

# MODFLOW-2005 Ground-Water Model – User Guide to the Adjoint State Based Sensitivity Process (ADJ)

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# Preface

This report describes a version of the MODFLOW-2005 modular ground-water model that uses the adjoint state method to calculate the sensitivity of observations to parameters. The sensitivity information provided by this program may be useful in many applications including parameter estimation. However, the program itself does not use the sensitivity in a parameter estimation process or for any other end use application. The program provides an alternative to calculating sensitivity information using the direct sensitivity approach implemented in MODFLOW-2000 or using a parameter perturbation method. The most popular optimization procedures require the Jacobian matrix of sensitivities with elements consisting of the sensitivity of each observation to each parameter. Other procedures use the gradient of an objective function with respect to the parameters. This program will calculate sensitivities needed to form the Jacobian matrix or the gradient of a weighted least-square-error objective function. The resulting sensitivity information is reported in the JUPITER API format or other optional formats. The program is based on the basic features of MODFLOW-2005 described in the MODFLOW-2000 user's manual. However, not all MODFLOW-2005 extension packages are supported. Most importantly, the calculations are limited to parameters defined using the Layer-Property Flow package or in one of the stress packages used with the Layer-Property Flow package.

This report presents a theoretical development of the adjoint state sensitivity method. The report documents input to the program to control the sensitivity calculations and the format of the sensitivity output files. This document does not provide of description of the input files needed to define the ground-water flow simulation. The reader should refer to the MODFLOW-2005 User's Guide for instructions on controlling the groundwater simulation (Harbaugh, 2005).

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# MODFLOW-2005 Ground-Water Model – User Guide to the Adjoint State based Sensitivity Process (ADJ)

By Tom Clemo

## **Abstract**

This report describes the adjoint state based sensitivity process for MODFLOW-2005 that calculates the sensitivity of observations to parameters. The process is composed of three basic components, described here for one observation and one parameter; first is the solution of the ground-water flow problem, next this solution is used to calculate the adjoint state for the observation, and finally the sensitivity of the of the observation to the parameter is determined by summing the product of the adjoint state with the derivative of the ground-water flow equations with respect to the parameter for each time step of the flow simulation. The theoretical development presents the mathematical basis for the second two steps in the process.

Sensitivity information is useful as part of a parameter estimation process, for reliability analysis, in uncertainty analysis, and to describe error propagation. The program described herein only determines the sensitivities. To implement any of the above analyses the program must be used in conjunction with other software. Sensitivity information can be determined using other approaches such as the direct sensitivity calculations of MODFLOW-2000 (Hill and Others, 2000) and the parameter perturbation method implemented in UCODE\_2005 (Poeter and others, 2005) and PEST (Doherty, 2004). This report describes when the adjoint sensitivity process can be expected to be more efficient than these other methods. As a general rule, but not always, adjoint sensitivities require the equivalent computational effort of a head solution simulation for each observation. The other approaches require the computational effort of a head solution for each parameter. If a full matrix of sensitivities is needed, the adjoint state based sensitivities is expected to be more efficient that the other approaches if there are more parameters than observations.

There are variations of the basic process that can significantly influence the efficiency of the calculations, depending on the use of the sensitivities and on the structure of the flow simulation. The highest efficiency is reached if the gradient of a weighted sum-of-square error is needed. Only a single adjoint state calculation is performed in this case. The gradient is used by truncated Newton, variable-metric, conjugate gradient, and quasi-Newton optimization procedures. The MODFLOWP (Hill, 1992) implemented parameter estimation using adjoint state based gradients with a conjugate gradient routine for an earlier version of MODFLOW (Harbaugh and McDonald, 1988). A different form of computational efficiency can be gained If the flow simulation has constant time steps. Significant increases in efficiency in determining the

full sensitivity matrix can then be gained by reusing the adjoint state calculation of an observation for other observations at the same observation location.

## Introduction

The adjoint state based sensitivity (ADJ) process for MODFLOW-2005 provides the sensitivity of calculated observations to model parameters. Throughout this user's guide, we assume that the reader is familiar with the use and terminology of MODFLOW-2005 (Harbaugh, 2005). In this document, the terms *observations* and *parameters* have formal meanings. Observations are defined for various MODFLOW packages and entered as such using the package input files. For example, observed seepage below a river, specified as a FLWOBS value in the river package, is a formal observation. MODFLOW-2005 will calculate a simulated value for the seepage. Parameters are defined either using an LPF input file or a within another package such as the WEL package. Sensitivity, then, is defined as the ratio of changes of the calculated observations with respect to small changes in the parameter values.

Computational demands of the adjoint state based sensitivity process are influenced less by the number of parameters than the number of observations. To take advantage of this aspect, parameters have two different interpretations. The first is consistent with the description of parameters in the MODFLOW-2005 manual. We refer to this interpretation as *lumped parameters*. The value of a lumped parameter is determined by the value supplied in the LPF file or in a specific package input. These values may be manipulated using multiplication matrices to specify different properties for different cells in the model. If the value of a lumped parameter is changed then the change influences all cells where that parameter is defined. The sensitivity to these parameters reflects the fact that the parameters influence many cells. We use the term *distributed parameter* to refer to a different interpretation of these same parameters. The key difference is that distributed parameters are defined on a cell-by-cell basis by using multiplication matrices. Typically, a value of one would be supplied as the parameter value in the LPF file so that the parameter value of a cell is the same as the value in the multiplication matrix. For distributed parameters, sensitivities are calculated with respect the multiplication matrix value for each cell in the model; not the value listed in the parameter definition statement. Thus, a distributed MODFLOW parameter actually represents a set of parameters, one for each cell where the parameter is defined. Only parameters that can be manipulated using multiplication arrays can also be distributed parameters. The two parameter interpretations can be used to define identical flow simulations.

The adjoint state based sensitivity process is, in large part, a modification of the previous MODFLOW codes MODFLOWP (Hill, 1992) and MODFLOW-2000 (Hill and Others, 2000). In these codes the sensitivity of observations to parameters could be used to estimate parameters. The current code is does not have a parameter estimation capability. The ADJ process only supplies sensitivities. There are many uses of the sensitivity information. Parameter estimation programs UCODE\_2005 (Poeter and others, 2005) and PEST (Doherty, 2000) require sensitivity information to define parameter update directions. The MODFLOWP user's guide (Hill, 1992) describes use of the objective function gradient in conjugate gradient optimization. Sensitivities can also be used to propagate uncertainty in parameter values to uncertainty in model prediction

(Tonkin and others, submitted). Jyrkama and Sykes (2006) used sensitivities calculated by the adjoint state method in a first order reliability analysis method to estimate the reliability of a pumping well to recharge uncertainty.

## 1.1 Overview of Capabilities

The current implementation of the adjoint sensitivity code has limited compatibility with respect to the MODFLOW-2005 packages. The LPF package must be used which excludes use of the BCF6 and HUF2 packages. All MODFLOW-2005 observation types are supported. These are; HOB, GBOB, DRNOB, RVOB, and CHOB. The following parameter types are supported; HK, VK, VKCB, HANI, VANI, SS, SY, CHD, GHB, RIV, RCH, WEL, DRN, EVT, and ETS. In addition, to overcome a difficulty in calculating the sensitivity to log-hydraulic conductivity for distributed parameters, two new parameter types have been introduced. These are YHK (log-horizontal conductivity) and YVK (log-vertical conductivity). The HFB parameter is not on this list. The HFB6 package is supported, but not the HFB parameters. We expect to include the HFB parameter in a future version. The HK parameter is limited to harmonic mean averaging. The alternate approaches for calculating horizontal conductance have not yet been implemented.

All of the basic stress packages are supported. The stress packages are; WEL, RCH, GHB, RIV, DRN, DRT, and EVT. Few of the MODFLOW extension packages (packages not described in the MODFLOW-2005 manual) have been implemented. Unsupported packages include; FHB, RES, STR, IBS, LAK, SFR, GAGE, SUB, UZF. We hope to add SFR2, LAK, GAGE, and UZF to the supported list in the near future. The adjoint code does not support local grid refinement. However, it has been written in anticipation of support for the LGR package.

The code can be used to calculate the sensitivity of each observation to each parameter creating a sensitivity (Jacobian) matrix. Alternately, the code can be used to calculate the gradient of a weighted sum-of-square-error objective function. To calculate the sensitivity matrix the adjoint state equations need to be solved for each observation. Only a single adjoint state calculation is needed for the gradient calculation. Weighting of the objective function requires assignment of weighting coefficients for the observations. The MODFLOW-2005 code has been “extended” to make it backward compatible with the observation weighting used in MODFLOW-2000. Section 3.5 describes how to add observation weights to the standard MODFLOW-2005 observation input files.

The sensitivity of an observation to a lumped parameter is a single number, whereas the sensitivity of an observation to a distributed parameter has a value for each cell where the parameter is defined. The sensitivity matrix for lumped parameters is reported in a form similar to the `_sc` and `_sc1` files of MODFLOW-2000. The user has the option of reporting unscaled or 1% scaled sensitivities (`_sc1`). The unscaled option does not apply any scaling to the sensitivities and thus are not the same as the sensitivities reported in the MODFLOW-2000 `_sc` files. There are four choices for reporting distributed parameter sensitivities. The formats are described in Section 4.3. Support programs to integrate the adjoint sensitivity code with the PEST program (Doherty, 2006) are included with the latest PEST distributions. Format 4 is intended for use with the JUPITER API (Banta and others, 2006).

If the flow problem can be simulated using constant time steps, then a variation in the method of calculating the adjoint states can be used to significantly reduce the computational

effort. The underlying method is described in Carrera and Medina (1994; Carrera and others, 1997) and in Section 2.7. With constant time steps and measurements that correspond to these time steps, only a single adjoint calculation is needed for all the observations made at a single location. The adjoint states for each observation can be inferred from this calculation. It should be evident that the location based adjoint state calculations can significantly reduce the computational effort to determine a sensitivity matrix. Constant time steps are not an absolute requirement. Temporally varying time steps will introduce an error into this method. However, the computational advantage of the location based method may make an approximate calculation of the sensitivity matrix useful for some applications.

Parallelization is another way to speed computation. The code supports a simple method of parallelization. An optional use of the code is to solve the flow problem without calculating sensitivities. This will produce a number of files that are needed in subsequent adjoint state calculations. The files resulting from the flow solution can be used for calculations of sensitivities, of individual observations, on separate processors.

The current release of the adjoint sensitivity code is a compromise between providing sensitivity calculations for the basic MODFLOW-2005 program and supporting the large number of processes that extend the capabilities of MODFLOW-2005. The intent to expand support to some packages has already been mentioned. In addition, some work to implementing adjoint sensitivity calculations in the transport code MT3DMS (Zheng and Wang, 1999) has been done. Support for adjoint calculations in MT3DMS has not been developed to a condition where formal release of a program is possible. However, the linkage to MODFLOW-2005 is complete and may be useful to some researchers.

