a)$$

$$S \frac{\partial h_c}{\partial t} = \nabla \cdot \mathbf{T} \nabla h_c - Q_{pc} \delta(x - x_w) \delta(y - y_w) + \frac{K_a}{b_a} (h_u - h_c), \quad (3.1b)$$

with boundary and initial conditions of

$$h_u(\mathbf{x}, t) = h_c(\mathbf{x}, t) = h_1 \text{ at } y = 0 \text{ and } h_u(\mathbf{x}, t) = h_c(\mathbf{x}, t) = h_2 \text{ at } y = L_y \quad (3.2a)$$

$$\nabla h_u \cdot \vec{n} = \nabla h_c \cdot \vec{n} = 0 \text{ at } x = 0 \text{ and } x = L_x \quad (3.2b)$$

$$h_u(\mathbf{x}, 0) = h_{0u}(\mathbf{x}) \text{ and } h_c(\mathbf{x}, 0) = h_{0c}(\mathbf{x}), \quad (3.2c)$$

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, \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 rate of natural recharge, Q_{pu} and Q_{pc} are the pumping rates for the unconfined and confined aquifers, respectively, (x_w, y_w) is the location of the pumping well, δ is the Dirac delta function, K_a and b_a are the hydraulic conductivity and the thickness of the aquitard, 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, $x = 0$ to $x = L_x$ and $y = 0$ to $y = L_y$ are the spatial bounds of the aquifer, \vec{n} is the outward unit normal vector, and $h_{0u}(\mathbf{x})$ and $h_{0c}(\mathbf{x})$ are the initial heads in the unconfined and confined aquifers, respectively.

Performing a mass balance on the river produces

$$\frac{\partial A_{riv}}{\partial t} + \frac{\partial Q_{riv}}{\partial s} = I/O, \quad (3.3)$$

where A_{riv} is the cross-sectional area of the river, Q_{riv} is the flow rate in the river, s is the spatial coordinate along the river channel in the direction of flow, and I/O are inflows and outflows per unit length of river channel. Inflows and outflows include precipitation (P), evaporation (ET), lateral inflows (I_L), and flow across the riverbed per unit length of riverbed, Q'_{rb} . As in section 2.1, Q'_{rb} is positive for a gaining river and negative for a losing river. Q'_{rb} is defined using Darcy's Law across the riverbed as

$$Q'_{rb} = -\frac{K_r}{b_r}(h_r - h_u)w, \quad (3.4)$$

where w is the channel width. (3.4) is analogous to the last term on the right hand side of (3.1a).

Accounting for these inflows and outflows, (3.3) can be rewritten as

$$\frac{\partial A_{riv}}{\partial t} + \frac{\partial Q_{riv}}{\partial s} = -\frac{K_r}{b_r}(h_r - h_u)w + Pw + I'_L, \quad (3.5)$$

where $I'_L = I_L/\Delta s$ is the lateral inflow per unit length. The STR package assumes that exchange with the river is the only source or sink of water to the river and neglects the transient storage term,

simplifying (3.5). Because we use the STR package, our derivation of the forward equation uses this simplified form, expressed as

$$\frac{\partial Q_{riv}}{\partial s} = -\frac{K_r}{b_r}(h_r - h_u)w. \quad (3.6)$$

We use Manning's equation to calculate Q_{riv} . While the flow in our river does not necessarily meet the assumption of uniform flow made by Manning's equation, we use it as a reasonable approximation. This assumption is also consistent with the approach used in the STR package.

Q_{riv} is given by

$$Q_{riv} = \frac{c}{n}R_h^{2/3}S_0^{1/2}A_{riv}, \quad (3.7)$$

where c is a constant, n is Manning's coefficient of roughness, R_h is the hydraulic radius, and S_0 is channel slope. For this work, we assume a wide rectangular channel with an area of $A_{riv} = w(h_r - z_r)$, where $h_r - z_r$ is the river depth and z_r is the elevation of the channel bottom. The channel width is much greater than the channel depth, which simplifies the hydraulic radius to $R_h \approx h_r - z_r$ and simplifies (3.7) to

$$Q_{riv} \approx \frac{c}{n}(h_r - z_r)^{5/3}S_0^{1/2}w. \quad (3.8)$$

By applying the definitions above, (3.6) becomes

$$\frac{\partial}{\partial s} \left[\frac{c}{n}(h_r - z_r)^{5/3}S_0^{1/2} \right] = -\frac{K_r}{b_r}(h_r - h_u). \quad (3.9)$$

Over the domain $0 < s < L_s$, the boundary condition for (3.9) is

$$Q_{riv} = Q_{riv_0} \text{ at } s = 0,$$

where Q_{riv_0} is the flow in the river at the upstream boundary.

To determine stream depletion using (3.1a), (3.1b), and (3.9), which we call the forward equations, a baseline simulation can be run to establish the rate of water that flows between the aquifer and the river, Q_{rb} , at a particular compliance time, t_c , without pumping. Another simulation can be then run with a pumping well activated at a specific location to obtain a new value of Q_{rb} .

The difference between the baseline value of Q_{rb} and the value of Q_{rb} found with pumping represents the stream depletion. To find depletion values that result from a well pumping at any arbitrary location in the aquifer, separate simulations are needed for each possible well location, which could potentially be any grid cell in the numerical model. As the number of grid cells increases, so does the calculation expense, making the forward approach computationally inefficient.

3.5 Adjoint equations for stream depletion

The adjoint methodology reduces the computational burden of the forward approach by providing the stream depletion caused by a pumping well anywhere in the domain with a single simulation. The first step in developing the adjoint methodology is deriving an expression for the sensitivity of river flow rate to changes in pumping rate, dQ_{riv}/dQ_p . Our definition of dQ_{riv}/dQ_p begins with examining Q'_{rb} . We define the flow across the riverbed as $Q_{rb} = \int_s Q'_{rb} ds$. We are interested in the sensitivity at a particular compliance time, t_c , and compliance location, (x_c, y_c) . We assume that pumping begins at $t = 0$ and use a Dirac delta function to evaluate Q_{rb} at t_c , resulting in

$$Q_{rb}(x_c, y_c, t_c) = - \iiint_{x,y,t} \frac{K_r}{b_r} (h_r - h_u) B(\mathbf{x}) \delta(t - t_c) dx dy dt. \quad (3.10)$$

We note that the travel time of water through a river segment is fast relative to the changes in head in the aquifer. Thus, any change in flow across the riverbed, Q_{rb} , due to changes in aquifer head can be assumed to propagate instantaneously throughout the river reach. The only change in the river flow that result from a change in the pumping rate is the change due to flow across the riverbed, thus, the sensitivity is rewritten as $dQ_{riv}/dQ_p = dQ_{rb}/dQ_p$, where Q_p is either Q_{pu} or Q_{pc} , depending on whether pumping occurs in the unconfined or confined aquifer. This sensitivity is found by differentiating (3.10) with respect to Q_p , yielding

$$\begin{aligned} \frac{dQ_{rb}(x_c, y_c, t_c)}{dQ_p(x_w, y_w)} &= - \frac{d}{dQ_p(x_w, y_w)} \iiint_{x,y,t} \frac{K_r}{b_r} (h_r - h_u) B(\mathbf{x}) \delta(t - t_c) dx dy dt \\ &= - \iiint_{x,y,t} \frac{K_r}{b_r} (\psi_r - \psi_u) B(\mathbf{x}) \delta(t - t_c) dx dy dt, \end{aligned} \quad (3.11)$$

where $\psi_u = \partial h_u / \partial Q_p$ and $\psi_r = \partial h_r / \partial Q_p$, with $Q_p = Q_{pu}$ or $Q_p = Q_{pc}$ depending on whether pumping occurs in the unconfined or confined aquifer, respectively. The sensitivity expressed in (3.11) provides the sensitivity of river flows at the compliance time, t_c , to pumping at a well located at (x_w, y_w) .

Equation (3.11) is not solved directly because doing so would require a separate simulation for each potential well location to obtain ψ_u , ψ_c , and ψ_r . Instead, we obtain a different form of (3.11) that is independent of ψ_u , ψ_c , and ψ_r . For the following derivation, we assume pumping occurs in the confined aquifer, thus $Q_p = Q_{pc}$. The derivation for pumping in the unconfined aquifer will follow the same process; the only difference is the pumping term is present in the unconfined aquifer equation and absent from the confined aquifer equation.

The first step in obtaining the new form of (3.11) is to take the derivative with respect to Q_{pc} of each term in (3.1a), (3.1b), and (3.9), resulting in

$$0 = -S_y \frac{\partial \psi_u}{\partial t} + \nabla \cdot [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u] - \frac{K_a}{b_a} (\psi_u - \psi_c) + \frac{K_r}{b_r} (\psi_r - \psi_u) B(\mathbf{x}) \quad (3.12a)$$

$$0 = -S \frac{\partial \psi_c}{\partial t} + \nabla \cdot \mathbf{T} \nabla \psi_c - \delta(x - x_w) \delta(y - y_w) + \frac{K_a}{b_a} (\psi_u - \psi_c) \quad (3.12b)$$

$$0 = -\frac{\partial}{\partial s} \left[\frac{5c}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \psi_r \right] - \frac{K_r}{b_r} (\psi_r - \psi_u), \quad (3.12c)$$

where $(h_{u0} - \zeta)$ is the initial saturated thickness. We assume the change in saturated thickness is small and thus we use the initial saturated thickness throughout our calculations. The variable N vanishes in (3.12a) because it is independent of Q_p . The boundary and initial conditions for (3.12a), (3.12b), and (3.12c) are

$$\psi_u = \psi_c = 0 \text{ at } y = 0 \text{ and } y = L_y$$

$$\nabla \psi_u \cdot \vec{n} = \nabla \psi_c \cdot \vec{n} = 0 \text{ at } x = 0 \text{ and } x = L_x$$

$$\frac{\partial Q_{riv}}{\partial Q_p} = 0 \text{ at } s = 0$$

$$\psi_u(\mathbf{x}, 0) = \psi_c(\mathbf{x}, 0) = 0$$

Next the inner product of each term in (3.12a) is taken with the arbitrary function ψ_u^* , the inner product of each term in (3.12b) is taken with the arbitrary function ψ_c^* , and the inner product

of each term in (3.12c) is taken with the arbitrary function ψ_r^* , yielding

$$0 = \iiint_{x,y,t} \left\{ -\psi_u^* S_y \frac{\partial \psi_u}{\partial t} + \psi_u^* \nabla \cdot [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u] - \psi_u^* \frac{K_a}{b_a} (\psi_u - \psi_c) \right. \\ \left. + \psi_u^* \frac{K_r}{b_r} (\psi_r - \psi_u) B(\mathbf{x}) \right\} dx dy dt \quad (3.14a)$$

$$0 = \iiint_{x,y,t} \left[-\psi_c^* S \frac{\partial \psi_c}{\partial t} + \psi_c^* \nabla \cdot \mathbf{T} \nabla \psi_c - \psi_c^* \delta(x - x_w) \delta(y - y_w) \right. \\ \left. + \psi_c^* \frac{K_a}{b_a} (\psi_u - \psi_c) \right] dx dy dt \quad (3.14b)$$

$$0 = \iiint_{x,y,t} \left\{ -\psi_r^* \frac{\partial}{\partial s} \left[\frac{5c}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \psi_r \right] - \psi_r^* \frac{K_r}{b_r} (\psi_r - \psi_u) \right\} B(\mathbf{x}) dx dy dt, \quad (3.14c)$$

with the definition of the inner product for the multi-dimensional domain given by

$$\langle f, g \rangle = \iiint_{x,y,t} fg dx dy dt.$$

The basis of an adjoint version of the sensitivity equation is constructed by adding (3.14a), (3.14b), and (3.14c) to (3.11) resulting in

$$\frac{dQ_{riv}(w_c, y_c, t_c)}{dQ_p(x_w, y_w)} = \iiint_{x,y,t} \left[-\psi_u^* S_y \frac{\partial \psi_u}{\partial t} + \psi_u^* \nabla \cdot [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u] - \psi_u^* \frac{K_a}{b_a} (\psi_u - \psi_c) \right. \\ \left. + \psi_u^* \frac{K_r}{b_r} (\psi_r - \psi_u) B(\mathbf{x}) - \psi_c^* S \frac{\partial \psi_c}{\partial t} + \psi_c^* \nabla \cdot \mathbf{T} \nabla \psi_c \right. \\ \left. - \psi_c^* \delta(x - x_w) \delta(y - y_w) + \psi_c^* \frac{K_a}{b_a} (\psi_u - \psi_c) \right. \\ \left. - \psi_r^* \frac{\partial}{\partial s} \left[\frac{5c}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \psi_r \right] B(\mathbf{x}) - \psi_r^* \frac{K_r}{b_r} (\psi_r - \psi_u) B(\mathbf{x}) \right. \\ \left. - \frac{K_r}{b_r} (\psi_r - \psi_u) B(\mathbf{x}) \delta(t - t_c) \right] dx dy dt, \quad (3.15)$$

The product rule is now applied on all terms of (3.15) containing derivatives of ψ_u , ψ_c , and

ψ_r to obtain derivatives of ψ_u^* , ψ_c^* , and ψ_r^* . The product rule expansions for these terms are

$$-\psi_u^* S_y \frac{\partial \psi_u}{\partial t} = -S_y \frac{\partial}{\partial t} (\psi_u^* \psi_u) + \psi_u S_y \frac{\partial \psi_u^*}{\partial t} \quad (3.16a)$$

$$\psi_u^* \nabla \cdot [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u] = \nabla \cdot (\psi_u^* [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u]) - [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u] \cdot \nabla \psi_u^* \quad (3.16b)$$

$$= \nabla \cdot (\psi_u^* [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u]) - \nabla \cdot (\psi_u [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u^*]) + \psi_u \nabla \cdot [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u^*]$$

$$-\psi_c^* S \frac{\partial \psi_c}{\partial t} = -S \frac{\partial}{\partial t} (\psi_c^* \psi_c) + \psi_c S \frac{\partial \psi_c^*}{\partial t} \quad (3.16c)$$

$$\psi_c^* \nabla \cdot \mathbf{T} \nabla \psi_c = \nabla \cdot (\psi_c^* \mathbf{T} \nabla \psi_c) - \mathbf{T} \nabla \psi_c \cdot \nabla \psi_c^* \quad (3.16d)$$

$$= \nabla \cdot (\psi_c^* \mathbf{T} \nabla \psi_c) - \nabla \cdot (\psi_c \mathbf{T} \nabla \psi_c^*) + \psi_c \nabla \cdot \mathbf{T} \nabla \psi_c^*$$

$$-\psi_r^* \frac{\partial}{\partial s} \left[\frac{5c}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \psi_r \right] B(\mathbf{x}) = -\frac{\partial}{\partial s} \left[\psi_r^* \frac{5c}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \psi_r \right] B(\mathbf{x}) \quad (3.16e)$$

$$+ \psi_r \frac{5c}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \frac{\partial \psi_r^*}{\partial s} B(\mathbf{x}).$$

