Sensitivity and uncertainty analysis of the recharge boundary condition

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[1] The reliability analysis method is integrated with MODFLOW to study the impact of recharge on the groundwater flow system at a study area in New Jersey. The performance function is formulated in terms of head or flow rate at a pumping well, while the recharge sensitivity vector is computed efficiently by implementing the adjoint method in MODFLOW. The developed methodology not only quantifies the reliability of head at the well in terms of uncertainties in the recharge boundary condition, but it also delineates areas of recharge that have the highest impact on the head and flow rate at the well. The results clearly identify the most important land use areas that should be protected in order to maintain the head and hence production at the pumping well. These areas extend far beyond the steady state well capture zone used for land use planning and management within traditional wellhead protection programs.

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1. Introduction

[2] The top or upper boundary of fully saturated groundwater flow models is usually described using the type II recharge flux boundary condition. Unlike saturated hydraulic conductivity which is a stationary system parameter, recharge is a dynamic process affected by a multitude of spatial and temporal factors [*Sharma*, 1989]. Both parameters are subject to a great deal of uncertainty because of scaling issues and are not only difficult to estimate, but also costly to measure in practice. While the flow solution is highly sensitive to the hydraulic conductivity distribution which can vary over several orders of magnitude, the recharge boundary condition also plays an important role in many modeling applications with studies in permeable unconfined aquifers being an example.

[3] In practice, the recharge boundary is typically characterized by a handful of zones with uniform recharge. The delineation of the recharge zones may be loosely based on the type of land use, soils, topography, or in larger-scale models, even climate. The recharge flux in each zone is seldom estimated explicitly, however, and is simply used as an adjustment parameter during model calibration [e.g., *Varni and Usunoff*, 1999; *Kirshen*, 2002]. This leads to nonunique model results due to the highly sensitive hydraulic conductivity distribution which is also routinely adjusted during model calibration, and furthermore to a potentially unrealistic description of the recharge boundary.

[4] Groundwater inverse modeling has been used extensively in model calibration [*Yeh*, 1986; *Carrera et al.*, 2005] and has been touted as an important if not essential step in many realistic field applications [*Poeter and Hill*, 1997]. The purpose of inverse modeling is to estimate the optimum spatial and temporal distribution of a particular model parameter or parameters, for example, hydraulic conductivity, on the basis of sparse measurements of hydraulic head and flow rates at a set of observation points (e.g., wells) in the domain. The optimal parameter set is determined by minimizing the error between the field observations and the computed values [e.g., *Poeter and Hill*, 1998; *Doherty*, 2002]. While the process of inverse groundwater modeling is an important calibration tool by facilitating parameterization and providing the "best" match between measured and simulated data, the solution is not necessarily unique [*Carrera and Neuman*, 1986]. This is especially true for the hydraulic conductivity and recharge distributions, which cannot be uniquely estimated using the inverse approach.

[5] The nonuniqueness problem can be resolved by estimating the recharge boundary condition explicitly using a separate hydrologic model that accounts for all the relevant hydrologic processes contributing to groundwater recharge. Estimating recharge explicitly using detailed site specific information on land use, soils, as well as temperature and precipitation, cannot only significantly improve groundwater model calibration, but may also be essential in certain modeling applications [*Jyrkama et al.*, 2002]. The traditional goal of minimizing the number of subjective recharge zones, hence fewer degrees of freedom, and adjusting the recharge rates during model calibration is therefore redundant and unnecessary.

[6] While the directly estimated recharge rates may provide a more realistic and reliable estimate of the recharge boundary condition than the traditional calibration approach, the results are still subject to error and uncertainty. The goal of this work therefore is not only to explore the sensitivity of the groundwater flow system to the recharge boundary condition, but also to investigate the impact of uncertainty in the estimated recharge rates on the flow solution, represented by head.

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[7] In this study, the recharge boundary condition is estimated using the method by *Jyrkama et al.* [2002]. The influence of uncertainty is investigated using the first-order reliability method (FORM), while the sensitivity analysis is accomplished by incorporating the adjoint method in MODFLOW [*McDonald and Harbaugh*, 1996]. Only the contribution of the uncertain recharge is considered in this work. All other parameters, such as hydraulic conductivities and sources/sinks are considered to be deterministic. The methodology is applied to a groundwater modeling study in New Jersey. Details of the modeling study have been published previously by *Jyrkama et al.* [2002].

[8] The first- and second-order reliability methods (FORM and SORM) were developed in the structural engineering field to evaluate the probability of failure of structural components and systems [e.g., *Hasofer and Lind*, 1974; *Ang and Tang*, 1984; *Madsen et al.*, 1986]. Reliability analysis considers the probabilistic nature of both random loads and resistances and seeks to find the limit state resulting in failure (and to evaluate its associated probability). However, violation of the limit state does not necessarily imply the catastrophic failure of a structure, and the performance function $g(\mathbf{X})$ can be formulated as any function of n-uncertain or random variables $\mathbf{X} = [x_1, \ldots, x_n]'$, where the prime indicates vector transpose.

