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Variation in parameter estimation using MODFLOWP

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VARIATION IN PARAMETER ESTIMATION USING MODFLOWP

A Thesis

Presented to

The Faculty of the Department of Civil and Environmental Engineering

San Jose State University

In Partial Fulfillment

of the Requirements for the Degree

Master of Science

by

Michael John Wanta

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ABSTRACT

VARIATION IN PARAMETER ESTIMATION USING MODFLOWP

by Michael John Wanta

This thesis discusses MODFLOWP (Hill, 1992; 1996), a modular, three-dimensional, finite difference groundwater flow model with the capability of using nonlinear regression to estimate model parameters. MODFLOWP calculates parameter sensitivities and statistics which allow the user to analyze the correlation between parameters, identify the most and least reliably-estimated parameters, and identify potential biases.

A test case was used to evaluate the parameter estimation capabilities of MODFLOWP. The model was modified by changing the number of parameters, the initial parameter estimates, and the constraints on the parameters. Results indicated that composite scaled sensitivities are a good indicator as to which parameters can be removed from the parameter estimation process, the standard deviation has a significant impact on the final parameter estimates, there appears to be a correlation between composite scaled sensitivities and parameter estimate reliability as measured by eigenvectors and eigenvalues, and some of the model runs were ill-posed and non-unique.

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1.0 Introduction

This thesis discusses the use of the groundwater parameter estimation and modeling program MODFLOWP (Hill, 1992; 1996). The purpose of this thesis is to evaluate MODFLOWP's parameter estimation capabilities. The evaluation was performed by determining how MODFLOWP results vary for the same physical groundwater system when varying the initial estimates of the parameters, constraints on the parameters, and by changing the number of parameters.

The remainder of this thesis consists of a description of MODFLOW in Section 2.0, a description of MODFLOWP in Section 3.0, test case results in Section 4.0, and conclusions of the work in Section 5.0.

1.1 Importance and Role of Groundwater Modeling

During the development of groundwater resource projects, information regarding the characteristics of the affected groundwater system is required to ensure proper planning of a particular project. There is also a need to characterize subsurface groundwater systems to predict the movement of contaminant plumes and to develop monitoring programs for sites which have the potential to pollute the groundwater.

Typically only one millionth of the subsurface groundwater system materials we are interested in are sampled (Poeter and McKenna, 1994). This leaves a large amount of uncertainty in using this limited amount of information as a basis for describing the entire subsurface system.

The importance and role of groundwater modeling is to assist with groundwater data interpretation and prediction of groundwater movement. A groundwater system is typically complex and difficult to predict without numerical modeling. Initial results of groundwater models can also act as a guide for further data collection.

1.2 Literature Review

A literature search was performed to identify published applications of MODFLOWP and related papers. A brief overview followed by a discussion of the content of selected published papers is included below.

Traditionally, determination of parameters in the groundwater flow problem has been performed using trial and error techniques, as is done with MODFLOW (McDonald and Harbaugh, 1988). With this method, parameters are first specified by the user and the resulting model-predicted heads are then compared to observed heads. Parameters are varied until the match between observed heads and calculated heads is acceptable to the user. MODFLOWP uses a method which is the inverse of the trial and error technique. In this method, which is referred to as the inverse method, the model input data includes observed heads and MODFLOWP then estimates the parameters based upon a user-specified convergence criterion.

The inverse problem of parameter estimation has been studied in depth since the 1960's. Various techniques have been developed to solve the inverse problem. The techniques have been classified as either direct or indirect (Yeh, 1986). The direct techniques handle the model parameters as dependent variables. The indirect techniques

are based upon a user-specified closure criterion, where the estimate of each parameter is iteratively modified until the user-specified closure criterion is met. MODFLOWP uses this indirect technique. Much of the following discussion can be referenced to Yeh (1986).

In the mid-1970's the non-uniqueness of the inverse problem was studied. Non-uniqueness occurs when the final parameter estimates vary with different initial estimates of the parameters (without constraints imposed on the parameters). Parameter uniqueness is related to parameter identifiability. An identifiable parameter is defined as a parameter which can be uniquely defined in all points of its domain using the groundwater model. An example of parameters which could not be identifiable is a pair of parameters with a very high correlation. It is difficult to identify specific values for either parameter, since the solution is the same for various combinations of the parameter values. For example, consider a simple one-cell one-layer model in which transmissivity and recharge are parameters. In this case, transmissivity doubles when recharge doubles without a change in head. These two parameters would not be identifiable in this simple case.

A number of models have been developed since the mid-1960's to solve the inverse problem. A large percentage of these models were used to determine the characteristics of oil reservoir flows. Earlier models were used to simulate two-dimensional flow in confined layers under transient conditions, and typically had the ability to estimate transmissivity and storage (Yeh, 1986). Numerical methods used to solve the flow equations included finite differences and finite elements. These models did not have the

capability to quantify the uncertainty of parameter estimates nor did they allow for prior information on the parameters.

Models in more recent years handle three-dimensional flow (MODFLOW and MODFLOWP are considered to be three-dimensional), transient and steady state flow, and a much wider variety of parameter types. Recent models, including MODFLOWP, also have the ability to allow for prior information on the parameters and to quantify the uncertainty of the initial parameter estimates.

Yager (1993) used MODFLOWP to simulate groundwater flow in a complex, fractured bedrock aquifer. MODFLOW was first used to model the groundwater system, with MODFLOWP being used to refine estimates of seven parameters after initial model calibration. The model consisted of 10 layers and covered an area of 110 square miles. The grid consisted of 1000-foot-square cells. The seven parameters were two transmissivity values, three vertical leakance values, and two areal recharge rates. Steady-state simulation results were compared with the observed heads in various layers and zones, low-flow rates of springs and streams and discharge flow rates from tunnels and excavations. The MODFLOWP model results suggested that a source of water not represented in the model was contributing to the majority of observed flow in the system. Results showed that MODFLOWP was effective in predicting parameter values and reduced the effort typically needed for model calibration.

Poeter and McKenna (1994) studied the effect of using groundwater modeling to reduce the uncertainty of groundwater system characteristics. A synthetic test case, in which existing conditions were known, was set up to assess modeling uncertainty.

MODFLOWP was used to estimate five parameters — all related to hydraulic conductivity. Final parameter estimates generated by MODFLOWP were lower than expected due to discontinuities of the geology. This led to a revision in the model set up. The revised model did not converge properly. Multiple runs were performed by slowly removing information from the model until the model converged with reasonable parameter values and head results. The study showed that groundwater system uncertainty can be substantially reduced using groundwater modeling.

Starn (1994) used MODFLOWP to estimate groundwater system characteristics and recharge for a two-dimensional test case. Six parameters were estimated: two transmissivity values, recharge, hydraulic conductivity, riverbed conductance (conductance $[L^2T^{-1}]$ is the product of the hydraulic conductivity and cross-sectional area of flow divided by the length of the flow path; in the case of a riverbed, conductance is hydraulic conductivity multiplied by the riverbed surface area and then divided by the thickness of the riverbed sediments), and conductance of a general head boundary. Starn set five criteria to determine these final parameters: (1) estimate as many parameters as possible; (2) the parameter estimation must converge; (3) correlation between parameters must be minimized; (4) variance of the estimates must be minimized; and (5) the weighted sum of square errors must be minimized. It was determined that all of these criteria could not be met and the above list of parameters, which was a reduction from the original number, was estimated. The study showed that nonlinear regression modeling was effective in predicting groundwater system characteristics and that using MODFLOWP is more efficient than trial and error modeling.

Giacinto (1994) used MODFLOWP to characterize the groundwater system for a Superfund site. The purpose of the modeling was to estimate parameter values, delineate zones of similar parameters and to predict hydraulic gradients. The model consisted of three layers and covered approximately eight square miles. Parameters were estimated for transmissivity, leakance, and areal recharge. Sensitivity analyses were used to modify the model. Results were used to prioritize further data collection at the site.

Anderman *et al.* (1994) used MODFLOWP to assist in tracking advective transport of a particle in a simulation representing groundwater contaminant transport. The MODFLOWP computer code was augmented to include special capabilities which assisted in particle tracking (advective-transport observations were added to the model). Five parameters were estimated: hydraulic conductivity, areal recharge, two flux values, and conductance. The modeling was performed in two steps. First, MODFLOWP was used to determine parameter composite scaled sensitivities (defined in Section 3.3.3), correlations and other information. Second, MODFLOWP was used to estimate the parameters. Results showed that the model produced unrealistic parameter estimates which may be attributed to a problem with the model set up or inaccurate head observations.

Anderman *et al.* (1996) continued their work using a modified version of MODFLOWP to investigate the importance of adding advective-transport observations to the model. This was done to reduce the problems associated with parameter insensitivity and correlations between parameters. Results indicated that adding advective-transport observations to the model produced more reasonable, precise and unique parameter

estimates than head-dependent flow observations alone. This occurred mainly due to the reduced correlation between parameters.

Ronan (1995) used parameter sensitivities calculated by MODFLOWP to examine parameter uncertainty for a model of a transient flow system. Model head data spanned an 11-year period during which hydraulic head varied by as much as 18 feet annually. The model consisted of three layers and was run under three steady state conditions to account for seasonal changes and the transient conditions of the aquifer system. Sensitivity results from MODFLOWP were compared to previously published sensitivity analyses and were found to be consistent with them. The paper suggested that MODFLOWP was a useful tool for estimating parameter sensitivities.

Of the papers reviewed, six papers cited time and effort efficiency gains when using MODFLOWP to aid in parameter estimation. All of the papers which discussed MODFLOWP indicated that relevant information is gained by groundwater modeling using MODFLOWP, although the success of each experience varied.

2.0 MODFLOW

2.1 Description of MODFLOW

MODFLOWP (Hill 1992; 1996) can be thought of as the MODFLOW program (McDonald and Harbaugh, 1988) with parameter estimation capabilities added.

Therefore, a discussion of MODFLOW provides a description of the fundamentals of MODFLOWP.

2.1.1 MODFLOW Packages/Modules

MODFLOW has been developed in a modular fashion, with various program modules or packages, each independent of one another. The modules in the original release of MODFLOW are: the basic input package, block-centered flow package, river package, recharge package, well package, general-head boundary package, drain package, evapotranspiration package, strongly implicit procedure package, slice successive overrelaxation package, and a few utility modules. Each program module has an associated input file. Modules relevant to this thesis are described below. Further information regarding these packages can be found in McDonald and Harbaugh (1988). Modules added after the original release of MODFLOW include the preconditioned conjugate-gradient package (Hill, 1990), and the stream flow routing package (Prudic, 1989). Please see the cited references for information on these packages.

A new version of MODFLOW (version 3.0) was released in December 1996. It is referred to as MODFLOW-96. Many new capabilities have been added to this newer version; they are not discussed in this thesis.

The basic input package is required for all models. It handles many of the administrative functions for MODFLOW. The numbers of rows, columns, layers and stress periods are read by the basic input package. This package also reads initial head data for each cell of the model and reads data determining whether each cell is variable-head, constant-head, or inactive. The package also calculates an overall water balance for the model.

The block-centered flow package is required for all models. The block-centered flow package computes the conductance components of the finite-difference equation which determines flow between adjacent cells in the discretized model. The block-centered flow package reads cell dimensions, layer thicknesses, storage coefficients, and transmissivity/hydraulic conductivity. It also calculates storage terms and handles the effects of adjacent cells becoming partially saturated during the computer simulation.

The river package is optional. It models flow between surface water and groundwater systems by calculating the conductance between these two systems. The package also reads the cell locations of the river, the head of the river at each cell, the conductance of the riverbed and the elevation of the riverbed.

The recharge package is optional. It is used to model areal surface recharge (typically from precipitation) and can also be used to simulate artificial or other types of

recharge. This package reads recharge fluxes for each cell and calculates the recharge flow at given cell locations.

The well package is optional. It is used to simulate the extraction or addition of water from or to specific cells. The package reads the cell location and well flow rate specified by the user.

The general-head boundary package is optional. It is used to calculate flow between model boundary cells and external sources. The package reads the head of the external source adjacent to the specified boundary cell, and the hydraulic conductance of the interface between the boundary cell and the external source.

2.1.2 Groundwater Flow System Representation

The groundwater flow system is represented in three dimensions. The vertical dimension is set up as various layers (one or more) of varying thickness. The horizontal dimension is set up by constructing a rectangular grid system over the horizontal plane.

To completely describe a groundwater flow system, the following are required (as applicable to each individual model) as input data by MODFLOW: transmissivity or hydraulic conductivity and layer bottom elevations, starting head elevations, storage coefficient of confined layers, specific yield of unconfined layers, pumping well rates and locations, vertical leakance between layers, horizontal anisotropy of each layer (ratio of column to row anisotropy), river location and conductance, surface recharge, evapotranspiration, and boundary conditions. For steady state models, the starting head

elevations are merely initial estimates of the head distribution; for transient models, the starting head elevations represent the actual head distribution at the start of the simulation.

2.2 Mathematical Model

The transient three-dimensional partial differential equation for groundwater flow is as follows (McDonald and Harbaugh, 1988):

$$\frac{\partial}{\partial x} (K_x \frac{\partial h}{\partial x}) + \frac{\partial}{\partial y} (K_y \frac{\partial h}{\partial y}) + \frac{\partial}{\partial z} (K_z \frac{\partial h}{\partial z}) - W = S_s \frac{\partial h}{\partial t} \quad (1)$$

where:

$K_{x,y,z}$ are values of hydraulic conductivity along the x, y and z axes (L/T)

h is the potentiometric or hydraulic head (L)

W is the volumetric flux per unit volume (sum of all sources and sinks) (T^{-1})

S_s is the specific storage (L^{-1})

t is time (T)

The steady-state form of the equation has zero as the right-hand term. The mathematical model flow equations are based upon Darcy's law and the continuity equation. Equation (1), when combined with initial conditions and boundary conditions, forms the mathematical description of the groundwater flow system.