Equations (3.16a)-(3.16e) are substituted into (3.15). (3.15) is then rearranged to isolate ψ_u , ψ_c , and ψ_r and the divergence terms, shown in (3.18), are separated from the main equation, resulting in

$$\begin{aligned} \frac{dQ_{riv}(w_c, y_c, t_c)}{dQ_p(x_w, y_w)} = & \iiint_{x,y,t} \left[\psi_u \left\{ S_y \frac{\partial \psi_u^*}{\partial t} + \nabla \cdot [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u^*] \right. \right. \\ & \left. \left. - \frac{K_a}{b_a} (\psi_u^* - \psi_c^*) + \frac{K_r}{b_r} [\psi_r^* - \psi_u^* + \delta(t - t_c)] B(\mathbf{x}) \right\} \right. \\ & \left. + \psi_c \left\{ S \frac{\partial \psi_c^*}{\partial t} + \nabla \cdot \mathbf{T} \nabla \psi_c^* + \frac{K_a}{b_a} (\psi_u^* - \psi_c^*) \right\} \right. \\ & \left. + \psi_r \left\{ \frac{5c}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \frac{\partial \psi_r^*}{\partial s} B(\mathbf{x}) \right. \right. \\ & \left. \left. - \frac{K_r}{b_r} [\psi_r^* - \psi_u^* + \delta(t - t_c)] B(\mathbf{x}) \right\} \right. \\ & \left. - \psi_c^* \delta(x - x_w) \delta(y - y_w) \right] dx dy dt + \text{Divergence terms}, \quad (3.17) \end{aligned}$$

where the divergence terms are

$$\begin{aligned} & \iiint_{x,y,t} \left\{ -S_y \frac{\partial}{\partial t} (\psi_u^* \psi_u) + \nabla \cdot (\psi_u^* [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u]) - \nabla \cdot (\psi_u [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u^*]) \right. \\ & \left. - S \frac{\partial}{\partial t} (\psi_c^* \psi_c) + \nabla \cdot (\psi_c^* \mathbf{T} \nabla \psi_c) - \nabla \cdot (\psi_c \mathbf{T} \nabla \psi_c^*) \right. \\ & \left. - \frac{\partial}{\partial s} \left[\psi_r^* \frac{5c}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \psi_r \right] B(\mathbf{x}) \right\} dx dy dt. \quad (3.18) \end{aligned}$$

The arbitrary functions ψ_u^* , ψ_c^* , and ψ_r^* are now defined so that ψ_u , ψ_c , and ψ_r are eliminated from (3.17), yielding

$$S_y \frac{\partial \psi_u^*}{\partial \tau} = \nabla \cdot [\mathbf{K}(h_{u0} - \zeta) \nabla \psi_u^*] - \frac{K_a}{b_a} (\psi_u^* - \psi_c^*) + \frac{K_r}{b_r} [\psi_r^* - \psi_u^* + \delta(\tau)] B(\mathbf{x}) \quad (3.19a)$$

$$S \frac{\partial \psi_c^*}{\partial \tau} = \nabla \cdot \mathbf{T} \nabla \psi_c^* + \frac{K_a}{b_a} (\psi_u^* - \psi_c^*) \quad (3.19b)$$

$$-\frac{5c}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \frac{\partial \psi_r^*}{\partial s} = -\frac{K_r}{b_r} [\psi_r^* - \psi_u^* + \delta(\tau)] \quad (3.19c)$$

where $\tau = t_c - t$ is backward time. To further simplify (3.17), the divergence terms are eliminated by defining initial conditions and boundary conditions on ψ_u^* , ψ_c^* , and ψ_r^* . The following initial and boundary conditions cause the divergence terms to vanish:

$$\psi_u^* = \psi_c^* = 0 \text{ at } y = 0 \text{ and } y = L_y, \quad (3.20a)$$

$$\nabla \psi_u^* \cdot \vec{n} = \nabla \psi_c^* \cdot \vec{n} = 0 \text{ at } x = 0 \text{ and } x = L_x, \quad (3.20b)$$

$$\psi_r^* = 0 \text{ at } s = L_s, \quad (3.20c)$$

$$\psi_u^*(\mathbf{x}, \tau = 0) = \psi_c^*(\mathbf{x}, \tau = 0) = 0, \quad (3.20d)$$

The variables ψ_u^* , ψ_c^* , and ψ_r^* are the adjoint states of h_u , h_c , and h_r , and (3.19a), (3.19b), and (3.19c) are the adjoints of (3.1a), (3.1b), and (3.9), respectively. The adjoint sensitivity equation resulting from the above simplifications of (3.17) is evaluated at the compliance time, $t = t_c$ ($\tau = 0$), and at the compliance location, (x_c, y_c) . After using (3.19a), (3.19b), and (3.19c) and the boundary and initial conditions above, (3.17) reduces to

$$\frac{dQ_{riv}(x_c, y_c, \tau = 0)}{dQ_p(x_w, y_w)} = \iiint_{x, y, \tau} -\psi_c^* \delta(x - x_w) \delta(y - y_w) dx dy d\tau = \int_{\tau=0}^{t_c} -\psi_c^*(x_w, y_w, \tau) d\tau. \quad (3.21)$$

Changing the variables (x_w, y_w) to (x, y) , (3.21) is written as

$$\frac{dQ_{riv}(x_c, y_c, \tau = 0)}{dQ_p(x, y)} = \int_{\tau=0}^{t_c} -\psi_c^*(x, y, \tau) d\tau. \quad (3.22)$$

Stream depletion is found using (3.19a), (3.19b), and (3.19c) to solve for ψ_c^* then integrating over time as indicated in (3.22) and multiplying by the pumping rate. Solving this system of equations provides stream depletion values for a well at any arbitrary location (x, y) in the confined

aquifer. The same approach can be used when pumping occurs in the unconfined aquifer, however, the $\psi_c^* \delta(x - x_w) \delta(y - y_w)$ term will be absent in the confined aquifer equations and it will be replaced by the term $\psi_u^* \delta(x - x_w) \delta(y - y_w)$ in the unconfined aquifer equations. The final adjoint equations for pumping in the unconfined aquifer is

$$\frac{dQ_{riv}(x_c, y_c, \tau = 0)}{dQ_p(x, y)} = \int_{\tau=0}^{\tau=t_c} -\psi_u^*(x, y, \tau) d\tau. \quad (3.23)$$

The adjoint equations are solved to obtain ψ_c^* and ψ_u^* , then ψ_c^* is used in (3.22) and ψ_u^* is used in (3.23) to find $\frac{dQ_{riv}}{dQ_p}$ due to pumping in the confined and unconfined aquifer, respectively, then multiplying by the pumping rate to obtain stream depletion, expressed as

$$\Delta Q_{riv} = \frac{dQ_{riv}}{dQ_p} Q_p, \quad (3.24)$$

where ΔQ_{riv} is stream depletion.

3.6 MODFLOW Modifications

To eliminate the need to run many forward simulations to calculate stream depletion, we adapt MODFLOW to solve equations (3.19a)-(3.19c), thus allowing us to model the stream depletion more efficiently. This is done by modifying the input values into MODFLOW and modifying the source code of the STR package.

3.6.1 Input Modifications

The adjoint equations, (3.19a), (3.19b), and (3.19c), have essentially the same form as the forward governing equations, (3.1a), (3.1b), and (3.9), so MODFLOW can be used to solve the adjoint equation. In the adjoint equations, the state variables are the adjoint states, ψ_u^* , ψ_c^* , and ψ_r^* , while in the forward equations the state variables are head. Thus when we use MODFLOW to solve the adjoint equations, “head” is a surrogate for the adjoint state. The adjoint equations are written in terms of τ , which is backwards time, so when we use MODFLOW to solves the adjoint equations, time becomes backward time, τ .

One of the first issues that arises in running an adjoint simulation based on equations (3.19a)-(3.19c) results from the initial condition in (3.20d), which indicates that $\psi_u^* = 0$ and $\psi_c^* = 0$ when $\tau = 0$ and would be entered into the MODFLOW input files as an initial condition of zero. In MODFLOW, when the head in a model cell drops below the bottom elevation of the cell, the cell “goes dry” and calculations are no longer performed on that cell. To avoid this, we define new state variables with magnitudes greater than the aquifer bottom elevation. These new state variables are defined as

$$\Psi_u^*(\mathbf{x}, \tau) = \beta + \psi_u^*(\mathbf{x}, \tau)/\gamma, \quad (3.25a)$$

$$\Psi_c^*(\mathbf{x}, \tau) = \beta + \psi_c^*(\mathbf{x}, \tau)/\gamma, \quad (3.25b)$$

$$\Psi_r^*(\mathbf{x}, \tau) = \beta + \psi_r^*(\mathbf{x}, \tau)/\gamma, \quad (3.25c)$$

where β is defined so that it is higher than the bottom elevation of all the aquifers in the model as well as the river bottom, yet lower than the land surface elevation. Setting the value of β to be greater than the bottom elevation of the aquifer ensures cells will not go dry due to the initial conditions. For a natural system, the value of β would be determined by finding the lowest point of land surface elevation throughout the domain and checking to make sure this is above the elevation of the bottom of the riverbed and the bottom elevation of the aquifer. The definition of γ is described below.

These new state variables are substituted into (3.19a)-(3.19c), yielding

$$S_y \frac{\partial \Psi_u^*}{\partial \tau} = \nabla \cdot [\mathbf{K}(h_{u0} - \zeta) \nabla \Psi_u^*] - \frac{K_a}{b_a} (\Psi_u^* - \Psi_c^*) + \frac{K_r}{b_r} [\Psi_r^* - \Psi_u^*] B(\mathbf{x}), \quad (3.26a)$$

$$S \frac{\partial \Psi_c^*}{\partial \tau} = \nabla \cdot \mathbf{T} \nabla \Psi_c^* + \frac{K_a}{b_a} (\Psi_u^* - \Psi_c^*), \quad (3.26b)$$

$$-\frac{5c}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \frac{\partial \Psi_r^*}{\partial s} = -\frac{K_r}{b_r} [\Psi_r^* - \Psi_u^*], \quad (3.26c)$$

with the following initial and boundary conditions:

$$\Psi_u^* = \Psi_c^* = \beta \text{ at } y = 0 \text{ and } y = L_y, \quad (3.27a)$$

$$\nabla \Psi_u^* \cdot \vec{n} = \nabla \Psi_c^* \cdot \vec{n} = 0 \text{ at } x = 0 \text{ and } x = L_x, \quad (3.27b)$$

$$\Psi_r^* = \beta \text{ at } s = L_s, \quad (3.27c)$$

$$\Psi_u^*(\mathbf{x}, \tau = 0) = \beta + \frac{K_r}{b_r S_y \gamma} B(\mathbf{x}), \quad (3.27d)$$

$$\Psi_c^*(\mathbf{x}, \tau = 0) = \beta. \quad (3.27e)$$

The $\delta(\tau)$ term in (3.19a) is now part of the initial condition in (3.27d). The $\delta(\tau)$ term in (3.19c) would be part of the initial condition on Ψ_r^* ; however, the temporal changes in Ψ_r^* are assumed to occur more rapidly than the changes in aquifer head and they are neglected here.

The purpose of γ is to ensure that the second term in (3.27d) is of the same order of magnitude as β . This second term is the load term to the adjoint simulation and represents an instantaneous perturbation at the river that is propagated into the aquifer over time. If the magnitude of this perturbation is too small, it will be on the same order of magnitude as the numerical error in the model and will not be noticeable in the simulation results. We use $\gamma \ll 1$ to prevent this. Using (3.25a) and (3.25b) in (3.23) and (3.22), the adjoint sensitivity equations become:

$$\frac{dQ_{riv}(x_c, y_c, \tau = 0)}{dQ_p(x, y)} = \int_{\tau=0}^{t_c} \gamma [-\Psi_u^*(x, y, \tau) - \beta] d\tau, \quad (3.28a)$$

$$\frac{dQ_{riv}(x_c, y_c, \tau = 0)}{dQ_p(x, y)} = \int_{\tau=0}^{t_c} \gamma [-\Psi_c^*(x, y, \tau) - \beta] d\tau. \quad (3.28b)$$

Another issue arises when attempting to model the first term on the right-hand side of the governing equation of groundwater flow (3.26a) in MODFLOW. The first term on the right-hand side of (3.1a) is non-linear in the state variable, while the first term on the right-hand side of (3.26a), the adjoint equation we want MODFLOW to solve, is linear in the adjoint state and depends on the initial head in the unconfined aquifer. For MODFLOW to handle this term, the unconfined aquifer is modeled as a **confined** aquifer with a transmissivity of $\mathbf{T} = \mathbf{K}(h_{u0} - \zeta)$. Doing so assumes that the drawdown in the unconfined aquifer is small compared to the saturated thickness.

Any terms that are independent of the pumping rate are not included in the adjoint simulation as they do not appear in the adjoint equations. For this test case, recharge is omitted from the adjoint model because it is not present in the adjoint equations.

Once the adjoint simulation has been run, the results for each time step are compiled. The time integrals in (3.28a) and (3.28b) are approximated as a summation, which we handle by post processing the MODFLOW results, and the temporal discretization of the MODFLOW simulation determines the accuracy of the results. For the adjoint simulation to correctly calculate stream depletion, the temporal discretization must be appropriately small.

3.6.2 STR Code Modifications and Input Modifications

In addition to modifying the MODFLOW input files, the STR code is also changed to solve (3.26c). The forward equations solved by MODFLOW are non-linear in the state variable, seen on the left-hand side term of (3.9). The adjoint version of this term, seen on the left-hand side of (3.26c), is linear in the adjoint state variable and depends on the forward state variable, h_r . Because of this, the STR code used to calculate flow between the river and the aquifer in MODFLOW cannot be used to directly calculate stream depletion. We modify the STR code to account for the differences between the form of the right hand side of (3.9) and that of (3.26c).