[9] Reliability analysis has also been applied to both surface water problems [e.g., *Melching*, 1992; *Maier et al.*, 2001; *Melching and Bauwens*, 2001] and groundwater studies [e.g., *Sitar et al.*, 1987; *Cawlfield and Wu*, 1993; *Jang et al.*, 1994; *Hamed et al.*, 1996b; *Hamed and Bedient*, 1999; *Skaggs and Barry*, 1997; *Xiang and Mishra*, 1997; *Boateng and Cawlfield*, 1999; *Boateng*, 2001]. The focus of the groundwater investigations has usually been in contaminant transport analysis, where the failure condition is formulated as the exceedance of a specified concentration threshold, for example, regulatory standard, at a specific time and location [e.g., *Sitar et al.*, 1987; *Jang et al.*, 1994]. In this paper, we express the performance function in terms of piezometric head and consider the recharge distribution (i.e., boundary condition) as random or uncertain. The goal of the reliability analysis therefore is to estimate the reliability of head at a selected location in the domain (i.e., pumping well) due to uncertainties in the estimated recharge boundary condition.

[10] The main advantage of the reliability method over other probabilistic modeling approaches, such as Monte Carlo simulation, is its high computational efficiency. Except for some simple problems (e.g., analytical expressions) with only a few random variables, however, the method may also become computationally demanding because of the evaluation of the first- or second-order derivatives in the solution algorithm [*Hamed et al.*, 1996a, 1996b]. In this paper, we eliminate the heavy computational burden by using the adjoint method to compute the sensitivity vectors efficiently.

[11] The adjoint sensitivity method has been applied to both groundwater flow and contaminant transport problems. *Sykes et al.* [1985] and *Wilson and Metcalfe* [1985] derived equations for steady groundwater flow, while *Samper and Neuman* [1986], *Ahlfeld et al.* [1988], and *Sun and Yeh* [1990] adopted the method for contaminant transport applications. The adjoint sensitivity method has also been utilized in reliability analysis. Both *Mok et al.* [1994] and *Skaggs and Barry* [1996] implemented the adjoint method in their finite element contaminant transport models and compared it with the perturbation method. They found the adjoint method to be considerably more efficient in evaluating the sensitivity of the performance function with respect to the uncertain variables, and furthermore showed that the computational savings would increase with the size of the problem.

[12] In this study, the adjoint method is implemented in MODFLOW to compute the sensitivity of head with respect to the recharge boundary condition. These sensitivities are required for the solution of the reliability problem, that is, to determine the location of the design point in the optimization algorithm.

[13] Both FORM and the adjoint method are well known and are applied to many problems in hydrogeology. However, the integration of these two methods and their use to analyze uncertainty for a large-scale complex field problem is unique. The adjoint method, as implemented in MODFLOW, is an essential aspect of this work. The traditional, cumbersome use of direct parameter sampling methods to determine the sensitivity coefficients in FORM do not provide the efficiency that is necessary for large field-scale problems. In fact, many of the uncertainty techniques that have been published cannot be adapted to field-scale problems because of computational limitations. This paper demonstrates how these limitations can be resolved without having to resort to simulation methods such as Monte Carlo and Latin Hypercube sampling.

2. Mathematical Development

2.1. Reliability Analysis

[14] The performance measure or limit state equation $g(\mathbf{X})$ is formulated as

$$M = g(\mathbf{X}) = w(\mathbf{u})\left[\mathbf{h} - \tilde{\mathbf{h}}\right] \tag{1}$$

where $\mathbf{X}$ represents the vector of boundary recharge fluxes, $\mathbf{u} = [x, y, z]'$ is a location vector, $w(\mathbf{u})$ is an arbitrary weighing function denoting the region of importance, $\mathbf{h}$ are the simulated heads, and $\tilde{\mathbf{h}}$ are the specified target heads. The limit state equation is therefore solely a function of the piezometric head and only indirectly related to recharge through the boundary value problem (i.e., the groundwater flow equation). To simplify the analysis, we select a single location of interest $\mathbf{u}_P$ coinciding with the location of a pumping well such that

$$w(\mathbf{u}) = \delta(\mathbf{u} - \mathbf{u}_P) \tag{2}$$

where δ denotes the Dirac delta. The failure condition associated with the limit state equation therefore indicates the probability that the head at the pumping well would fall below a certain specified level $\tilde{h}_P$ because of uncertainties in the estimated recharge boundary condition. Or in other words, the probability associated with exceeding a specified drawdown at the well.

[15] The probability content associated with the failure region is obtained by integrating the joint probability density function (PDF) for the limit state equation as

$$P[g(\mathbf{X}) \le 0] = \int_{g(\mathbf{X}) \le 0} f_x(\mathbf{x}) \mathrm{d}x \tag{3}$$

where $f_x(\mathbf{x})$ is the joint PDF of $\mathbf{X}$, integrated over the entire failure domain. Because the joint PDF for the model parameters is practically always unknown, either simulation methods or approximation methods such as FORM and SORM must be used.