2.2.1 Discretization

The groundwater flow system is broken into a series of cubic blocks which form a three-dimensional grid over the area and depth to be modeled. The conventions used by MODFLOW are as follows: *i* is the row designator, *j* is the column designator, and *k* is the layer designator. The length, width and depth (unless transmissivity is provided) may be specified for each grid block. Each block contains a node at the center. The node is the point at which head in the block is calculated. The system may have multiple layers with specified thicknesses; the layers are normally hydrogeologic units. A hypothetical discretized system is shown in Figure 1.

Using the groundwater flow equations and groundwater system input data, MODFLOW calculates heads for each active node over the grid system. The heads are calculated for transient or steady state solutions, as specified by the user.

Explanation

----- Aquifer Boundary

● Active Cell

○ Inactive Cell

Δr_j Dimension of Cell Along the Row Direction. Subscript (J) Indicates the Number of the Column

Δc_i Dimension of Cell Along the Column Direction. Subscript (I) Indicates the Number of the Row

Δv_k Dimension of the Cell Along the Vertical Direction. Subscript (K) Indicates the Number of the Layer

Figure 1.—A discretized hypothetical aquifer system.

(Source: McDonald and Harbaugh, 1988)

MODFLOW utilizes a finite-difference form of equation (1) to calculate hydraulic heads at discrete locations and times for heterogenous, anisotropic and transient conditions. The finite difference form of equation (1), which is centered in space and implicit in time, is (McDonald and Harbaugh, 1988):

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

where:

$CR_{i,j,k}$ is the row conductance, which is the product of the hydraulic conductivity and cross-sectional area of flow divided by the length of the flow path at a specific point in the three-dimensional i,j,k grid along the row direction (L^2T^{-1})

$h_{i,j,k}^m$ is the head in cell i,j,k at time t_m (L)

$CC_{i,j,k}$ is the column conductance, which is the product of the hydraulic conductivity and cross-sectional area of flow divided by the length of the flow path at a specific point in the three-dimensional i,j,k grid along the column direction (L^2T^{-1})

$CV_{i,j,k}$ is the vertical conductance, which is the product of the hydraulic conductivity and cross-sectional area of flow divided by the length of the flow path at a specific point in the three-dimensional i,j,k grid along the vertical direction (L^2T^{-1})

$P_{i,j,k}$ is the summation of conductances from external sources (L^2T^{-1})

$Q_{i,j,k}$ is the summation of flows from external sources (L^3T^{-1})

$\Delta r_j \Delta c_i \Delta v_k$ is the volume of cell i,j,k (L^3) where Δr_j is the distance between rows, Δc_i is the distance between columns, and Δv_k is the distance between layers (L)

$SS_{i,j,k}$ is the specific storage of cell i,j,k (L^{-1})

t_m is the time at the end of time step m (T)

The subscript $\frac{1}{2}$ in equation (2) can be best explained by example: $CR_{i,j-\frac{1}{2},k}$ is the conductance in row i and layer k between nodes $i,j-1,k$ and i,j,k . The subscript $j-\frac{1}{2}$ should be thought of as the total region between nodes and not a specific point.

2.3 Boundary Conditions

Four types of boundary conditions can be used in the MODFLOW computer program: specified head, no-flow, head-dependent and specified flux. The boundary conditions are typically applied at the outer limits of the grid, but may also be specified within the grid.

Since the model grid does not necessarily need to correspond to the physical limits of the aquifer being modeled, boundary conditions can be specified within the aquifer or along physical aquifer boundaries. The main reason for specifying grid boundaries within an aquifer is to reduce the size of the model area and data collection effort, allowing the user to focus in on a specific area of interest.

The different types of boundary conditions are discussed in the following sections.

2.3.1 Specified Head Boundaries

Specified head boundaries are boundaries at which the head is held constant, at a user specified value, for the duration of the computer simulation. A model domain adjacent to a large water body with a static water level could cause this type of boundary condition.

2.3.2 No-Flow Boundaries

No-flow boundaries are boundaries which do not allow flow to pass between the no-flow boundary cell and the adjacent active cell inside the model domain. This boundary condition would occur at physical boundaries where an aquifer is adjacent to a very low permeability material or at model boundaries coincident with stream lines or flow lines, or at groundwater divides.

MODFLOW provides two ways of modeling no-flow boundaries: (1) the user specifies inactive (no-flow) cells for which no calculations are performed; and (2) automatically assuming no flow along model grid boundaries which do not have any other type of boundary condition specified.

2.3.3 Specified Flux Boundaries

Specified flux boundaries allow a constant flux into or out of the boundary cells and to or from an external source outside the model domain. This boundary condition would be imposed where the subsurface flow across the model grid boundary can be estimated.

This type of boundary condition is typically modeled using MODFLOWP's well package. It can also be simulated by using the recharge package.

2.3.4 Head-Dependent Boundaries

Head-dependent boundaries are boundaries at which flux varies with head. For example, a river would act as a head-dependent boundary condition where the amount of flow into or out of the aquifer would be dependent upon the difference in head elevations between the river and the aquifer. If the head in the river is higher, flow would enter the aquifer at a rate based on the conductance of the riverbed.

This type of boundary condition is simulated by using the river package. The head in the river and the riverbed conductance are user-specified.

This boundary condition is also simulated in the drain, streamflow routing and general head boundary packages. The drain package allows flow out of the aquifer if head in the aquifer is above the elevation of the drain. If head in the aquifer is below the elevation of the drain, no flow out of the aquifer occurs. The elevation of the drain and the conductance between the drain and the aquifer are user-specified. The streamflow routing package is very similar to the river package, although it also models river flow and stage. The head in the stream, the streambed conductance, and hydraulic parameters for the stream are user-specified. The general head boundary package is the most general package which allows flow into or out of a cell in proportion to the head difference between the cell and the adjacent external fixed source. User input for this case is the

external head and the conductance of the zone between the source and the cell at which the general head boundary is specified.

2.4 Initial Conditions

For steady state conditions, which are the only conditions this thesis discusses, initial conditions are not required. However, MODFLOW requires the user to provide “initial guesses” for heads. These values are only used as initial estimated heads, a starting point for the iterative solution process as described below.

2.5 Solution Algorithms

The backward difference equation represented by equation (2) is always numerically stable (McDonald and Harbaugh, 1988). The set of linear equations resulting from equation (2) is solved at each time step using iterative methods. For steady state models the set of linear equations is solved once, using the same iterative methods.

The original version of MODFLOW (McDonald and Harbaugh, 1988) gave the user the option of using the Strongly Implicit Procedure (SIP) or Slice-Successive Overrelaxation (SSOR) methods for solving large systems of linear equations by iteration. Recent releases of MODFLOW include another iterative linear equation solver, the Principal Conjugate Gradient Method (PCG2; Hill, 1990). Further information regarding these solvers can be found in the references cited.

The iterative approach is used since it can solve the linear equations more quickly and has low roundoff error. The process is started by selecting an estimated head value

for each node. The estimated head values are modified through the use of the solution equations, producing new head values. The newly calculated values will more closely “fit” the mathematical model of the groundwater system. This process occurs through multiple iterations until the closure criterion is met. The closure criterion is user-specified and is the absolute value of the computed head change from one iteration to the next.

2.5.1 General Matrix Equation

MODFLOW uses equation (2) to obtain the solution to equation (1), as mentioned above. Equation (2), written in matrix form, is:

$$[A] \underline{h}_m = \underline{r} \quad (3)$$

where:

[A] is a matrix of the coefficients of head (all matrices will be defined using brackets [] in this thesis)

$\underline{h}_m$ is a vector of head values at the end of a time step for all nodes in the model

$\underline{r}$ is a vector of the constant terms for all nodes in the model

Vector $\underline{r}$ and matrix [A] are used to solve for vector $\underline{h}_m$ using iterative methods found in one of the three solvers discussed above.

2.5.2 Iterative Process for Head Calculation

The iterative process used to calculate heads at each node in the model starts with user-specified initial values of head at each node (vector h_m). The heads are then changed by the user-specified solver. The changed head values should be closer to satisfying the system of equations. The new head values then take the place of the previous head values, thus ending one iteration. This process continues until changes made to the head values become very small, satisfying a user-defined convergence criterion, or when reaching a user-defined maximum number of iterations.

The convergence criterion is satisfied when the absolute change in head at all nodes is less than the user-defined convergence criterion value. This value is normally specified to be an order of magnitude smaller than the level of accuracy required in the head results.

Ideally, the user would like to specify a convergence criterion to be met when the calculated heads are very close to the exact solution satisfying the system of equations. Unfortunately, this is not possible since the actual solution is not known. Therefore, an indirect method must be used — indirect method refers to estimating heads first and then checking if the estimated heads satisfy the flow equations. Normally, this method of specifying convergence criterion is adequate (McDonald and Harbaugh, 1988); however, the user should be aware that the calculated head values are not necessarily calculated to a level of accuracy related to the closure criterion. For example, if the closure criterion is specified as 0.01 feet, convergence will occur when heads are changed by less than 0.01 feet. This does not indicate that estimated heads have an accuracy of 0.01 feet.

3.0 MODFLOWP

3.1 Description of MODFLOWP

MODFLOWP is a new version of MODFLOW as documented in Hill (1992), and as revised in Hill (1996). It functions essentially the same as MODFLOW with the added ability to estimate parameters using nonlinear regression. (A parameter is a factor that is used to describe a physical characteristic or property of a specific model which may be estimated by MODFLOWP; for example, transmissivity or hydraulic conductivity of an aquifer could be parameters.) It can be run without parameter estimation, in which case it functions nearly identical to MODFLOW (McDonald and Harbaugh, 1988). The program can perform parameter estimation for transient and steady-state simulations. Version 1.9 of MODFLOWP was used for all analyses performed for this thesis. Use of different MODFLOWP versions should not impact the test case results.

MODFLOWP can be used as an aid in the calibration of models using MODFLOW. In some cases it can be thought of as a pre- and post-processor to MODFLOW (Hill, undated). This use would reduce time and effort spent on trial and error calibration and on sensitivity analyses. For example, MODFLOWP could be used as a pre-processor to calculate MODFLOW input values. The gain in efficiency comes from two factors: (1) the ability to easily change parameter values that may affect an array of values by changing one value (factor) in one input file, and (2) the automated parameter estimation capability which calculates parameter values which best fit measured heads. Post-processing capabilities of MODFLOWP include the calculation of various output

measures to assist the user in determining the accuracy of the model results.

Unfortunately, MODFLOWP does not print out mass balance results when being used to estimate parameters.

MODFLOWP also calculates sensitivities which can be used to optimize data acquisition (Hill, undated). Parameter sensitivities (defined in Section 3.2.3) can indicate whether existing data adequately allow one to estimate the parameter values with MODFLOWP and where additional data may be useful (Hill, undated). Problems in groundwater flow calibration can also be better identified using MODFLOWP (Anderman, *et al.*, 1994), since MODFLOWP has the ability to determine whether parameters are precisely estimated.

3.2 Parameter Estimation

A parameter is a variable which is to be estimated by MODFLOWP by using nonlinear regression. The program allows the user to specify up to 14 different types of parameters: well pump rates, river conductance, drain conductance, streamflow conductance, general head boundary conductance, constant heads, transmissivity or hydraulic conductivity, horizontal anisotropy of each layer (ratio of column to row anisotropy), leakance, storage coefficients, specific yield, areal recharge, and evapotranspiration.

Parameters can be assigned initial estimates by the user. These estimates consist of an initial parameter value and the approximate uncertainty of the estimate (expressed as a standard deviation, variance or coefficient of variation) which is used to calculate the

weight (defined in Section 3.2.5) of the parameter in the resulting regression equations.

The weight assigned to parameters is used to indicate the reliability of each initial parameter estimate relative to the others. The weight must also be adjusted to correct for different units between parameter values.

MODFLOWP then calculates estimated values for each parameter by solving a set of nonlinear regression equations. The regression problem is typically solved using PCG2, other preconditioned gradient methods, or a direct solver. SIP is not recommended (Hill, 1992). A discussion of the MODFLOWP solution algorithm follows.

3.2.1 Parameter Estimation Using Nonlinear Regression

Hydraulic head is a nonlinear function of many of the parameters in the groundwater flow equation (Hill, 1992). For example, hydraulic head is a nonlinear function of hydraulic conductivity. Therefore, nonlinear regression needs to be used for solving the groundwater flow inverse problem.

Nonlinear regression is used to calculate parameter values. When only head data are available, the sum-of-squares objective function is defined as:

$$\begin{aligned} S(\underline{b}) &= \sum_{q=1}^{ND} [h_q - h'_q]^2 \\ &= \underline{e}^T \underline{e} \end{aligned} \quad (4)$$

where:

$S(\underline{b})$ is a scalar function of the parameter values

- $\underline{b}$ is the vector of parameter values
- ND is the number of hydraulic head observations
- h_q is the measured hydraulic head at observation point q
- h'_q is the calculated hydraulic head at observation point q based upon the estimated parameter values
- $\underline{e}$ is the vector of residuals

The purpose of nonlinear regression is to minimize the value of $S(\underline{b})$, ultimately finding the global minimum of the objective function (refer to Section 4.3.3 for further discussion). The global minimum can be calculated by solving equation (5) below.

$$\frac{\partial S(\underline{b})}{\partial \underline{b}} = 0 \quad (5)$$

It is possible for there to be multiple solutions to equation (5). This would occur in models that are not well conditioned — a model without a unique, well defined minimum.

MODFLOWP cannot solve equation (5) directly for nonlinear problems. Two procedures are available: (1) a modified Gauss-Newton method; and (2) a conjugate direction optimization method. Only the first method is described in this thesis.