We developed (3.26c) from equations in which the width of the river, w , had been canceled out for simplicity. The STR package includes the width of the river in its calculation of flow, thus we rewrite (3.26c) to include the width, yielding

$$-\frac{5cw}{3n}S_0^{1/2}(h_r - z_r)^{2/3}\frac{\partial\Psi_r^*}{\partial s} = -\frac{K_r w}{b_r}[\Psi_r^* - \Psi_u^*]. \quad (3.29)$$

Next we manipulate (3.29), rewriting the left hand side using the product rule expansion, to obtain

$$-\frac{5cw}{3n}S_0^{1/2}(h_r - z_r)^{2/3}\frac{\partial\Psi_r^*}{\partial s} = -\frac{\partial}{\partial s}\left[\frac{5cw}{3n}S_0^{1/2}(h_r - z_r)^{2/3}\Psi_r^*\right] + \Psi_r^*\frac{\partial}{\partial s}\left[\frac{5cw}{3n}S_0^{1/2}(h_r - z_r)^{2/3}\right]. \quad (3.30)$$

Expanding the derivative of last term in (3.30) results in

$$\begin{aligned} \Psi_r^* \frac{\partial}{\partial s} \left[\frac{5cw}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \right] &= \Psi_r^* \frac{5c}{3} \left[-\frac{w}{n^2} S_0^{1/2} (h_r - z_r)^{2/3} \frac{\partial n}{\partial s} + \frac{w}{2n} S_0^{-1/2} (h_r - z_r)^{2/3} \frac{\partial S_0}{\partial s} \right. \\ &\quad \left. + \frac{2w}{3n} S_0^{1/2} (h_r - z_r)^{-1/3} \frac{\partial (h_r - z_r)}{\partial s} + \frac{1}{n} S_0^{1/2} (h_r - z_r)^{2/3} \frac{\partial w}{\partial s} \right]. \end{aligned} \quad (3.31)$$

Substituting (3.30) and (3.31) into (3.26c), we rewrite (3.26c) as

$$\begin{aligned} -\frac{\partial}{\partial s} \left[\frac{5cw}{3n} S_0^{1/2} (h_r - z_r)^{2/3} \Psi_r^* \right] + \Psi_r^* \frac{5c}{3} \left[-\frac{w}{n^2} S_0^{1/2} (h_r - z_r)^{2/3} \frac{\partial n}{\partial s} + \frac{w}{2n} S_0^{-1/2} (h_r - z_r)^{2/3} \frac{\partial S_0}{\partial s} \right. \\ \left. + \frac{2w}{3n} S_0^{1/2} (h_r - z_r)^{-1/3} \frac{\partial (h_r - z_r)}{\partial s} + \frac{1}{n} S_0^{1/2} (h_r - z_r)^{2/3} \frac{\partial w}{\partial s} \right] = -\frac{K_r w}{b_r} [\Psi_r^* - \Psi_u^*]. \end{aligned} \quad (3.32)$$

For comparison, the forward equation for the river mass balance, shown in (3.9), is repeated here, with the river width included,

$$\frac{\partial}{\partial s} \left[\frac{wc}{n} S_0^{1/2} (h_r - z_r)^{5/3} \right] = -\frac{K_r w}{b_r} (h_r - h_u). \quad (3.33)$$

This is the equation that is solved in the STR packages, thus, we modify the STR package to solve (3.32) instead and call the modified version STRADJ.

The first term on the left-hand side of (3.32) is similar to the term on the left-hand side of (3.33). The adjoint version is linear in the state variable, Ψ_r^* , while the forward equation is non-linear, so the code is changed to handle this difference along with the different constant for the adjoint version. The presence of the forward river head, h_r , in the adjoint version of the equation must also be accounted for in the STRADJ code. To obtain results for h_r , additional simulations would need to be run for every cell in the model domain, thus eliminating any computational advantage provided by the adjoint approach. We avoid this by using a constant value in place of h_r , which we call h_{rc} . If h_{rc} is set to the initial head in the river, the term $(h_r - z_r)^{2/3}$ in the first term of the left-hand side of (3.32) would represent no change in the river head due to depletion, so the stream depletion values calculated in this case would likely be lower than actual values. Another approach would be to set h_{rc} according the river level associated with some maximum

depletion, for instance, the stream depletion that defines non-tributary groundwater discussed in Section 1.3.5. The calculated stream depletion values in this case would likely be higher than the actual values. Because h_{rc} does not exist in the STR code, it is added into the STRADJ input file and the $(h_r - z_r)^{2/3}$ term accounted for in the STRADJ code.

The second term on the left-hand side of (3.32) does not exist in (3.33) and is added to the STRADJ code. In order for the STRADJ code to calculate the derivatives with respect to s in this term, the length of each reach must be specified to calculate ds . In the STR package, reach length is lumped together with other parameters in the streambed hydraulic conductance term. For STRADJ, the reach length is added to the STRADJ input file to aid in the code's execution.

The order in which the STRADJ code is changed to account for the river flow being reversed in the adjoint simulation. For the forward model, calculations begin in the first reach, which is the upstream-most reach, and proceed in a downstream manner. The STRADJ is modified to perform calculations in the reverse order, beginning at the downstream-most reach and working upstream.

The boundary conditions must be modified because the river flow is reversed in the adjoint simulation and the order of calculations of the STRADJ code is reversed. For the forward model, the boundary condition in the river is handled by the STR package as an inflow that corresponds to head in the farthest upstream reach and enters at the uppermost reach in the model. Recall from (3.27c) that the adjoint version of the river mass balance has its boundary on the lowest reach in the system because the adjoint equations begin at L_s , the downstream end of the river. The STRADJ code is modified so that the boundary condition enters at the lowest reach in the model. The value of this boundary condition, which is a surrogate for inflow, is calculated from the first term of the right hand side of (3.32) as

$$\Phi = \frac{5cw}{3n} S_0^{1/2} (h_{rc} - z_r)^{2/3} D_{adj}, \quad (3.34)$$

where Φ is the surrogate for inflow and $D_{adj} = \Psi_r^* - z_r$ is the surrogate for river depth. The value of Φ is entered in the STRADJ input file as flow for the last reach in the model, and the value of the flow for the first reach in the model is set to zero.

The STRADJ code can be found in Appendix A. For reference, Table 3.1 shows a list of the variables used for the STR and STRADJ package input file, the corresponding variable in the STR package code, and the corresponding variable used in our notation throughout this work.

Table 3.1: Variables used in the STR and STRADJ model

Description	STR input	STRADJ code	Our notation
Channel width	Width	STRM(6)	w
Channel slope	Slope	STRM(7)	S_0
Channel roughness	Rough	STRM(8)	n
Constant for Manning's Equation	CONST	CONST	c
Streambed hydraulic conductivity	none	none	K_r
Streambed thickness	Sbot-Stop	STRM(5) - STRM(4)	b_r
Streambed hydraulic conductance	Cond	CSTR, STRM(3)	wK_r/b_r
Elevation of top of streambed	Stop	STRM(5)	z_r
Elevation of bottom of streambed	Sbot	STRM(4)	$z_r - b_r$
Stream stage	Stage	STRM(2), HSTR	h_r
Aquifer head	none	H, HNEW	h
Flow into segment	none	STRM(1)	Q_{rivin}
Flow into reach	none	STRM(10)	Q_{rivin}
Flow out of reach	none	STRM(9)	Q_{rivout}
Flow across streambed (leakage)	none	FLOWBOT, STRM(11)	Q_{rb}
River head constant	none	STRM(12)	h_{rc}
Reach length	none	STRM(13)	ds

Chapter 4

Test Case

In order to verify the adjoint methodology developed in the previous chapter, we run a test case using MODFLOW to compare the stream depletion results calculated using the standard forward approach to those found with the adjoint method. We show the results from the forward test case in Section 4.2 and compare these with the results from the adjoint test case in Section 4.3.

4.1 Conceptual Model

We develop a model for the test case based on the hypothetical aquifer described in Section 3.1 and shown in Figure 3.1. It has two 20 m thick layers, an unconfined aquifer on top and a confined aquifer on bottom, with a simulated confining layer between them. The model domain spans from $x = 0$ m to $x = L_x = 1600$ m in the x -direction and from $y = 0$ m to $y = L_y = 2000$ m in the y -direction. No flow boundary conditions exist at $x = 0$ m and $x = 1600$ m and constant head boundary conditions of $h = 10$ m and $h = 9$ m exist at $y = 0$ m and $y = L_y = 2000$ m, respectively. The model discretization is $\Delta x = 50$ m by $\Delta y = 50$ m, yielding 40 rows and 32 columns. We employ the Dupuit assumptions in the unconfined aquifer and assume the flow in the confined aquifer is essentially horizontal as well. Additionally, we assume both the confined and unconfined aquifers are isotropic. A meandering river flows from $y = L_y$ to $y = 0$ m and penetrates 10 m into the unconfined aquifer, with a path defined by the equation

$$x_{cl} = 775 \text{ m} + 250 \text{ m} \sin \left(2\pi \frac{y - dy/2}{y_{max} - dy} \right), \quad (4.1)$$

where x_{cl} is the x coordinate of the centerline of the river, $dy = 50$ m is the spatial discretization in the y -direction, and $y_{max} = 2000$ m is the length of the model domain in the y -direction. A pumping well can extract water from either the confined or unconfined aquifer at a rate of $Q_p = 10$ m³/d.

We use MODFLOW to simulate the model, with the river modeled using the STR package, pumping wells modeled using the well (WEL) package, and recharge modeled with the recharge (RCH) package. The model also employs the preconditioned partial-gradient (PCG) package and block-centered flow (BCF) packages to solve the finite difference equations. Table 4.1 lists the values used to construct the model.

4.2 Forward Simulations

For the standard forward model, calculating stream depletion for each potential well location in the hypothetical aquifer system requires an initial model run to determine the flow rate across the riverbed in the absence of pumping. Next, a separate model run finds the flow rate across the riverbed as a result of pumping in the cell located in the first row and column of the unconfined aquifer. The difference in flow rates across the riverbed between the initial simulation and the simulation with pumping is calculated and saved. Additional simulations are run to cycle the pumping well through each cell of the model domain, with a separate simulation required for each cell and the difference in flow rates saved for each simulation. The stream depletion for each possible well location is shown in Figure 4.1 c,d. Figure 4.1 c,d shows higher stream depletion values for wells located near the river and lower values for wells further from the river. The low stream depletion values near $y = L_y$ and $y = 0$ m are caused by the constant head boundaries at $y = L_y$ and $y = 0$ m. A well located near these boundaries will draw all of its water from the fixed head boundary rather than from the aquifer in the model domain and the river. For our hypothetical aquifer, a total of 2560 simulations are needed in addition to the initial simulation to determine stream depletion for a well located at the center of every grid block in the model domain. The runtime required to perform all simulation runs and compile the results is 4 hours 36 minutes

Table 4.1: Forward aquifer and model parameters.

Description	Value
Head at north boundary, $h_u(\mathbf{x}, t)$ and $h_c(\mathbf{x}, t)$ at $y = 2000$ m	20 m
Head at south boundary, $h_u(\mathbf{x}, t)$ and $h_c(\mathbf{x}, t)$ at $y = 0$ m	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, \mathbf{K}	0.2 m/d
Hydraulic conductivity of aquitard, K_a	0.02 m/d
Transmissivity of confined aquifer, \mathbf{T}	1.0 m ² /d
Specific yield, S_y	0.2
Storage coefficient in aquitard	0
Storage coefficient in confined aquifer, S	1×10^{-3}
Recharge rate, N	4×10^{-7} m/d
River bottom elevation, z_r	15.125 m
Riverbed thickness, b_r	0.125 m
River width, w	25 m
Hydraulic conductivity of the riverbed, K_r	2.5×10^{-5} m/d
Manning's coefficient of roughness for the riverbed, n	0.04
Riverbed slope, S_0	0.001
Spatial discretization	50×50 m
Temporal discretization	1 d
Compliance time, t_c	1825 d
Pumping rate, Q_w	10 m ³ /d
Initial head in unconfined aquifer, $h_{u0}(\mathbf{x})$	16 m
Initial head in confined aquifer, $h_{c0}(\mathbf{x})$	16 m
Initial river stage, h_r	19 m
River flow, Q_{r0}	16,325,000 m ³ /d

(16,560 seconds) on a HP Workstation XW4100 with a Dual core 2.4 GHz processor and 1.5 Gb of RAM.

4.3 Adjoint Simulation

Using the modifications to MODFLOW described in Sections 3.6.1 and 3.6.2, we run an adjoint simulation based on the same hypothetical aquifer with a partially penetration meandering stream used in the forward simulation. Several of the same MODFLOW input files are used to run the adjoint simulation; however, some of them are modified. These include the basic (BAS), discretization (DIS), and block centered flow (BCF) package files. The MODFLOW code is recompiled to include the STRADJ version of the STR package in place of the regular STR package and the inputs to the STR package are also modified. The well (WEL) package and recharge (RCH) package are not used in the adjoint simulation.

The basic package file is modified from the forward model by setting the initial head throughout the unconfined and confined aquifer to $\beta = 16$. Additionally, the model cells directly below the river in the unconfined aquifer are set to according to the initial condition shown in (3.27d). To account for cases where the river doesn't occupy an entire cell, this initial condition is slightly modified by dividing the area of the river by the area of the cell, and this term is used to replace the $B(\mathbf{x})$ term in (3.27d), resulting in

$$\Psi_u^*(\mathbf{x}, \tau = 0) = \beta + \frac{K_r}{b_r S_y \gamma} \frac{A_{riv}}{A_{tot}}, \quad (4.2)$$

where A_{riv} is the area of the river in a model cell and A_{tot} is the area of of the cell the river passes through.

The block centered flow package file is changed so that the unconfined aquifer is modeled as a confined aquifer with a primary storage coefficient of S_y and a transmissivity of $\mathbf{T} = \mathbf{K}(h_{r0} - \zeta)$.