2.1.1. First-Order Reliability Method

[16] The principle of the first-order reliability method (FORM) is to transform the problem from the space of the basic random variables $\mathbf{X}$ into the space of uncorrelated standard normal variables $\mathbf{Y}$. The transformation depends on the nature and availability of statistical information and any underlying correlation between the basic random variables.

[17] Assuming the correlation structure, the first two moments, and marginal distributions for each of the random variables are known, the problem is first transformed into *correlated* standard normal variates $\mathbf{Z}$ as

$$\mathbf{Z} = \begin{Bmatrix} \Phi^{-1}[F_{x_1}(x_1)] \\ \vdots \\ \Phi^{-1}[F_{x_n}(x_n)] \end{Bmatrix} \tag{4}$$

where Φ^{-1} is the inverse of the standard normal distribution and F_{x_1} is the cumulative distribution function of the uncertain variable x_1. The *correlated* standard normal variates are then transformed into *uncorrelated* standard normal variates as

$$\mathbf{Y} = \boldsymbol{\Gamma}_o \mathbf{Z} \tag{5}$$

where $\boldsymbol{\Gamma}_o$ is the lower triangular matrix resulting from the Cholesky decomposition of the correlation matrix $\mathbf{R}_o$, that is, $\boldsymbol{\Gamma}_o = \mathbf{L}_o^{-1}$. The transformation also maps the limit state surface into standard normal space such that $g(\mathbf{X}) \equiv G(\mathbf{Y})$. The elements of the correlation matrix $\mathbf{R_o}$ for the correlated standard normal variates $\mathbf{Z}$ are related to the basic variables $\mathbf{X}$ through the Nataf transformation [*Der Kiureghian and Liu*, 1986]. In the case of no correlation between the basic random variables, the solution is obtained using a single transformation.

[18] The closest point to the origin on the transformed n-dimensional failure surface is referred to as the design point $\mathbf{Y}^*$ which is also the most likely point leading to $P[G(\mathbf{Y}) = 0]$. In this case, this represents the most likely realization of recharge values that results in the exceedance of a specified drawdown at the pumping well.

[19] In FORM, the limit state surface is approximated by a tangent hyperplane using a first-order Taylor series expansion at the design point

$$G(\mathbf{Y}) \approx G(\mathbf{Y}^*) + \nabla_{\mathbf{Y}} G(\mathbf{Y})' \cdot (\mathbf{Y} - \mathbf{Y}^*) \tag{6}$$

where $\nabla_{\mathbf{Y}} G(\mathbf{Y})' = \left[\frac{\partial G(\mathbf{Y})}{\partial y_1}, \ldots, \frac{\partial G(\mathbf{Y})}{\partial y_n} \right]$. The gradients can be related to the basic variables through the chain rule

$$\nabla_{\mathbf{Y}} G(\mathbf{Y}) = \nabla_{\mathbf{X}} g(\mathbf{X})' \cdot \mathbf{J}_{\mathbf{Y,X}}^{-1} \tag{7}$$

where $\mathbf{J_{Y,X}}$ is the Jacobian of the transformation from $\mathbf{X}$ to $\mathbf{Y}$ defined in (5).

[20] The distance from the origin to the design point is referred to as the reliability index β [*Hasofer and Lind*, 1974] and is given as the inner vector product

$$\beta = -\boldsymbol{\alpha}^* \cdot \mathbf{Y}^* \tag{8}$$

where $\boldsymbol{\alpha}^*$ is the unit outward normal to the limit state surface. The first-order approximation of the probability integral (3) is expressed as

$$P_f \approx \Phi(-\beta) \tag{9}$$

[21] The FORM approximation is reasonable as long as the limit state surface is relatively flat near the design point [*Sitar et al.*, 1987]. Higher-order methods such as SORM may provide better approximation to the limit state surface, however, the added improvement comes at a significantly higher computation cost [*Rackwitz*, 2001].

2.1.2. Probabilistic Sensitivity Factors

[22] The direction cosines α_i describe the sensitivity of the reliability index with respect to variations in each of the standard variates. The sensitivity of β with respect to the basic variables is described by the unit gamma sensitivity vector

$$\boldsymbol{\gamma} = \frac{(\nabla_{\mathbf{X}^*}\beta)\mathbf{D}}{|(\nabla_{\mathbf{X}^*}\beta)\mathbf{D}|} \tag{10}$$

which can also be written as

$$\boldsymbol{\gamma} = \frac{\boldsymbol{\Gamma}_o' \boldsymbol{\alpha}^*}{|\boldsymbol{\Gamma}_o' \boldsymbol{\alpha}^*|} \tag{11}$$

where $\mathbf{D}$ is the diagonal matrix of standard deviations. The unit gamma sensitivities therefore describe the relative importance of each of the input parameters, that is, the recharge boundary condition, on the probabilistic outcome.