3.2.2 Modified Gauss-Newton Optimization Method

The modified Gauss-Newton optimization method for parameter estimation is typically used in MODFLOWP (Hill, 1992). This iterative process uses equations (6) and (7) to solve for the parameter estimates.

$$([C]^T [X_r]^T [\omega'] [X_r] [C] + [I] \mu_r) [C]^{-1} \underline{d}_r = [C]^T [X_r]^T [\omega'] (\underline{h} - \underline{h}'_r) \quad (6)$$

$$\underline{b}_{r+1} = \rho_r \underline{d}_r + \underline{b}_r \quad (7)$$

where:

$[C]$ is a diagonal scaling matrix with element c_{ii} equal to $([X_r]^T [\omega'] [X_r])_{ii}^{-1/2}$

$[X_r]$ is the sensitivity matrix at parameter estimates $\underline{b}_r$

r is the parameter estimation iteration number

$[\omega']$ is the estimated weight matrix

$\underline{d}_r$ is a vector used to update the parameter estimates

μ_r is the Marquardt parameter (Hill, 1992)

ρ_r is a damping parameter

$\underline{h}$ is the vector of all head observations

$\underline{h}'_r$ is the vector of model-predicted heads using parameters $\underline{b}_r$

Section 3.2.3 discusses the sensitivity matrix $[X]$, or $[X_r]$ as shown in equation (6), and Sections 3.2.4 and 3.2.5 discuss the weight matrix $[\omega']$.

Two convergence criteria are applied when using the Gauss-Newton iterative solution method. The first convergence criterion applies when the largest absolute value of d_r/b_r is less than a user-specified value. This condition occurs as the parameter estimates (b_r) approach the values which minimize the sum-of-squares objective function and d_r approaches zero. The second convergence criterion applies when the sum of squared weighted residuals does not change by more than a user-specified percentage for three consecutive iterations. The parameter estimation iterative process stops when either of the two criteria is satisfied.

3.2.3 Sensitivities in Nonlinear Regression

Sensitivities are required to calculate $\underline{b}$ in equation (5). They are defined by:

$$[X] = \frac{\partial h'}{\partial \underline{b}} \quad (8)$$

where:

$[X]$ is the matrix of sensitivities. Each term of $[X]$ represents the sensitivity of head at a measurement location to one of the model parameters.

Sensitivities in nonlinear groundwater flow models are dependent upon parameter values. For example, $\partial h' / \partial b$ would be constant for parameter values between 1 and 3 as represented in Figure 2. As the parameter value increases beyond 3, $\partial h' / \partial b$ changes.

Figure 2 - Head with respect to parameter value
(Sensitivity is the slope of the curve).

In order for MODFLOWP to calculate sensitivities, a linear problem is assumed to exist at the point of concern. Assuming a linear problem, equation (8) can be rewritten as:

$$[X]^T [X] \underline{b} = [X]^T \underline{h} \quad (9)$$

3.2.4 Weighting of Observations

Weighting of observations is required to produce a valid regression model for three potential conditions (Hill, 1992). The first condition occurs when the observations are not equally reliable. For example, some measurements may be made to a greater level

of accuracy than others. The more accurate measurements should therefore be required to have smaller residuals in the regression model, requiring a larger weight. The second condition occurs if the observations have correlated errors. If hydraulic head measurements all had similar errors, weighting would be used to indicate that these measurements were correlated.

The third condition occurs if the observations have different units. For example, the accuracy of a hydraulic head observation (L) would be different than that of stream-flow gains or losses (L³/T). A unit change between the two parameters may need to be weighted differently.

Weighting of observations in the least-squares regression problem is handled by using a symmetric weight matrix in equation (9). The resulting equation is given as equation (10).

$$[X]^T [\omega'] [X] \underline{b} = [X]^T [\omega'] \underline{h} \quad (10)$$

3.2.5 Weighting of Parameters or Prior Information on Parameter Estimates

Prior information on parameter estimates, or parameter weights (constraints), can also be incorporated into the MODFLOWP model. Prior information is defined as data on model parameters that is independent of the hydraulic head observations. Prior parameter estimates are incorporated into the solution by adding a term to the sum-of-squares objective function.

$$S(\underline{b}) = \sum_{q=1}^{ND} [h_q - h'_q]^2 + \sum_{p=1}^{NPR} [P_p - P'_p]^2 \quad (11)$$

where:

P_p is the independent parameter estimate

P'_p is the calculated parameter estimate

NPR is the number of parameters with prior estimates

Although equation (11) shows the simpler unweighted form of the least squares objective function, MODFLOWP allows the estimated weight matrix, $[\omega']$, to be augmented to include parameter weights based upon prior information.

3.3 Output

MODFLOWP calculates statistical and non-statistical output including: parameter estimates with the standard deviation and coefficient of variation of the estimate, calculated heads (which can be compared to measured heads), parameter sensitivities with respect to heads at specified data points (measured head locations), eigenvalues and eigenvectors, and correlations between parameters. Example output from the baseline run described in Section 4.3.1 is shown in the following sections. Output tables are formatted as in the MODFLOWP output file so that this part of the thesis can be used to interpret additional output files.

3.3.1 Parameter Estimates and Statistics

The partial output shown in Table 1 lists the final parameter estimates, and standard deviation and coefficient of variation of the estimates calculated by MODFLOWP. The first two rows indicate the parameters of concern. Values in the following sections of the table indicating parameter statistics correspond to the positions of the parameters as listed in the first two rows.

Table 1 - Final Parameter Estimates and Related Data

PARAMETER ID :

Q_{B1} W_2	Q_{B2} T_3	Q_1 W_3	Q_2 R_2	h_{B1}
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FINAL PARAMETER ESTIMATE :

0.845E+02	0.944E+03	-0.969E+05	-0.510E+05	0.102E+02
-0.128E-03	0.129E+02	0.131E-03	0.805E-01	

STANDARD DEVIATION:

0.250E+02	0.480E+03	0.179E+04	0.942E+03	0.775E+00
0.737E-04	0.364E+01	0.363E-04	0.793E-02	

COEFFICIENT OF VARIATION:

0.295E+00	0.508E+00	0.184E-01	0.185E-01	0.763E-01
0.574E+00	0.282E+00	0.276E+00	0.986E-01	

Variance of the final parameter estimate is calculated using equation (12).

$$[V(b')] = S^2 ([X]^T [\omega'] [X])^{-1} \quad (12)$$

where:

$[V(b')]$ is the variance-covariance matrix containing the variances of the final parameter estimates

S^2 is the estimated error variance, which is the minimized value of the objective function divided by [the number of observations plus the number of parameters with prior estimates, minus the number of parameters]

$[X]$ is the sensitivity matrix

$[\omega']$ is the estimated weight matrix

The standard deviation, S , is the square root of the variance of each estimate. For the i^{th} parameter estimate, $S_i = \sqrt{v_i}$. The standard deviation gives an indication of the magnitude of the estimated error for each final parameter estimate and should be compared to the final parameter estimate, not necessarily to the standard deviations for the other parameters. The coefficient of variation is used for this comparison. The coefficient of variation is calculated as $COV_i = S_i \div b'_i$, where b'_i is the final estimate of parameter i and S_i is its standard deviation. The coefficient of variation provides an indication of the reliability of the parameter estimate and normally provides indications equivalent to that of the eigenvalues and eigenvectors (Carrera and Neuman, 1986; refer to Section 3.3.4).

The parameters with the smallest coefficients of variation are considered to be the most

reliable. The coefficients of variation shown in the output in Table 1 indicate that the reliability of q_{B2} is much lower than that of Q_1 , because Q_1 has a coefficient of variation equal to 0.184E-01 and the coefficient of variation of q_{B2} is equal to 0.508E+00.

3.3.2 Model Predictions at Head Locations

Data at measured head locations are compared to heads calculated for each location by MODFLOWP, as shown in Table 2. The difference between the two values is the residual at each head location. A weighting factor, which is specified by the user, is applied to each residual to calculate a weighted residual.

The columns in Table 2 indicate, from left to right: the hydraulic head observation number; the hydraulic head measured at the observation point; the MODFLOWP model prediction of hydraulic head at the observation point; the residual; the user-specified weight of the observation; and the weighted residual.

The goal of the solution algorithm for MODFLOWP is to minimize the sum of the squares of the weighted residuals. Minimizing this sum generates the closest match of calculated heads to measured heads. The weight for each measured head can be used to indicate the level of confidence in the measured head data. For example, if observation 1 was not considered to be as reliable as the other data points, a lower weight would be applied to the residual. This would have the effect of lowering the sum of the squares of the weighted residuals, thereby not constraining the solution to match the head at this data point as closely. The partial output shown in Table 2 has the same weight for each observation, which would indicate equal confidence in each measured head.

Table 2 - Residual Data

OBS #	MEAS. HEAD	CALC. HEAD	RESIDUAL	WEIGHT** .5	WEIGHTED RESIDUAL
1	69.220	67.880	1.34	1.00	1.34
2	80.580	81.593	-1.01	1.00	-1.01
3	72.660	72.280	0.380	1.00	0.380
4	49.550	50.195	-0.645	1.00	-0.645
5	10.040	10.500	-0.460	1.00	-0.460

3.3.3 Sensitivities

The unscaled sensitivity of head to an estimated parameter is equal to $\partial h / \partial b$ where h is equal to head and b is equal to the parameter estimate. The larger the absolute value of the sensitivity, the more the head will vary per unit change in the parameter value. Parameter sensitivities should be scaled when comparing parameters with different units, because a unit change in one parameter may be much more significant than a unit change in another parameter. In MODFLOWP, scaled sensitivities are calculated by multiplying each unscaled sensitivity by the parameter value and the square root of the weight. They represent the percent change in head corresponding to a one percent change in the parameter. For example, a unit change in Q_1 (see Table 1) would be equivalent to a one one-thousand of a percent change ($1 \div 96,900$). This would likely have little impact to the head. A unit change in W_3 (see Table 1) would be much more significant, changing the

value of W_3 from 0.000131 to 1.000131 (over 763,000 percent). Scaled sensitivities will be reported in this thesis.

The sensitivity of each parameter with respect to the head at each observation point is calculated by MODFLOWP. The user has the option of printing scaled or unscaled sensitivities. Table 3 shows output of both types of sensitivities. The upper half shows unscaled sensitivities and the lower half shows scaled sensitivities.

Sensitivities of the head observations to the shown parameters (listed in the first two rows) are given in the last four columns of Table 3. The sensitivities for each head observation are spread over two rows due to space limitations. For example, the unscaled sensitivity of head at observation point 1 to q_{B1} is 0.132E-02 and the unscaled sensitivity of the same head to T_3 is -4.780E+00.

The scaled sensitivities in Table 3 show that heads at locations one through five are most sensitive to changes in T_3 and W_3 . Also, heads at locations one through five are not sensitive to q_{B2} .

There are two valuable pieces of information, related to the MODFLOWP model setup, that can be obtained from analyzing parameter sensitivities. First, MODFLOWP provides a composite scaled sensitivity value for each parameter, which is calculated by taking the square root of the sum of the square of all scaled sensitivity values for each head observation and dividing by the number of observations. These values indicate the overall sensitivity of all measured heads to a parameter in the model. These values have

Table 3 - Sensitivities and Scaled Sensitivities of Observation Point Heads with Respect to Parameters

Unscaled				
PARAMETER ID :	Q_{B1} W_2	Q_{B2} T_3	Q_1 W_3	Q_2 R_2
OBS#				
1	0.132E-02 0.666E+04	0.650E-06 -4.780E+00	0.200E-06 0.489E+06	0.401E-06 0.611E+00
2	0.340E-03 0.248E+04	0.211E-06 -5.860E+00	0.156E-06 0.587E+06	0.468E-06 0.630E+00
3	0.472E-03 0.308E+04	0.257E-06 -5.150E+00	0.177E-06 0.518E+06	0.518E-06 0.726E+00
4	0.801E-03 0.451E+04	0.421E-06 -3.440E+00	0.199E-06 0.353E+06	0.502E-06 0.744E+00
5	0.206E-02 0.983E+04	0.972E-06 -0.340E+00	0.207E-06 0.564E+05	0.274E-06 0.455E+00
Scaled				
1	0.112E+00 -0.855E+00	0.613E-03 -0.617E+02	-0.193E-01 0.641E+02	-0.204E-01 0.491E-01
2	0.287E-01 -0.318E+00	0.199E-03 -0.757E+02	-0.151E-01 0.771E+02	-0.239E-01 0.507E-01
3	0.399E-01 -0.396E+00	0.259E-03 -0.665E+02	-0.172E-01 0.680E+02	-0.264E-01 0.584E-01
4	0.677E-01 -0.578E+00	0.397E-03 -0.444E+02	-0.193E-01 0.463E+02	-0.256E-01 0.598E-01
5	0.174E+00 -1.260E+00	0.918E-03 -4.390E+00	-0.200E-01 7.400E+00	-0.140E-01 0.366E-01

been termed “composite scaled sensitivities” by Anderman *et al.* (1994). Parameters with comparatively low composite scaled sensitivity values would not need to be included in

the parameter estimation process, since a relatively large change in the parameter would make very little difference to the resulting hydraulic head at observation points.

Therefore, these composite scaled sensitivity values assist the user in determining which parameters need to be kept in the modeling process. Secondly, parameter sensitivities at all model grid points can be calculated and plotted (Wanta and Ronan, 1996). This allows the user to identify zones, if any exist, in which parameter sensitivities are, on the average, higher or lower than the composite scaled parameter sensitivity value. This information can be used to separate parameters into multiple zones for better model accuracy.