The STR package input file is modified by setting the initial flow in the furthest upstream reach to zero and setting the initial flow in the furthest downstream reach to Φ . The additional inputs, the river head constant h_{rc} and the reach length ds , are added to the input file for each

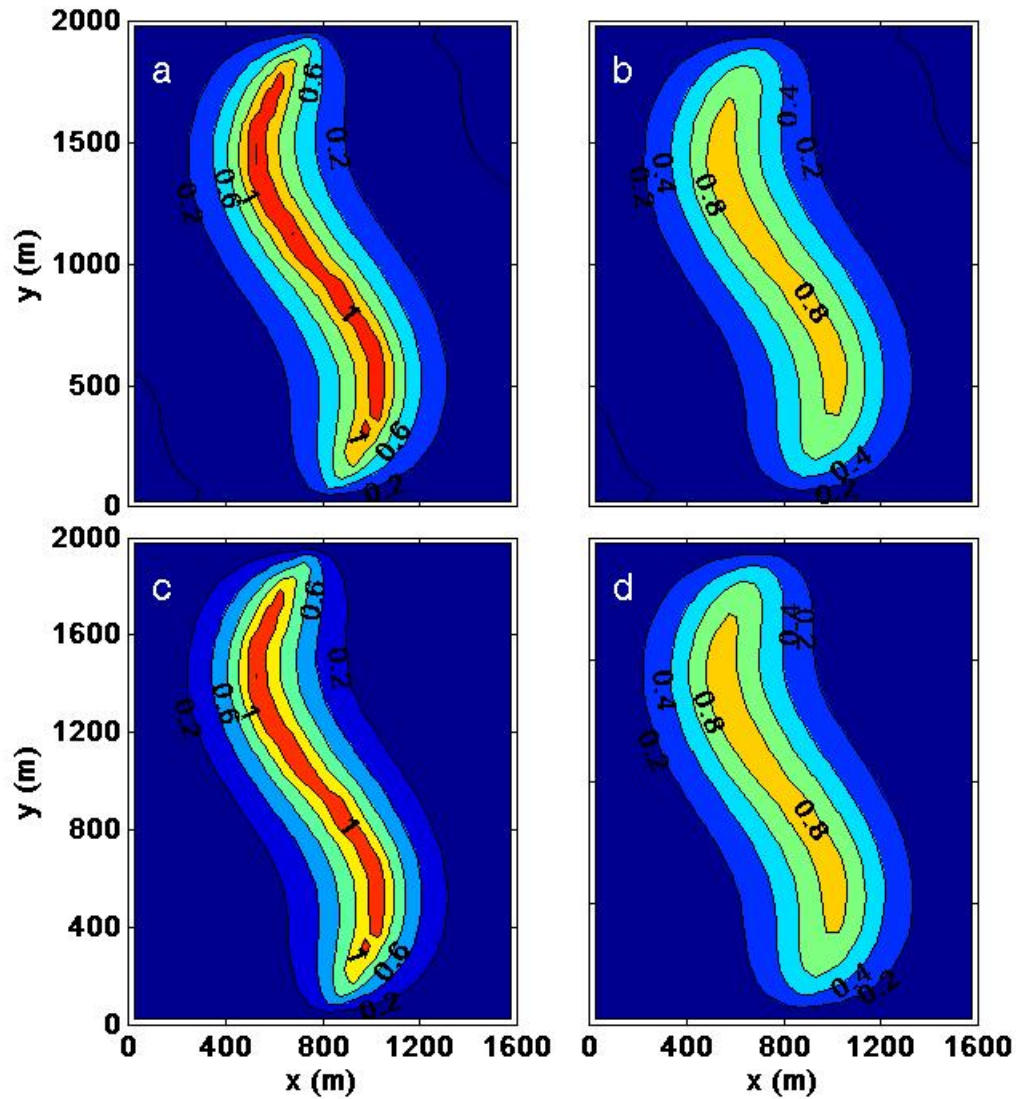


Figure 4.1: Stream depletion (m^3/d) from forward and adjoint simulations (a) Adjoint results with pumping in the unconfined aquifer. (b) Adjoint results with pumping in the confined aquifer. (c) Forward results with pumping in the unconfined aquifer. (d) Forward results with pumping in the confined aquifer.

Table 4.2: Adjoint aquifer and model parameters.

Description	Value
$\psi_u^*(\mathbf{x}, \tau)$ and $\psi_c^*(\mathbf{x}, \tau)$ at north and south boundary, $y = 2000$ m and $y = 0$ m	16 d^{-1}
β	16 d^{-1}
γ	1×10^{-5}
Initial adjoint state in unconfined aquifer, $\psi_u^*(\mathbf{x}, \tau = 0)$	$\beta + \frac{K_r}{b_r S_y \gamma} B(\mathbf{x})$
Initial adjoint state in lower confined aquifer, $\psi_c^*(\mathbf{x}, \tau = 0)$	16 d^{-1}
Adjoint “river flow”, Φ	$6,143,724 \text{ m}^3/\text{d}$
River head constant, h_{rc}	19 m

reach of the river. For this simulation, the river head constant, h_{rc} , is set to 19 m, representing a scenario with minimum depletion.

Table 4.2 lists the values used to construct the adjoint model. If a parameter is not listed it has not changed from the forward model.

Only one adjoint simulation is required to obtain stream depletion values that correspond to a pumping well located anywhere in the model domain. Equations (3.26a)-(3.26c) are solved in MODFLOW and the results are used in (3.28a), (3.28b) and (3.24) to calculate stream depletion based on a pumping rate of $Q_p=10 \text{ m}^3/\text{d}$. Figure 4.1 a,b shows the adjoint stream depletion results above the forward results for both unconfined and confined aquifers. As with the forward simulation, the stream depletion is higher for a pumping well located near the river and the depletion is lower the further from the river the pumping well is located. The results of the adjoint simulations are visually indistinguishable from forward simulation results, indicating the adjoint methodology accurately calculates stream depletion.

The runtime required to complete the MODFLOW adjoint simulation was 22.9 seconds on a HP Workstation XW4100 with a Dual core 2.4 GHz processor and 1.5 Gb of RAM, and the required time to post process the results was 29 seconds, resulting in a total time required to calculate the adjoint stream depletion of 52 seconds. This is three orders of magnitude less than the computation time required to run the forward simulations. Clearly, the adjoint method provides a much more efficient approach to quantifying stream depletion.

The error between the forward and adjoint simulation varied spatially, with the error near the river greater than the error further from the river. The spatial behavior of the absolute error, calculated as the adjoint stream depletion minus the forward stream depletion, is shown in Figure 4.2. The adjoint results are higher than those of the forward simulations for the majority of the domain, with the exception of a few cells that lie directly below the river in the unconfined aquifer. The maximum absolute error in the unconfined aquifer is $0.0116 \text{ m}^3/\text{d}$ and occurs in row 35, $y=300$ m, and column 10, $x=500$ m, of the domain, while the maximum absolute error for the confined aquifer is $0.0102 \text{ m}^3/\text{d}$ and occurs at row 23, $y=900$ m, and column 19, $x=950$ m, of the domain. The relative error at these two locations is 2.14% and 2.34% for the unconfined and confined aquifer, respectively. The relative error is lowest near the river and increases as the location of the pumping well moves away from the river, as seen in Figure 4.3. The behavior of the relative error becomes erratic in locations further away from the river where the values of the forward stream depletion approach zero. In these location, the absolute error is divided by infinitesimally small values of the forward stream depletion. The relative error in the unconfined aquifer is also negative in the cells underlying the river, shown in white in Figure 4.3. In areas where the depletion values are above $0.1 \text{ m}^3/\text{d}$, the relative error is less than 10%. On the whole, the adjoint results are relatively accurate, especially considering the assumptions made to solve the adjoint equation that theoretically depends on the forward model results.

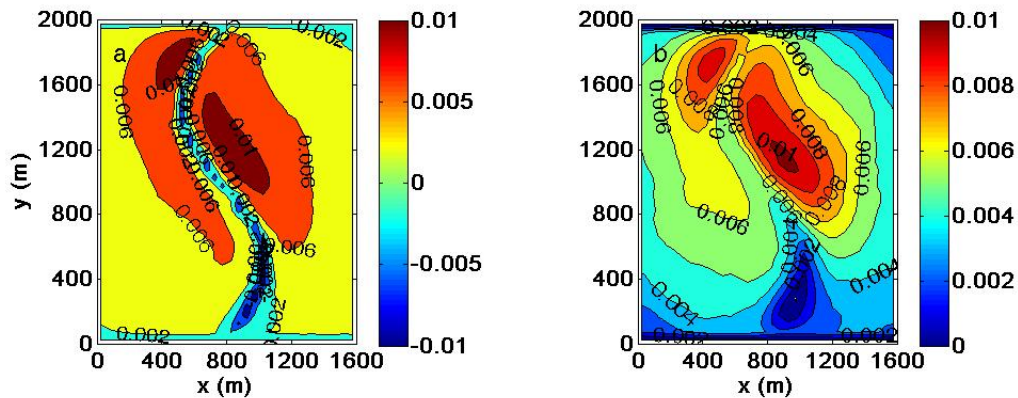


Figure 4.2: Absolute error between the adjoint and forward simulations calculated as the adjoint stream depletion minus the forward stream depletion for (a) the unconfined aquifer and (b) the confined aquifer.

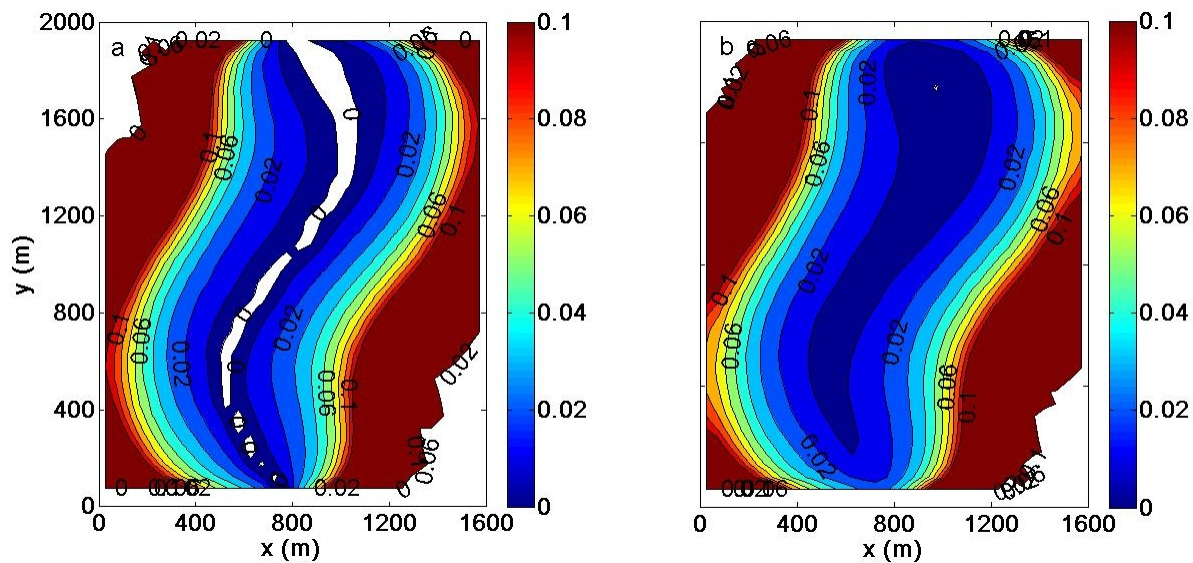


Figure 4.3: Relative error between the adjoint and forward simulations for the unconfined aquifer, (a), and the confined aquifer, (b).

Chapter 5

Discussion

The results of the forward and adjoint simulations show the adjoint methodology works well and provides a great deal of stream depletion information with much less computational expense. In this chapter, we investigate the assumptions of the approach and the limitations of this method.

5.1 Assumptions

In developing the forward and adjoint models, we make several common assumptions about the behavior of groundwater flow in the model domain and the geometry of the river as well as assumptions that simplify our calculations. We employ the Dupuit assumption, which assumes groundwater flows horizontally in unconfined aquifers, and we also assume flow is horizontal in the confined aquifer.

One assumption we make is that drawdown in the unconfined aquifer is small compared to aquifer thickness. We approximate the saturated thickness in the unconfined aquifer, $(h_u - \zeta)$, using the initial head as $(h_{u0} - \zeta)$, as seen in (3.12a). To test this assumption, we compared the heads in the unconfined aquifer before and after pumping using a pumping well located away from the model boundaries and from the river, all of which might cause less drawdown. When pumping from the unconfined aquifer at the location $(x, y) = (400 \text{ m}, 1000 \text{ m})$ at a pumping rate of $Q_p = 10 \text{ m}^3/\text{d}$, the largest difference between the initial head in the aquifer and the head after pumping for 5 years (1825 days) occurs at the pumping location, as seen in Figure 5.1. This difference at the pumping well is 1.377 m, which is 6.89% of the 20 m thickness of the unconfined aquifer. This

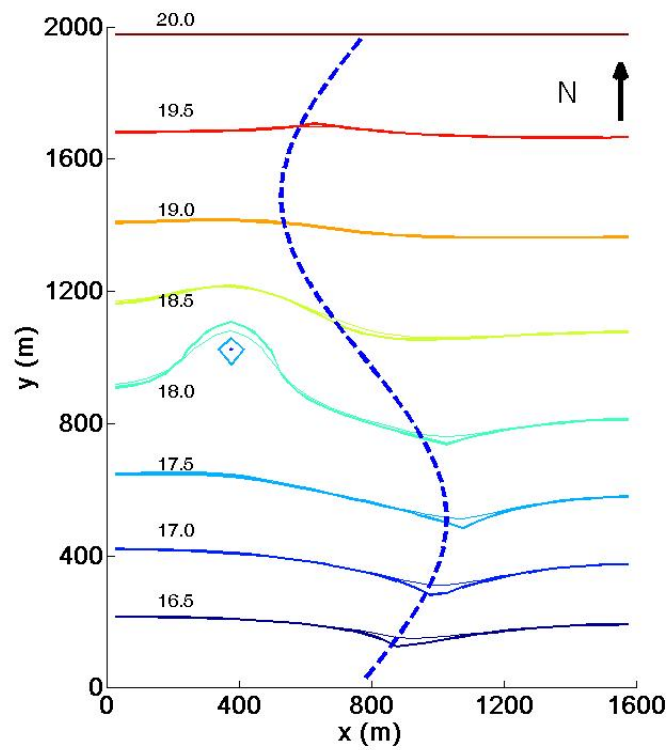


Figure 5.1: Head (m) in the model domain when pumping occurs in the unconfined aquifer at $(x, y)=(400 \text{ m}, 1000 \text{ m})$. Thick contour lines represent head in the unconfined aquifer and thin contour lines represent head in the confined aquifer.

maximum drawdown only impacts the model heads in the vicinity of the pumping well with an area with a radius of about 200 m from the well. The average difference between initial heads and heads after pumping across the unconfined aquifer is 0.023 m, which is 0.11% of the 20 m thickness of the unconfined aquifer. While drawdown in the immediate vicinity of the well might cause some vertical flow, the average drawdown is several orders of magnitude less than the aquifer thickness, indicating the assumption that drawdown in the unconfined aquifer is small compared to the aquifer thickness appropriately represents the behavior of the head. Cases where this assumption might not hold true include instances when the pumping rate is very high, causing higher depletions, especially in the vicinity of the pumping well, or in case where the unconfined aquifer is not very thick compared to the drawdown.