2.1.3. Method of Solution

[23] The most challenging part of the reliability analysis is in finding the coordinates of the design point on the failure surface. The location of the design point is obtained by solving the nonlinear constrained optimization problem

$$\min(\beta) \tag{12}$$

subject to

$$G(\mathbf{Y}) = 0 \tag{13}$$

[24] Applying the Lagrange multiplier method to (6) results in a sequential linearization algorithm [*Hasofer and Lind*, 1974; *Rackwitz and Fiessler*, 1978]

$$\mathbf{Y}_{k+1} = \frac{1}{|\nabla_{\mathbf{Y}} G(\mathbf{Y}_k)|^2} \left[\nabla_{\mathbf{Y}} G(\mathbf{Y}_k)' \cdot \mathbf{Y}_k - G(\mathbf{Y}_k) \right] \nabla_{\mathbf{Y}} G(\mathbf{Y}_k) \tag{14}$$

Either the mean point in the original variable space or the origin in the standard normal space is often taken as the first point in the iteration sequence. To ensure convergence, the nonnegative merit function introduced by *Liu and Der Kiureghian* [1991] is used

$$m(\mathbf{Y}) = \frac{1}{2}\left|\mathbf{Y} - \frac{\nabla_{\mathbf{Y}} G(\mathbf{Y})' \cdot \mathbf{Y}}{|\nabla_{\mathbf{Y}} G(\mathbf{Y})|^2} \nabla_{\mathbf{Y}} G(\mathbf{Y})^2\right| + \frac{1}{2} c G(\mathbf{Y})^2 \qquad (15)$$

where c is a positive constant. A new point $\mathbf{Y}_{k+1}$ is selected if the new merit function is less than the old value, that is, if $m(\mathbf{Y}_{k+1}) < m(\mathbf{Y}_k)$, otherwise midpoint approximation between the old and the new point is used.

[25] For complex performance functions without closed form expressions for the first-order derivatives, the gradient vector can be approximated using the small perturbation or finite difference approach [e.g., *Hamed et al.*, 1996a]

$$\nabla_{\mathbf{X}} g(\mathbf{X}) = \frac{\partial g(\mathbf{X})}{\partial x_i} \approx \frac{g(x_i + \Delta x_i) - g(x_i - \Delta x_i)}{2\Delta x_i} \qquad (16)$$

for a selected small step size Δx_i. For numerical problems, however, the evaluation of the gradient vector using finite differences can become very demanding computationally because of the large number of random variables resulting from model discretization. This computational limitation has often restricted the use of FORM to applications with relatively few parameters; large-scale problems with spatially distributed parameters have presented a challenge. This challenge is overcome in this paper using the adjoint method.

2.2. Adjoint Method

[26] Transient three-dimensional saturated groundwater flow in heterogeneous anisotropic porous media is expressed as [*Bear*, 1972]

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial h}{\partial x_j}\right) \pm Q = S_s \frac{\partial h}{\partial t} \qquad (17)$$

where K_{ij} is the hydraulic conductivity tensor, h is the hydraulic head, Q represents sources or sinks from pumping and recharge, and S_s is the specific storage. Because fully saturated models only describe groundwater flow below the water table, the specification of either the location of the water table (Dirichlet, type I) or the recharge flux (Neumann, type II) is required as the top or upper boundary.

[27] The above problem can be described in matrix form as

$$\mathbf{A}(\boldsymbol{\theta}, \mathbf{h})\mathbf{h} = \mathbf{q}(\hat{\boldsymbol{\eta}}) \qquad (18)$$

where $\mathbf{A}$ is the symmetric matrix of head coefficients, $\boldsymbol{\theta}$ are system parameters, $\mathbf{h}$ are the head values, and $\mathbf{q}$ is the vector of constant terms, or **RHS**, which is a function of the model boundary conditions $\hat{\boldsymbol{\eta}}$ [*McDonald and Harbaugh*, 1996]. Because the objective of this study is to investigate the impact of the recharge boundary condition on the groundwater flow system, only the recharge rates are assumed to be random or uncertain, while all other model parameters are assumed to be deterministic.

[28] The solution of the first-order reliability problem requires the sensitivity of the limit state equation $g(\mathbf{X})$ with respect to the recharge boundary condition. The marginal sensitivity of a specified performance measure M with respect to the recharge rate vector $\mathbf{X}$ is

$$\frac{\partial M}{\partial \mathbf{X}'} = \frac{\partial M(\mathbf{h})}{\partial \mathbf{h}'}\frac{\partial \mathbf{h}}{\partial \mathbf{X}'} \qquad (19)$$

[29] Expressing the flow problem (18) in terms of head and recharge only, and differentiating with respect to vector $\mathbf{X}$ gives

$$\frac{\partial \mathbf{A}(\mathbf{h})}{\partial \mathbf{h}'}\frac{\partial \mathbf{h}}{\partial \mathbf{X}'}[\mathbf{I} * \mathbf{h}] + \mathbf{A}(\mathbf{h})\frac{\partial \mathbf{h}}{\partial \mathbf{X}'} = \frac{\partial \mathbf{q}(\mathbf{X})}{\partial \mathbf{X}'} \qquad (20)$$

where $\mathbf{I}$ is the identity matrix and $*$ denotes the Kronecker or outer product.