3.3.4 Eigenvalues and Eigenvectors

Eigenvalues and eigenvectors of the variance-covariance matrix are calculated for each parameter. Eigenvalues and eigenvectors are used to determine the reliability of parameter estimates for a given run (Carrera and Neuman, 1986). Parameter reliability can be thought of as the accuracy of the final parameter estimate calculated by MODFLOWP. The eigenvalues and eigenvectors are scaled so that the results are not affected by the final parameter values (Hill, 1992). Using eigenvalues and eigenvectors produces similar results as using the coefficient of variation values calculated by MODFLOWP to check parameter reliability (Hill, 1992).

The least reliable parameter estimates are identified by the largest elements (sign of the eigenvector does not affect the interpretation) of the eigenvectors associated with the largest eigenvalues. The most reliable parameter estimates are identified by the largest elements of the eigenvectors associated with the smallest eigenvalues (Hill, 1992). The

number of eigenvalues (scalars) corresponds to the number of parameters (NP) as do the number of eigenvectors, each of which has NP elements.

Table 4 shows the lowest and highest eigenvalues, and associated eigenvectors from a MODFLOWP output file. Parameter identifiers are listed on the left hand side of the table. For the smallest eigenvalue, 0.2993D-04, the largest eigenvector element (with a value of -0.6967D-00), corresponds to parameter T_3 , which is therefore deemed the most reliably estimated parameter. The least reliable parameters are q_{B1} and q_{B2} (the largest eigenvalue of 0.6286D+00 is associated with the largest eigenvectors -0.3123D+00 and -0.4765D+00 for these parameters, respectively).

Table 4 - Eigenvalues and Eigenvectors

EIGENVALUES¹

0.2993D-04 0.6286D+00

EIGENVECTORS

α_{B1} 0.2156D-02 -0.3123D+00

α_{B2} -0.2593D-04 -0.4765D+00

Q_1 0.4347D-02 -0.5070D+03

Q_2 0.1360D-02 0.2212D-03

h_{B1} -0.2149D-03 -0.1466D-01

T_3 -0.6967D-00 -0.2036D+00

W_1 0.2708D-02 -0.1931D+00

R_2 0.5731D-03 -0.1315D-02

¹ Eigenvalues correspond to eigenvectors with NP entries, where NP is the numbers of parameters

3.3.5 Correlation

The partial output shown in Table 5 lists the correlation between some pairs of parameters. The correlations are printed in two rows due to space limitations. The parameter identifiers listed in the top two rows of the table correspond to the two rows listed for each parameter in the left hand column.

Table 5 - Parameter Pair Correlations

	Q_1 T_3	Q_2 W_3	h_{B1} R_2
q_{B1}	-1.00000 1.00000	-1.00000 1.00000	-0.05813 1.00000
q_{B2}	-1.00000 1.00000	-1.00000 1.00000	-0.05813 1.00000
Q_1	1.00000 -1.00000	1.00000 -1.00000	0.05813 -1.00000
Q_2	1.00000 -1.00000	1.00000 -1.00000	0.05813 -1.00000
h_{B1}	0.05813 -0.05813	0.05813 -0.05813	1.00000 -0.05813

Correlation between parameters indicates the interdependency of the various parameters being estimated. Correlation ranges from -1.0 to 1.0. A value of 1.0 indicates that the parameters are directly correlated. For example, Q_1 and Q_2 are directly correlated, when Q_1 increases so does Q_2 . A value of -1.0 indicates that the parameters are inversely correlated. For example, when T_3 increases Q_1 decreases. Values between 1.0 and -1.0 indicate that the parameters are less correlated, with a value of 0 being uncorrelated. A parameter will always have a correlation of 1.0 with itself.

4.0 Test Case

This test case is based on an example model presented in the MODFLOWP documentation (Hill, 1992; pp. 193-221) and in an earlier paper by Cooley (1985). The model was used to test the functionality of MODFLOWP with a site in which all information was “known”.

4.1 Physical System Description

This test case models a system which consists of one confined aquifer which is separated into three transmissivity zones (T_1 , T_2 and T_3) as shown in Figure 3. The system is bounded by no-flow, specified-flux, and specified-head boundaries. A leaky riverbed and two pumping wells are located in Zone 2. There are three areal recharge zones (W_1 , W_2 and W_3) which correspond to the transmissivity zones.

Boundary conditions consist of specified-flow boundaries (q_{B1} and q_{B2}) on the north boundary of the model and no-flow boundaries on the west, south and southeastern boundaries of the model. A specified hydraulic head boundary (described in terms of h_{B1} , h_{B2} , and h_{B3}) is on the east side of the model. Two pumping wells (Q_1 and Q_2) are located in Zone 2.

Figure 3. - Physical System for Test Case One. (Source: Hill, 1992)

4.2 Model Setup

The domain is an irregular L-shape. The majority of the domain is discretized into square 1,000-foot by 1,000-foot cells. Cells are 200 feet wide across the river and 50 feet wide adjacent to the specified-flow and specified-head boundaries. The specified hydraulic head boundary on the east side of the model is linearly interpolated between heads at three locations (h_{B1} , h_{B2} , and h_{B3}). Specified-flow boundaries are modeled using surface recharge over cells which are 1000 feet wide and 50 feet long (top to bottom). Two wells, Q_1 and Q_2 , which model the effects of pumping from the aquifer, are located in the center of cell (row 7, column 11) and in the center of cell (row 9, column 12), respectively. Heads for each grid cell are shown in Figure 4. These heads were generated by MODFLOWP for Run 1 as discussed in Section 4.3.1, but approximate the “known” heads. Shaded cells indicate the location of the river which had a stage elevation equal to 4.5.

The system is modeled in steady state. Fourteen parameters are estimated in this test case. The parameters are listed in Table 6.

All of the parameter values are known, since this is a synthetic test case. To replicate real world conditions, the hydraulic head was “sampled” at 32 locations, which are shown as hollow circles on Figure 3. These 32 hydraulic head “observations” were perturbed by adding a small error to each value. The errors were normally distributed with a mean of zero and a standard deviation of one foot.

	Column															
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	87.61	84.77	78.78	68.96	54.08	31.86	7.88	4.74	4.37	3.44	1.33	0.75	1.99	4.74	8.40	10.20
2	81.01	78.18	72.21	62.42	47.61	25.71	7.29	4.61	4.48	2.88	0.72	0.14	1.38	4.14	7.84	9.91
3	66.78	64.27	59.01	50.49	37.86	20.03	6.50	4.57	4.39	1.63	-1.76	-2.61	-1.02	2.34	6.78	9.35
4	50.57	48.62	44.59	38.16	28.81	15.84	5.93	4.53	4.29	-0.59	-6.49	-7.54	-4.95	-0.26	5.51	8.80
5	31.79	30.57	28.08	24.24	18.90	11.65	5.56	4.50	4.11	-4.77	-15.84	-15.82	-10.71	-3.70	4.02	8.25
6	19.27	18.47	16.90	14.64	11.80	8.67	5.79	4.46	3.78	-12.41	-36.00	-28.95	-18.12	-7.57	2.46	7.69
7	17.33	16.60	15.19	13.16	10.66	7.96	5.60	4.40	3.33	-23.18	-86.56	-45.58	-24.98	-10.65	1.21	7.14
8	16.38	15.69	14.34	12.41	10.00	7.18	5.32	4.43	3.59	-14.49	-42.63	-41.59	-25.29	-11.01	0.78	6.58
9						5.69	4.93	4.45	3.98	-7.70	-27.64	-52.58	-23.34	-8.60	1.35	6.03
10						5.23	4.82	4.49	4.30	-0.19	-7.37	-12.99	-6.64	-1.11	3.20	5.47
11						5.35	5.01	4.52	4.49	4.30	4.00	3.76	4.03	4.26	4.45	5.14
12						5.42	5.10	4.55	4.52	4.49	4.45	4.42	4.46	4.49	4.52	5.14
13						5.68	5.48	5.12	5.04	4.89	4.86	4.87	4.91	4.97	5.07	5.22
14						6.59	6.76	9.15	12.22	18.81	22.28	23.66	24.31	24.61	24.65	24.41
15						26.19	29.06	35.78	37.81	43.29	48.19	50.84	52.29	52.99	53.11	52.86
16						51.36	54.02	57.35	58.48	61.87	66.17	69.08	70.87	71.80	72.01	71.76
17						63.71	65.91	68.28	69.10	71.62	75.40	78.26	80.16	81.19	81.44	81.19

= the river limits

Figure 4 - Test case hydraulic heads.

Table 6 - Test Case Parameters

Zone	Parameter	Parameter Description	"Known" Parameter Value
1	q_{B1}	Specified flux at the north boundary of Zone 1	50 ft/d
	T_1	Transmissivity of Zone 1	50 ft ² /d
	W_1	Recharge of Zone 1, except where q_{B1} occurs	3×10^{-4} ft/d
2	q_{B2}	Specified flux at the north boundary of Zone 2	500 ft/d
	h_{B1}	Specified hydraulic head boundary at the upper right boundary of Zone 2	10.0 ft
	h_{B2}	Specified hydraulic head boundary at the river in Zone 2	5.0 ft
	h_{B3}	Specified hydraulic head boundary at the rightmost boundary between Zones 2 and 3	5.5 ft
	T_2	Transmissivity of Zone 2	500 ft ² /d
	W_2	Recharge of Zone 2, except at where q_{B2} occurs	-1×10^{-4} ft/d
	R_2	Conductance of the riverbed in Zone 2; (hydraulic conductance for the riverbed is equal to the product of vertical hydraulic conductivity and the area of the riverbed divided by the thickness of the riverbed)	0.1 ft ² /d
	Q_1	Pumping well number one in Zone 2	-100,000 ft ³ /d
	Q_2	Pumping well number two in Zone 2	-50,000 ft ³ /d
3	T_3	Transmissivity of Zone 3	20 ft ² /d
	W_3	Recharge of Zone 3	2×10^{-4} ft/d

4.3 MODFLOWP Test Runs and Results

The following scenarios were run for this test case:

- the standard run with parameter estimation (the base run MODFLOWP simulation as presented in Hill (1992), Test Case 2)
- multiple runs with varying numbers of parameters
- multiple runs with varying initial estimates of the parameters
- a run with no weights on the initial estimates of the parameters

- multiple runs with varying weights on the initial estimates of the parameters
- combinations of the above.

The purpose of performing these runs was to examine the parameter estimation capabilities of MODFLOWP using the input variations listed above on the same physical groundwater system.

4.3.1 Standard (Baseline) Run (Run 1)

The unmodified run of the model with parameter estimation as described in the MODFLOWP documentation (Hill, 1992) is considered the standard or baseline run. Results from other runs described below will be compared to the output of this run.

Model characteristics are described in Section 4.2. Input data for the parameters and final parameter estimates generated by the MODFLOWP run are shown in Table 7. The weight (constraint) applied to each of the initial estimates is given as both a standard deviation and as a percentage of the initial estimate (similar to a coefficient of variation). A large coefficient of variation would allow a final parameter estimate to vary more than a parameter with a lower coefficient of variation.

Shaded cells in the table indicate parameters that were not weighted. The percent change from the known value and initial estimate are calculated as shown below.

Percent Change from Known Value (col. 7) = $[(\text{Final Estimate}) - (\text{Known Value})] \div [\text{Known Value}] \times 100$

Percent Change from Initial Estimate (col. 8) = $[(\text{Final Estimate}) - (\text{Initial Estimate})] \div [\text{Initial Estimate}] \times 100$

Table 7 - Standard Run Input Data and Results for Run 1

Parameter Description	Known Value	Initial Estimate	Standard Deviation	Standard Deviation ÷ Initial Est.	Final Estimate generated by MODFLOWP	Percent Change from Known Value// Initial Estimate	
q_{B1}	50	45	NS	NS	84.5	69%	88%
q_{B2}	500	420	NS	NS	944	89%	125%
Q_1	-100,000	-97,000	1940	2%	-96,900	-3%	0%
Q_2	-50,000	-51,000	1020	2%	-51,000	2%	0%
h_{B1}	10.0	10.4	1.04	10%	10.2	2%	-2%
h_{B2}	5.0	4.8	0.48	10%	5.14	3%	7%
h_{B3}	5.5	5.1	0.51	10%	5.22	-5%	2%
T_1	50	70	NS	NS	66.5	33%	-5%
W_1	0.0003	0.0004	0.00012	30%	0.000299	0%	-28%
T_2	500	420	84	20%	488	-3%	16%
W_2	-0.0001	-0.0002	NS	NS	-0.000128	28%	-36%
T_3	20	15	NS	NS	12.9	-65%	-14%
W_3	0.0002	0.00017	0.000051	30%	0.000131	-34%	-23%
R_2	0.1	0.08	0.008	10%	0.0805	-19%	1%

NS = not specified, therefore no weights to the parameter estimate are applied

In general, the results show that MODFLOWP may change parameter values from the initial estimates by large amounts where no weights are specified, and will hold parameter values within specified constraints (a constraint is defined as [standard deviation] ÷ [initial parameter estimate] in this thesis). For example, in the baseline case, q_{B1} , q_{B2} , T_1 , W_2 , and T_3 are not constrained parameters. The differences between the initial estimate and the final values selected by MODFLOWP for these parameters range from 5% to 125% (absolute values), and average approximately 54% (absolute values).

The differences between the initial estimate and the final values selected by MODFLOWP for parameters with weights range from 0% to 28% (absolute values), and average approximately 9% (absolute values) — constraints range from 2% to 30% and average approximately 14%. It is not surprising that the final estimated parameter values do not match the known values since the weights on the parameters varied and errors representing field measurement error were introduced into the “measured” heads. Therefore, a different solution is expected.

Zone 1 had a large increase in specified boundary flow (q_{B1}) and transmissivity (T_1). Other factors remained relatively constant. These increases counteract each other and seem reasonable. Zone 2 had a large increase in specified boundary flow (q_{B2}) and in negative recharge (W_2). Other factors remained relatively constant. These increases also counteract each other and seem reasonable. Zone 3 had a large decrease in transmissivity (T_3) and recharge (W_3). These decreases also counteract each other and seem reasonable. As discussed below, these parameter pairs have a high correlation with each other (see the discussion on correlation below).