The linkage has the capability of transforming sensitivity of observations to Darcy velocity to sensitivity of the observations to MODFLOW parameters. Darcy velocity sensitivity must be supplied as a set of arrays which contain the sensitivity of each component of velocity for each cell in the domain. Each time step of the simulation should have an associated velocity sensitivity array. Presumably, the sensitivity to Darcy velocity will have been calculated using a transport code. However, it may be possible to define sensitivities along specific path lines, analytically or with simple numerical calculations. The Darcy velocity sensitivity does not need to be determined using the adjoint state approach. A paper by Samper and Nueman (1986) provided the theoretical basis for our implementation of the transformation.

Use of the code for transforming Darcy velocity sensitivities requires significantly more information than other uses of the code. Therefore, we have relegated description of this aspect of the code to Section 6. This section is essentially a mini-manual about using the code for transport problems. Section 6 is strictly limited to the transformation of Darcy velocity sensitivities. The issue of calculating velocity sensitivities is not addressed.

## **Theory**

Sykes, Wilson, and Andrews (1985) introduced the use of adjoint calculations the use of adjoint calculations to the groundwater literature. Their development of the equations remains an excellent source and is recommended as a complement to the development presented here. A more in depth development, in a non-groundwater context, is presented in Cacuci (2003; Cacuci and others, 2003). Cacuci derives the adjoint equations for general physical systems. His book

also covers uncertainty analysis using sensitivity information. The development of the equations presented here follows Bryson and Ho (1976).

We start with an abstraction of MODFLOW-2005 as a non-linear operator ( $F$ ) that calculates vector of observations ( $d$ ) as using a vector of parameters ( $p$ ) (property values that are not formal parameters are embedded in  $F$ ),

$$d = F(p) \quad (2-1)$$

The first step is to expand the operator in a Taylor series about nominal parameter values ( $p_0$ ) and then truncate it at the first term to get;

$$d = F(p_0) + Gdp \quad (2-2)$$

$G$  is the sensitivity matrix composed of elements  $\frac{dd_l}{dp_n}$  where indices  $l$  and  $n$  identify particular elements of the observation and parameter vectors. The parameter  $p_n$  could be either a lumped parameter or a single cell of a distributed parameter. Using the chain rule of calculus, we now decompose  $G$  into the product of two terms;

$$G_{l,n} = \frac{dd_l}{df} \frac{df}{dp_n} \quad (2-3)$$

The variable  $f$  represents the discrete flow equations solved by MODFLOW-2005 (See equations 2-1, 2-2 and 2-24 of the MODFLOW-2005 manual (Harbaugh, 2005)). The meaning of  $f$  is made more explicit in Equation 2-4 below. We will show later that  $\frac{dd_l}{df}$  are the adjoint states,  $\lambda_l$ , and that they can be calculated using the computational equivalent of a simulation of the original flow problem.  $\frac{df}{dp_n}$  is the derivative of the flow equations with respect to parameter  $n$ . The calculation of  $\frac{df}{dp_n}$  is relatively fast compared to calculation of the adjoint states. Calculation of  $\frac{df}{dp_n}$  is described in Section 2.10. The concept of using adjoint states to calculate sensitivities is not intuitively obvious. Our description begins with a related problem, optimization of a function.

## 2.1 Adjoint states for constrained optimization

We now take a detour to provide intuition of why the adjoint state approach works. Let  $L(h, m)$  be a function. A common function is the error in matching an observation

$$L(h, p) = F(p) - d \quad (2-4)$$

$h$  is the hydraulic head solution throughout the model. Clearly,  $h$  is a function of  $p$  and often  $d_i$  will be equal to  $h$  for a cell at some particular time. Now, take  $f$  to represent the set of discrete flow equations 2-2 of the MODFLOW-2005 manual rewritten as

$$f(h, p) = \sum Q - SS \frac{\Delta h}{\Delta t} \Delta V = 0 \quad (2-5)$$

The set of equations  $f(h, p)$  has one equation at each time step (or steady state calculation) for each active cell in the model domain. Because  $f = 0$ , the function  $L(h, p)$  can be augmented with  $f$  without changing its value

$$H(h, p) = L(h, p) + \lambda f(h, p) \quad (2-6)$$

At this point,  $\lambda$  is arbitrary. Equation 2-6 is the equation formed if we wanted to constrain  $h$  to be the correct solution to the flow equations, using  $\lambda$  as a Lagrange multiplier. Because  $H = L$ ,

$$dH = \frac{\partial H}{\partial h} dh + \frac{\partial H}{\partial p} dp \quad (2-7)$$

and

$$\frac{\partial H}{\partial h} = \frac{\partial L}{\partial h} + \lambda \frac{\partial f}{\partial h} \quad (2-8)$$

Now set  $\lambda$  such that  $\frac{\partial H}{\partial h} = 0$ .

$$\lambda = \frac{\partial L}{\partial h} \left( \frac{\partial f}{\partial h} \right)^{-1} \quad (2-9)$$

By doing so, the dependence of  $H$  on  $h$  is eliminated from Equation 2-8 and  $H$  can be minimized with respect to  $m$  without worrying about the influence of  $m$  on  $h$ . Minimizing  $H$  also minimizes  $L$  because  $H = L$ .

### 2.1.1 Simple example of constrained optimization

To reinforce the concept of how the adjoint state can be used to simplify a problem, we present an example introduced in Bryson and Ho (1976).

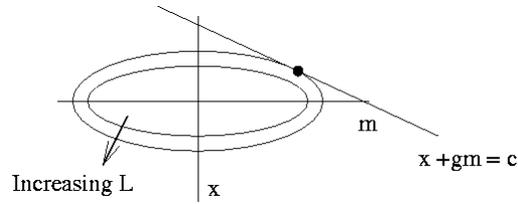
Define  $L$  as

$$L(x, m) = \frac{1}{2} \left( \frac{x^2}{a^2} + \frac{m^2}{b^2} \right) \quad (2-10)$$

Subject to

$$f(x, m) = x + gm - c = 0 \quad (2-11)$$

As shown in Figure 2-1



**Figure 2-1: Minimization example**

Define

$$H = \frac{1}{2} \left( \frac{x^2}{a^2} + \frac{m^2}{b^2} \right) + \lambda(x + gm - c) \quad (2-12)$$

The resulting equations to solve are;

$$\begin{aligned} f = 0 &\rightarrow x + gm - c = 0 \\ \frac{\partial H}{\partial x} = 0 &\rightarrow \frac{x}{a^2} + \lambda = 0 \\ \frac{\partial H}{\partial m} = 0 &\rightarrow \frac{m}{b^2} + \lambda g = 0 \end{aligned} \quad (2-13)$$

The solution to these three equations with three unknowns is;

$$\begin{aligned} \lambda &= \frac{-c}{a^2 + g^2 b^2} \\ m &= \frac{b^2 g c}{a^2 + g^2 b^2} \\ x &= \frac{a^2 c}{a^2 + g^2 b^2} \\ L_o &= \frac{1}{2} \frac{c^2}{a^2 + g^2 b^2} \end{aligned} \quad (2-14)$$

Note that  $\frac{\partial f}{\partial c} = 1$  and

$$\lambda = \frac{\partial L_o}{\partial c} = \frac{\partial L_o}{\partial f} \quad (2-15)$$

## 2.2 A one time step transient for a constant property model

The adjoint sensitivity calculation for a one step transient solution is presented in this section. The MODFLOW-2005 manual presents a development of the set of equations that are used to

calculate the head distribution in MODFLOW. Equation 2-25 of the MODFLOW-2005 manual is

$$\begin{aligned}
& CR_{i,j-1/2,k} (h_{i,j-1,k}^1 - h_{i,j,k}^1) + CR_{i,j+1/2,k} (h_{i,j+1,k}^1 - h_{i,j,k}^1) + CC_{i-1/2,,k} (h_{i-1,j,k}^1 - h_{i,j,k}^1) + \\
& CC_{i+1/2,j,k} (h_{i+1,j,k}^1 - h_{i,j,k}^1) + CV_{i,j,k-1/2} (h_{i,j,k-1}^1 - h_{i,j,k}^1) + \\
& CV_{i,j,k+1/2} (h_{i,j,k+1}^1 - h_{i,j,k}^1) + P_{i,j,k} h_{i,j,k}^1 + Q_{i,j,k} = SS_{i,j,k} (\Delta r_j \Delta c_i \Delta v_k) \frac{h_{i,j,k}^1 - h_{i,j,k}^0}{t^1 - t^0}
\end{aligned} \tag{2-16}$$

Where,  $h^0$  is head in the cell before the time step and  $h^1$  are the head values after the time step. The  $CR$  matrices are hydraulic conductance between model cells along columns,  $CC$  are conductance between model cells along rows, and  $CV$  are conductance between model cells in adjacent layers. The matrices  $P$ , and some entries in  $Q$ , are a result of head dependent flow boundary conditions to a cell such as flow from a river.  $Q$  may also represent flow sources that are not head dependent such as pumping rate.  $SS$  is the specific storage of a cell,  $\Delta r_j, \Delta c_i, \Delta v_k$  are the row, column and layer thicknesses of the cell and  $t^1 - t^0$  is the time step increment. To simplify the development of the adjoint equations, the hydraulic conductance matrices are assumed to be insensitive to changes the hydraulic head. The assumption is relaxed in Section 2.6.

If we collect all terms that include  $h^1$  on the left hand side of the equation and all terms that include  $h^0$  on the right hand side along with the  $Q$  terms we can write the flow equations in matrix form as

$$Ah^1 = Bh^0 + C \tag{2-17}$$

If the equations have the correct solution,  $f = Bh^0 + C - Ah^1 = 0$ . In this development,  $A$  and  $B$  depend on model parameters  $p$ , but not on  $h^0$  or  $h^1$ . The model equivalent of the observation is a function of head at a single cell at the end of the time step which is represented as  $L = L(h_{i,j,k}^1)$ .

Augment  $L$  with  $f$  to form

$$\begin{aligned}
J &= L(h_{i,j,k}^1, p) + \lambda^T (Bh^0 + C - Ah^1) \\
H &= \lambda^T (Bh^0 + C) \\
J &= H(h^0, p, \lambda) + L^1(h_{i,j,k}^1, p) - \lambda^T Ah^1 \\
dJ &= \left( \frac{\partial H}{\partial h^0} \right)^T dh^0 + \left( \frac{\partial H}{\partial p} \right)^T dp + \left( \frac{\partial L}{\partial p} \right)^T dp - \lambda^T \frac{\partial A}{\partial p} h^1 dp + \left[ \left( \frac{\partial L}{\partial h^1} \right)^T - \lambda^T A \right] dh^1
\end{aligned} \tag{2-18}$$

For this one step example,  $h^0$  is known and hence  $dh^0 = 0$ . To eliminate the dependence of  $J$  on  $h^1$  we choose

$$\lambda^T A = \left( \frac{\partial L}{\partial h^1} \right)^T \quad (2-19)$$

Now, we want to manipulate this equation to be the same form as the ground water flow equation

$$A\lambda = B \cdot 0 + \frac{\partial L}{\partial h^1} \Big|_{i,j,k} \quad (2-20)$$

Where we have taken advantage of the symmetry of the discrete groundwater flow equations;  $A^T = A$ . The line and subscript to the right of the last term indicates that the derivative is non-zero only at the location of the observation. MODFLOW can be used to solve this equation where the initial conditions for  $\lambda$  are zero and  $\frac{\partial L}{\partial h^1}$  is taken as the only external source term. If the function  $L$  is the error of a calculated head measurement  $h_{i,j,k} - d_l$  located at the center of a cell then  $\frac{\partial L}{\partial h^1} \Big|_{i,j,k} = \delta(i - i_l, j - j_l, k - k_l)$ .