[30] Designating the state sensitivity $\partial \mathbf{h}/\partial \mathbf{X}'$ with ψ, the adjoint equations of the partial differential equations are formulated by multiplying (20) by an arbitrary differentiable constant $\tilde{\psi}$ and subtracting the result from (19) to give

$$\frac{\partial M}{\partial \mathbf{X}'} = \left[\frac{\partial M(\mathbf{h})}{\partial \mathbf{h}'}\right]\psi - \tilde{\psi}'\left[\frac{\partial \mathbf{A}(\mathbf{h})}{\partial \mathbf{h}'}\psi[\mathbf{I} * \mathbf{h}]\right] - \tilde{\psi}'\mathbf{A}(\mathbf{h})\psi + \tilde{\psi}'\frac{\partial \mathbf{q}(\mathbf{X})}{\partial \mathbf{X}'} \qquad (21)$$

[31] Collecting terms,

$$\frac{\partial M}{\partial \mathbf{X}'} = \left(\left[\frac{\partial M(\mathbf{h})}{\partial \mathbf{h}'}\right] - \tilde{\psi}'\left[\frac{\partial \mathbf{A}(\mathbf{h})}{\partial \mathbf{h}'}[\mathbf{I} * \mathbf{h}]\right] - \tilde{\psi}'\mathbf{A}(\mathbf{h})\right)\psi + \tilde{\psi}'\frac{\partial \mathbf{q}(\mathbf{X})}{\partial \mathbf{X}'} \qquad (22)$$

Since $\tilde{\psi}$ is arbitrary, we let

$$\left[\frac{\partial M(\mathbf{h})}{\partial \mathbf{h}'}\right] - \tilde{\psi}'\left[\frac{\partial \mathbf{A}(\mathbf{h})}{\partial \mathbf{h}'}[\mathbf{I} * \mathbf{h}]\right] - \tilde{\psi}'\mathbf{A}(\mathbf{h}) = 0 \qquad (23)$$

which yields

$$\left[\mathbf{A}(\mathbf{h}) + \frac{\partial \mathbf{A}(\mathbf{h})}{\partial \mathbf{h}'}[\mathbf{I} * \mathbf{h}]\right]'\tilde{\psi} = \frac{\partial M(\mathbf{h})}{\partial \mathbf{h}'} \qquad (24)$$

where $\tilde{\psi}$ represents the adjoint state or importance function [*Sykes et al.*, 1985]. The second term on the left hand side of (24) will be shown to have a negligible impact on the reliability solution for the system investigated in this study, and is therefore ignored. However, it may be the case that the term is important for other systems. Equation (24) thus becomes

$$[\mathbf{A}(\mathbf{h})]'\tilde{\psi} = \frac{\partial M(\mathbf{h})}{\partial \mathbf{h}'} \qquad (25)$$

which is also termed the adjoint or backward problem.

[32] Using the definition of the performance measure given in (1) the load term on the right hand side of (25) becomes

$$\frac{\partial M(\mathbf{h})}{\partial \mathbf{h}'} = w(\mathbf{u}) \qquad (26)$$

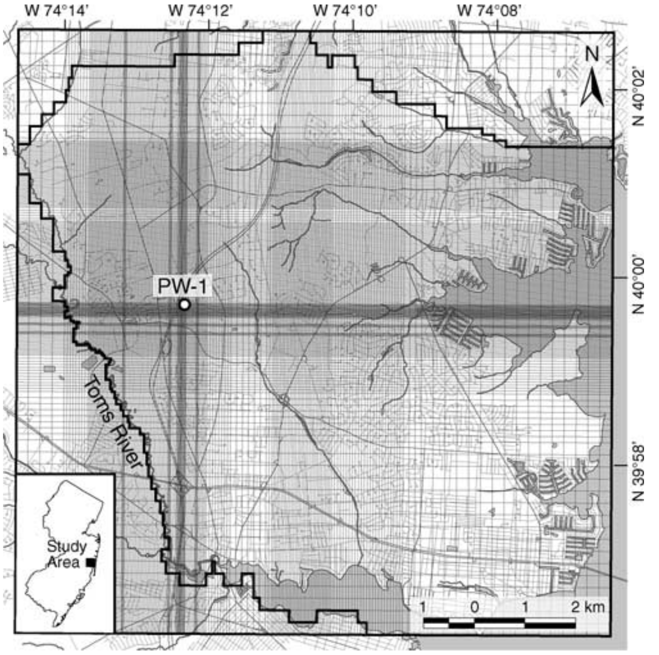

Figure 1. Study area location and MODFLOW finite difference grid.

resulting in the final form of the backward problem

$$[\mathbf{A}(\mathbf{h})]'\tilde{\psi} = w(\mathbf{u}) \tag{27}$$

where the weighing function is equal to 1 at the location of interest $\mathbf{u}_P$, and is zero elsewhere. The importance function in (27) therefore represents the increase of head at all locations in the domain due to a unit volumetric influx of water at the selected location $\mathbf{u}_P$ (i.e., the pumping well). Similar to the use of direct parameter sampling for the determination of the marginal sensitivities, the adjoint method also yields local derivatives.