4.3.1.1 Additional Output for Run 1

Residuals - Run 1

For the baseline run, the maximum and minimum residuals are 2.5 feet (observation 20) and -1.28 feet (observation 19), respectively. The average residual is 0.145 feet. The sum of square weighted residuals is 24.146. (All residuals reported for all runs in this thesis have a weight equal to 1.0.)

The magnitude of the maximum and minimum residuals appears to be significant, considering that the sum of square weighted residuals for these two observations alone accounts for over 32 percent of the sum of square weighted residuals. Although, considering that the sum of square weighted residuals for all observations is less than 25, the number of observations is 32, and that all measured observations have up to a one-foot introduced error, the overall sum of square weighted residuals is not significant.

Composite Scaled Sensitivities - Run 1

Composite scaled sensitivities range from 0.0383 (for R_2) to 4.07 (for W_3) and average approximately 1.47 as shown in Figure 5. The parameters with the largest composite scaled sensitivities are transmissivity for Zones 1, 2 and 3, and recharge for Zone 3 with the composite scaled sensitivity for each parameter being approximately 2.44, 2.78, 3.96, and 4.07 respectively. These were the only parameters whose composite scaled sensitivities were consistently higher than those of other parameters for all runs in this thesis.

The large magnitude of the composite scaled sensitivity for transmissivity and W_3 indicates that changes in the transmissivity parameters combined with W_3 have, by far, the greatest impact on head across the model domain. It is also evident that the riverbed conductance parameter (R_2) has the least impact on heads in the domain and could be excluded as a parameter without a significant impact to the final model results.

Figure 5 - Run 1 composite scaled sensitivities.

Eigenvalues and Eigenvectors - Run 1

The eigenvalue and eigenvector output indicates that transmissivity for Zone 3 (T_3) and recharge for Zone 3 (W_3) are the parameters estimated most reliably. The smallest eigenvalue was 0.2993E-4. The eigenvectors of T_3 and W_3 that correspond to the smallest eigenvalue were -0.6967 and 0.7170, respectively. These two parameters also had the highest composite scaled sensitivities. This is important, since the user would want the parameters which have the greatest effect on hydraulic heads per unit of change, to be the most reliably estimated parameters. These two parameters also had significant variations from the known values and lesser variations from the initial estimates. This may cause one to be concerned about the eigenvalue and eigenvector data which indicates that these parameters are estimated most reliably. However, the head residuals are relatively small, other results discussed in this section indicate a good model run with the exception of highly correlated parameter pairs (see correlation discussion below), and it appears that

the final parameter estimates are reasonable. Possible reasons for these variations are related to the perturbed head data which causes Run 1 to be different from the known model run, correlation between parameter pairs, and the constraints on the parameters. Parameter T_3 has no constraint and W_3 has a loose constraint. This allows the model to satisfy convergence criteria without constraining the parameter close to its initial estimate. Since these two parameters are perfectly correlated and W_3 is constrained to an initial estimate which is lower than its known value, variations from the known values and initial estimates are not unexpected.

The eigenvalue and eigenvector output further indicates that specified flux at the north boundary of Zone 2 (q_{B2}) and recharge for Zone 2 (W_2) were the parameters estimated least reliably. The largest eigenvalue was 0.6286. The eigenvectors of q_{B2} and W_2 that correspond to the largest eigenvalue were -0.4765 and -0.6926, respectively. These two parameters also had low composite scaled sensitivities compared to the other parameters.

Correlation - Run 1

MODFLOWP provides output for parameter pairs with correlation values of 0.85 and greater, and -0.85 and lower. Three parameter pairs fit within this range for the fourteen-parameter baseline run: q_{b1} and T_1 have a correlation of 0.96, T_3 and W_3 have a correlation of 1.00, and $[T_1 \text{ and } W_2]$ and $[W_1 \text{ and } W_2]$ have a correlation of -0.92. (Negative correlation between W_2 and other parameters is due to the negative recharge value of W_2 .) This shows that recharge and transmissivity parameters are the most

correlated parameter pairs for this run. Highly correlated parameters are difficult to independently estimate and lead to non-unique model solutions (Yeh, 1986).

Water Mass Balance - Run 1

The volumetric flux into and out of the model is compared in Figures 6 and 7. Figure 6 shows the distribution of water into the model and Figure 7 shows distribution out of the model. The region labeled “wells” in Figure 6 represents the flux in along the specified flux boundaries (which are modeled using the well package in MODFLOWP).

The total volumetric flux of water into and out of the site is equal at 164,380 ft³/day. As shown in Figures 6 and 7, the majority of water entering the model is from riverbed leakage (110,080 ft³/day or 67 percent), and 90 percent (147,900 ft³/day) of the water exits the model through the two pumping wells.

4.3.2 Varied Number of Parameters (Runs 2 to 8)

Several runs were performed with varying numbers and types of parameters estimated in each run to determine the impact these changes had on the final parameter estimates. The number of parameters used ranged from 9 to 14. Final parameter estimates generated by MODFLOWP are shown in Table 8.

The parameters excluded from the various runs do not have final results listed and the corresponding cells are darkly shaded in the following tables. These parameter values were held at the known values for the runs from which they were excluded.

Figure 6 - Run 1 water balance in.

Figure 7 - Run 1 water balance out.

Table 8 - Comparison of Number of Parameters vs. Parameter Final Values - Runs 1 to 8

Parameter Description	Known Value	Initial Estimate	Std. Dev. ÷ Init. Estimate	Parameter Final Values							
				Run Number							
				1	2	3	4	5	6	7	8
q_{a1}	50	45	NS	84.5	84.5	95.3	84.6	279	72.8	104	95.4
q_{a2}	500	420	NS	944	944	1090	946	2720		1190	1320
Q_1	-100,000	-97,000	2%	-96,900	-96,900	-96,900		-97,700		-98,100	-85,800
Q_2	-50,000	-51,000	2%	-51,000	-51,000	-51,100		-51,200		-51,400	-47,900
h_{m1}	10.0	10.4	10%	10.2	10.2	10.3	10.2	11.3	10.3	10.3	10.9
h_{m2}	5.0	4.8	10%	5.14	5.14	5.15	5.14	5.28	5.13	5.14	5.33
h_{m3}	5.5	5.1	10%	5.22	5.22	5.21	5.22	4.59	5.23	4.43	4.39
T_1	50	70	NS	66.5	66.5	74.2	66.6	187	58.1	80.5	73.5
W_1	0.0003	0.0004	30%	2.99E-4	2.99E-4	3.24E-4	3.00E-4	5.17E-4	2.70E-4	3.48E-4	3.12E-4
T_2	500	420	20%	488	488	490	488	521	486	500	
W_2	-0.0001	-0.0002	NS	-1.28E-4	-1.28E-4	-1.68E-4	-1.28E-4	-6.2E-4	-0.84E-4		
T_3	20	15	NS	12.9	12.9	16.8	12.9		11.8		
W_3	0.0002	0.00017	30%	1.31E-4	1.31E-4		1.30E-4		1.20E-4		
R_3	0.1	0.08	10%	0.0805			0.0805		0.0804		

NS = not specified, therefore no weights to the parameter estimate are applied

The remainder of this section describes Runs 2 through 8. The descriptions are followed by a summary of results in terms of each of the following categories: residuals, sensitivities, eigenvalues and eigenvectors, and correlations.

The results indicate that varying the number and type of parameters estimated can make a large difference in the final estimated parameter values. As before, the largest deviations from the original known values or initial estimates occur for the parameters which have been constrained the least. Run 1 in Table 8 is the baseline case.

Run 2

One parameter is removed (from the list of parameters to be estimated) from the baseline case for Run 2. The removed parameter is hydraulic conductance of the riverbed in Zone 2 (R_2). The results from this run are identical to the baseline run. This indicates that the riverbed conductance has little impact on the model or that the specified conductance is nearly the same value as that estimated by MODFLOWP when used as a parameter. The standard deviation on riverbed conductance is low compared to other parameters. The final parameter estimate for riverbed conductance only changes one percent from the initial estimate for Run 1. For Run 2, R_2 was set at 0.1, which is 19 percent greater than the final value estimated by MODFLOWP in Run 1. It appears that riverbed conductance does not significantly impact other parameters, since a 19 percent increase in an important parameter would have some impact on the parameter estimates. Therefore, it will not be further addressed. This result is also consistent with the riverbed conductance parameter having the lowest composite scaled sensitivity as discussed earlier.

Run 3

Both recharge in Zone 3 (W_3) and hydraulic conductance of the riverbed in Zone 2 (R_2) were removed to create Run 3. The largest impacts occurred to parameters q_{B1} , q_{B2} , T_1 , W_2 , and T_3 . Recharge for Zone 3 had one of the looser constraints of the listed parameters and, for Run 1, changed -23 percent from the initial estimate. When this parameter was removed from the MODFLOWP run, the value for recharge in Zone 3 was set at 0.0002 — an increase of 34 percent from the final estimate generated by MODFLOWP for the baseline run. In order to keep calculated heads close to the measured heads, it would be expected that transmissivity for Zone 3 would also increase by a large amount to account for the increased recharge. Transmissivity for Zone 3 did increase by over 30 percent. To account for the added flow to the system, negative recharge in Zone 2 must increase (towards the negative) or the pumping wells must pump more. Considering that the constraints on the pumping wells are very tight (small standard deviation) and no constraint is placed on recharge for Zone 2, it would be expected that recharge for Zone 2 would change dramatically. As shown in Table 8, this is the case, although it is surprising to see that the pumping well rates were not at all affected. This may be due to the fact that the wells produce steep localized variations in the heads and that increasing the pumping rates, given the tight constraints, did not provide a better solution. The increase in transmissivity in Zone 3 also affects recharge at the specified flow boundary. In order to keep heads relatively similar for a higher transmissivity, the specified flow condition must also increase accordingly as well as there being slight

increases in transmissivity and specified flow for Zones 1 and 2. The results are consistent with expectations as indicated in Table 8.

Run 4

Flow rates at the two pumping wells, Q_1 and Q_2 , were removed to create Run 4. These two parameters were selected since they did not change much in any of the previous varied number of parameter runs (likely because of the small standard deviations, or tight constraints, specified). Therefore, removing these two parameters should have little affect on the estimated values of other parameters from their values in Run 1. As can be seen in Table 8, this assumption is correct. The values of the 12 parameters left in the model had little to no change from the baseline run estimates.

Run 5

Transmissivity for Zone 3 (T_3), recharge for Zone 3 (W_3) and hydraulic conductance of the riverbed in Zone 2 (R_2) were removed to create Run 5. At this point, all parameters from Zone 3 have been removed from the parameter estimation analysis of MODFLOWP. The results from this run indicate that most parameters, except flow from the pumping wells which is highly constrained, changed significantly from the baseline run. The largest impacts occurred to parameters q_{B1} , q_{B2} , T_1 , W_1 , and W_2 . For this run, transmissivity for Zone 3 was set at 20 — an increase of 65 percent from the final value estimated by MODFLOWP in the baseline run. Other removed parameters were set as previously discussed. Considering the large increase in Zone 3 transmissivity and

recharge, it is likely that the parameter estimates for the adjacent zones would significantly increase as shown in Table 8. The parameters which are not constrained varied greatly, from approximately one to five times the value of the estimates calculated in the baseline run. Recharge in Zone 2 had the largest increase, over 480 percent toward the negative from the baseline run, which is directly related to the increases in recharge and transmissivity in Zone 3. A slight increase in flow rates from the pumping wells was also estimated by MODFLOWP. The change in these two parameters allows the excess flow to be removed from Zone 2. The increase in negative recharge and pumping rates from Zone 2 would likely increase specified flux in Zone 2, and transmissivity and recharge in Zone 1. These results were realized as shown in Table 8. (The mass balance is further discussed below.)

Run 6

Flow rates at the two pumping wells (Q_1 and Q_2) and specified flux at the north boundary of Zone 2 (q_{B2}) were removed to create Run 6. Values used for the removed parameters are those indicated as known values in Table 8. For parameters Q_1 and Q_2 , there should be little impact as discussed in Run 4. However, the known value of q_{B2} used for this run is nearly half of the value estimated by MODFLOWP in the baseline run. Therefore, one would expect there to be a noticeable impact from removing this parameter, even though its composite scaled sensitivity is very low compared to that of other parameters.

Results for this run show that specified flux at the north boundary of Zone 1 (q_{B1}) decreased by approximately 14 percent, and transmissivity in Zone 1 (T_1) decreased by approximately 13 percent. Recharge of Zone 2 (W_2) also decreased by approximately 34 percent. Other parameter estimates did not change significantly. Considering that the specified flux at the north boundary of Zone 2 (q_{B2}) was cut in half and the pumping well rates remained the same, one would expect transmissivity of Zone 2 to decrease or recharge over Zone 2 (W_2) to increase based on the parameter correlations discussed earlier. This is not the case as can be seen in Table 8. The results are not as predictable as earlier runs. Parameter T_2 does not change and W_2 decreases. Since W_2 is unconstrained (see Table 8) and head is not very sensitive to changes in W_2 for Run 6 (see Section 4.3.2.1), this result is not unexpected. The correlation between parameters, discussed earlier, may give the best prediction of the results in Table 8. The correlations between q_{B1} and T_1 are high, and the correlations between T_1 and W_2 are also high. These parameters had the highest percent changes relative to the other parameters estimates as shown in Table 8.