Returning to the augmented performance measure

$$\begin{aligned} \frac{dJ}{dp} &= \frac{\partial L}{\partial p} + \frac{\partial H}{\partial p} - \lambda^T \frac{\partial A}{\partial p} h^1 \\ \frac{dJ}{dp} &= \frac{\partial L}{\partial p} + \lambda^T \frac{\partial(Bh^0 + C - Ah^1)}{\partial p} \\ \frac{dJ}{dp} &= \frac{\partial L}{\partial p} + \lambda^T \left[ \frac{\partial B}{\partial p} h^0 + \frac{\partial C}{\partial p} - \frac{\partial A}{\partial p} h^1 \right] \end{aligned} \quad (2-21)$$

If the observation does not depend directly on the parameter, the first term in Equation 2-21 is zero. If the parameter is not storage then the term involving the matrix  $B$  is zero. If there are no source terms or head dependent boundary conditions that depend directly on the parameter, then the derivative of the matrix  $C$  with respect to the parameter is zero. For these conditions, the sensitivity equation reduces to

$$\frac{dJ}{dp} = -\lambda^T \frac{\partial A}{\partial p} \quad (2-22)$$

## 2.3 Multi-step transient

For a multi-step transient we have a series of time step equations

$$A^m h^m = B^m h^{m-1} + C^m \quad (2-23)$$

and a performance measure composed of matching a single observation made at time step  $N$ . The performance measure is augmented with each of the time step equations

$$J = L(h^N, p) + \sum_{m=1}^N (\lambda^m)^T [B^m h^{m-1} + C^m - A^m h^m] \quad (2-24)$$

Collecting terms of similar  $h^m$  together

$$J = L(h^N, p) + (\lambda^N)^T h^N + \sum_{m=1}^N (\lambda^m)^T C^m + \sum_{m=1}^{N-1} [(\lambda^{m+1})^T B^{m+1} - (\lambda^m)^T A^m] h^m + (\lambda^1)^T B^1 h^0 \quad (2-25)$$

$$dJ = (\lambda^1)^T B^1 dh^0 + \sum_{m=1}^{N-1} [\lambda^{m+1} B^m - \lambda^m A^m] dh^m + \left[ \left( \frac{\partial L}{\partial h^N} \right)^T - (\lambda^N)^T A \right] dh^N + \left( \frac{\partial L}{\partial p} \right)^T dp + \sum_{m=1}^N (\lambda^m)^T \left[ \frac{\partial B^m}{\partial p} h^{m-1} + \frac{C^m}{\partial p} - \frac{\partial A^m}{\partial p} h^m \right] dp \quad (2-26)$$

To eliminate the dependency of  $J$  on  $h$  the  $\lambda$  are constrained such that

$$A^N \lambda^N = \frac{\partial L}{\partial h^N} \quad (2-27)$$

and for each time step before  $N$

$$A^m \lambda^m = B^{m+1} \lambda^{m+1} \quad (2-28)$$

These equations can be solved by MODFLOW using the  $A$  and  $B$  matrices of the head solution and with boundary conditions set to 0, except for possible matrix  $P$  terms. The equation for the adjoint state after time step  $N$ ,  $\lambda^N$ , is solved first and the adjoint steps for each other time step are solved in order of decreasing time steps. The adjoint equations are solved backwards in time.

For specified initial conditions, the resulting sensitivity is given by

$$\frac{dJ}{dp} = \frac{\partial L}{\partial p} + \sum_{m=1}^N (\lambda^m)^T \left[ \frac{\partial B^m}{\partial p} h^{m-1} + \frac{\partial C^m}{\partial p} - \frac{\partial A^m}{\partial p} h^m \right] \quad (2-29)$$

The calculation of the adjoint state does not depend on what parameter is involved. Therefore, once the head and adjoint state solutions are calculated the sensitivity of  $J$  to each parameter can be calculated relatively quickly.

## 2.4 Observations between time steps

Some observations may occur at times that do not coincided with the end of time steps. MODFLOW-2005 uses linear interpolation of calculated observations at the time steps to determine the observation at the proper time. Interpolation is in effect a weighted sum of calculated observations before and after the time step that bounds the observation time. The two weighting factors are given by;

$$\begin{aligned}
F &= W_{N-1}F_l^{N-1} + W_N F_l^N \\
W_{N-1} &= \frac{t^N - t_l}{t^N - t^{N-1}} \\
W_N &= \frac{t_l - t^{N-1}}{t^N - t^{N-1}}
\end{aligned} \tag{2-30}$$

Where  $N$  references the time at the end of the time step that bounds the observation time,  $t_l$ .

The performance measure for an observation that does not fall on a time step is  $L = W_{N-1}F_l^{N-1} + W_N F_l^N - d_l$ . The following equations result from using this performance measure to calculating the adjoint states for Equation 2-26.

$$\begin{aligned}
A^N \lambda^N &= W_N \frac{\partial F_l^N}{\partial h^N} \\
A^{N-1} \lambda^{N-1} &= B^N \lambda^N + W_{N-1} \frac{\partial F_l^{N-1}}{\partial h^{N-1}}
\end{aligned} \tag{2-31}$$

and for each time step before  $N-1$

$$A^m \lambda^m = B^{m+1} \lambda^{m+1} \tag{2-32}$$

## 2.5 Multi-cell observations

If a head observation is offset from the center of the specified cell and/or composed from more than one layer, then the simulated head is the weighted sum of multiple calculated head values. Calculated observations offset from the center of a cell use weighting factors,  $R(i_l, j_l)$ , which are calculated by linear interpolation between the cell and its neighbors (See file OBS.pdf). The factors  $R$  are non-zero for at most four head values and sum to 1.0. Multi-layer head observations, which might represent a piezometer open over multiple layers, also have weighting factors,  $P(k_l)$ , to represent the fraction contribution of each layer to the observation. The factors  $P$  are obtained from the HOB file describing the observations. In the case of multi-cell head observations the adjoint state source equation source term becomes;

$$\frac{\partial L}{\partial h^N} = \sum_j \sum_i \sum_k R(i_l, j_l) P(k_l) \tag{2-33}$$

Flow observations may represent the flow from many cells. Flow observations can be defined by

$$F_l = \sum_n f_n q_n \tag{2-34}$$

where  $n$  is the index of the cells that are used to define the observation and  $q_n$  are the appropriate flows for each cell. The  $f$  factors are defined in the input file describing the observations. The  $f$  factors are not proportionality factors which represent fractional contributions of the cells to the observation. The fractional contribution of the cells is

$$P_n = \frac{f_n}{\sum_n f_n} \quad (2-35)$$

The adjoint state equation source term as can be written as

$$\frac{\partial L}{\partial h^N} = \sum_n \sum_j \sum_i \sum_k P_n \delta(i - i_n, j - j_n, k - k_n) \quad (2-36)$$

## 2.6 Multi-step transient after a steady state calculation

If a steady state stress period proceeds a transient stress period then  $h^0$  may depend on the parameters. In this case, we add an additional adjoint state to remove the dependence in Equation 2-21 on the steady state head solution. The constraint is

$$C^0 - A^0 h^0 = 0 \quad (2-37)$$

where  $A^0$  does not include the storage term on the right hand side of Equation 2-15. This creates an additional equation to solve for the time zero adjoint state.

$$A^0 \lambda^0 = B^1 \lambda^1 \quad (2-38)$$

And results in

$$\frac{dJ}{dp} = \frac{\partial L}{\partial p} + \sum_{m=1}^N (\lambda^m)^T \left[ \frac{\partial B^m}{\partial p} h^{m-1} + \frac{\partial C^m}{\partial p} - \frac{\partial A^m}{\partial p} h^m \right] + (\lambda^0)^T \left[ \frac{\partial C^0}{\partial p} - \frac{\partial A^0}{\partial p} h^0 \right] \quad (2-39)$$

The steady state adjoint,  $\lambda_0^0$ , can be defined equivalently by either of the following equations (Carrera and Medina, 1994).

$$\lambda_0^0 = \sum_{m=0}^N \lambda^m \quad (2-40)$$

or

$$A^0 \lambda_0^0 = \frac{\partial L}{\partial h^N} \quad (2-41)$$

The steady state adjoint is not the same as the adjoint for a steady state period prior to a transient. For a single steady state stress period, then, the second form defines the adjoint state equation.

$$\frac{dJ}{dp} = \frac{\partial L}{\partial p} + (\lambda_0^0)^T \left[ \frac{\partial C^0}{\partial p} - \frac{\partial A^0}{\partial p} h^0 \right] \quad (2-42)$$

## 2.7 Location based adjoint state calculations

Carrera and Medina (1994) and Carrera and others (1997) present a technique that reduces the number of adjoint solutions from the number of observations to the number of measurement locations if a transient simulation has constant  $A$  and  $B$  matrices. Constant  $A$  and  $B$  matrices require; 1) constant time steps, 2) insensitivity of  $A$  and  $B$  to head changes, and 3) no head dependent boundary conditions that change with time.

We introduce a series of objective functions  $L_l = (h^l)$  corresponding to observations at times  $l$ , all at the same location. Corresponding adjoint states  $\lambda_l^m$  are for time step  $m$  of observation  $l$ . The  $\lambda_l^m$  are zero if time step  $m$  is after time step  $l$  ( $m > l$ ). The adjoint states  $\lambda_N^m$  are for the last observation at the location. For each other observation, the solutions to Equation 2-28 result in  $\lambda_l^m = \lambda_N^{m+(N-l)}$ . This equivalence does not apply to the time zero adjoint because the time zero adjoint equation differs from the transient adjoint calculations. To find the time zero adjoint we make use of Equation 2-33.