2.3. MODFLOW Implementation

[33] Evaluation of the gradient sensitivity vector requires the solution of (18) which is termed the forward problem and is solved first for the coefficient matrix **A** and the head distribution **h**, while the backward problem (27) is used to calculate the importance function $\tilde{\psi}$ for the performance measure M.

[34] The marginal sensitivity of the performance measure with respect to the system parameters is obtained from (22) as

$$\frac{\partial M}{\partial \mathbf{X}'} = \tilde{\psi}' \frac{\partial \mathbf{q}(\mathbf{X})}{\partial \mathbf{X}'} \tag{28}$$

In MODFLOW, **q** is formulated in terms of the recharge volume; that is, **q** is the product of recharge rate and grid block area. Since **X** is the vector of recharge rates, the derivative $\frac{\partial \mathbf{q}(\mathbf{X})}{\partial \mathbf{X}'}$ in (28) simply reduces to the grid block area, leading to

$$\frac{\partial M}{\partial \mathbf{X}'} = \nabla_x g(\mathbf{X}) = \tilde{\psi}' \Delta\mathbf{r}\Delta\mathbf{c} \tag{29}$$

where $\Delta\mathbf{r}$ and $\Delta\mathbf{c}$ denote the dimensions of the finite difference grid blocks in the row and column directions, respectively. The sensitivity of head with respect to the recharge boundary condition $\nabla_{\mathbf{X}} g(\mathbf{X})$ is therefore simply equal to the value of the importance function $\tilde{\psi}$ in each grid block multiplied by the horizontal grid block area.

[35] The adjoint problem can be readily solved using MODFLOW with only minor changes to the original code. The solution is obtained by (1) running MODFLOW (forward problem) to obtain the **A** matrix, (2) setting the **RHS** vector equal to zero, except for the grid cell containing the head of interest, which is set to one, and (3) rerunning MODFLOW using the new **RHS** to obtain the importance function $\tilde{\psi}$.

[36] While the forward problem is nonlinear, the adjoint problem is linear with passive boundary conditions. That is, there is no loading except at the node of interest. The method was implemented in MODFLOW-96 [*McDonald and Harbaugh*, 1996].

[37] The sensitivities could also be calculated alternatively similar to MODFLOWP as implemented in MODFLOW-2000 [*Harbaugh et al.*, 2000]. MODFLOW-2000 calculates sensitivities for hydraulic head throughout the model using the sensitivity equation method [*Hill et al.*, 2000]. As discussed previously, however, the main advantage of the adjoint method is that it allows computationally efficient evaluation of all the sensitivities in a single model run.

3. Model Application

3.1. Study Area

[38] The study area is located in Toms River, New Jersey, and is shown in Figure 1 along with the MODFLOW grid and the location of the pumping well PW-1 investigated in this study. The model domain covers approximately 139 km^2 of fairly flat coastal topography typical of New Jersey. The groundwater model was used as a forensic tool for investigating the historical origin of a contaminant plume and its impact on a municipal wellfield. Details of the model have previously been published by *Jyrkama et al.* [2002].

[39] The model domain was discretized into 208 rows by 200 columns with 4 vertical layers. The computational grid was refined around pumping areas. The permeable Cohansey-Kirkwood unit forms the primary aquifer in the area [e.g., *Vyas et al.*, 2004], and is underlain by the basal clay Kirkwood formation. The hydraulic conductivity distribution was estimated from numerous well records and ranged from 1.5 m/day to 50 m/day across the domain. The general direction of groundwater flow is toward the southeast corner of the domain.

3.2. Recharge Boundary Condition

[40] Whereas the clay Kirkwood formation forms the type II, no-flow bottom boundary for the groundwater model, the top or upper boundary of the model was described using the General Head Boundary (GHB), River (RIV) and Recharge (RCH) packages in MODFLOW. The lateral model boundaries were described using rivers and surface water divides. The estimation of the recharge boundary is described in detail by *Jyrkama et al.* [2002]. The recharge distribution for the study area was derived by running a physically based hydrologic model for each