To test our assumption that the stream depletion will scale linearly with the pumping rate, we run several forward simulations using different pumping rates. We use a pumping well located at $(x, y) = (400 \text{ m}, 1000 \text{ m})$, and stream depletion was calculated using the forward approach in the same manner described in Section 4.2. The range of pumping rates we use is limited by the numerical precision of the model and the thickness of the unconfined aquifer. If the pumping rate is too low, the stream depletion will be on the same order as the model precision and it will appear there is no stream depletion. If the pumping rate is too high, the head in the cell containing the pumping well will drop below the bottom elevation of the unconfined aquifer, causing the cell to go dry and no longer be included in model calculations, resulting in the model calculating stream depletion inaccurately. For our model, the range of pumping rates that provide meaningful stream depletion results are $2 \text{ m}^3/\text{d} \leq Q_p \leq 62 \text{ m}^3/\text{d}$. Figure 5.2 shows the forward stream depletion plotted over this range of pumping rates. The behavior of the stream depletion is linear, indicating that this assumption is correct.

We also assume that using a value 19 m for h_{rc} in the adjoint simulation will not underestimate the forward values for stream depletion. After completing the adjoint simulation, we ran additional adjoint simulations with different values of h_{rc} to test how sensitive the adjoint stream depletion results were to h_{rc} and found no difference in depletion between $h_{rc} = 18 \text{ m}$, a river head constant

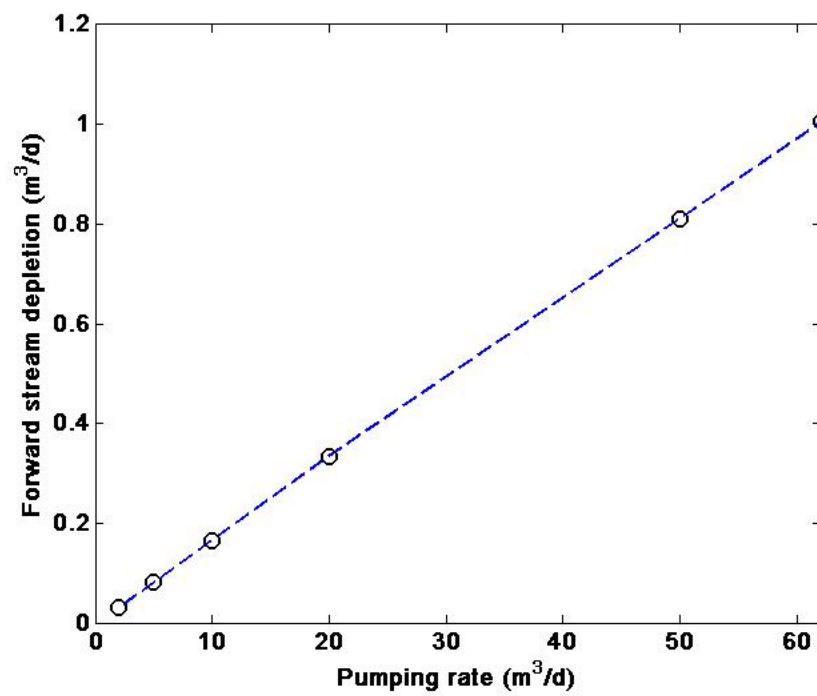


Figure 5.2: Linear scaling of forward stream depletion with pumping rate.

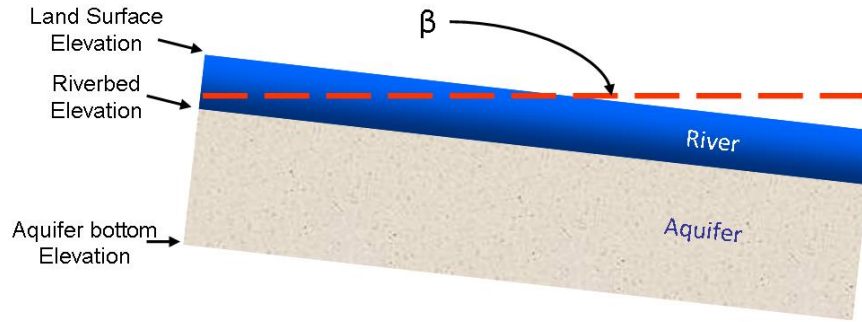


Figure 5.3: An aquifer underlying a slope where a single value of β does not remain above the elevation of the bottom of the aquifer and the river and below the land surface elevation.

representing high depletion, and $h_{rc} = 19$ m. We also found the difference in depletion between $h_{rc} = 15.25$ m, a river head constant representing a case where the river has almost run dry, and $h_{rc} = 19$ m was less than 2×10^{-7} m. From these results we conclude that a river head constant of $h_{rc} = 19$ m does not cause the adjoint depletion to underestimate the actual depletion.

5.2 Limitations

While this work provides an efficient method for determining stream depletion resulting from a new well at an unspecified location, it does have a few limitations. One of the main limitations lies in the bounds on the parameter β . Recall that β is used to prevent cells from going dry in the adjoint simulation and must be greater than the elevation of the bottom of the aquifer and the bottom of the riverbed but below the land surface elevation. These bounds are easily met if an aquifer and the overlying land surface are fairly flat; however, if an aquifer underlies a steep slope the bounds on β may not be able to be met throughout the model domain. Figure 5.3 represents a case where no single value of β can be used throughout the aquifer and this method of determining stream depletion can not be used to find stream depletion in this domain.

Another limitation of this method is that it cannot be used to site multiple wells based on

the the lowest possible stream depletion. Several cases where more than one well might be desired or required exist, such as required emergency wells or well fields that employ several wells; however, this work develops adjoint equation based on a single pumping well.

This method is also limited by its inability to handle situations where aquifer head drops below the river bottom the aquifer is no longer hydraulically connected to the river. In this instance, no additional stream depletion will occur. The adjoint method is not simulating head; it simulates the adjoint state and is not able to determine if the aquifer head drops below the river bottom. If the head does drop below the aquifer bottom, the adjoint method will continue calculating depletion that is not physically occurring and will over predict stream depletion, making it a conservative estimate. To avoid this, forward simulations can be run at selected locations with high depletion afterwards to determine if the aquifer has become disconnected from the river.

This work also assumes the river can be approximated as a wide rectangular channel where the width is much greater than the depth, allowing us to simplify Manning's equation. Most rivers and streams have different channel geometries and may not be well represented by a wide rectangular channel.

The revised STRADJ code is not currently set up to handle named parameters or diversions. This is not a limitation of the adjoint methodology, it is simply a limitation of the current implementation and will be addressed in future work.

Chapter 6

Conclusion & Future Work

In this final chapter, we present our conclusions and discuss areas of future work for the adjoint method of quantifying stream depletion.

6.1 Conclusions

This work develops an adjoint method for finding stream depletion caused by pumping in an aquifer that is hydraulically connected to a river using the adjoint approach. With only one simulation, the adjoint method provides the stream depletion associated with a pumping well located anywhere in the model domain. This information is useful for identifying locations for new wells that minimize stream depletion or for understanding what areas along a river section are most sensitive to pumping.

The adjoint method we develop in this work accurately approximates the stream depletion values for simulations that adhere to the assumptions we use to develop the adjoint approach. For a test case using a hypothetical aquifer, the adjoint stream depletion values are visually indistinguishable from the forward stream depletion values. The relative error between the adjoint and forward simulations is small.

The adjoint simulation proved to be far more computationally efficient than the forward simulations. Adjoint stream depletions for the model domain were found in 52 seconds, while the stream depletions results for the forward model took 4 hours and 36 minutes. The adjoint approach provides an accurate approximation of stream depletion in several orders of magnitude less time.

6.2 Future Work

This work proves the value of an adjoint approach to quantifying stream depletion and it also highlights areas of future work. While the method has proved effective when applied to a hypothetical aquifer, a case study comparing the adjoint stream depletion found using the method described in this work to the stream found from a model of an actual aquifer will provide insight into how the method works in a more complex model. A case study we intend to investigate is the model of the Upper San Pedro Basin in southern Arizona and northern Mexico that was developed by the USGS (Leake 2010).

In our development of the adjoint method, we did not investigate how the adjoint method behaves when used in conjunction with other sources or sinks, such as evapotranspiration. Additional work developing the adjoint method to accommodate additional sources and sinks that exist in natural systems will further the applicability of this work.

Another area of future work lies in Type III boundary conditions. Neupauer and Griebeling (2011) developed the adjoint theory for Type III boundary conditions of the form $\alpha h + \beta \Delta h \cdot n = g_3(t)$. This theory needs to be tested with the coupled version of the adjoint equations presented in this work.

Many of the limitations listed in Section 5.2 can be addressed by developing an adjoint version of the SFR package. The STR package is not designed to calculate unsaturated flow between the aquifer and the riverbed; however the stream flow routing (SFR) package has the capability of modeling unsaturated zone flow (Niswogner and Prudic 2005). To find stream depletion for cases where the aquifer head drops below the riverbed and unsaturated flow occurs, adjoint equations for unsaturated zone flow must be developed along with an adjoint version of the SFR package designed to handle these equations. The SFR package is also able to handle multiple channel geometries based on an eight point cross section, so the adjoint equations can be modified to account for an eight point channel geometry and the SFR package modified to calculate these equations (Prudic et al. 2004). Another capability of the SFR package is an alternate approach to calculating

stream depth and width from depth-discharge and width-discharge functions based on streamflow gage regressions. An adjoint version of the regression equations could be developed in place of the depth to flow relationship based on Manning's equation used in this work.

Another area of future work involves adapting this work to handle situations where stream depletion information is desired in systems with multiple wells. One approach to handling multiples wells is an optimization method that identifies a well configuration that minimized stream depletion.

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Appendix A

Adjoint Version of STR Code

Below is the modified version of the STR package code, which we call STRADJ, written in fortran.

```
C! Time of File Save by ERB: 3/9/2006 5:28PM
C   Last change:  ERB  12 Sep 2002   4:49 pm
C   ADJOINT VERSION of STR CODE
C   MODIFIED by SAG
C   MODIFIED by RMN, 3/17/2012, ADJOINT TRIBUTARY CALCULATIONS
C   SUBROUTINE GWF1STR6ALP(ISUM,ISUMI,LCSTRM,ICSTRM,MXSTRM,NSTREM,IN,
1       IOUT,ISTCB1,ISTCB2,NSS,NTRIB,NDIV,ICALC,CONST,
2       LCTBAR,LCTTRIB,LCIVAR,LCFGAR,NPSTR,ISTRPB)
C
C-----VERSION 15APRIL1998 GWF1STR6ALP
C-----VERSION 12MAR1999 -- modified to use character strings longer
C-----than 4 characters and to change VBVL and VBNM DIMENSION to MSUM
C   *****
C   ALLOCATE ARRAY STORAGE FOR STREAMS
C   *****
C
C   SPECIFICATIONS:
C   -----
C   CHARACTER*200 LINE
C   -----
C
C1-----IDENTIFY PACKAGE AND INITIALIZE NSTREM.
C   WRITE(IOUT,1) IN
C   1 FORMAT(1X,/1X,'STRM -- STREAM PACKAGE, VERSION 6, 6/98 ',
C   1'INPUT READ FROM UNIT ',I4)
C   NSTREM=0
C
C2----- READ MXACTS, NSS, NTRIB, ISTCB1, AND ISTCB2.
```



```

CALL URDCOM(IN,IOUT,LINE)
CALL UPARLSTAL(IN,IOUT,LINE,NPSTR,MXPS)
READ(LINE,3)MXACTS,NSS,NTRIB,NDIV,ICALC,CONST,ISTCB1,ISTCB2
3 FORMAT(5I10,F10.0,2I10)
  IF(MXACTS.LT.0)MXACTS=0
  IF(NSS.LT.0)NSS=0
  WRITE(IOUT,4)MXACTS,NSS,NTRIB
4 FORMAT(1X,'MAXIMUM OF ',I6,' ACTIVE STREAM NODES AT ONE TIME',/
1 1X,'NUMBER OF STREAM SEGMENTS IS ',I6,/
2 1X,'NUMBER OF STREAM TRIBUTARIES IS ',I6)
  IF(NDIV.GT.0) WRITE(IOUT,5)
5 FORMAT(1H ,'DIVERSIONS FROM STREAMS HAVE BEEN SPECIFIED')
  IF(ICALC.GT.0) WRITE(IOUT,6) CONST
6 FORMAT(1X,'STREAM STAGES WILL BE CALCULATED USING A CONSTANT OF '
1 ,F10.4)
  IF(ISTCB1.GT.0) WRITE(IOUT,7) ISTCB1,ISTCB2
7 FORMAT(1X,'CELL BUDGETS WILL BE SAVED ON UNITS ',I4,' AND ',I4)
C
C3-----SET LCSTRM EQUAL TO ADDRESS OF FIRST UNUSED SPACE IN RX.
  ISTRPB=MXACTS+1
  MXSTRM=MXACTS+MXPS
  LCSTRM=ISUM
C
C4-----CALCULATE AMOUNT OF SPACE NEEDED FOR STRM LIST.
C   ++++ADJOINT MODIFICATION++++
  ISPA=12*MXSTRM
C   ++++ADJOINT MODIFICATION++++
  ISUM=ISUM+ISPA
C
C5-----CALCULATE AMOUNT OF SPACE NEEDED FOR ISTRM LIST.
  ICSTRM=ISUMI
  ISPB=5*MXSTRM
  ISUMI=ISUMI+ISPB
C
C6-----CALCULATE AMOUNT OF SPACE NEEDED FOR ITRBAR LIST.
  LCTBAR=ISUMI
  ISPC=NSS*NTRIB
  ISUMI=ISUMI+ISPC
C
C7-----CALCULATE AMOUNT OF SPACE NEEDED FOR ARTRIB LIST.
  LCTRIB=ISUM
  ISPD=NSS
  ISUM=ISUM+ISPD
C
C   ++++++ ADJOINT MODIFICATION ++++++ RMN
C7-----CALCULATE AMOUNT OF SPACE NEEDED FOR MXRCH LIST.
  LCMXRC=ISUM