Once  $\lambda_0^0$  has been defined using Equation 2-33 with the  $\lambda_N$  then  $\lambda_l^0$  is found by

$$\begin{aligned}\lambda_l^0 &= \lambda_0^0 - \sum_{m=1}^l \lambda_l^m \\ &= \lambda_0^0 - \sum_{m=1}^l \lambda_N^{m+(N-l)}\end{aligned}\tag{2-43}$$

## 2.8 Multi-step transient for head dependent flow equations

If the  $A$ ,  $B$ , and  $C$  matrices of the flow equations are head dependent then the full derivative of Equation 2-25 becomes

$$\begin{aligned}dJ &= (\lambda^1)^T B^1 dh^0 + \sum_{m=1}^{N-1} \left[ \lambda^{m+1} \left[ B^m + \frac{\partial B^m}{\partial h^m} h^m \right] - \lambda^m \left[ A^m + \frac{\partial A^m}{\partial h^m} h^m \right] \right] dh^m + \\ &\left[ \left( \frac{\partial L}{\partial h^N} \right)^T - (\lambda^N)^T \left[ A^N + \frac{\partial A^N}{\partial h^N} h^N \right] \right] dh^N + \left( \frac{\partial L}{\partial p} \right)^T dp + \sum_{m=1}^N (\lambda^m)^T \left[ \frac{\partial B^m}{\partial p} h^{m-1} + \frac{C^m}{\partial p} - \frac{\partial A^m}{\partial p} h^m \right] dp\end{aligned}\tag{2-44}$$

The  $B$  matrix does not depend on  $h$ , therefore  $\frac{\partial B^m}{\partial h^m} = 0$ , resulting in adjoint update equations of the form

$$\left[ A^N + \left( \frac{\partial A^N}{\partial h^N} h^N \right)^T \right] \lambda^N = \frac{\partial L}{\partial h^N} \quad (2-45)$$

and for each time step before N

$$\left[ A^m + \left( \frac{\partial A^m}{\partial h^m} h^m \right)^T \right] \lambda^m = B^{m+1} \lambda^{m+1} \quad (2-46)$$

Primarily, head dependent conditions arise from variable saturated thickness of a cell. Details for the derivative of  $A$  with respect to head are given in Section 2-10. The term  $\left( \frac{\partial A^m}{\partial h^m} h^m \right)^T \lambda^m$  makes the adjoint state equation asymmetric. To avoid solving unsymmetric equations  $\left( \frac{\partial A^m}{\partial h^m} h^m \right)^T \lambda^m$  is shifted to the right hand side producing a system of equations that is solved iteratively

$$A^m \lambda^m = B^{m+1} \lambda^{m+1} + \left( \frac{\partial A^m}{\partial h^m} h^m \right)^T \lambda^{m*} \quad (2-47)$$

$$A^m \lambda^m = B^{m+1} \lambda^{m+1} + h^m{}^T \frac{\partial A^m}{\partial h^m} \lambda^{m*} \quad (2-48)$$

Where  $m^*$  indicates the adjoint state solution in the last iteration. The effect of transposition in the final term on the right hand side is that the adjoint state of location  $i, j, k$  multiplies derivatives of  $A$  with respect to the head at locations  $i, j, k$  but does not multiply the derivatives of  $A$  with respect to any other head.

## 2.9 Gradient of a weighted sum of squares objective function

MODFLOWP (Hill, 1992) provides two options for parameter estimation. One option is to calculate the parameter sensitivity matrix using parameter perturbations for use in the Levenburg-Marquart non-linear optimization procedure. The objective function used to define the parameter estimation problem is the weighted sum of squares of mismatch of the observations. The second option is to calculate the gradient of the objective function using the adjoint state method for use in a conjugate gradient solution procedure. A very attractive feature of this second approach is that the gradient of the objective function can be calculated using a single adjoint state solution. A problem with the approach is that the conjugate gradient procedure requires many more iterations than the Levenburg-Marquart procedure to converge.

Carrera and Medina found that the long convergence sequence for the conjugate gradient procedure made the approach inferior to Levenburg-Marquart for typical ground water problems. (Carrera and Medina, 1994). However, Zhang and others (2005) found that preconditioning of

the limited-memory Broyden-Fletcher-Goldfarb-Shanno (LBFGS) algorithm significantly reduces the convergence sequence making the LBFGS algorithm more efficient than Levenburg-Marquart for their highly non-linear two-phase flow problem. Rama Rao and others (1995) produced an efficient method of estimating transmissivity using both transmissivity estimates from pump tests and temporal head measurements. Their approach used the gradient of the objective function to select optimal pilot point locations.

The weighted sum-of-square-error objective function contains measurements from possibly many times.

$$L(h, m) = \frac{1}{2} \sum W_i (d_i - F_i(m))^2 \quad (2-49)$$

Following the development of a multi-step transient  $L$  in the augmented objective function similar to equation 2-25 becomes a function of  $h$  rather than a single measurement time  $h^N$ .

$$J = L(h, p) + \sum_{m=1}^N (\lambda^m)^T [B^m h^{m-1} + C^m - A^m h^m] \quad (2-50)$$

Collecting terms and multiplying the heads at each time step results in

$$\begin{aligned} dJ = & (\lambda^1)^T B^1 dh^0 + \sum_{m=1}^{N-1} \left[ \left( \frac{\partial L}{\partial h^m} \right)^T + \lambda^{m+1} B^m - \lambda^m A^m \right] dh^m + \left[ \left( \frac{\partial L}{\partial h^N} \right)^T - (\lambda^N)^T A \right] dh^N + \\ & \left( \frac{\partial L}{\partial p} \right)^T dp + \sum_{m=1}^N (\lambda^m)^T \left[ \frac{\partial B^m}{\partial p} h^{m-1} + \frac{C^m}{\partial p} - \frac{\partial A^m}{\partial p} h^m \right] dp \end{aligned} \quad (2-51)$$

with adjoint state equations

$$A^N \lambda^N = \frac{\partial L}{\partial h^N} \quad (2-52)$$

and for each time step before N

$$A^m \lambda^m = B^{m+1} \lambda^{m+1} + \left( \frac{\partial L}{\partial h^m} \right) \quad (2-53)$$

$\left( \frac{\partial L}{\partial h^m} \right)$  has non-zero terms at the location of each measurement made during the time step.

If the observations represent cell-centered head measurements then  $\left( \frac{\partial L}{\partial h^m} \right)$  becomes a series of terms  $W_i (F_i - d_i) \delta(i - i_l, j - j_l, k - k_l)$ . There is one term for each observation at time step  $m$ .

## 2.10 Evaluation of matrix derivatives

Evaluation of the matrix derivative with respect to parameters is presented by two examples rather than being inclusive of all cases. For simplicity, the presentation is made with respect a single cell of a distributed parameter. The sensitivity to lumped parameters is just the sum of sensitivities to each cell where the parameter is defined so the extension from a single distributed parameter to a lumped parameter is trivial.

### 2.10.1 Matrix Derivatives with Respect to Parameters

#### Hydraulic Conductivity Parameter

An interesting example is horizontal conductivity. For harmonic mean averaging of conductivity (the only averaging method supported by the adjoint code), the MODFLOW-2005 manual (Equation 5-16) defines the horizontal conductance terms as

$$\begin{aligned} CR_{i,j+1/2,k} &= 2DEL C_i \frac{TR_{i,j,k} TR_{i,j+1,k}}{TR_{i,j,k} DELR_j + TR_{i,j+1,k} DELR_{j+1}} \\ CC_{i+1/2,j,k} &= 2DELR_j \frac{TC_{i,j,k} TC_{i+1,j,k}}{TC_{i,j,k} DELC_i + TC_{i+1,j,k} DELC_{i+1}} \end{aligned} \quad (2-54)$$

where

$$\begin{aligned} TR_{i,j,k} &= \Delta v_{i,j,k} HK_{i,j,k} \\ TC_{i,j,k} &= \Delta v_{i,j,k} HK_{i,j,k} HANI_{i,j,k} \end{aligned} \quad (2-55)$$

$\Delta v$  is the saturated thickness for a cell,  $HK$  is the horizontal hydraulic conductivity, and  $HANI$  is the ratio of conductivity in the column direction to conductivity in the row direction.

The derivatives of the  $CR_{i,j+1/2,k}$  and  $CC_{i+1/2,j,k}$  terms of Equation 2.15 with respect to  $HK_{i,j,k}$  are

$$\begin{aligned} \frac{\partial CR_{i,j+1/2,k}}{\partial HK_{i,j,k}} &= 2\Delta v_{i,j,k} DELC_i \left[ \frac{TR_{i,j+1,k}}{TR_{i,j,k} DELR_j + TR_{i,j+1,k} DELR_{j+1}} + \frac{TR_{i,j,k} TR_{i,j+1,k} DELR_j}{(TR_{i,j,k} DELR_j + TR_{i,j+1,k} DELR_{j+1})^2} \right] \\ \frac{\partial CC_{i+1/2,j,k}}{\partial HK_{i,j,k}} &= 2\Delta v_{i,j,k} HANI_{i,j,k} DELR_j \left[ \frac{TC_{i+1,j,k}}{TC_{i,j,k} DELC_i + TC_{i+1,j,k} DELC_{i+1}} + \frac{TC_{i,j,k} TC_{i+1,j,k} DELC_i}{(TC_{i,j,k} DELC_i + TC_{i+1,j,k} DELC_{i+1})^2} \right] \end{aligned} \quad (2-56)$$

#### Drain Conductivity Parameter

The DRT parameter influences the boundary conditions of the model. These influences are represented in matrices  $P$  and  $Q$  of Equation 2-16. Equation 6-11 of the MODFLOW-2005 user guide presents the drain boundary condition as

$$\begin{aligned} QD_n &= CD_n (HD_n - h_{i,j,k}) & h_{i,j,k} > HD_n \\ QD_n &= 0. & h_{i,j,k} \leq HD_n \end{aligned} \quad (2-57)$$

Where  $QD_n$  is the flow from the drain to the aquifer ( $QD_n$  will always be less than or equal to zero),  $CD_n$  is the drain conductance, and  $HD_n$  is the drain elevation. When the drain is active

( $h_{i,j,k} > HD_n$ ), matrices  $P$  and  $C$  have an element along the diagonal for cell  $i, j, k$  consisting of  $-CD_n$  and  $-CD_nHD_n$ , respectively. When  $CD_n$  is defined by a drain parameter it is composed of two terms multiplied together, a multiplication factor,  $RTF$ , for each cell and the parameter value. Thus for any cell where a drain defined by a parameter is active, the derivative of  $A$  with respect to the parameter value is  $RTF$ , and  $RTF \cdot HD_n$  in the case of matrix  $C$ .

A drain return reintroduces a fixed proportion,  $RFPROP$ , of the flow to a drain back into the aquifer at another cell location. The returned flow is not dependent on the head at the other location. For return flow the matrices  $P$  and  $C$  have an off-diagonal element in the row of the return cell location aligned with location  $i, j, k$  of  $RFPROP \cdot RTF$ , and  $RFPROP \cdot RTF \cdot HD_n$ , respectively.

## 2.10.2 Matrix Derivatives with Respect to Head

### Derivative of Conductance with Respect to Head

By inspection of Equation 2-55 we can see that the derivation of the conductance terms with respect to head are very similar to the conductance terms with respect to hydraulic conductivity if the saturated thickness of a cell is dependent on the hydraulic head in the cell. If the head in a cell is between the top and bottom elevation of the cell then  $\frac{\partial \Delta v}{\partial h} = 1$ . For this circumstance the derivatives of  $CR$  and  $CC$  with respect to head are

$$\frac{\partial CR_{i,j+1/2,k}}{\partial h_{i,j,k}} = 2HK_{i,j,k} DELC_i \left[ \frac{TR_{i,j+1,k}}{TR_{i,j,k} DELR_j + TR_{i,j+1,k} DELR_{j+1}} + \frac{TR_{i,j,k} TR_{i,j+1,k} DELR_j}{(TR_{i,j,k} DELR_j + TR_{i,j+1,k} DELR_{j+1})^2} \right]$$

$$\frac{\partial CC_{i+1/2,j,k}}{\partial h_{i,j,k}} = 2HK_{i,j,k} HANI_{i,j,k} DELR_j \left[ \frac{TC_{i+1,j,k}}{TC_{i,j,k} DELC_i + TC_{i+1,j,k} DELC_{i+1}} + \frac{TC_{i,j,k} TC_{i+1,j,k} DELC_i}{(TC_{i,j,k} DELC_i + TC_{i+1,j,k} DELC_{i+1})^2} \right]$$

(2-58)

with similar terms for the derivatives with respect to  $h_{i+1,j,k}$  and  $h_{i,j+1,k}$ .