Run 7

Recharge for Zones 2 and 3 (W_2 and W_3), transmissivity for Zone 3 (T_3), and hydraulic conductance of the riverbed in Zone 2 (R_2) were removed for Run 7. Zone 3 parameters have been set with a significant increase, and a slight decrease has been set in recharge for Zone 2 compared to the final parameter estimates from the baseline run. In general, the results from this run indicate that most parameters changed significantly from

the baseline run. At this point, three of the five unconstrained parameters remain in the model — specified flux in Zones 1 and 2 (q_{B1} , q_{B2}) and transmissivity in Zone 1 (T_1) — and four of the fourteen parameters are set equal to the known values. This would give an indication that the parameter estimates generated by MODFLOWP may start to approach the known values — assuming the parameter constraints did not restrict a parameter otherwise. As shown in Table 8, the estimated value for transmissivity in Zone 2 (T_2) is equal to the known value. Parameters q_{B1} and q_{B2} are both two times greater than their known values and T_1 is 60 percent greater than its known value. As discussed in Section 4.3.2.1, the results of this run indicate that the final parameter estimates do not provide an accurate representation of the physical groundwater system characteristics. Even though the run converged, head residuals were very high in Zone 3.

Run 8

Recharge for Zones 2 and 3 (W_2 and W_3), transmissivity for Zones 2 and 3 (T_2 and T_3), and hydraulic conductance of the riverbed in Zone 2 (R_2) were removed for Run 8. Zone 3 parameters have been set with a significant increase, and a decrease has been set for Zone 2 parameters compared to the results from the baseline run. In general, the results from this run indicate that most parameters changed significantly from Run 1. A third of the parameters in this model run were unconstrained — specified flux in Zones 1 and 2 (q_{B1} and q_{B2}) and transmissivity in Zone 1 (T_1), and five of the fourteen parameters were set equal to the known values. As shown in previous runs, the parameters which are

not constrained tend to deviate farther from the expected values, than those parameters which are constrained.

4.3.2.1 Additional Output for Runs 2 to 8

The number of significant figures in the tables used throughout the remainder of the thesis is high to permit comparison of small changes in similar runs.

Residuals - Runs 2 to 8

The average residual, maximum and minimum residual, and sum of the squared residual results for all of the runs in which the number of parameters was varied were compared to each other. Residual data from Runs 2 through 8 are shown in Table 9.

The residual data for Runs 2 through 4 and Run 6 were similar. This indicates that the final parameter values, when used in the flow equations, produced similar hydraulic head values at all of the 32 measured head locations. This does not guarantee exact agreement in heads at locations where measurements were not available. However, the observation points span the entire model, indicating that there most likely was a close match of head values.

The residual data from Runs 5, 7 and 8 indicate that the final solution of the flow equations did not match heads nearly as closely as did the other runs. Even though approximately 25 percent of the sum of the squared residuals is related to the minimum residual, the average residual is much greater than for the other runs. One interesting

Table 9 - Residuals for Runs 2 to 8

Run Number	Average Residual	Min. Residual (Observation Number)	Max Residual (Observation Number)	Sum of Squared Residuals
Run 1	0.145	-1.28 (19)	2.50 (20)	24.146
Run 2	0.145	-1.28 (19)	2.50 (20)	24.151
Run 3	0.130	-1.54 (5)	2.51 (20)	26.114
Run 4	0.145	-1.28 (19)	2.50 (20)	24.161
Run 5	-0.363	-8.72 (2)	3.05 (23)	205.38
Run 6	0.152	-1.18 (5)	2.49 (20)	24.607
Run 7	-0.830	-9.65 (2)	2.60 (20)	249.47
Run 8	-0.617	-9.89 (2)	3.04 (11)	291.15

difference between these three runs and the others is that the average residual for these is negative whereas the average residual for all other runs is positive. Nearly the entire additional increase in the sum of squared residuals comes from the observation points in Zone 3. These residuals indicate that final head elevations are much higher in Zone 3 for these runs than for the other runs. This is represented in Figure 8, which shows estimated heads for Run 7. It is likely that this occurs because Runs 5, 7 and 8 are the only runs to have all parameters from Zone 3 removed from the parameter estimation. The remaining parameters are apparently too “remote” to have sufficient effect on heads in Zone 3, especially at Observation Point 2.

	Column															
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	87.59	84.78	78.85	69.14	54.46	32.54	8.44	4.79	4.89	3.56	1.41	0.82	2.07	4.86	8.59	10.30
2	80.88	78.07	72.16	62.49	47.87	26.28	7.72	4.83	4.45	2.87	0.67	0.07	1.33	4.13	7.90	10.00
3	66.58	64.09	58.88	50.43	37.96	20.38	6.77	4.68	4.36	1.53	-1.93	-2.82	-1.23	2.20	6.75	9.44
4	50.46	48.52	44.49	38.09	28.83	16.03	6.08	4.54	4.26	-0.71	-6.71	-7.80	-5.22	-0.47	5.45	8.87
5	31.95	30.70	28.17	24.29	18.91	11.69	5.61	4.50	4.10	-4.86	-15.98	-16.05	-10.97	-3.92	3.94	8.31
6	19.41	18.59	16.97	14.63	11.72	8.54	5.71	4.46	3.76	-12.42	-35.92	-29.03	-18.31	-7.76	2.38	7.74
7	17.17	16.42	14.98	12.92	10.40	7.73	5.47	4.39	3.30	-23.06	-85.86	-45.44	-25.07	-10.81	1.13	7.18
8	16.06	15.36	14.00	12.05	9.65	6.89	5.17	4.42	3.67	-14.45	-42.40	-41.41	-25.32	-11.12	0.71	6.61
9						5.43	4.78	4.44	3.97	-7.70	-27.49	-52.07	-23.28	-8.67	1.28	6.04
10						5.01	4.70	4.48	4.29	-0.22	-7.37	-12.91	-6.66	-1.18	3.15	5.48
11						5.19	4.92	4.52	4.49	4.30	3.93	3.74	4.01	4.25	4.45	5.14
12						5.27	5.02	4.55	4.52	4.49	4.45	4.42	4.48	4.49	4.51	5.14
13						5.61	5.45	5.10	5.03	4.91	4.91	4.92	4.95	4.93	4.76	4.43
14						6.73	6.97	9.68	13.11	20.49	24.40	25.93	26.63	26.89	26.78	26.49
15						28.70	31.92	39.42	41.69	47.81	53.28	56.23	57.83	58.56	58.64	58.35
16						56.79	59.77	63.49	64.76	68.53	73.33	76.57	78.55	79.56	79.77	79.49
17						70.59	73.04	75.69	76.60	79.41	83.63	86.81	88.91	90.04	90.31	90.03

0.0000 = the river limits

Figure 8 - Estimated heads for Run 8

Composite Scaled Sensitivities - Runs 2 to 8

The composite scaled sensitivity results for all of the runs in which the number of parameters was varied are shown in Table 10.

Table 10 - Composite Scaled Sensitivities for Runs 2 to 8

Parameter	Run 1	Run 2	Run 3	Run 4	Run 5	Run 6	Run 7	Run 8
q_{B1}	1.64	1.64	1.69	1.64	2.40	1.59	1.71	1.75
q_{B2}	0.0805	0.0805	0.0922	0.0806	0.217		0.0986	0.130
Q_1	2.06	2.06	2.05		1.95		2.03	2.12
Q_2	0.999	0.999	0.994		0.938		0.980	1.09
h_{B1}	0.354	0.354	0.357	0.354	0.394	0.358	0.358	0.381
h_{B2}	0.185	0.185	0.186	0.185	0.190	0.185	0.185	0.192
h_{B3}	0.133	0.133	0.132	0.133	0.117	0.133	0.113	0.112
T_1	2.44	2.44	2.43	2.44	2.34	2.45	2.43	2.42
W_1	1.55	1.55	1.56	1.55	1.41	1.53	1.58	1.59
T_2	2.78	2.78	2.78	2.78	2.80	2.78	2.76	
W_2	0.305	0.305	0.391	0.305	1.18	0.203		
T_3	3.96	3.96	3.94	3.96		3.96		
W_3	4.07	4.07		4.07		4.06		
R_2	0.0383			0.0383		0.0381		

The majority of the runs had similar composite scaled sensitivity values for each parameter, with the exception of Run 5. Referring back to Table 8, specified flux in Zones 1 and 2 (q_{B1} and q_{B2}), transmissivity in Zone 1 (T_1) and recharge for Zone 2 (W_2) in

Run 5 varied significantly from those of the other runs. Specifically, these parameters were all larger for Run 5. Since the composite scaled sensitivity is scaled by the parameter value, one would expect larger composite scaled sensitivities for larger parameter values. This is the case for all but T_1 . The reason for T_1 having a lower sensitivity in this run may be related to the possible non-linearity of the sensitivity for this parameter at its final value for Run 5. One may also expect the final estimates of parameters, which are highly correlated to these parameters, to vary more significantly from those of the other runs. Based on the results presented in Table 8, this is the case.

Eigenvalues and Eigenvectors - Runs 2 to 8

The eigenvalues and eigenvectors were used to determine which parameters were most and least reliably estimated. The results for all of the runs in which the number of parameters was varied were compared to each other and are shown in Table 11.

The eigenvalue and eigenvector output indicates that transmissivity for Zone 3 (T_3) and recharge for Zone 3 (W_3) were the most reliable parameters for Runs 2, 4 and 6, the only runs to include both parameters. These two parameters also had the highest composite scaled sensitivities in these runs. In general, for all runs, the parameters with the higher composite scaled sensitivities were the most reliably estimated and the parameters with the lower composite scaled sensitivities were the least reliably estimated.

Table 11 - Summary of Parameter Reliability as determined by Evaluation of Eigenvalues and Eigenvectors for Runs 2 to 8

Run Number	Most Reliable Parameters	Least Reliable Parameters
Run 1	T_3, W_3	q_{B2}, W_2
Run 2	T_3, W_3	q_{B2}, W_2
Run 3	T_3	q_{B2}, W_2
Run 4	T_3, W_3	q_{B2}, W_2
Run 5	q_{B1}, T_1, T_2	q_{B1}, q_{B2}, T_1
Run 6	T_3, W_3	W_2
Run 7	Q_1, T_2	q_{B2}
Run 8	q_{B1}, T_1, W_1	q_{B2}

One unusual result occurred in Run 5, where q_{B1} and T_1 were estimated both most and least reliable as determined by the eigenvalue and eigenvector output. One possible explanation for this is that these two parameters had high composite scaled sensitivities, but were also highly correlated and unconstrained. Run 5 also had a very high sum of squared residuals, indicating that the estimated model did not fit the observed model well, and no parameters in Zone 3. These factors combined may have caused inaccurate eigenvalue and eigenvector output. The estimated parameters for Run 5 would be considered to poorly describe the observed physical system, as would the results for Runs 7 and 8.

Correlation - Runs 2 to 8

Results of correlation values equal to or greater than 0.85 or equal to or less than -0.85 for all of the runs in which the number of parameters was varied were compared to each other. Results are shown in Table 12. Of course, where parameters were removed from the run, no correlation was calculated by MODFLOWP. The parameter pairs which were highly correlated (greater than 0.85 or less than -0.85) for the majority of the runs are: q_{B1} and T_1 , T_3 and W_3 , T_1 and W_2 , and W_1 and W_2 .

This correlation between parameter pairs can be seen in Table 8. For example, the increases and decreases in final parameter estimates for q_{B1} and T_1 are nearly proportional, with similar results for other highly correlated parameter pairs.

Water Mass Balance

Water mass balance results are not part of the standard output of MODFLOWP. MODFLOWP must be run without parameter estimation in order to produce these data. The mass balance results are included in this thesis to provide further information about the model runs. Table 13 shows the water mass balance information as percentages of the total flow of water into and out of the site. The fluxes into and out of the model were equal to within 0.01 percent for all runs shown in Table 13.

Table 12 - Correlation of Parameter Pairs for Runs 2 to 8

Run Number	Parameter Pair	Correlation Value
Run 1	q_{B1}, T_1	0.96
	T_3, W_3	1.00
	T_1, W_2 and W_1, W_2	-0.92
Run 2	q_{B1}, T_1	0.96
	T_3, W_3	1.00
	T_1, W_2 and W_1, W_2	-0.92
Run 3	q_{B1}, T_1	0.96
	T_1, W_2	-0.90
	W_1, W_2	-0.87
Run 4	q_{B1}, T_1	0.96
	T_3, W_3	1.00
	T_1, W_2	-0.93
	W_1, W_2	-0.92
Run 5	q_{B1}, T_1	0.96
Run 6	q_{B1}, T_1	0.96
	T_3, W_3	1.00
	T_1, W_2	-0.91
	W_1, W_2	-0.92
Run 7	q_{B1}, T_1	0.93
Run 8	q_{B1}, T_1	0.93

For Runs 1 through 4 and Runs 6 through 8, the majority of water enters the model through river leakage. The river is entirely in Zone 2 and is adjacent to the two pumping wells (Q_1 and Q_2). Twenty percent of the water also enters through the constant head boundaries. Approximately 90 percent of the water leaves through the pumping wells. In Run 5, a large amount of water exits the system through negative recharge.

Table 13 - Water Mass Balance Data for Runs 1 to 8, as Percentages of Total Flow

		Run 1	Run 2	Run 3	Run 4	Run 5	Run 6	Run 7	Run 8
I N	Constant Head	21	21	21	21	20	21	21	20
	Q_{B1}, Q_{B2}	5	5	6	5	13	4	6	7
	W_1, W_3	7	7	8	7	8	6	8	8
	River Leakage	67	67	65	67	59	69	65	65
O U T	Constant Head	< 1	< 1	< 1	< 1	< 1	< 1	< 1	< 1
	Q_1, Q_2	90	90	88	90	69	93	86	85
	W_2	7	7	9	7	27	5	11	12
	River Leakage	3	3	3	3	4	2	3	3
Total Flow (ft ³ /day)		164,380	164,370	168,760	164,490	216,900	159,640	173,550	157,770

This result is not surprising, since the value of recharge in Zone 2 (W_2) as shown in Table 8 is approximately five times greater than for the other runs. However, the greatly increased negative recharge value is not realistic, since evapotranspiration would not likely have such a large impact on a groundwater system. Since this parameter is not constrained, MODFLOWP allows it to vary unrealistically while attempting to match observed heads. As mentioned previously, Run 5 does not represent the observed physical system well.