```

```

      ISPDA=NSS
      ISUM=ISUM+ISPDA
C
C8A-----CALCULATE AMOUNT OF SPACE NEEDED FOR IDIVAR LIST.
      LCIVAR=ISUMI
      ISPE=NSS
      ISUMI=ISUMI+ISPE
C
C8B-----CALCULATE AMOUNT IF SPACE NEEDED FOR NDFGAR LIST.
      LCFGAR=ISUMI
      ISPF=NSS
      ISUMI=ISUMI+ISPF
C
C9-----PRINT AMOUNT OF SPACE USED BY STREAM PACKAGE.
      ISP=ISPA+ISPD
      WRITE (IOUT,8)ISP
      8 FORMAT(1X,I10,' ELEMENTS IN RX ARRAY ARE USED FOR STREAMS')
      ISP=ISPB+ISPC+ISPE+ISPF
      WRITE (IOUT,9)ISP
      9 FORMAT(1X,I10,' ELEMENTS IN IR ARRAY ARE USED FOR STREAMS')
C
C10-----RETURN.
      RETURN
      END
      SUBROUTINE GWF1STR6RPPD(IN,IOUT,NCOL,NROW,NLAY,NPSTR,STRM,ISTRM,
&          ISTRPB,MXSTRM,ITERP,INAMLOC)
C
C-----VERSION 20011108 GWF1STR6RPPD
C *****
C READ STREAM PARAMETERS
C *****
C Modified 11/8/2001 to support parameter instances - ERB
C
C SPECIFICATIONS:
C -----
C Original code: DIMENSION STRM(11,MXSTRM),ISTRM(5,MXSTRM)
C ++++ADJOINT MODIFICATION++++
C DIMENSION STRM(12,MXSTRM),ISTRM(5,MXSTRM)
C ++++ADJOINT MODIFICATION++++
C -----
C
C-----READ NAMED PARAMETERS.
      IF (ITERP.EQ.1) THEN
          IRDFLG = 0
          WRITE(IOUT,1000) NPSTR
1000  FORMAT(1X,//1X,I5,' Stream parameters')
      ELSE

```

```

        IRDFLG = 1
    ENDIF
    IF(NPSTR.GT.0) THEN
        LSTSUM=ISTRPB
        DO 20 K=1,NPSTR
            LSTBEG=LSTSUM
            CALL UPARLSTRP(LSTSUM,MXSTRM,IN,IOUT,IP,'STR','STR',ITERP,
&                NUMINST,INAMLOC)
            NLST=LSTSUM-LSTBEG
            IF (NUMINST.GT.1) NLST = NLST/NUMINST
C        ASSIGN STARTING INDEX FOR READING INSTANCES
            IF (NUMINST.EQ.0) THEN
                IB=0
            ELSE
                IB=1
            ENDIF
C        READ LIST(S) OF CELLS, PRECEDED BY INSTANCE NAME IF NUMINST>0
            LB=LSTBEG
            DO 10 I=IB,NUMINST
                IF (I.GT.0) THEN
                    CALL UINSRP(I,IN,IOUT,IP,ITERP)
                ENDIF
                CALL SGWF1STR6R(NLST,MXSTRM,STRM,ISTRM,IB,IN,
&                IOUT,NCOL,NROW,NLAY,IRDFLG)
                LB=LB+NLST
            10    CONTINUE
            20    CONTINUE
            END IF
C
C6-----RETURN
            RETURN
            END
C        ORIGINAL CODE
C        SUBROUTINE GWF1STR6RPSS(STRM,ISTRM,NSTREM,MXSTRM,IN,IOUT,ITRBAR,
C        1        NDIV,NSS,NTRIB,IDIVAR,ICALC,IPTFLG,NCOL,NROW,NLAY,NPSTR,
C        2        ISTRPB)
C        ++++++++ ADJOINT MODIFICATION ++++++++ RMN
C        SUBROUTINE GWF1STR6RPSS(STRM,ISTRM,NSTREM,MXSTRM,IN,IOUT,ITRBAR,
C        1        NDIV,NSS,NTRIB,IDIVAR,ICALC,IPTFLG,NCOL,NROW,NLAY,NPSTR,
C        2        ISTRPB,MXRCH)
C        ++++++++ ADJOINT MODIFICATION ++++++++ RMN

C-----VERSION 15APRIL1998 GWF1STR6RPSS
C        *****
C        READ STREAM DATA:  INCLUDES SEGMENT AND REACH NUMBERS, CELL
C        SEQUENCE OF SEGMENT AND REACH, FLOW INTO MODEL AT BOUNDARY,
C        STREAM STAGE, STREAMBED CONDUCTANCE, AND STREAMBED TOP AND

```

```

C          BOTTOM ELEVATIONS
C          *****
C
C          SPECIFICATIONS:
C          -----
C          Original code: DIMENSION STRM(11,MXSTRM),ISTRM(5,MXSTRM),ITRBAR(NSS,NTRIB),
C          1          IDIVAR(NSS)
C          ++++ADJOINT MODIFICATION++++ RMN
C          DIMENSION STRM(12,MXSTRM),ISTRM(5,MXSTRM),ITRBAR(NSS,NTRIB),
C          1          IDIVAR(NSS),MXRCH(NSS)
C          ++++ADJOINT MODIFICATION++++ RMN
C          -----
C
C1A-----IF MXSTREAM IS LESS THAN 1 THEN STREAM IS INACTIVE. RETURN.
C          IF(MXSTRM.LT.1) RETURN
C
C1B-----READ ITMP(NUMBER OF STREAM CELLS OR PARAMETERS).
C          READ(IN,1)ITMP,IRDFLG,IPTFLG
C          1 FORMAT(4I10)
C
C          MXACTS=ISTRPB-1
C          IF(NPSTR.LE.0) THEN
C
C2A-----IF ITMP <0 THEN REUSE NON-PARAMETER DATA FROM LAST STRESS PERIOD.
C          IF(ITMP.LT.0) THEN
C              WRITE(IOUT,2)
C          2          FORMAT(/,'REUSING STREAM NODES FROM LAST STRESS PERIOD')
C              RETURN
C          ELSE
C
C3A-----IF THERE ARE NEW NON-PARAMETER STREAM CELLS, READ THEM
C          NSTREM=ITMP
C          IF(NSTREM.GT.MXACTS) THEN
C              WRITE(IOUT,99) NSTREM,MXACTS
C          99          FORMAT(1X,/1X,'THE NUMBER OF ACTIVE STREAM CELLS (',
C          1          I6,') IS GREATER THAN MXACTS(',I6,')')
C              CALL USTOP(' ')
C          END IF
C          +++++++ ADJOINT MODEIFICATION +++++++ RMN
C              CALL SGWF1STR6R(NSTREM,MXSTRM,STRM,ISTRM,1,IN,IOUT,NCOL,
C          1          NROW,NLAY,IRDFLG,MXRCH,NSS)
C          +++++++ ADJOINT MODEIFICATION +++++++ RMN
C              END IF
C          ELSE
C
C1C-----IF THERE ARE ACTIVE STR PARAMETERS, READ THEM AND SUBSTITUTE

```

```

NSTREM=0
CALL PRESET('STR')
IF(ITMP.GT.0) THEN
  DO 100 N=1,ITMP
    CALL UPARLSTLOC(IN,'STR',IOUT,'STR',IBEG,IEND,PV)
    NLST=IEND-IBEG+1
    NSTREM=NSTREM+NLST
    IF(NLST.GT.MXACTS) THEN
      WRITE(IOUT,99) NLST,MXACTS
      CALL USTOP(' ')
    END IF
    DO 50 I=1,NLST
      II=NSTREM-NLST+I
      III=IBEG+I-1
      DO 40 J=1,5
        STRM(J,II)=STRM(J,III)
        ISTRM(J,II)=ISTRM(J,III)
40      CONTINUE
        STRM(3,II)=STRM(3,II)*PV
        IF(IRDFLG.EQ.0) THEN
          IF (N.EQ.1 .AND. I.EQ.1) WRITE(IOUT,4)
4          FORMAT(/,4X,'LAYER  ROW    COL    SEGMENT  REACH  STREAMFLOW',
16X,'STREAM  STREAMBED  STREAMBED BOT  STREAMBED TOP',/27X,
2'NUMBER  NUMBER                                STAGE  CONDUCTANCE',6X,
3'ELEVATION  ELEVATION',/3X,110('-'))
          WRITE(IOUT,6) (ISTRM(J,II),J=1,5), (STRM(J,II),J=1,5)
        ENDIF
6          FORMAT(1X,1X,I6,2I7,2I9,7X,G11.4,G12.4,G11.4,4X,2G13.4)
50      CONTINUE
C
100     CONTINUE
      END IF
    END IF
C
C3-----PRINT NUMBER OF REACHES IN CURRENT STRESS PERIOD.
      WRITE (IOUT,101) NSTREM
101  FORMAT(1X,/1X,I6,' STREAM REACHES')
C
C4-----IF THERE ARE NO STREAM REACHES THEN RETURN.
      IF(NSTREM.EQ.0) RETURN
C
C6----READ AND PRINT DATA IF STREAM STAGE IS CALCULATED.
      IF(ICALC.LE.0) GO TO 300
      IF(IRDFLG.EQ.0) WRITE(IOUT,7)
7  FORMAT(/,4X,'LAYER',3X,'ROW',4X,'COL  ',',', 'SEGMENT',3X,
1'REACH',8X,'STREAM',13X,'STREAM',10X,'ROUGH',/27X,'NUMBER',3X,
2 'NUMBER',8X,'WIDTH',14X,'SLOPE',10X,'COEF.',/3X,110('-'))

```

```

      DO 280 II=1,NSTREM
      READ(IN,8) STRM(6,II),STRM(7,II),STRM(8,II)
8  FORMAT(3F10.0)
      IF(IRDFLG.EQ.0) WRITE(IOUT,9) ISTRM(1,II),
&   ISTRM(2,II),ISTRM(3,II),ISTRM(4,II),ISTRM(5,II),
1   STRM(6,II),STRM(7,II),STRM(8,II)
      9  FORMAT(2X,I6,2I7,2I9,7X,G12.4,4X,G13.4,4X,G12.4)
280  CONTINUE
C
C7-----INITIALIZE ALL TRIBUTARY SEGMENTS TO ZERO.
300  DO 320 IK=1,NSS
      DO 320 JK=1,NTRIB
      ITRBAR(IK,JK)=0
320  CONTINUE
C
C8-----INITIALIZE DIVERSION SEGMENT ARRAY TO ZERO.
      DO 325 IK=1,NSS
      IDIVAR(IK)=0
325  CONTINUE
C
C9-----READ AND PRINT TRIBUTARY SEGMENTS.
      IF(NTRIB.LE.0) GO TO 343
      IF(IRDFLG.EQ.0) WRITE(IOUT,10)NTRIB
10  FORMAT(/,30X,'MAXIMUM NUMBER OF TRIBUTARY STREAMS IS ',I6,//1X,
1   20X,'STREAM SEGMENT',15X,'TRIBUTARY STREAM SEGMENT NUMBERS')
      DO 340 IK=1,NSS
      READ(IN,11) (ITRBAR(IK,JK),JK=1,NTRIB)
11  FORMAT(10I5)
      IF(IRDFLG.EQ.0) WRITE(IOUT,12) IK,(ITRBAR(IK,JK),JK=1,NTRIB)
12  FORMAT(19X,I6,20X,10I5)
340  CONTINUE
C
C10----READ AND PRINT DIVERSION SEGMENTS NUMBERS.
343  IF(NDIV.LE.0) GO TO 350
      IF(IRDFLG.EQ.0) WRITE(IOUT,13)
13  FORMAT(/,10X,'DIVERSION SEGMENT NUMBER',10X,
1   'UPSTREAM SEGMENT NUMBER')
      DO 345 IK=1,NSS
      READ(IN,14) IDIVAR(IK)
14  FORMAT(I10)
      IF(IRDFLG.EQ.0) WRITE(IOUT,15) IK,IDIVAR(IK)
15  FORMAT(19X,I6,27X,I6)
345  CONTINUE
C
C11----SET FLOW OUT OF REACH, FLOW INTO REACH, AND FLOW THROUGH
C   STREAM BED TO ZERO.
350  DO 360 II =1,NSTREM

```

```

        STRM(9,II)=0.0
        STRM(10,II)=0.0
        STRM(11,II)=0.0
360 CONTINUE
C
C12-----RETURN
        RETURN
        END
C ORIGINAL CODE
C SUBROUTINE GWF1STR6FM(NSTREM,STRM,ISTRM,HNEW,HCOF,RHS,IBOUND,
C 1 MXSTRM,NCOL,NROW,NLAY,NSS,ITRBAR,NTRIB,ARTRIB,
C 2 IDIVAR,NDFGAR,ICALC,CONST)
C ++++++++ ADJOINT MODIFICIATION ++++++++ RMN
        SUBROUTINE GWF1STR6FM(NSTREM,STRM,ISTRM,HNEW,HCOF,RHS,IBOUND,
1 MXSTRM,NCOL,NROW,NLAY,NSS,ITRBAR,NTRIB,ARTRIB,
2 IDIVAR,NDFGAR,ICALC,CONST,MXRCH)
C ++++++++ ADJOINT MODIFICIATION ++++++++ RMN
C
C-----VERSION 15APRIL1998 GWF1STR6FM
C
C *****C
C ADD STREAM TERMS TO RHS AND HCOF IF FLOW OCCURS IN MODEL CELL C
C *****C
C
C SPECIFICATIONS: C
C -----C
C
C DOUBLE PRECISION HNEW
C Original code: DIMENSION STRM(11,MXSTRM),ISTRM(5,MXSTRM),HNEW(NCOL,NROW,NLAY),
C 1 HCOF(NCOL,NROW,NLAY),RHS(NCOL,NROW,NLAY),
C 2 IBOUND(NCOL,NROW,NLAY),ITRBAR(NSS,NTRIB),ARTRIB(NSS),
C 3 IDIVAR(NSS),NDFGAR(NSS)
C
C ++++ADJOINT MODIFICATION++++ RMN
        DIMENSION STRM(12,MXSTRM),ISTRM(5,MXSTRM),HNEW(NCOL,NROW,NLAY),
1 HCOF(NCOL,NROW,NLAY),RHS(NCOL,NROW,NLAY),
2 IBOUND(NCOL,NROW,NLAY),ITRBAR(NSS,NTRIB),ARTRIB(NSS),
3 IDIVAR(NSS),NDFGAR(NSS),MXRCH(NSS)
C ++++ADJOINT MODIFICATION++++ RMN
C
C -----C
C
C1-----IF NSTREM<=0 THERE ARE NO STREAMS. RETURN. C
        IF(NSTREM.LE.0)RETURN
C
C2A-----PROCESS EACH CELL IN THE STREAM LIST. C
C2B-----INITIALIZE NDFGAR ARRAY TO ZERO. C