## Input Instructions

### 3.1 ADJ file type in MODFLOW Names File

The input file for MODFLOW that assigns file names to FORTRAN unit numbers is referred to in this report as the MODFLOW Names File. This file is used to identify which packages are to be used in the MODFLOW simulation. Two new file types have been added to the MODFLOW Names File. These are type ADJ which signals the use of the adjoint based sensitivity package and file type COBS which signals that the adjoint package will be used to calculate parameter sensitivities from Darcy velocity sensitivities that presumably have been calculated using a transport code. Section 6 describes this special use of the adjoint sensitivity code. If the ADJ file specification is missing then the program will behave very similarly to Version 1.1 of MODFLOW-2005 (Released May 18, 2006).

Four other files for the adjoint code can be defined in the names file. The optional observation map (Section 4.1) assigned unit number IUOBSMAP in the ADJ file must be defined as type DATA. The optional solver control for the solution to the adjoint states must also be type DATA. The same solver used for the head solution must be used for adjoint states solution, but use of this file provides separate control of the solver specifically for the adjoint state solution. The unit number for the solver control file is specified using IUSOLV in the ADJ file. Sensitivities to lumped and distributed parameters will be written to unit numbers IADJSU and IADJXDU respectively. File IADJSU must be defined as type DATA. File IADJXDU can be defined either as type DATA or DATA(BINARY).

### 3.2 Type ADJ input file

These input instructions assume that a calculation of parameter sensitivities from velocity sensitivities is not being requested. See Section 6 if such a calculation is desired. Input for the adjoint sensitivity calculations is read from a file that is specified with "ADJ" as the file type in the MODFLOW Name File. [] indicate optional input data

1. [#Text]

Text is optional and can include as many text lines as desired as long as they begin with #.

2. OPERATION, [MODE or WEIGHTS or IUPAROBS]

3. [PREFIX]

PREFIX is read only if OPERATION has a value of 3 or 4.

4. IADJSU IADJFM IADJSCL IADJPC

5. IUOBSMAP

6. IUSOLV

7. NPE NPARDIS

8. IADJXDU IAFORM DISCUT PVALUEOUT

Read only if NPARDIS is greater than zero.

9. [IPDISP(1) IPDISP(2), ...]

IPDISP is a NPARDIS long integer list read only if NPARDIS is greater than zero.

10. PARNAM LN

Read NPE times

#### Explanation of Variables

OPERATION - Defines the mode of operation of the adjoint sensitivity code. OPERATION is an integer value between 1 and 4. The following lists how OPERATION controls the program.

- 1) Sensitivities will be calculated for each observation creating a Jacobian matrix of sensitivities of each observation to each parameter.

- 2) Gradient of the weighted sum of squares errors of all observations is calculated.
- 3) Only the solution for hydraulic heads will be performed. Sensitivity calculations will not be done. The resulting heads and necessary boundary condition information will be stored in a series of files starting with the PREFIX character string.
- 4) Sensitivities will be calculated for a single observation that will be obtained from file unit IUPAROBNS defined in the MODFLOW Names File. Head and boundary condition information will be read from files starting with the PREFIX character string.

MODE - Read only if OPERATION=1. If MODE is greater than zero then adjoint states are solved for the last observation at a location. The adjoint states for earlier observations are calculated from this solution. If the simulation does not have constant time steps then these calculated adjoint states are an approximation. Care is required to ensure that observation times correspond to the time step times. Observation time data needs to be within 1% of the time step duration.

WEIGHTS – Read only if OPERATION=2. If WEIGHTS is non-zero then observations are weighted in the calculation of the sum-of-squares gradient. Otherwise all observations are assigned a weight of 1. Setting WEIGHTS to a non-zero value changes the input requirements for observations so that observation data must be entered using the instructions indicated in Section 3.5 for head observations and 3.6 for flow observations. If WEIGHTS is zero then the standard MODFLOW-2005 input instructions apply.

IUPAROBNS - Read only if OPERATION=4. IUPAROBNS defines the unit number from which to read the active observation. This unit number must be defined as a DATA file type in the MODFLOW Names File.

PREFIX - A character string without blanks used to define the names of head solution and boundary condition files created using OPERATION =3 or read using OPERATION=4. Only the first 70 characters will be used.

IADJSU - File unit number of lumped parameter sensitivities. File name should be supplied in the MODFLOW Name File. The file must be type DATA.

IADJFM - Print Format for IADJSU; Section 3.4 describes the influence of IADJFM on the output format.

IADJSCL – a value of 1 causes 1% scaled sensitivities to be output to file IADJSU. If IADJSCL is set to 1 then the reported sensitivities are multiplied by the parameter value and divided by 100. If IADJSCL is not set to 1 then the sensitivities are not scaled. They are not scaled by the parameter value.

IADJPC - a non-zero value causes observation and parameter names to be added to file IADJSU.

IUOBSMAP - File unit number for mapping of observations of all types to output observation number. File name should be supplied in the MODFLOW Name File using type DATA.

IUSOLV - File unit number for adjoint calculation solver control. File name should be supplied in the MODFLOW Name File using type DATA. The file supplies separate solver control information for the adjoint solution. The solver must be the same as used in the head calculations. If IUSOLV is zero then the solver control used for the head calculations is used to control the adjoint state calculations. It would be a rare situation where using the same control parameters for both the head solution and the adjoint calculations would be appropriate.

NPE - Number of lumped parameters to be used to calculate sensitivity information. Any distributed parameters must be included as lumped parameters also.

NPARDIS - Number of distributed parameters to calculate sensitivities for. Each distributed parameter must have a corresponding lumped parameter.

IADJXDU - File unit number for distributed parameter sensitivity output. File name should be supplied in the MODFLOW Name File. Type of file (DATA or DATA(BINARY)) controls whether the file is formatted or binary. The type of binary file can be controlled using the openspec.inc file prior to compilation of the program.

IAFORM - controls the format of the distributed parameter sensitivity output. Briefly, the value must be 1-4. See Section 4.3 Distributed Sensitivity Output for more detail.

- 1) Option 1 causes single column of sensitivities to be output with the following cycle pattern. The columns of the grid are the inner most cycle, then rows, layers, parameters, with observations as the outer cycle. Comment lines starting with # are written prior to each new distributed parameter. All columns, rows and layer are included which means that both active and inactive cells are included. Inactive cells are listed with a sensitivity of zero.
- 2) Option 2 creates a row of sensitivities for each distributed parameter-observation pair using the same cycling as for option 1. Formatted output (file type DATA) uses 20(1PG16.7) for each line. No text lines are included. Each new parameter will cause a new line in the output.
- 3) Option 3 compresses the output to eliminate small sensitivity values. After a header that lists each distributed parameter and each observation in the orders in which they are cycled, each line of the output lists numbers for the distributed parameter identification, column, row, layer, observation, and sensitivity only for sensitivity values larger than DISCUT (See below).
- 4) Option 4 compresses the output into distributed parameter matrices in way readable using JUPITER UTL\_READMATRIX. The sensitivities of each parameter-observation pair are written in compressed format. For each pair a line is written with the text COMPRESSEDMATRIX and a name composed of the parameter name and the observation name separated with an underscore ( \_ ). The next line lists the total number of printed elements followed by the product of NCOL\*NROW and then the number of layers. After this each line contains a pointer to the column, row, and layer plus the sensitivity value. The pointer uses the column, row, layer cycling as

described for option 1. To read the file created using option 4 the sensitivity data for each distributed parameter-observation pair would be read using sequential calls to UTL\_READMATRIX. The sequence would be one call for each distributed parameter in order parameters listed in the top of the file, which is repeated for each observation listed.

DISCUT - DISCUT is a relative cutoff criterion for compressed output options 3 and 4. Only sensitivities with relative sensitivities greater the DISCUT are written. Relative sensitivity is in comparison to the largest cell sensitivity of an observation to a parameter.

PVALUEOUT - If PVALUEOUT is 1 then the parameter value of a cell is added after the cell sensitivity is listed in the distributed parameter sensitivity output. This option is not allowed for IAFORM formats 2 or 4. The value listed is the product of the value listed in the LPF file and the multiplication matrix, whereas the sensitivity is to the value in the sensitivity matrix. If the value in the LPF file is 1.0 then the sensitivity and parameter value are consistent.

IPDISP(1), IPDISP(2) is an integer list (all on one line if desired) corresponding to the PARNAM names read next. 2 would correspond to the second PARNAM entry.

PARNAM - read NPE times. PARNAM must be identical to a parameter name supplied in the "LPF" input file. PARNAM identifies which parameters are used to calculate lumped parameter sensitivities. IPDISP identifies which lumped parameters are also distributed parameters.

LN - If LN is 1 the sensitivities are calculated with respect to the natural log of the parameter. Use YHK and YVK for natural log of conductivity. For YHK and YVK parameters only, an LN value of 0 in the ADJ file indicates dimensional values in the multiplier arrays and an LN value of 1 indicates log parameter values in the multiplier arrays.

### 3.3 Format control of the lumped parameter sensitivity output

IADJFM controls the length of each line and format of the reported sensitivities using the following corresponding formats:

Output longer than 80 characters		Output less than 80 characters	
IADJFM	FORMAT	IADJFM	FORMAT
1	11G10.3	13	10F6.0
2	9G13.6	14	10F6.1
3	15F7.1	15	10F6.2
4	15F7.2	16	10F6.3
5	15F7.3	17	10F6.4
6	15F7.4	18	10F6.5
7	20F5.0	19	5G12.5
8	20F5.1	20	6G11.4

9	20F5.2	21	7G9.2
10	20F5.3		
11	20F5.4		
12	10G11.4		

### 3.5 Observation weights for gradient calculation

There is no need for observation weights in the standard usage of MODFLOW-2005. However, the calculation of the gradient of the sum-of-square observation error requires weights. The adjoint code re-implements the assignment of observation weights used in MODFLOW-2000. However, observation weights are optional. If weighting of the gradient calculation is not requested, input files for standard MODFLOW-2005 simulations do not need to be modified. The following description replaces the input instructions for observations. Further detail regarding the concepts of observations in MODFLOW-2005 can be obtained from the file OBS.pdf distributed with this software.

#### 3.5.1 Weighted Head Observations

1. [#Text]

Text is optional and can include as many text lines as desired as long as they begin with #.

2. NH MOBS MAXM IUHOBSV HOBDRY

3. TOMULT **EVF**

4. OBSNAM LAYER ROW COLUMN IREFSP TOFFSET ROFF COFF HOBS **STATISTIC**  
**STAT-FLAG**

5. [MLAY(1), PR(1), MALY(2), PR(2), ...]

6. [ITT]

7. [OBSNAM IREFSP TOFFSET HOBS **STATISTIC STAT-FLAG**]

#### Definition of Variables

Variables that are needed in addition to the standard MODFLOW-2005 head observation data are STATISTIC and STAT-FLAG. These are listed in **bold** type.

NH – Number of head observations.

MOBS – Number of head observations that are multilayer.

MAXM – Maximum number of layers use for any multilayer observation.