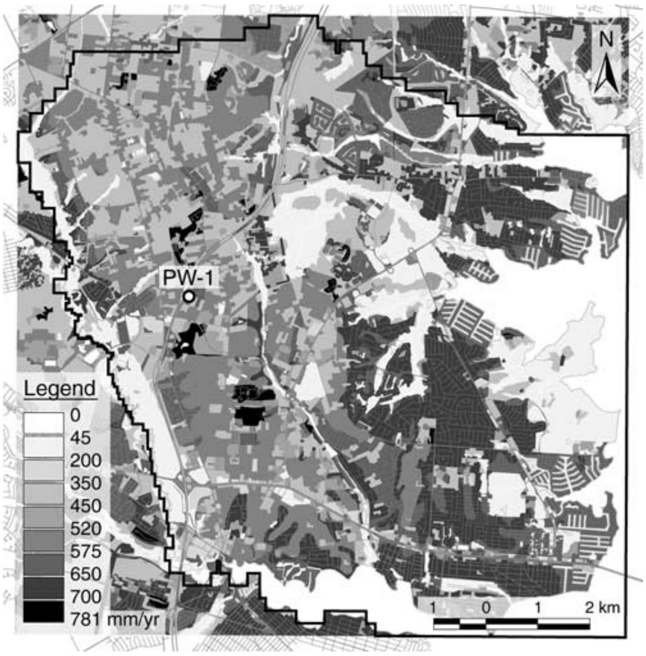

Figure 2. Average annual recharge rates for the elementary units.

combination of unique land use, soil, and the level of surface imperviousness in the area. The unique combinations, also referred to as elementary units (EU) or the smallest possible modeling units which could be considered quasi-homogeneous [*Lahmer et al.*, 1999], were identified by overlaying detailed spatial data maps in the GIS environment. Unlike aggregation methods such as the hydrological response unit (HRU) concept [e.g., *Bormann et al.*, 1999] which seek computational savings by combining the hydrologic processes (e.g., recharge) into similar groups, the recharge rates were estimated exclusively for each of the EUs. The analysis was therefore conducted at the scale of the input data, with the only limitation being the number and spatial resolution of the independent data maps.

[41] The average annual (or steady state) recharge rates for the elementary units are shown in Figure 2. The recharge map clearly reflects the strong influence of different land uses and soils on the recharge process in the study area. The recharge flux boundary condition for the groundwater model was computed using areal averages, that is, on the basis of the areal contribution of EUs within each boundary grid block.

3.3. Initializing FORM

[42] While equation (29) describes the sensitivity of head with respect to each of the recharge boundary grid blocks in the groundwater flow model, the sensitivities can also be related back to each of the elementary units through the chain rule as

$$\frac{\partial M}{\partial \mathbf{R}'} = \frac{\partial M}{\partial \mathbf{X}'}\frac{\partial \mathbf{X}}{\partial \mathbf{R}'} = \sum_{i=1}^{n} \tilde{\psi}_i \Delta r_i \Delta c_i \hat{a}_i \qquad (30)$$

where $\mathbf{R}$ are the recharge rates for each of the unique landcover combinations, n is the number of grid blocks intersecting each combination, and $\hat{a}$ is the proportion of the area within each of the intersected grid blocks i. Equation (30) therefore allows the assessment of the impact of recharge on the groundwater flow system independent of the groundwater model discretization. That is, the sensitivity of the performance measure is related back to the recharge rates and areas derived explicitly from the physically based recharge methodology.

[43] The estimated recharge rates for each of the elementary units were considered uncertain in the reliability analysis, resulting in a total of 8883 random variables or individual areas of recharge. All other model parameters were considered deterministic, as established from a detailed transient model calibration to nearly 410,000 discrete water level measurements of more than 100 monitoring wells over a 30 year period [*Jyrkama et al.*, 2002].

[44] The uncertain recharge rates were assumed to be lognormally distributed with the mean condition described by the average annual values illustrated in Figure 2. The coefficient of variation (COV), which is the ratio of standard deviation to the mean, was used to reflect uncertainty in the estimates. The same COV was assumed for all recharge rates in each simulation and no correlation was assumed between the parameters. The determination of correlation, if any, between the recharge EUs is beyond the scope of this study.

[45] The objective of the reliability analysis was to find the distribution of recharge (with a specified level of uncertainty) that would cause the head in the well to be less than or equal to a selected target level. Simulations were conducted for various COVs and target head levels. All simulations were run until the limit state equation (1); that is, the head difference in the well was less than 0.001 m. The algorithm was computationally very efficient as convergence in each simulation was generally obtained in only a few iterations. The mean point in the standard normal

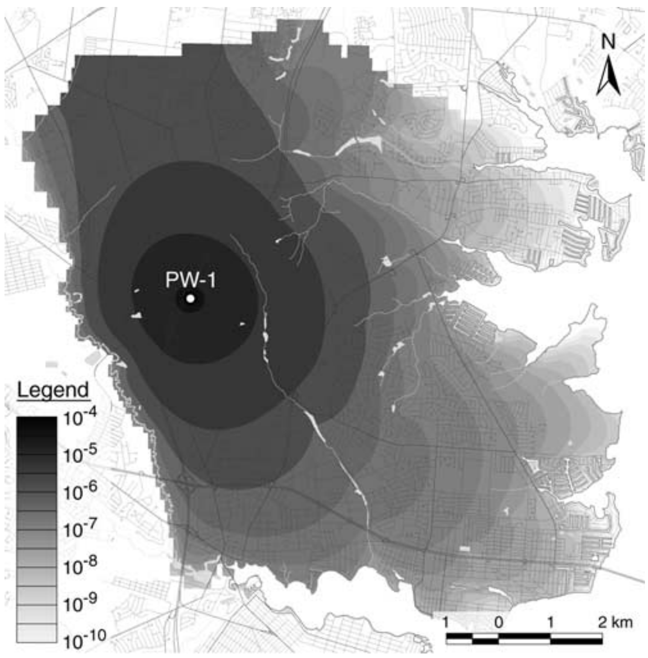

Figure 3. Importance function obtained from the solution of the adjoint problem.