Runs 5, 7 and 8 have larger total flux deviations from the baseline run than do the other runs. This deviation is related to the large fluctuations in specified flux (q_{B1} and q_{B2}), the pumping rates of wells Q_1 and Q_2 , and negative recharge in Zone 2 (W_2).

The general direction of the flow of water (refer to Figures 4 and 8) is from the perimeter of the system to the pumping wells, and from the river towards the pumping wells. The majority of the water enters the model through the constant head boundaries and through river leakage, and exits through the pumping wells and through negative recharge. The steepest gradients occur along the northwest and southeast no-flow boundaries. It is evident from Figures 4 and 8 how water enters and leaves the river, based on the heads of adjacent cells.

4.3.3 Varying Initial Estimates

Several runs were performed with different initial parameter estimates in each run to determine the impact these changes had on the final parameter estimates. The purpose of these runs was to determine if a global or local minimum has been reached. Either a global or local minimum of the objective function may cause the model to converge as long as the convergence criteria are met. Referring to Figure 9, varying the initial parameter estimates may force the initial value of the objective function to the right of the local minimum or to the left of the inflection point.

The initial parameter estimates of unconstrained parameters were varied by up to an order of magnitude in either direction. Only small changes to constrained parameters were made, since a greatly constrained parameter would be kept close to its initial

Figure 9 - Hypothetical Objective Function Surface. (Source: Hill, 1992)

estimate. Several parameters had their initial estimates modified in each run. The final parameter estimates did not change; neither did the other output. Therefore, it appears that a global minimum of the objective function was reached in the previous model solution, and that there are no local minimums of the objective function that would cause MODFLOWP to converge with incorrect final parameter estimates.

4.3.4 Varying Standard Deviations (Parameter Constraints; Runs 9 to 12)

Several runs were performed varying the standard deviation (constraint) on the recharge in Zone 3 (parameter W_3) to determine the impact these varied standard deviations had on the final parameter estimates. The results of these runs are shown in Table 14. The standard deviation percentage is defined as the standard deviation divided by the initial parameter estimate (similar to a coefficient of variation).

The initial parameter estimates for these runs are the same used for the baseline run. The initial parameter estimate for W_3 is 1.7×10^{-4} and the final parameter estimate for the baseline run was 1.31×10^{-4} . The lower the standard deviation value, the tighter the constraint, so the more likely the final parameter estimate for W_3 will be closer to the initial estimate than for runs with higher standard deviation values for W_3 . Parameter W_3 was selected for these runs, since it was determined to be a reliable parameter on the basis of its eigenvalue and eigenvector relationships, and it also had strong correlations with other parameters. Therefore, changes made to this parameter should have noticeable effects on the run results.

Runs 9 to 12

The standard deviation percentage on recharge of Zone 3 (W_3) was modified to 10, 20, 40 and 50 percent, from its original value of 30 percent in the baseline run.

Expected results would be that the final parameter estimate would be closer to the initial parameter estimate for W_3 when the standard deviation percentage was low, and that parameters correlated with W_3 having high standard deviation percentage values (or having no standard deviation) would vary from the baseline run more than the other parameters.

Table 14 indicates that the final parameter estimates fall within reasonable ranges. Parameter W_3 is closer to its initial value when the standard deviation percentage is low and farther from the initial value when the standard deviation percentage is high. Also, the parameters with no standard deviation (q_{B1} , q_{B2} , T_1 , W_2 and T_3) vary much more from the baseline run than the other parameter final estimates.

Table 14 - Comparison of Standard Deviation Percentage of Parameter W_3 vs. Parameter Final Values

Parameter Description	Known Value	Baseline Case Estimates with 30% Standard Deviation Percentage of W_3	Standard Deviation Percentage of Parameter W_3 – Run Number			
			10% – Run 9	20% – Run 10	40% – Run 11	50% – Run 12
q_{B1}	50	84.5	93.2	88.7	81.5	79.4
q_{B2}	500	944	1,060	1,000	902	874
Q_1	-100,000	-96,900	-96,900	-96,900	-96,900	-96,800
Q_2	-50,000	-51,000	-51,100	-51,000	-51,000	-51,000
h_{B1}	10.0	10.2	10.2	10.2	10.1	10.1
h_{B2}	5.0	5.14	5.15	5.15	5.14	5.14
h_{B3}	5.5	5.22	5.21	5.22	5.23	5.23
T_1	50	66.5	72.7	69.5	64.3	62.9
W_1	0.0003	0.000299	0.000319	0.000309	0.000291	0.000286
T_2	500	488	490	489	487	486
W_2	-0.0001	-0.000128	-0.000160	-0.000144	-0.000117	-0.000109
T_3	20	12.9	16.1	14.5	11.8	11.0
W_3	0.0002	0.000131	0.000163	0.000146	0.000120	0.000112
R_2	0.1	0.0805	0.0805	0.0805	0.0805	0.0804

4.3.4.1 Additional Output for Runs 9 to 12

There is an obvious trend in the final parameter estimate values. All the estimated values have trends away from the baseline run final estimate as the standard deviation on parameter W_3 is increased.

Residuals - Runs 9 to 12

The residual results for all of the runs in which the constraint on parameter W_3 was varied are summarized in Table 15.

The residual data for Runs 9 through 12 are similar. This indicates that the final parameter values, when used in the flow equations, produced similar hydraulic head values at all of the 32 measured head locations. As shown in Table 15, the sum of the squared residuals decreased slightly as the constraint on W_3 was loosened. A possible reason for the better match in heads is that MODFLOWP was able to modify W_3 by larger amounts to match head observations as the constraint on W_3 was loosened.

Table 15 - Residuals for Runs 9 to 12

Run Number	Average Residual	Min. Residual (Observation Number)	Max Residual (Observation Number)	Sum of Squared Residuals
Run 9	0.133	-1.45 (5)	2.50 (20)	25.658
Run 10	0.139	-1.31 (19)	2.50 (20)	24.808
Run 1	0.145	-1.28 (19)	2.50 (20)	24.146
Run 11	0.149	-1.25 (19)	2.49 (20)	23.752
Run 12	0.152	-1.24 (19)	2.49 (20)	23.531

Composite Scaled Sensitivities - Runs 9 to 12

The final composite scaled sensitivities (based on final parameter estimates) for all of the runs in which the standard deviation of parameter W_3 was varied are shown in Table 16.

Table 16 - Composite Scaled Sensitivities for Runs 9 to 12

Parameter	Run 9	Run 10	Run 1	Run 11	Run 12
q_{B1}	1.68	1.66	1.64	1.63	1.62
q_{B2}	0.0900	0.0851	0.0805	0.0771	0.0747
Q_1	2.05	2.06	2.06	2.06	2.06
Q_2	0.995	0.997	0.999	1.00	1.00
h_{B1}	0.357	0.355	0.354	0.353	0.352
h_{B2}	0.186	0.186	0.185	0.185	0.185
h_{B3}	0.133	0.133	0.133	0.133	0.133
T_1	2.43	2.44	2.44	2.44	2.44
W_1	1.56	1.55	1.55	1.54	1.54
T_2	2.78	2.78	2.78	2.78	2.78
W_2	0.375	0.339	0.305	0.279	0.261
T_3	3.94	3.95	3.96	3.97	3.97
W_3	4.08	4.08	4.07	4.07	4.07
R_2	0.0385	0.0384	0.0383	0.0383	0.0382

The composite scaled sensitivities of each parameter for Runs 9 through 12 had little variation. The only two parameters which varied significantly were q_{B2} and W_2 . These two parameters are also considered to be least reliably estimated as discussed below.

The composite scaled sensitivities should remain constant for all parameters whose final values do not change or that have a linear relationship between head and the parameter value (see Figure 2). Composite scaled sensitivities which change based upon

the parameter value have a non-linear relationship with respect to head. For example, parameters T_1 , T_3 and W_3 have nearly constant composite scaled sensitivities while their final estimates vary for each run, but parameters q_{B1} , q_{B2} and W_2 have a trend in their composite scaled sensitivities as their final estimates vary.

Eigenvalues and Eigenvectors - Runs 9 to 12

The eigenvalue and eigenvector results for all of the runs in which the constraint of parameter W_3 was varied are summarized in Table 17. The eigenvalue and eigenvector output indicate that transmissivity for Zone 3 (T_3) and recharge for Zone 3 (W_3) were the most reliable parameters for the runs. Specified flux at the north boundary of Zone 2 (q_{B2}) and recharge for Zone 2 (W_2) were the parameters estimated least reliably. This is consistent for all runs and does not differ from the results of the baseline run.

Correlation - Runs 9 to 12

Results of correlation values equal to or greater than 0.85 or equal to or less than -0.85 for Runs 9 through 12 were compared to each other. There is little variation in the correlation results which are shown in Table 18.

Water Mass Balance - Runs 9 to 12

Table 19 shows the water mass balance information as percentages of the total flow of water into and out of the site. The fluxes into and out of the model were equal to within 0.01 percent for all runs shown in Table 19.

Table 17 - Summary of Parameter Reliability as determined by Evaluation of Eigenvalues and Eigenvectors for Runs 9 to 12

Run Number	Most Reliable Parameters	Least Reliable Parameters
Run 1	T_3, W_3	q_{B2}, W_2
Run 9	T_3, W_3	q_{B2}, W_2
Run 10	T_3, W_3	q_{B2}, W_2
Run 11	T_3, W_3	q_{B2}, W_2
Run 12	T_3, W_3	q_{B2}, W_2

Table 18 - Correlation of Parameter Pairs for Runs 9 to 12

Run Number	Parameter Pair	Correlation Value
Run 9	q_{B1}, T_1	0.96
	T_3, W_3	1.00
	T_1, W_2	-0.90
	W_1, W_2	-0.88
Run 10	q_{B1}, T_1	0.96
	T_3, W_3	1.00
	T_1, W_2	-0.92
	W_1, W_2	-0.90
Run 1	q_{B1}, T_1	0.96
	T_3, W_3	1.00
	T_1, W_2 and W_1, W_2	-0.92
Run 11	q_{B1}, T_1	0.97
	T_3, W_3	1.00
	T_1, W_2 and W_1, W_2	-0.93
Run 12	q_{B1}, T_1	0.97
	T_3, W_3	1.00
	T_1, W_2 and W_1, W_2	-0.93

The water mass balance data for Runs 9 through 12 does not vary significantly from that of the baseline run. As shown in Table 19, as the constraint on W_3 was relaxed and its final estimate decreased, the percent contribution of total flux by parameters W_2 and W_3 into the model also decreased as did the total flux. These trends caused a slight increase in the percent flux into the model by river leakage over each run, as the river leakage contribution remained nearly constant.

Table 19 - Water Mass Balance Data for Runs 9 to 12, as Percentages of Total Flow

		Run 9	Run 10	Run 1	Run 11	Run 12
IN	Constant Head	20	21	21	21	21
	q_{B1}, q_{B2}	6	6	5	5	5
	W_1, W_3	8	7	7	7	6
	River Leakage	66	66	67	67	68
OUT	Constant Head	< 1	< 1	< 1	< 1	< 1
	Q_1, Q_2	88	89	90	91	91
	W_2	9	8	7	7	6
	River Leakage	3	3	3	2	3
Total Flow (ft ³ /day)		167,910	166,090	164,380	163,190	162,230

4.3.5 Various Runs with no Parameter Standard Deviation (Runs 13 to 15)

Several runs were performed in which the standard deviation assigned to each parameter was removed to determine the impact these changes had on the final parameter estimates. This is equivalent to removing constraints from all parameters — letting the parameter estimation algorithm vary parameters significantly from the initial parameter estimates. The results of these runs are shown in Table 20.

Run 13

Standard deviations on all of the parameters were removed. The purpose of this run was to see the impact that parameter constraints had on the final parameter estimates.

Most final parameter estimates varied significantly from their values in the baseline run. Only a few parameter estimates remained relatively close to their baseline run values. As shown in Table 20, the final estimates of Q_1 and Q_2 vary significantly from the known values and initial estimates. Considering that one would have a realistic estimate of these parameter values, this run indicates the importance of placing constraints on parameter initial estimates.

Run 14

Standard deviations on all of the parameters were removed and the initial flow rate value at pumping well number one (Q_1) was reduced to -87,000 from its original value of -97,000. The remaining data in the model were kept at the original initial values as in the

baseline run. The purpose of this run was to see the combined impact that parameter standard deviations and initial values had on the final parameter estimates.

Table 20 - Comparison of Parameters with no Standard Deviation vs. Parameter Final Values for Runs 13 to 15

Parameter Description	Known Value	Baseline Run Final Estimate	Run Number/Description		
			13 / No Standard Deviations	14 / No Standard Deviations, Q_1 Modified	15 / No Standard Deviations, T_2 Modified
q_{B1}	50	84.5	104	104	79.2
q_{B2}	500	944	1,280	1,280	982
Q_1	-100,000	-96,900	-175,000	-176,000	-134,000
Q_2	-50,000	-51,000	-93,400	-93,600	-71,500
h_{B1}	10.0	10.2	8.25	8.25	8.25
h_{B2}	5.0	5.14	6.89	6.89	6.89
h_{B3}	5.5	5.22	6.15	6.14	6.15
T_1	50	66.5	83.0	83.2	63.5
W_1	0.0003	0.000299	0.000395	0.000396	0.000302
T_2	500	488	870	871	665
W_2	-0.0001	-0.000128	-0.0000354	-0.0000355	-0.0000271
T_3	20	12.9	11.0	11.1	8.45
W_3	0.0002	0.000131	0.000113	0.000113	0.0000864
R_2	0.1	0.0805	0.293	0.294	0.224

The final parameter estimates for Runs 13 to 15 varied only slightly from those in Run 1. This may indicate that there is a local or global solution minimum in which small variations of the parameter estimates meet the convergence criterion.