IUHOBVS – The file unit number for reporting calculated equivalents to the observations. The file type must be listed as DATA.

HOBDRY – The value written to file IUHOBVS when a cell needed to calculate the observation is dry at the time of observation.

TOMULT – TOMULT is used to convert the time scale of TOFFSET to the time scale used in the calculations. The product TOMULT\*TOFFSET must have time units specified in the DIS file.

**EVF** – EVF works as a divisor of the observation weights. It provides a convenient mechanism to change the relative weighting of all head observations to weighting of flow observations with a single change to the input.

OBSNAM - Name of the observation. OBSNAM is a string of up to 12 characters. After the OSNAM entry enough blank characters must be used to fill the first twelve spaces of the line. OBSNAM should be unique. However the OBSNAM supplied for input item 4 is not used if the IRESP of that entry is negative, which indicates multiple observations at the specified location. The OBSNAM for the observations at this location are entered using item 7.

LAYER – the layer index for the location. If LAYER is less than zero then multiple layers are used to calculate the observation. The indexes for these layers are entered using item 5.

ROW – the row index of the observation location.

COLUMN – the column index of the observation location.

IREFSP – is the stress period to which the observation time is referenced. The reference point is the beginning of the stress period. If the value of IREFSP is negative then there are multiple observations at the observation location. If IREFSP is negative then  $||\text{IREFSP}|$  observations must be using the item 7 format.

TOFFSET – the observation time measured from the beginning of the reference stress period. The reference stress period is defined by IREFSP. TOFFSET can be specified using time scale units that differ from the simulation time scale. TOMULT is used to convert TOFFSET time units to the simulation time scale. The product of TOMULT \* TOFFSET must have the same units as specified in the DIS file.

ROFF – This is the row offset used to locate the observation location relative to the center of the ROW. Row offset may vary from -0.5 to 0.5. If ROFF is not zero then multiple calculated head values contribute to the calculated observation. See the file OBS.PDF for a more detailed explanation of ROFF.

COFF – This is the column offset used to locate the observation location relative to the center of the COLUMN. Column offset may vary from -0.5 to 0.5. If COFF is not zero then

multiple calculated head values contribute to the calculated observation. See the file OBS.PDF for a more detailed explanation of COFF.

HOBS – The observation head value. As with OBSNAM, the observation value is not used if multiple observations are entered for the location.

MLAY(i) – The  $i^{\text{th}}$  layer used for a multi-layer head observation.

PR(i) – The proportion of the calculated head of layer MLAY(i) used to determine the calculated observation value. The sum of all for an observation PR should equal 1.0.

ITT – Indicator of head observation type. If ITT is 1 then the head values given as HOBS are used as the observation values. If ITT is 2 then the first observation of the list is treated as a reference head value. Subsequent observations are calculated as changes from the reference observation. The HOBS values for these observations are still entered as head values. The change in head from the reference observation is calculated within the code.

**STATISTIC** – Observation STATISTIC. If STAT-FLAG is 3 then STATISTIC is used as the observation weighting factor. For values of STAT-FLAG less than 3 then STATISTIC interpreted as a measurement error statistic.

**STAT-FLAG** – STAT-FLAG is used in the following manner to determine the observation weighting factor.

If **STAT-FLAG** = 0 – the weight is  $\frac{1}{\text{EVF} * \text{WEIGHT}}$ . **STATISTIC** is treated as a variance observation measure.

If **STAT-FLAG** = 1 – the weight is  $\frac{1}{\text{EVF} * \text{WEIGHT}^2}$ . **STATISTIC** is treated as an observation standard deviation measure.

If **STAT-FLAG** = 2 – the weight is  $\frac{1}{\text{EVF} * (\text{WEIGHT} * \text{HOBS})^2}$ . **STATISTIC** is treated as an observation coefficient of variation measure.

If **STAT-FLAG** = 3 – the weight is STATISTIC/EVF

### 3.5.2 Flow Observations

Flow observations have similar input formats. Each observation type requires a separate observation definition input file. The specific meaning of the input variable FLOWOBS changes with observation type. The other variables have consistent meanings.

1. [#Text]

2. NQ NQC NQT IUOBSV
3. **TMULT EVF**
4. NQOB NQCL – Item 4 through 6 are listed NQC times.
5. OBSNAM IREFSP TOFFSET FLOWOBS **STATISTIC STAT-FLAG** – Item 5 read NQOB times after item 4.
6. LAYER ROW COLUMN FACTOR – Item 6 is read NQCL times after the last item 5.

### **Definition of Variables**

NQ – The number of cell groups that define the observation locations.

NQC – The total number of cells for all observations listed in the input file.

NQT – The number of observations listed in the file.

IUOBSV – a FORTRAN unit number defining the output file used to report the calculated observation values. The file name of the unit must be specified in the MODFLOW Names File as type DATA.

TMULT - used to convert the time scale of TOFFSET to the time scale used in the calculations. The product TOMULTH\*TOFFSET must have time units specified in the DIS file.

**EVF** – EVF works as a divisor of the observation weights. It provides a convenient mechanism to change the relative weighting of all observations of this type to weighting of other observations with a single change to the input.

NQOB – The number of observations listed for this cell group.

NQCL – The number of cells in this cell group.

OBSNAM – the observation name. The observation name can have up to 12 characters. After the OBSNAM entry enough blank characters must be used to fill the first twelve spaces of the line.

TOFFSET – the observation time measured from the beginning of the reference stress period. The reference stress period is defined by IREFSP. TOFFSET can be specified using time scale units that differ from the simulation time scale. TOMULT to convert TOFFSET time units to the simulation time scale. The product of TOMULT\*TOFFSET must have the same units as specified in the DIS file.

FLOWOBS – The value of the observation.

**STATISTIC** – Observation STATISTIC. If STAT-FLAG is 3 then STATISTIC is used as the observation weighting factor. For values of STAT-FLAG less than 3 then STATISTIC interpreted as a measurement error statistic.

**STAT-FLAG** – STAT-FLAG is used in the following manner to determine the observation weighting factor:

If **STAT-FLAG** = 0 – the weight is  $\frac{1}{\text{EVF} * \text{WEIGHT}}$ . **STATISTIC** is treated as a variance observation measure.

If **STAT-FLAG** = 1 – the weight is  $\frac{1}{\text{EVF} * \text{WEIGHT}^2}$ . **STATISTIC** is treated as an observation standard deviation measure.

If **STAT-FLAG** = 2 – the weight is  $\frac{1}{\text{EVF} * (\text{WEIGHT} * \text{HOBS})^2}$ . **STATISTIC** is treated as an observation coefficient of variation measure.

If **STAT-FLAG** = 3 – the weight is STATISTIC/EVF.

**LAYER** – the layer index for the location.

**ROW** – the row index of the observation location.

**COLUMN** – the column index of the observation location.

**FACTOR** – The proportion of this cell's contribution to the total calculation of the simulated FLOWOBS equivalent. Usually the sum of FACTORs for each cell group should sum to 1.0. However, if the observation results from measuring only a portion of the flow, then the FACTORs may sum to less than 1.0. See Equation 2-34 or Equation 5 of the file OBS.pdf.

## Output Files

### 4.1 Observation Map

The observation map relates individual observations to a global observation list. An ordered listing of the observations is also included in the header of both the lumped and distributed parameter sensitivity files. The unit number of the observation map is specified by input variable IUOBSMAP. If this value is less than or equal to 0 then the map will not be printed. The file name should be defined in the MODFLOW Names File as type DATA. The observation map will contain a line for each observation type such as:

Head observations of grid 1 are global observations 1 to 3  
River flow observations of grid 1 are global observations 4 to 6

The file anticipates support for the local grid refinement (LGR) package. However, the LGR package cannot be used with this version of the adjoint sensitivity code.

## 4.2 Lumped Parameter Sensitivity Output

The unit number for the lumped parameter output file is defined by input variable IADJSU. This file should be defined in the MODFLOW Names file as type DATA.

### File Listing Format

```
NOBS
Obsnum OBSNAM Misfit - One line for each observation.
...
          PARNAM PARNAM PARNAM PARNAM PARNAM ...*
OBSNAM* Sensitivity† Sensitivity Sensitivity Sensitivity Sensitivity Sensitivity ...
...
```

\* The printing of observation and parameter names is optional and are included if the input variable IADJPC is not zero.

† The format of the sensitivity values is controlled by input variable IADJFM using the specifications listed in Section 3.4.

### Definition of Variables

NPE - Number of parameters.

NOBS - Number of observations represented in this file.

PARNAM - Name of the parameter. PARNAM corresponds to PARNAM in the LPF file.

OBSNAM - Name of observation.

Misfit – Input observation value – Calculated Observation value

Sensitivity – The sensitivity of observations to lumped parameters. The sensitivity of distributed parameters is listed as zero in this file.

## 4.3 Distributed Parameter Sensitivity Output

The unit number for distributed parameter sensitivity files is defined by input variable IADJXDU. This unit number can be defined as either type DATA or DATA(BINARY) in the MODFLOW Names File. All format options use a common header which lists the distributed parameters and observations represented in the file.

## Common Header Format

IAFORM PVALUEOUT  
THRESH  
NPARDIS  
PARNAM – One entry per line. One line for each distributed Parameter.  
....  
NOBS  
OBSNAM – One entry per line. One line for each observation.  
...

## Definition of Variables

IAFORM – An IAFORM value of three indicates that Format Option 3 is being used to report the distributed parameter sensitivities.

PVALUEOUT – If PVALUEOUT is 1 then Parameter\_Cell\_Values are printed. Otherwise no Parameter\_Cell\_Values are printed.

Threshold - The sensitivity threshold below which sensitivity is not printed. THRESH is the product of DISCUT times the largest sensitivity for the parameter-observation pair.

NPARDIS - Number of distributed parameters.

NOBS - Number of observations represented in this file.

PARNAM - Name of the distributed parameter. PARNAM corresponds to PARNAM in the LPF file.

OBSNAM - Name of observation.

### 4.3.1 Format Option 1

Option 1 causes single column of sensitivities to be output with the following cycle pattern. The columns of the grid are the inner most cycle, then rows, layers, parameters, with observations as the outer cycle. Comment lines starting with # are written prior to each new distributed parameter if the file is type DATA, but not if the file type is DATA(BINARY). All columns, rows and layer are included which means that both active and inactive cells are included. Inactive cells are listed with a sensitivity of zero. If the PVALUEOUT variable is set to 1 then the parameter value for each cell is also included. These values are defined through the LPF and multiplication array input files.

## File Listing Format

IAFORM PVALUEOUT  
THRESH  
NPARDIS  
PARNAM – One entry per line. One line for each distributed Parameter.  
....

NOBS  
OBSNAM – One entry per line. One line for each observation.  
...  
NCOL NROW NLAY  
# SENSITIVITY MATRIX FOR OBSERVATION OBSNAM  
# PARAMETER PARNAM – These two # lines are listed for each parameter-observation pair. If DATA(BINARY) is used to define the file type the # lines will not be printed.  
Sensitivity Parameter\_Cell\_Value\* – Sensitivities for all NCOL\*NROW\*NLAY cells are written.  
...  
# SENSITIVITY MATRIX FOR OBSERVATION OBSNAM  
# PARAMETER PARNAM  
Sensitivity Parameter\_Cell\_Value\*

### Definition of Variables

Sensitivity – Sensitivity of the observation to the value for the cell listed in the appropriate multiplication array defined in the LPF file.