```

```

DO 5 I=1,NSS
NDFGAR(I)=0
5 CONTINUE
C
C
C3-----DETERMINE LAYER, ROW, COLUMN OF EACH REACH.
C
C   Original Code:
C   DO 500 L=1,NSTREM
C   LL=L-1
C   ++++ADJOINT MODIFICATION++++
C   DO 500 LNEW=1,NSTREM
C     L=NSTREM-LNEW+1
C     LL=L+1
C   ++++ADJOINT MODIFICATION++++
C     IL=ISTRM(1,L)
C     IR=ISTRM(2,L)
C     IC=ISTRM(3,L)
C
C
C4----06FEB1990, CHECK FOR CELLS OUTSIDE MOVED TO C12, C16 AND C18.
C
C5-----DETERMINE STREAM SEGMENT AND REACH NUMBER.
C     ISTSG=ISTRM(4,L)
C     NREACH=ISTRM(5,L)
C
C
C6-----SET FLOWIN EQUAL TO STREAM SEGMENT INFLOW IF FIRST REACH.
C
C   ORIGINAL CODE:
C   IF(NREACH.GT.1) GO TO 200
C   FLOWIN=STRM(1,L)
C   ++++ADJOINT MODIFICATION++++ RMN
C     IF (NREACH.LT.MXRCH(ISTSG)) GO TO 200
C     FLOWIN=STRM(1,L)
C   ++++ADJOINT MODIFICATION++++ RMN
C
C
C7-----STORE OUTFLOW FROM PREVIOUS SEGMENT IN ARTRIB IF SEGMENT >1.
C
C   ORIGINAL CODE:
C   IF(ISTSG.EQ.1)GO TO 50
C   IFLG = ISTRM(4,LL)
C   ARTRIB(IFLG)=STRM(9,LL)
C   ++++ADJOINT MODIFICATION++++ RMN
C     IFLG = ISTRM(4,LL)
C   ++++ADJOINT MODIFICATION++++ RMN
C
C
C8A-----CHECK UPSTREAM SEGMENT FOR DIVERSIONS.
C
C   DO 40 NSFLG = 1,NSS
C   IF(IFLG.NE.IDIVAR(NSFLG)) GO TO 40
C
C
C8B-----DETERMINE AMOUNT OF FLOW TO BE DIVERTED.
C
C   DO 20 IDL=1,NSTREM

```



```

        IF(NSFLG.NE.ISTRM(4,IDL)) GO TO 20
        IF(ISTRM(5,IDL).NE.1) GO TO 20
        DUM=ARTRIB(IFLG)-STRM(1,IDL)
C
C8C-----SUBTRACT FLOW FROM UPSTREAM SEGMENT IF THERE IS ENOUGH FLOW
C-----IN UPSTREAM SEGMENT.
        IF(DUM.GE.0.0) ARTRIB(IFLG)=DUM
        IF(DUM.LT.0.0) NDFGAR(IFLG)=1
        20 CONTINUE
        40 CONTINUE
        50 IF(IDIVAR(ISTSG).LE.0) GO TO 60
            NDFLG=IDIVAR(ISTSG)
            IF(NDFGAR(NDFLG).EQ.1) FLOWIN=0.0
        60 IF(FLOWIN.GE.0.0) GO TO 300
C
C9-----SUM TRIBUTARY OUTFLOW AND USE AS INFLOW INTO DOWNSTREAM SEGMENT.
C ORIGINAL CODE
C FLOWIN =0.
C DO 100 ITRIB=1,NTRIB
C INODE=ITRIBAR(ISTSG,ITRIB)
C IF(INODE.LE.0) GO TO 100
C FLOWIN=FLOWIN+ARTRIB(INODE)
C 100 CONTINUE
C ++++ADJOINT MODIFICATION++++ RMN
C FLOWIN=ARTRIB(ISTSG)
C ++++ADJOINT MODIFICATION++++ RMN
C
C10-----IF REACH >1, SET INFLOW EQUAL TO OUTFLOW FROM UPSTREAM REACH.
C ORIGINAL CODE:
C 200 IF(NREACH.GT.1) FLOWIN=STRM(9,LL)
C ++++ ADJOINT MODIFICATION +++++ RMN
C 200 IF (NREACH.LT.MXRCH(ISTSG)) FLOWIN=STRM(9,LL)
C ++++ ADJOINT MODIFICATION +++++ RMN
C
C11-----COMPUTE STREAM STAGE IN REACH IF ICALC IS GREATER THAN 1.
        300 IF(ICALC.LE.0) GO TO 310
C Original code:
C XNUM=((FLOWIN+STRM(9,L))/2.0)*STRM(8,L)
C DNOM=CONST*STRM(6,L)*(SQRT(STRM(7,L)))
C DEPTH=(XNUM/DNOM)**0.6
C
C ++++Adjoint Modification++++
C XNUM=3.0*((FLOWIN+STRM(9,L))/2.0)*STRM(8,L)
C DNOMA=5.0*CONST*STRM(6,L)*(SQRT(STRM(7,L)))
C DNOMB=(STRM(12,L)-STRM(5,L))**(2.0/3.0)
        DNOM=DNOMA*DNOMB
        DEPTH=XNUM/DNOM

```

```

C   ++++Adjoint Modification++++
      IF(DEPTH.LE.0.) DEPTH=0.
      STRM(2,L)=DEPTH+STRM(5,L)
310 HSTR=STRM(2,L)
C
C12----DETERMINE LEAKAGE THROUGH STREAMBED.
      IF(IBOUND(IC,IR,IL).LE.0) GO TO 315
      IF(FLOWIN.LE.0.) HSTR=STRM(5,L)
      CSTR=STRM(3,L)
      SBOT=STRM(4,L)
      H=HNEW(IC,IR,IL)
      T=HSTR-SBOT
C
C13----COMPUTE LEAKAGE AS A FUNCTION OF STREAM STAGE AND HEAD IN CELL.
C      Original code: FLOBOT=CSTR*(HSTR-H)
C
C   ++++Adjoint Modification++++
      FLOBOT=(CSTR*(HSTR-H))
C   ++++Adjoint Modification++++
C
C14----RECOMPUTE LEAKAGE IF HEAD IN CELL IS BELOW STREAMBED BOTTOM.
      IQFLG=0
      IF(H.GT.SBOT) GO TO 312
      IQFLG=1
      FLOBOT=CSTR*T
C
C15----SET LEAKAGE EQUAL TO STREAM INFLOW IF LEAKAGE MORE THAN INFLOW.
312 IF(FLOBOT.LE.FLOWIN) GO TO 320
      IQFLG=1
      FLOBOT=FLOWIN
C
C16-----STREAMFLOW OUT EQUALS STREAMFLOW IN MINUS LEAKAGE.
315 IF(IBOUND(IC,IR,IL).LE.0) FLOBOT=0.
320 FLOWOT=FLOWIN-FLOBOT
C      ORIGINAL CODE (DELETED FROM ADJOINT MODIFICATIONS) RMN
C      IF((ISTSG.GT.1).AND.(NREACH.EQ.1)) STRM(9,LL)=ARTRIB(IFLG)
C
C17----STORE STREAM INFLOW, OUTFLOW AND LEAKAGE FOR EACH REACH.
      STRM(9,L)=FLOWOT
      STRM(10,L)=FLOWIN
      STRM(11,L)=FLOBOT
C   ++++ADJOINT MODIFICATION++++ RMN
      IF (NREACH.GT.1) GO TO 201
      DO 30 ITRIB=1,NTRIB
          INODE=ITRIBAR(ISTSG,ITRIB)
          IF (INODE.NE.0) ARTRIB(INODE)=STRM(9,L)
30      CONTINUE

```

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201      CONTINUE
C      ++++ADJOINT MODIFICATION++++  RMN
C
C18----RETURN TO STEP 3 IF STREAM INFLOW IS LESS THAN OR EQUAL TO ZERO C
C      AND LEAKAGE IS GREATER THAN OR EQUAL TO ZERO OR IF CELL C
C      IS NOT ACTIVE--IBOUND IS LESS THAN OR EQUAL TO ZERO. C
      IF(IBOUND(IC,IR,IL).LE.0) GO TO 500
      IF((FLOWIN.LE.0.0).AND.(FLOBOT.GE.0.0)) GO TO 500
C
C19-----IF HEAD > BOTTOM THEN ADD TERMS TO RHS AND HCOF. C
      IF(IQFLG.GT.0) GO TO 400
      RHS(IC,IR,IL)=RHS(IC,IR,IL)-CSTR*HSTR
      HCOF(IC,IR,IL)=HCOF(IC,IR,IL)-CSTR
      GO TO 500
C
C20-----IF HEAD < BOTTOM THEN ADD TERM ONLY TO RHS. C
      400 RHS(IC,IR,IL)=RHS(IC,IR,IL)-FLOBOT
      500 CONTINUE
C
C21-----RETURN. C
      RETURN
      END
C      ORIGINAL CODE
C      SUBROUTINE GWF1STR6BD(NSTREM,STRM,ISTRM,IBOUND,MXSTRM,HNEW,NCOL,
C      1  NROW,NLAY,DELT,VBVL,VBNM,MSUM,KSTP,KPER,ISTCB1,ISTCB2,ICBCFL,
C      2  BUFF,IOUT,NTRIB,NSS,ARTRIB,ITRBAR,IDIVAR,NDFGAR,ICALC,CONST,
C      3  IPTFLG)
C      ++++++++ ADJOINT MODIFICIATION ++++++++ RMN
      SUBROUTINE GWF1STR6BD(NSTREM,STRM,ISTRM,IBOUND,MXSTRM,HNEW,NCOL,
      1  NROW,NLAY,DELT,VBVL,VBNM,MSUM,KSTP,KPER,ISTCB1,ISTCB2,ICBCFL,
      2  BUFF,IOUT,NTRIB,NSS,ARTRIB,ITRBAR,IDIVAR,NDFGAR,ICALC,CONST,
      3  IPTFLG,MXRCH)
C      ++++++++ ADJOINT MODIFICIATION ++++++++ RMN

C-----VERSION 2 18DEC1990 GWF1STR6BD C
C
C      *****C
C      CALCULATE VOLUMETRIC BUDGET FOR STREAMS C
C      *****C
C
C      SPECIFICATIONS: C
C      -----C
      CHARACTER*16 VBNM(MSUM),TEXT,STRTXT
      DOUBLE PRECISION HNEW
C      Original Code: DIMENSION STRM(11,MXSTRM),ISTRM(5,MXSTRM),IBOUND(NCOL,NROW,NLAY),
C      1      HNEW(NCOL,NROW,NLAY),VBVL(4,MSUM),
C      2      BUFF(NCOL,NROW,NLAY),ARTRIB(NSS),ITRBAR(NSS,NTRIB),

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C      3          IDIVAR(NSS),NDFGAR(NSS)
C      ++++ADJOINT MODIFICATION++++
        DIMENSION STRM(12,MXSTRM),ISTRM(5,MXSTRM),IBOUND(NCOL,NROW,NLAY),
1         HNEW(NCOL,NROW,NLAY),VBVL(4,MSUM),
2         BUFF(NCOL,NROW,NLAY),ARTRIB(NSS),ITRBAR(NSS,NTRIB),
3         IDIVAR(NSS),NDFGAR(NSS),MXRCH(NSS)
C      ++++ADJOINT MODIFICATION++++
        DATA TEXT/' STREAM LEAKAGE'/
        DATA STRTXT/'STREAM FLOW OUT '/
C      -----C
C
        WRITE(IOUT,*) ISTRM(1,10),ISTRM(2,10),ISTRM(3,10), ISTRM(4,10)
C1-----SET IBD=1 IF BUDGET TERMS SHOULD BE SAVED ON DISK.      C
        IBD=0
        RATIN = 0.
        RATOUT = 0.
C
C2-----IF NO REACHES, KEEP ZEROS IN ACCUMULATORS.            C
        IF(NSTREM.EQ.0) GO TO 600
C
C3A-----TEST TO SEE IF CELL-BY-CELL TERMS ARE NEEDED.        C
        IF((ICBCFL.EQ.0).OR.(ISTCB1.LE.0)) GO TO 10
C
C3B-----CELL-BY-CELL TERMS ARE NEEDED, SET IBD AND CLEAR BUFFER. C
        IBD = 1
        DO 5 IL=1,NLAY
        DO 5 IR=1,NROW
        DO 5 IC=1,NCOL
        BUFF(IC,IR,IL)=0.
        5 CONTINUE
C
C3C-----INITIALIZE NDFGAR ARRAY TO ZERO.                        C
        DO 7 I=1,NSS
        NDFGAR(I)=0
        7 CONTINUE
C
        WRITE(*,*) NSTREM
C4-----IF THERE ARE STREAMS THEN ACCUMULATE LEAKAGE TO OR FROM THEM. C
C      Original Code:
C      10 DO 500 L=1,NSTREM
C          LL=L-1
C      ++++ADJOINT MODIFICATION++++
C      10 DO 500 LNEW=1,NSTREM
C          L=NSTREM-LNEW+1
C          LL=L+1
C      ++++ADJOINT MODIFICATION++++
C

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C5---DETERMINE REACH LOCATION. C
      IL=ISTRM(1,L)
      IR=ISTRM(2,L)
      IC=ISTRM(3,L)
C C
C6----06FEB1990, CHECK FOR CELLS OUTSIDE MOVED TO C14, C18 AND C29. C
C C
C7-----DETERMINE SEGMENT AND REACH NUMBER. C
      ISTSG=ISTRM(4,L)
      NREACH=ISTRM(5,L)
C ORIGINAL CODE:
C   IF(NREACH.GT.1) GO TO 200
C C
C8-----SET FLOWIN EQUAL TO SEGMENT INFLOW IF FIRST REACH. C
C   FLOWIN=STRM(1,L)
C   ++++ADJOINT MODIFICATION++++ RMN
C     IF (NREACH.LT.MXRCH(ISTSG)) GO TO 200
C     FLOWIN=STRM(1,L)
C   ++++ADJOINT MODIFICATION++++ RMN
C C
C9-----STORE OUTFLOW FROM PREVIOUS SEGMENT IN ARTRIB IF SEGMENT >1. C
C   ORIGINAL CODE:
C   IF(ISTSG.EQ.1) GO TO 50
C   IFLG = ISTRM(4,LL)
C   ARTRIB(IFLG)=STRM(9,LL)
C   ++++ADJOINT MODIFICATION++++ RMN
C     IFLG = ISTRM(4,LL)
C   ++++ADJOINT MODIFICATION++++ RMN
C C
C10A----CHECK UPSTREAM SEGMENT FOR DIVERSIONS. C
      DO 40 NSFLG = 1,NSS
      IF(IFLG.NE.IDIVAR(NSFLG)) GO TO 40
C C
C10B----DETERMINE AMOUNT OF FLOW TO BE DIVERTED. C
      DO 20 IDL=1,NSTREM
      IF(NSFLG.NE.ISTRM(4,IDL)) GO TO 20
      IF(ISTRM(5,IDL).NE.1) GO TO 20
      DUM=ARTRIB(IFLG)-STRM(1,IDL)
C C
C10C----SUBTRACT FLOW FROM UPSTREAM SEGMENT IF THERE IS ENOUGH FLOW C
C   IN UPSTREAM SEGMENT. C
      IF(DUM.GE.0.0) ARTRIB(IFLG)=DUM
      IF(DUM.LT.0.0) NDFGAR(IFLG)=1
      20 CONTINUE
      40 CONTINUE
      50 IF(IDIVAR(ISTSG).LE.0) GO TO 60
      NDFLG=IDIVAR(ISTSG)