Run 15

Standard deviations on all of the parameters were removed and the initial value of transmissivity in Zone 2 (T_2) was halved to 210 from its original value of 420. The remaining data in the model were kept at the original initial values as in the baseline run. This was a second attempt to evaluate the combined impact that parameter standard deviations and initial values had on the final parameter estimates.

In this case, the final parameter estimates varied significantly from Runs 13 and 14, as shown in Table 20. This indicates that the initial parameter estimates specified by the user can have a large impact on the final parameter estimates calculated by MODFLOWP.

Based upon the large difference in final parameter estimates between Runs 13 and 14 and Run 15, it is likely that Runs 13 and 14 converged on nearly the same local minimum while Run 15 converged on a much different local minimum (refer to Figure 9). These unusual results are analyzed further in the following section.

4.3.5.1 Additional Output for Runs 13 to 15

Residuals - Runs 13 to 15

The residuals at observed head locations for Runs 13 to 15 are presented in Table 21. The residual data for each run was nearly the same at all observation locations. The variation at observed heads was not different within the number of significant figures shown in Table 21. This results was not expected. Considering that the final parameter estimates were different for each run, this indicates that the model is not unique. This is

further evidence of the non-uniqueness of inverse solutions of the groundwater flow equation (Yeh, 1986).

Table 21 - Residuals for Runs 13 to 15

Run Number	Average Residual	Min. Residual (Observation Number)	Max. Residual (Observation Number)	Sum of Squared Residuals
Run 1	0.1450	-1.28 (19)	2.50 (20)	24.146
Run 13	0.0715	-1.16 (14)	2.50 (20)	18.826
Run 14	0.0715	-1.16 (14)	2.50 (20)	18.826
Run 15	0.0715	-1.16 (14)	2.50 (20)	18.826

Composite Scaled Sensitivities - Runs 13 to 15

The composite scaled sensitivities for Runs 13 to 15 are represented in Figure 10. All of the composite scaled sensitivities for Runs 13 through 15 were exactly the same and were close to the values of the baseline run. Given that sensitivities were constant over different parameter estimates indicates that the hydraulic head is approximated by a linear function of these parameters over the range of final parameter estimates in these runs (see Figure 2).

Eigenvalues and Eigenvectors - Runs 13 to 15

The eigenvalues and eigenvectors results for runs 13 through 15 are summarized in Table 22.

Figure 10 - Composite scaled sensitivities of Run 1 and Runs 13 to 15.

Table 22 - Summary of Parameter Reliability as Determined by Evaluation of Eigenvalues and Eigenvectors for Runs 13 to 15

Run Number	Most Reliably Estimated Parameters	Least Reliably Estimated Parameters
Run 1	T_3, W_3	q_{B2}, W_2
Run 13	R_2	$q_{B1}, q_{B2}, Q_1, Q_2, T_1, T_2, T_3, W_1, W_2, W_3, R_2$
Run 14	T_2, W_2, W_3, R_2	$q_{B1}, q_{B2}, Q_1, Q_2, T_1, T_2, T_3, W_1, W_2, W_3, R_2$
Run 15	T_1, W_1, T_2, W_2, R_2	$q_{B1}, q_{B2}, Q_1, Q_2, T_1, T_2, T_3, W_1, W_2, W_3, R_2$

The results for the most reliably estimated parameter are not consistent for these runs as compared to results presented for Runs 1 through 12. Furthermore, some of the

most reliably estimated parameters also were indicated to be estimated least reliably. Of the parameters which were determined to be equally unreliable, each parameter had the same exact eigenvector associated with the same exact highest eigenvalue. These results indicate that Runs 13 through 15 are ill-posed.

Correlation - Runs 13 to 15

The correlation coefficients for Runs 13 to 15 in Table 20 were compared to each other. All three runs had identical data, but did not match any of the runs previously discussed. There were 55 parameter pairs, out of a possible 84, which had correlation values equal to 1.0 or -1.0. This would indicate that there is not enough information in the model in order to estimate the parameters independently.

Water Mass Balance - Runs 13 to 15

Table 23 shows the water mass balance information as percentages of the total flow of water into and out of the site. The fluxes into and out of the model were nearly equal for Runs 13 and 14, but had a large decrease in Run 15 as shown in Table 23. The percent contributions in and out of the model by all parameters were identical (within the number of significant figures shown) for all runs. The decrease in flux for Run 15 can be attributed to the decrease in flow rate of river leakage from Runs 13 and 14 to Run 15. There was a corresponding decrease in flux out from the pumping wells to match observed heads.

The total flux into and out of the model for Runs 13 to 15 was much higher than that of Run 1. Since there is no constraint on the amount of flux through the majority of the model, it is not surprising to see large variations in these values. This is not realistic of what may occur in a real system. In order for this situation to be minimized, one would need to specify and constrain flux through cells within the model. MODFLOWP does allow the user to set up the model to include specified flux through cells as a parameter.

Table 23 - Water Mass Balance Data for Runs 13 to 15 as Percentages of Total Flow

		Run 1	Run 13	Run 14	Run 15
IN	Constant Head	21	21	21	22
	q_{B1}, q_{B2}	5	4	4	4
	W_1, W_3	7	5	5	4
	River Leakage	67	70	70	70
OUT	Constant Head	< 1	< 1	< 1	< 1
	Q_1, Q_2	90	95	95	95
	W_2	7	1	1	1
	River Leakage	3	4	4	4
Total Flow (ft ³ /day)		164,380	281,600	282,790	215,570

5.0 Conclusions

The evaluation of MODFLOWP's parameter estimation capabilities was performed by determining how MODFLOWP results vary for the same physical groundwater system (test case) when varying the initial estimates of the parameters, constraints on the parameters, and by changing the number of parameters. The conclusions based on this research are presented below.

Composite scaled sensitivities are a good indicator as to which parameters can be removed from the parameter estimation process. Since parameters with low composite scaled sensitivities have been shown to have final estimates very close to the initial parameter estimates in nearly all model runs in this thesis, removing these parameters from the estimation process has little impact on the model results as long as the other parameters are reasonably well-constrained. This result has occurred in Run 2 in which river leakance (R_2) was removed from the run while not affecting other parameter values. The constant head parameters in Runs 2 through 8 also varied only slightly in most of the runs presented in this thesis. These results are logical, since parameters with low composite scaled sensitivities have little effect on heads. One must also be aware that a parameter value may vary by a large amount even if its composite scaled sensitivity is low. Therefore, composite scaled sensitivities should not be solely used for the purpose of reducing the number of parameters estimated. When parameters with high composite scaled sensitivities are removed from the parameter estimation process, it is likely that the

final parameter estimates for other parameters in the model will be different. This assumes that the final estimate for the removed parameter was different than its initial estimate.

There appears to be a correlation between composite scaled sensitivities and parameter estimate reliability as measured by eigenvectors and eigenvalues. In the majority of model runs in this thesis, the parameters with high composite scaled sensitivities have typically been estimated most reliably. There were no cases in which a model with reasonable results had a parameter with a low composite scaled sensitivity which was estimated most reliably. The opposite is also true, but to a lesser extent. Parameters with low composite scaled sensitivities have typically been estimated least reliably. This is likely due to the fact that parameters with low composite scaled sensitivities could vary by large amounts without affecting head residuals at observation points. Also, parameters with high composite scaled sensitivities cannot vary by large amounts without affecting head residuals at observation points. This has the tendency to force parameter estimates within certain reasonable ranges, although many other factors such as specified standard deviation and correlation also affect results.

The standard deviation (parameter constraint) has a significant impact on the final parameter estimate. The standard deviation can be used to allow a large or small difference between the final parameter estimate and initial estimate. The standard deviation is used to weight the squared residuals in the objective function MODFLOWP minimizes and, therefore, has a large influence on final parameter estimates at model convergence. For example, if a parameter has a small standard deviation specified for its

initial estimate, the larger the difference in the initial estimate and the calculated parameter value, the larger the objective function value (see Equation 11).

Runs 13 through 15 for the test case presented in this thesis are examples of model runs with high parameter correlations. For example, these runs with no standard deviations imposed on the parameters (Section 4.3.5) have 55 parameter pairs (65 percent of all possible parameter pairs) with correlations of 1.0 or -1.0. Since these parameter pairs are correlated, it is unlikely that MODFLOWP can independently estimate these parameters accurately. These same model runs have parameters with no imposed standard deviations in which changes to the initial estimate cause large differences in the final parameter estimates. Eigenvector and eigenvalue results for these model runs show that the majority of parameters have the same eigenvector value associated with the largest eigenvalue, indicating that the parameters were all equally unreliable. Since this model is known to be non-unique, it is possible that the results of the eigenvectors and eigenvalues indicate that the model is non-unique. A recommended method (Hill 1992) to reduce the number of highly correlated parameter pairs is to simply remove one of the parameters which is highly correlated with another parameter. It would be best to eliminate a parameter which is estimated to have a relatively accurate initial estimate, since the value of a parameter removed from the parameter estimation routine of MODFLOWP will not be allowed to vary.

There are a variety of possible methods to determine whether a model is ill-posed. Ill-posedness in a groundwater model is generally defined by Yeh (1986) as having parameters which are non-unique and unstable. Non-uniqueness of parameters can be

identified by parameter pairs with high correlations, parameters with large standard deviations whose final estimates vary due to modest changes in the initial parameter estimate, and possibly by parameters which are estimated to be equally unreliable as indicated by eigenvalues and eigenvectors.

In summary, it is very important to put a MODFLOWP groundwater model through the rigorous tests (varied model runs) performed in this thesis. It will allow the user to identify parameters which can be or need to be removed from the estimation process, determine the sensitivity of heads to parameter variations, determine the sensitivity of final parameter estimates to the standard deviation imposed on the parameters, and assess how close the final heads of the calculated model are to the observed heads.

Bibliography

- Anderman, E. R., M. C. Hill, and E. P. Poeter, 1994, Two-Dimensional Advective Transport in Nonlinear Regression: Sensitivities and Uncertainty of Plume-Front Observations, Proceedings of the 1994 Groundwater Modeling Conference, Department of Civil Engineering, Colorado State University Campus, August 10-12.
- Anderman, E. R., M. C. Hill, and E. P. Poeter, 1996, Two-Dimensional Advective Transport in Ground-Water Flow Parameter Estimation, *Ground Water*, 34 (November-December): 1001-1009.
- Carrera, Jesus, and S. P. Neuman, 1986, Estimation of aquifer parameters under transient and steady state conditions, Applications to synthetic and field data, *Water Resources Research*, 22, No. 2: 228-242.
- Cooley, Richard L., 1985, A Comparison of Several Methods of Solving Nonlinear Regression of Groundwater Flow Problems, *Water Resources Research*, 21, (October): 1525-1538.
- Giacinto, Joseph F., 1994, An Application of MODFLOWP to a Superfund Case Study, Proceedings of the 1994 Groundwater Modeling Conference, Department of Civil Engineering, Colorado State University Campus, August 10-12.
- Hill, Mary, 1990, Preconditioned Conjugate-Gradient 2 (PCG2), A Computer Program for Solving Ground-Water Flow Equations; *United States Geological Survey, Water Resources Investigations Report 90-4048*.
- Hill, Mary, 1992, A Computer Program (MODFLOWP) for Estimating Parameters of a Transient, Three-Dimensional, Ground-Water Flow Model Using Nonlinear Regression, *United States Geological Survey, Open-File Report 91-484*.
- Hill, Mary, 1996, MODFLOWP Revision 2.8.
- Hill, Mary, Undated, Using Nonlinear Regression in Groundwater Flow Model Calibration with MODFLOWP.
- McDonald, Michael G., and Arlen W. Harbaugh, 1988, Techniques of Water-Resources Investigations of the United States Geological Survey, A Modular Three-Dimensional Finite Difference Ground-Water Flow Model, U.S. Geological Survey. Book 6, Chapter A1.

- Poeter, Eileen P., and Sean A. McKenna, 1994, Geostatistical Simulation and Inverse Flow Modeling to Reduce Uncertainty Associated with Flow and Transport Predictions, Proceedings of the 1994 Groundwater Modeling Conference, Department of Civil Engineering, Colorado State University Campus, August 10-12.
- Prudic, D. E., 1989, Documentation of a Computer Program to Simulate Stream-Aquifer Relations Using a Modular, Finite-Difference, Ground-Water Flow Model; *United States Geological Survey Open File Report 88-729* as modified with updates from February and December, 1990.
- Ronan, A. D., 1995, Flow Parameter Uncertainty in the Pajaro Valley Aquifer System: A Case Study using MODFLOWP, Proceedings of the International Symposium, American Society of Civil Engineers, San Antonio, Texas, Pages 211-216.
- Starn, J. Jeffrey, 1994, Application of Nonlinear Regression to Estimate Parameters of a Two-, Dimensional Groundwater Flow Model, Proceedings of the 1994 Groundwater Modeling Conference, Department of Civil Engineering, Colorado State University Campus, August 10-12.
- Wanta, M. J., and A. D. Ronan, 1996, Automated Parameter Estimation Using MODFLOWP - A Case Study, *Eos Trans. AGU*, 77(46): F278
- Yager, Richard M., 1993, Simulated Three-Dimensional Groundwater Flow in the Lockport Group, A Fractured Dolomite Aquifer near Niagara Falls, New York, United States Geological Survey, *Water Resources Investigations Report 92-4189*.
- Yeh, William W-G., 1986, Review of parameter identification procedures in groundwater hydrology: the inverse problem, *Water Resources Research*, 22, 2: 95-108.

IMAGE EVALUATION TEST TARGET (QA-3)

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