Parameter\_Cell\_Value\* – the value of the parameter in the cell. This value is the product of the parameter value listed in the LPF file and the value for the cell listed in the appropriate multiplication array defined in the LPF file. The parameter cell value is printed only if the PVALUEOUT variable is set to 1.

...

#### 4.3.2 Format Option 2

Option 2 creates a row of sensitivities for each distributed parameter-observation pair using the same cycling as for option 1. Formatted output uses 20(1PG16.7) for each line. No text lines are included. Each new parameter will cause a new line in the output.

### File Listing Format

IAFORM PVALUEOUT  
THRESH  
NPARDIS  
PARNAM – One entry per line. One line for each distributed Parameter.  
....  
NOBS  
OBSNAM – One entry per line. One line for each observation.  
...  
NCOL NROW NLAY  
Sensitivity Sensitivity Sensitivity ... - One list per parameter-observation pair

...

### 4.3.3 Format Option 3

Option 3 compresses the output to eliminate small sensitivity values. After a header that lists each distributed parameter and each observation in the orders in which they are cycled, each line of the output lists numbers for the distributed parameter identification, column, row, layer, observation, and sensitivity only for sensitivity values larger than DISCUT. Output for option 3 contains two possible extra data that the options 2 and 4. The misfit between the input observation value and the calculated observation value is reported. The misfit can also be obtained from the MOFLOW-2005 output files defined for observations in the MODFLOW Names File. If the PVALUEOUT variable is set to 1 then the parameter value for each cell is also included. These values are defined through the LPF and multiplication array input files.

#### File Listing Format

```
IAFORM PVALUEOUT
THRESH
NPARDIS
PARNAM – One entry per line. One line for each distributed Parameter.
....
NOBS
OBSNAM – One entry per line. One line for each observation.
...
Nument PARNAM OBSNAM Misfit Cutoff – One for each parameter-observation pair.
icol irow ilay Sensitivity Parameter_Cell_Value – Nument lines are printed.
...
Nument PARNAM OBSNAM Misfit Cutoff
icol irow ilay Sensitivity Parameter_Cell_Value
...
```

#### Definition of Variables

Nument - Number of entries to follow for that particular distributed parameter-observation pair. If sensitivities for an observation cannot be calculated because the cell in which the observation lies has gone dry, then the NUMENT entry will be zero.

Misfit - Difference between observed observation and calculated observation. If the observation cannot be calculated because the cell in which the observation lies has gone dry, then the Misfit entry will be -999.

Cutoff – The absolute value of the smallest sensitivity that would be printed for this observation-parameter pair. Cutoff is the product of THRESH and the largest absolute sensitivity of any cell.

Sensitivity – Sensitivity of the observation to the value for the cell listed in the appropriate multiplication array defined in the LPF file.

Parameter\_Cell\_Value – the value of the parameter in the cell. This value is the product of the parameter value listed in the LPF file and the value for the cell listed in the appropriate multiplication array defined in the LPF file. The parameter cell value is printed only if the PVALUEOUT variable is set to 1.

#### 4.3.4 Format Option 4

Option 4 compresses the output into distributed parameter matrices in way readable using JUPITER UTL\_READMATRIX. The sensitivities of each parameter-observation pair are written in compressed format. To read the file created using option 4 the sensitivity data for each distributed parameter-observation pair would be read using sequential calls to UTL\_READMATRIX. The sequence would be one call for each distributed parameter in order of parameters listed in the top of the file, which is repeated for each observation listed.

#### File Listing Format

IAFORM PVALUEOUT  
THRESH  
NPARDIS  
PARNAM – One entry per line. One line for each distributed Parameter.  
....  
NOBS  
OBSNAM – One entry per line. One line for each observation.  
...  
COMPRESSEDMATRIX PARNAM\_OBSNAM – One per parameter-observation pair.  
NNZ NROW\*NCOL NLAY  
IPOS Sensitivity – repeated NNZ times  
...  
COMPRESSEDMATRIX PARNAM\_OBSNAM  
Nnz NCOL\*NROW NLAY  
Ipos Sensitivity  
...

#### Definition of Variables

COMPRESSEDMATRIX - an ASCII string

PARNAM\_OBSNAM - a concatenation of the parameter name and the observation name connected by an underscore “\_”.

Nnz – The number of sensitivity values printed for the parameter-observation pair. Only sensitivities that are equal or greater than Threshold are printed.

Ipos – The location index for the associated sensitivity. Ipos identifies the location of the associated sensitivity in the model domain. The counting cycles columns first, then rows then layers. For example, Ipos=6 in a 5 column by 5 row by 5 layer model would indicate the first column of the second row in the top layer.

## Usage Notes

### 5.1 WARNING - RATE DISCREPANCIES

Some error checking of the adjoint state calculations is done by calculating a “mass balance” of net incoming “flow” and outgoing “flow” during a simulation. This is similar to the familiar flow budget of MODFLOW. An imbalance is referred to as a rate discrepancy. If any rate discrepancy is larger than  $1 \times 10^{-6}$  percent of the influx to the cell then a warning message is printed to the GLOBAL file at the end of the time step that reports the discrepancy calculated during the time step. A typical warning message looks like:

```
SUM OF POSITIVE RATES= 2.89639E-10    SUM OF NEGATIVE RATES= 2.89639E-10  
PERCENT DISCREPANCY = -9.85E-05
```

At the end of a simulation in which any discrepancy was more than  $1 \times 10^{-4}$ , a final message listing the largest discrepancy encountered is printed to both the GLOBAL file and the screen (standard out). A discrepancy of  $1 \times 10^{-4}$  percent would rarely indicate a significant problem with the simulation. A discrepancy of  $1 \times 10^{-2}$  percent may be significant. Significance depends on the use of the sensitivity information and on when the discrepancy occurs. If the positive and negative rates are small compared to the adjoint states then a large percentage error in the rates is not significant. Rate discrepancies may be controlled by solver control variables for the adjoint state calculations.

### Parameter Sensitivities from Velocity Sensitivity

This section describes a capability that is a significant variation from other capabilities of the code. If the reader is not interested in using the code to calculate sensitivities from previously determined observation sensitivities to Darcy velocity then this section can be safely ignored. Transport codes such as MT3DMS (Zheng and Wang, 1999) and RT3D (Clement, 1997) can use the flow results from MODFLOW simulations to define the flow velocities for transport simulations. Velocity sensitivity refers to the sensitivity of transport related calculation to the flow results from MODFLOW transformed Darcy velocity. Since porosity is not a property that is represented in a MODFLOW calculation, the sensitivity to fluid velocity can not be used directly. How the sensitivity to Darcy velocity is calculated is beyond the scope of this document. We simply assume that the sensitivity to Darcy velocity is available in the form of an input file.

A paper by Samper and Neuman (1986) has been used as the basis of the development of the velocity sensitivity capability. The presentation below, however, uses the conventions adopted in Section 2.

### 6.1 Theory

In effect, the Darcy velocity sensitivity becomes a pseudo-observation that is distributed throughout the model domain and may also be distributed in time. Henceforth Darcy velocity will be shortened to velocity. Applying the chain rule to the sensitivity of an observation  $C$  to a MODFLOW parameter,  $p$ , a representation similar to Equation 2.2 can be formed

$$\frac{dC}{dp} = \frac{dC}{dV} \frac{dV}{dp} = \frac{dC}{dV} \frac{dV}{df} \frac{df}{dp} \quad (6.1)$$

where  $V$  is velocity and, as in section 2,  $f$  represents the flow equations. The velocity has components defined across each cell boundary.  $V_{r,j,i,k}$  would be the velocity along a row across the face common to cell  $j, i, k$  and cell  $j, i+1, k$ . Equation 6.1 shows that  $\frac{dC}{dV}$  is a scaling factor that multiplies the sensitivity of velocity to the parameter. As before, the factor  $\frac{df}{dp}$  is applied after solving for adjoint states,  $\lambda \equiv \frac{dC}{dV} \frac{dV}{df}$ . By multiplying  $\frac{dV}{df}$  by  $\frac{dC}{dV}$  we are taking advantage of the fact that the adjoint state equations are linear even for non-linear flow problems. The equations are linear because the  $A$  and  $B$  matrices are fixed once the head solution is known. Using this definition of the adjoint states, we can solve for  $\frac{dC}{dp}$  with a single adjoint state solution. Following the conventions used in Section 2 we define the function  $L$  as  $\frac{dC}{dV} V$ .

$V$  represents every velocity in the model domain calculated throughout the flow solution including the possibility of a steady state velocity. Thus each element of the five dimensional matrix  $V$  contributes to the source term in the adjoint state equations except where  $\frac{dC}{dV}$  is zero. (The five dimensions are the three spatial coordinates that define a cell location plus a dimension to represent the three directions of flow and a time dimension). The function  $L$  augmented by the flow equations becomes

$$J = L(h, p) + (\lambda^0)^T [C^0 - A^0 h^0] + \sum_{m=1}^N (\lambda^m)^T [B^m h^{m-1} + C^m - A^m h^m] \quad (6.2)$$

$$\begin{aligned} dJ = & \left[ \left( \frac{\partial L}{\partial h^0} \right)^T + (\lambda^1)^T B^1 - (\lambda^0)^T A^0 \right] dh^0 + \sum_{m=1}^{N-1} \left[ \left( \frac{\partial L}{\partial h^m} \right)^T + (\lambda^{m+1})^T B^m - (\lambda^m)^T A^m \right] dh^m + \\ & \left[ \left( \frac{\partial L}{\partial h^N} \right)^T - (\lambda^N)^T A \right] dh^N + \left( \frac{\partial L}{\partial p} \right)^T dp + (\lambda^0)^T \left[ \frac{C^0}{\partial p} - \frac{\partial A^0}{\partial p} h^0 \right] + \sum_{m=1}^N (\lambda^m)^T \left[ \frac{\partial B^m}{\partial p} h^{m-1} + \frac{C^m}{\partial p} - \frac{\partial A^m}{\partial p} h^m \right] dp \end{aligned} \quad (6.3)$$

The terms  $\frac{\partial L}{\partial h^m}$  are evaluated for each component of velocity as follows;

$$\frac{\partial L_{j,i,k}}{\partial h^m} = \frac{dC}{dV^m} \frac{\partial V^m_{c,j,i,k}}{\partial h^m} + \frac{dC}{dV^m} \frac{\partial V^m_{r,j,i,k}}{\partial h^m} + \frac{dC}{dV^m} \frac{\partial V^m_{v,j,i,k}}{\partial h^m} \quad (6.4)$$

where

$$\frac{\partial V^m_{c,j,i,k}}{\partial h^m} = CR^m_{j,i,k} [\delta(j^* - j, i^* - i, k^* - k) - \delta(j^* - j + 1, i^* - i, k^* - k)] \quad (6.5)$$

$$\frac{\partial V^m_{r,j,i,k}}{\partial h^m} = CC^m_{j,i,k} [\delta(j^* - j, i^* - i, k^* - k) - \delta(j^* - j, i^* - i + 1, k^* - k)] \quad (6.6)$$

$$\frac{\partial V^m_{v,j,i,k}}{\partial h^m} = CV^m_{j,i,k} [\delta(j^* - j, i^* - i, k^* - k) - \delta(j^* - j, i^* - i, k^* - k + 1)] \quad (6.7)$$

Similarly, if the parameter is a lumped hydraulic conductivity parameter the direct term  $\frac{\partial L}{\partial p}$  contributes to the sensitivity for each non-zero term in  $\frac{dC}{dV}$ . Sensitivity of a cell for a distributed hydraulic conductivity parameter will have a direct term only when the cell is used to calculate one of the conductance terms. That is only for the cell or neighboring cells.