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        IF(NDFGAR(NDFLG).EQ.1) FLOWIN=0.0
    60 IF(FLOWIN.GE.0.0) GO TO 300
C
C11--SUM TRIBUTARY OUTFLOW AND USE AS INFLOW INTO DOWNSTREAM SEGMENT. C
C    ORIGINAL CODE:
C    FLOWIN =0.
C    DO 100 ITRIB=1,NTRIB
C    INODE=ITRBAR(ISTSG,ITRIB)
C    IF(INODE.LE.0) GO TO 100
C    FLOWIN=FLOWIN+ARTRIB(INODE)
C 100 CONTINUE
C    ++++ADJOINT MODIFICATION++++    RMN
C    FLOWIN=ARTRIB(ISTSG)
C    ++++ADJOINT MODIFICATION++++    RMN
C
C12-----IF REACH >1, SET INFLOW EQUAL TO OUTFLOW FROM UPSTREAM REACH. C
C    ORIGINAL CODE:
C 200 IF(NREACH.GT.1) FLOWIN=STRM(9,LL)
C ++++ ADJOINT MODIFICATION ++++++ RMN
C 200 IF (NREACH.LT.MXRCH(ISTSG)) FLOWIN=STRM(9,LL)
C ++++ ADJOINT MODIFICATION ++++++ RMN
C
C13----COMPUTE STREAM STAGE IN REACH IF ICALC > 1. C
C 300 IF(ICALC.LE.0) GO TO 310
C    Original Code:
C    XNUM=((FLOWIN+STRM(9,L))/2.0)*STRM(8,L)
C    DNOM=CONST*STRM(6,L)*(SQRT(STRM(7,L)))
C    DEPTH=(XNUM/DNOM)**0.6
C
C    ++++Adjoint Modification++++
C    XNUM=3.0*((FLOWIN+STRM(9,L))/2.0)*STRM(8,L)
C    DNOMA=5.0*CONST*STRM(6,L)*(SQRT(STRM(7,L)))
C    DNOMB=(STRM(12,L)-STRM(5,L))*(2.0/3.0)
C    DNOM=DNOMA*DNOMB
C    DEPTH=XNUM/DNOM
C    ++++Adjoint Modification++++
C    IF((DEPTH).LE.0) DEPTH=0.
C    STRM(2,L)=DEPTH+STRM(5,L)
C 310 HSTR=STRM(2,L)
C
C14----DETERMINE LEAKAGE THROUGH STREAMBED. C
C    IF(IBOUND(IC,IR,IL).LE.0) GO TO 315
C    IF(FLOWIN.LE.0.0) HSTR=STRM(5,L)
C    CSTR=STRM(3,L)
C    SBOT=STRM(4,L)
C    H=HNEW(IC,IR,IL)
C    T=HSTR-SBOT

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C                                                    C
C15----COMPUTE LEAKAGE AS A FUNCTION OF STREAM STAGE AND HEAD IN CELL. C
C      Original code: FLOBOT=CSTR*(HSTR-H)
C      ++++Adjoint Modification++++
C      FLOBOT=(CSTR*(HSTR-H))
C      ++++Adjoint Modification++++
C                                                    C
C16----RECOMPUTE LEAKAGE IF HEAD IN CELL IS BELOW STREAMBED BOTTOM. C
C      IF(H.GT.SBOT) GO TO 312
C      FLOBOT=CSTR*T
C                                                    C
C17----SET LEAKAGE EQUAL TO STREAM INFLOW IF LEAKAGE MORE THAN INFLOW. C
C      312 IF(FLOBOT.LE.FLOWIN) GO TO 320
C      FLOBOT=FLOWIN
C                                                    C
C18----STREAMFLOW OUT EQUALS STREAMFLOW IN MINUS LEAKAGE. C
C      315 IF(BOUND(IC,IR,IL).LE.0) FLOBOT=0.
C      320 FLOWOT=FLOWIN-FLOBOT
C      ORIGINAL CODE (DELETED FROM ADJOINT MODIFICATIONS) RMN
C      IF((ISTSG.GT.1).AND.(NREACH.EQ.1)) STRM(9,LL)=ARTRIB(IFLG)
C                                                    C
C19----STORE STREAM INFLOW, OUTFLOW AND LEAKAGE FOR EACH REACH. C
C      STRM(9,L)=FLOWOT
C      STRM(10,L)=FLOWIN
C      STRM(11,L)=FLOBOT
C                                                    C
C      ++++ADJOINT MODIFICATION++++ RMN
C      IF (NREACH.GT.1) GO TO 201
C      DO 30 ITRIB=1,NTRIB
C      INODE=ITRIBAR(ISTSG,ITRIB)
C      IF (INODE.NE.0) ARTRIB(INODE)=STRM(9,L)
C      30 CONTINUE
C      201 CONTINUE
C      ++++ADJOINT MODIFICATION++++ RMN
C20----IF LEAKAGE FROM STREAMS IS TO BE SAVED THEN ADD RATE TO BUFFER. C
C      IF(IBD.EQ.1) BUFF(IC,IR,IL)=BUFF(IC,IR,IL)+FLOBOT
C                                                    C
C21----DETERMINE IF FLOW IS INTO OR OUT OF MODEL CELL. C
C      SKIP ESTIMATE OF LEAKAGE FROM STREAM IF LEAKAGE IS ZERO. C
C      IF(FLOBOT)494,500,496
C                                                    C
C22-----SUBTRACT FLOW RATE FROM RATOUT IF AQUIFER DISCHARGES TO STREAM.C
C      494 RATOUT=RATOUT-FLOBOT
C      GO TO 500
C                                                    C
C23-----ADD FLOW RATE TO RATIN IF STREAM DISCHARGES TO AQUIFER. C
C      496 RATIN=RATIN+FLOBOT

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500 CONTINUE
C
C24-----IF BUDGET TERMS WILL BE SAVED THEN WRITE TO DISK.
      IF(IBD.EQ.1) CALL UBUDSV(KSTP,KPER,TEXT,ISTCB1,BUFF,NCOL,NROW,
1          NLAY,IOUT)
C
C25A-----MOVE RATES INTO VBVL FOR PRINTING BY MODULE BAS_OT.
      600 VBVL(3,MSUM)=RATIN
          VBVL(4,MSUM)=RATOUT
C
C25B-----MOVE PRODUCT OF RATE AND TIME STEP INTO VBVL ACCUMULATORS.
      VBVL(1,MSUM)=VBVL(1,MSUM)+RATIN*DELT
      VBVL(2,MSUM)=VBVL(2,MSUM)+RATOUT*DELT
C
C25C-----MOVE BUDGET TERM LABELS INTO VBNM FOR PRINTING BY BAS_OT.
      VBNM(MSUM)=TEXT
C
C26-----INCREASE BUDGET TERM COUNTER BY ONE.
      MSUM=MSUM+1
C
C27-----RESET IBD COUNTER TO ZERO.
      IBD=0
C28----IF STREAM OUTFLOW FROM EACH REACH IS TO BE STORED ON DISK
C      THEN STORE OUTFLOW RATES TO BUFFER.
      IF((ICBCFL.EQ.0).OR.(ISTCB2.LE.0)) GO TO 625
      IBD = 1
      DO 605 IL=1,NLAY
      DO 605 IR=1,NROW
      DO 605 IC=1,NCOL
      605 BUFF(IC,IR,IL)=0.
C
C29-----SAVE STREAMFLOWS OUT OF EACH REACH ON DISK.
      DO 615 L=1,NSTREM
      IC=ISTRM(3,L)
      IR=ISTRM(2,L)
      IL=ISTRM(1,L)
      IF(IBOUND(IC,IR,IL).LE.0) GO TO 615
      BUFF(IC,IR,IL)=BUFF(IC,IR,IL)+STRM(9,L)
      615 CONTINUE
      CALL UBUDSV(KSTP,KPER,STRTXT,ISTCB2,BUFF,NCOL,NROW,NLAY,IOUT)
C
C30-----PRINT STREAMFLOW RATES AND LEAKAGE FOR EACH REACH.
      625 IF((ISTCB1.GE.0).OR.(ICBCFL.LE.0)) GO TO 800
          IF(IPTFLG.GT.0) GO TO 800
          IF(ICALC.GT.0) GO TO 700
          WRITE(IOUT,650)
      650 FORMAT(/,12X,'LAYER',6X,'ROW',5X,'COLUMN',5X,'STREAM',4X,

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1 'REACH',6X,'FLOW INTO',5X,'FLOW INTO',5X,'FLOW OUT OF'/42X,
2   'NUMBER',4X,'NUMBER',4X,'STREAM REACH',4X,'AQUIFER',
3   6X,'STREAM REACH'//)
  DO 690 L=1,NSTREM
    IL=ISTRM(1,L)
    IR=ISTRM(2,L)
    IC=ISTRM(3,L)
    WRITE(IOUT,675)IL,IR,IC,ISTRM(4,L),ISTRM(5,L),
1     STRM(10,L),STRM(11,L),STRM(9,L)
c 675 FORMAT(1X,5X,5I10,8X,G9.3,5X,G9.3,8X,G9.3) ! Changed 3/9/06 ERB
675 FORMAT(1X,5X,5I10,4X,G14.7,1X,G14.7,1X,G14.7)
690 CONTINUE
    GO TO 800
700 WRITE(IOUT,710)
710 FORMAT(/,12X,'LAYER',6X,'ROW',5X,'COLUMN',5X,'STREAM',4X,
1 'REACH',6X,'FLOW INTO',5X,'FLOW INTO',5X,'FLOW OUT OF',5X,
2 'HEAD IN'/42X, 'NUMBER',4X,'NUMBER',4X,'STREAM REACH',
3 4X,'AQUIFER',6X,'STREAM REACH',5X,'STREAM'//)
  DO 750 L=1,NSTREM
    IL=ISTRM(1,L)
    IR=ISTRM(2,L)
    IC=ISTRM(3,L)
    WRITE(IOUT,775)IL,IR,IC,ISTRM(4,L),ISTRM(5,L),
1     STRM(10,L),STRM(11,L),STRM(9,L),STRM(2,L)
c 775 FORMAT(1X,5X,5I10,8X,G9.3,5X,G9.3,7X,G9.3,4X,F9.2) ! Changed 3/9/06 ERB
775 FORMAT(1X,5X,5I10,4X,G14.7,1X,G14.7,1X,G14.7,2X,F9.2)
750 CONTINUE
800 CONTINUE

C
C31-----RETURN. C
      RETURN C
      END
C ORIGINAL CODE
C SUBROUTINE SGWF1STR6R(NLST,MXSTRM,STRM,ISTRM,LSTBEG,IN,
C 1 IOUT,NCOL,NROW,NLAY,IRDFLG)
C ++++++++ ADJOINT MODIFICATION ++++++++ RMN
C SUBROUTINE SGWF1STR6R(NLST,MXSTRM,STRM,ISTRM,LSTBEG,IN,
C 1 IOUT,NCOL,NROW,NLAY,IRDFLG,MXRCH,NSS)
C ++++++++ ADJOINT MODIFICATION ++++++++ RMN
C-----VERSION 15APRIL1998 SGWF1STR6R
C
C *****C
C READ STRM AND ISTRM
C *****
C
C SPECIFICATIONS:
C -----

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C      Original code: DIMENSION STRM(11,MXSTRM),ISTRM(5,MXSTRM)
C      ADJOINT MODIFICATION*****
C      DIMENSION STRM(12,MXSTRM),ISTRM(5,MXSTRM),MXRCH(NSS)
C      ADJOINT MODIFICATION*****
C      -----
C
C5-----READ AND PRINT DATA FOR EACH STREAM CELL.
      IF(IRDFLG.EQ.0) WRITE(IOUT,4)
      4 FORMAT(/,4X,'LAYER   ROW       COL       SEGMENT   REACH   STREAMFLOW',
        16X,'STREAM   STREAMBED   STREAMBED BOT   STREAMBED TOP',/27X,
        2'NUMBER   NUMBER                               STAGE   CONDUCTANCE',6X,
        3'ELEVATION   ELEVATION',/3X,110(' '))
      N=NLST+LSTBEG-1
      DO 250 II=LSTBEG,N
C      Original code: READ(IN,5)K,I,J,ISTRM(4,II),ISTRM(5,II),STRM(1,II),STRM(2,II),
C      1STRM(3,II),STRM(4,II),STRM(5,II)
C      5 FORMAT(5I5,F15.0,4F10.0)
C      IF(IRDFLG.EQ.0) WRITE(IOUT,6)K,I,J,ISTRM(4,II),
C      1ISTRM(5,II),STRM(1,II),STRM(2,II),STRM(3,II),STRM(4,II),STRM(5,II)
C      6 FORMAT(1X,1X,I6,2I7,2I9,7X,G11.4,G12.4,G11.4,4X,2G13.4)
C      ++++ADJOINT MODIFICATION++++
      READ(IN,5)K,I,J,ISTRM(4,II),ISTRM(5,II),STRM(1,II),STRM(2,II),
      1STRM(3,II),STRM(4,II),STRM(5,II),STRM(12,II)
C      ++++ FOLLOWING LINE ADDED FOR TRIBUTARY ADJOINT MODIFICATION ++++ RMN
      MXRCH(ISTRM(4,II))=ISTRM(5,II)
      5 FORMAT(5I5,F15.0,5F10.0)
      IF(IRDFLG.EQ.0) WRITE(IOUT,6)K,I,J,ISTRM(4,II),ISTRM(5,II),
      1STRM(1,II),STRM(2,II),STRM(3,II),STRM(4,II),STRM(5,II),STRM(6,II)
      6 FORMAT(1X,1X,I6,2I7,2I9,7X,G11.4,G12.4,G11.4,4X,3G13.4)
C      ++++ADJOINT MODIFICATION++++
      ISTRM(1,II)=K
      ISTRM(2,II)=I
      ISTRM(3,II)=J
C
C      Check for illegal grid location
      IF(K.LT.1 .OR. K.GT.NLAY) THEN
        WRITE(IOUT,*) ' Layer number in list is outside of the grid'
        CALL USTOP(' ')
      END IF
      IF(I.LT.1 .OR. I.GT.NROW) THEN
        WRITE(IOUT,*) ' Row number in list is outside of the grid'
        CALL USTOP(' ')
      END IF
      IF(J.LT.1 .OR. J.GT.NCOL) THEN
        WRITE(IOUT,*) ' Column number in list is outside of the grid'
        CALL USTOP(' ')
      END IF

```

```
250 CONTINUE  
C  
   RETURN  
   END
```