## 6.2 ADJ input file for velocity sensitivity data

Specification of an input file of type COBS in the MODFLOW Names File signals the calculation of parameter sensitivities from velocity sensitivity data. Input for the adjoint sensitivity calculations is read from a file that is specified with "ADJ" as the file type in the MODFLOW Name File. The use of bracket, [], indicates optional input data

### File Listing Format

1. [#Text]

Text is optional and can include as many text lines as desired as long as they begin with #.

2. OPERATION, [MODE or WEIGHTS or IUPAROBS]

3. NCONCMX

4. [PREFIX]

PREFIX is read only if OPERATION has a value of 3 or 4.

5. IADJSU IADJFM IADJSCL IADJPC

6. IUOBSMAP

7. CFNAME

8. VSNAM

9. IUSOLV

10. NPE NPARDIS

11. IADJXDU IAFORM DISCUT PVALUEOUT

Read only if NPARDIS is greater than zero.

12. [IPDISP(1) IPDISP(2), ...]

IPDISP is a NPARDIS long integer list read only if NPARDIS is greater than zero.

13. PARNAM LN

Read NPE times

### **Explanation of Variables**

**OPERATION** - Defines the mode of operation of the adjoint sensitivity code. OPERATION is an integer value between 1 and 4. The following lists how OPERATION controls the program.

- 1) Sensitivities will be calculated for each observation creating a Jacobian matrix of sensitivities of each observation to each parameter.
- 2) Gradient of the weighted sum of squares errors of all observations is calculated.
- 3) Only the solution for hydraulic heads will be performed. Sensitivity calculations will not be done. The resulting heads and necessary boundary condition information will be stored in a series of files starting with the PREFIX character string.
- 4) Sensitivities will be calculated for a single observation that will be obtained from file unit IUPAROBS defined in the MODFLOW Names File. Head and boundary condition information will be read from files starting with the PREFIX character string.

**MODE** - Read only if OPERATION=1. If MODE is greater than zero then adjoint states are solved for the last observation at a location. The adjoint states for earlier observations are calculated from this solution. If the simulation does not have constant time steps then these calculated adjoint states are an approximation.

**WEIGHTS** – Read only if OPERATION=2. If WEIGHTS is non-zero then observations are weights in the calculation of the sum-of-squares gradient. Otherwise all observations are assigned a weight of 1. Setting WEIGHTS to a non-zero value, changes the input requirements for observations. In this case, observation data must be entered using the instructions indicated in Section 3.5 for head observations and 3.6 for flow observations.

**IUPAROBS** - Read only if OPERATION=4. IUPAROBS defines the unit number from which to read the active observation. This unit number must be defined as a DATA file type in the MODFLOW Names File.

**NCONCMX** - Maximum number of concentration measurements used to calculate velocity sensitivities in transport code.

- PREFIX – A character string without blanks used to define the names of head solution and boundary condition files created using OPERATION =3 or read using OPERATION=4. Only the first 70 characters will be used.
- IADJSU – File unit number of lumped parameter sensitivities. File name should be supplied in the MODFLOW Name File. The file must be type DATA.
- IADJFM – Print Format for IADJSU; Section 3.4 describes the influence of IADJFM on the output format.
- IADJSCL – a value of 1 causes 1% scaled sensitivities to be output to file IADJSU. If IADJSCL is set to 1 then the reported sensitivities are multiplied by the parameter value and divided by 100. If IADJSCL is not set to 1 then the sensitivities are not scaled. They are not scaled by the parameter value.
- IADJPC – a non-zero value causes row (measurement) and column (parameter) numbers to be added to file IADJSU.
- IUOBSMAP – File unit number for mapping of observations of all types to output observation number. File name should be supplied in the MODFLOW Name File using type DATA.
- CFNAME – File name for concentration location and time data. This name is supplied only if velocity sensitivity data has been calculated for a transport model.
- VSNAME – File name from velocity sensitivity data. This name is supplied only if velocity sensitivity data has been calculated for a transport model.
- IUSOLV – File unit number for adjoint calculation solver control. File name should be supplied in the MODFLOW Name File using type DATA. The file supplies separate solver control information for the adjoint solution. The solver must be the same as used in the head calculations. If IUSOLV is zero then the solver control used for the head calculations is used to control the adjoint state calculations. It would be a rare situation where using the same control parameters for both the head solution and the adjoint calculations would be appropriate.
- NPE – Number of lumped parameters to be used to calculate sensitivity information. Any distributed parameters must be included as lumped parameters also.
- NPARDIS – Number of distributed parameters to calculate sensitivities for. Each distributed parameter must have a corresponding lumped parameter.
- IADJXDU – File unit number for distributed parameter sensitivity output. File name should be supplied in the MODFLOW Name File. Type of file (DATA or DATA(BINARY)) controls whether the file is formatted or binary. The type of binary file can be controlled using the openspec.inc file prior to compilation of the program.
- IAFORM – controls the format of the distributed parameter sensitivity output. Briefly, the value must be 1-4. See Section 3.5 Distributed Sensitivity Output for more detail.
- 1) Option 1 causes single column of sensitivities to be output with the following cycle pattern. The columns of the grid are the inner most cycle, then rows, layers, parameters, with observations as the outer cycle. Comment lines starting with # are written prior to each new distributed parameter. All columns, rows and layers are

included, which means that both active and inactive cells are included. Inactive cells are listed with a sensitivity of zero.

- 2) Option 2 creates a row of sensitivities for each distributed parameter-observation pair using the same cycling as for option 1. Formatted output (file type DATA) uses 20(1PG16.7) for each line. No text lines are included. Each new parameter will cause a new line in the output.
- 3) Option 3 compresses the output to eliminate small sensitivity values. After a header that lists each distributed parameter and each observation in the orders in which they are cycled, each line of the output lists numbers for the distributed parameter identification, column, row, layer, observation, and sensitivity only for sensitivity values larger than DISCUT (See below).
- 4) Option 4 compresses the output into distributed parameter matrices in way readable using JUPITER UTL\_READMATRIX. The sensitivities of each parameter-observation pair are written in compressed format. For each pair a line is written with the text COMPRESSEDMATRIX and a name composed of the parameter name and the observation name separated with and underscore ( \_ ). The next line lists the total number of printed elements followed by the product of NCOL\*NROW and then the number of layers. After this each line contains a pointer to the column, row, and layer plus the sensitivity value. The pointer uses the column, row, layer cycling as described for option 1. To read the file created using option 4 the sensitivity data for each distributed parameter-observation pair would be read using sequential calls to UTL\_READMATRIX. The sequence would be one call for each distributed parameter in order parameters listed in the top of the file, which is repeated for each observation listed.

DISCUT – DISCUT is a relative cutoff criterion for compressed output options 3 and 4. Only sensitivities with relative sensitivities greater the DISCUT are written. Relative sensitivity is in comparison to the largest cell sensitivity of an observation to a parameter.

PVALUEOUT – If PVALUEOUT is 1 then the parameter value of a cell is added after the cell sensitivity is listed in the distributed parameter sensitivity output. This option is not allowed for IAFORM formats 2 or 4. The value listed is the product of the value listed in the LPF file and the multiplication matrix, whereas the sensitivity is to the value in the sensitivity matrix. If the value in the LPF file is 1.0 then the sensitivity and parameter value are consistent.

IPDISP(1), IPDISP(2) is an integer list (all on one line) corresponding to the PARNAM names read next. 2 would correspond to the second PARNAM entry.

PARNAM – read NPE times. PARNAM must be identical to a parameter name supplied in the “LPF” input file. PARNAM identifies which parameters are used to calculate lumped parameter sensitivities. IPDISP identifies which lumped parameters are also distributed parameters.

LN – If LN is 1 the sensitivities are calculated with respect to the natural log of the parameter. Use YHK and YVK for natural log of conductivity. For YHK and YVK parameters only, an LN value of 0 in the ADJ file indicates dimensional values in the

multiplier arrays and an LN value of 1 indicates log parameter values in the multiplier arrays.

## 6.3 Input Instructions for velocity sensitivity data

### File Listing Format for File CFNAME

NUMLOC NUMMEAS

COLUMN ROW LAYER IEND ISTART – NUMLOC sets of data

IPER ISTEP TOFF – IEND-ISTART+1 lines per location

↓

COLUMN ROW LAYER IEND ISTART – second data set

IPER ISTEP TOFF – IEND-ISTART+1 lines per location

### Explanation of Variables

NUMLOC – Number of observation locations

NUMMEAS – Total number of observations

COLUMN – The column index of the observation location.

ROW – The row index of the observation location.

LAYER – The layer index for the location.

IEND – Observation number for last observation at location.

ISTART – Observation number for first observation at location.

IPER – Stress period number when observation occurred.

ISTEP – Time step in the stress period when observation occurred.

TOFF – Fraction of time step completed when observation occurred.

### File Listing Format for File VSNAM

The sensitivity data file requires a very restrictive format. The file has been created using FORTRAN DIRECT ACCESS format. This is accomplished with an OPEN statement similar to

```
OPEN(UNIT=Unit number, NAME=name, FORM='UNFORMATTED',  
      ACCESS='DIRECT', RECL=Len)
```

Where, Len is the record length of the sensitivity data.  $Len=4*(3*NCOL*NROW*NLAY)$ . The stored sensitivities are single precision, e.g. 4 bytes long. A single record contains the array VELSENS(3,NCOL,NROW,NLAY). There are three directions with indices; column direction=1, row direction=2, vertical=3. This record contains the velocity sensitivity for a single observation at a one time step. The data are stored with the direction index cycling first, then column, then row, and finally layer. This order is consistent with the default order when an entire array is written. Note the all indices are included, even inactive cells.

The openspec.inc file can be used to make the UNFORMATTED style compatible with the code. See Chapter 9 of the MODFLOW-2005 manual and the file openspec.inc for more details. The MODFLOW-2000 guide to linking MT3DMS to MODFLOW-2000 (Zheng and others, 2001) may also provide insight into adjusting the openspec.inc file and writing the velocity sensitivity file.

Direct access files are written and read by record number. A unique record number for a velocity sensitivity array is given by

$$\text{Record number} = (\text{IOBS} - 1) * \text{NTIMES} + \text{KSTP} \quad (6-8)$$

where IOBS is the index of the observations in the order listed in file CFNAME, NTIMES is the total number of time steps in the simulation (NTIMES is the sum of the time steps for each period), and KSTP is the current time step of the adjoint state calculation. This time step is the time step of the head solution. Both NTIMES and KSTP include the steady state period if applicable.

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