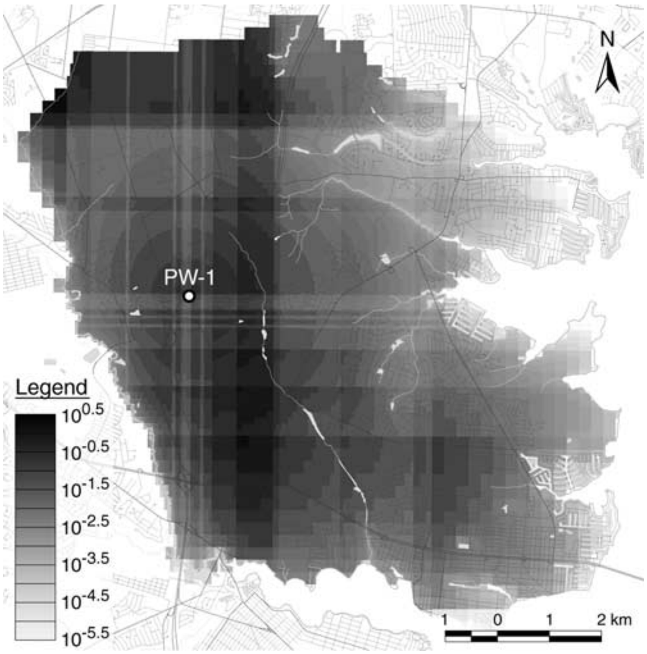

Figure 4. Marginal sensitivity of head at the well with respect to the MODFLOW recharge boundary condition.

space was used as the starting point for all simulations. The overall analysis was conducted using Visual Basic programming, while MODFLOW was used solely for the computation of the head distribution and importance function at each iteration cycle of the optimization algorithm.

4. Model Results

4.1. Adjoint Sensitivities

[46] The adjoint state variable or importance function $\tilde{\psi}$ from the backward problem is shown in Figure 3. The value of the function decreases exponentially with distance from the selected well as a result of the unit injection of water into the system at the well. Multiplying the value of the function with the horizontal grid block areas according to equation (29) yields the sensitivity of the head at the well with respect to recharge in each of the MODFLOW boundary grid blocks. These marginal sensitivities are shown in Figure 4. As expected, the sensitivities are positive indicating that recharge has a positive influence on the head at the well (i.e., increasing recharge will increase the head).

[47] As indicated by Figure 4, the head in the well may not necessarily be influenced by recharge changes in the closest grid blocks, but it can be highly sensitive to areas farther away. The marginal sensitivities are shown by equation (29) to be only dependent on the importance function and the grid block areas. Therefore there is no direct contribution from the estimated recharge boundary fluxes on the sensitivity gradients. The importance function in (29) does depend on recharge, but only very weakly, as the **A** matrix from the forward problem (18) depends on the heads which, in turn, are influenced by the boundary conditions. Equation (29) and Figure 4 therefore demonstrate that the sensitivity of head with respect to recharge is essentially independent of the actual recharge rates, thereby exposing the central weakness of arbitrariness in the traditional approach of recharge calibration in a handful of subjective areas or zones.

[48] The main advantage of the adjoint sensitivity analysis is demonstrated in Figure 5 which shows the marginal sensitivity of head at the well with respect to the recharge rate in each of the elementary areas as calculated using (30). Figure 5 identifies the sensitivities on the basis of the delineation of land use and soils in the study area and therefore allows the assessment of the impact of recharge on the groundwater flow system independent of the groundwater model discretization. The sensitivities were furthermore obtained in a single MODFLOW run (i.e., forward and back) as opposed to $208 \times 200 = 41{,}600$ runs that would be required by the small perturbation approach. Although Figure 5 only gives the sensitivity of head in a single location to the recharge boundary condition, other performance measures could also be readily considered.

4.2. Reliability Analysis

[49] A typical result of the reliability analysis is illustrated in Figure 6. In this case, the target head at the well was assumed to be 0.5 m below the initial mean value, with a COV of 0.3 for the 8883 uncertain recharge rates (other COVs and target heads were also used and will be discussed later). The plot illustrates the percent difference in recharge between the mean condition (i.e., average annual recharge distribution) and the distribution of recharge that resulted in failure (i.e., the most likely realization of recharge that resulted in the head being equal to 0.5 m below the mean level at the well).

[50] As expected, Figure 6 appears to be very similar to Figure 5. Because of the nature of the gradient optimization algorithm, the recharge rates are changed the most for areas that have the highest influence on the head at the well (darker areas in Figure 5) while the less sensitive areas are

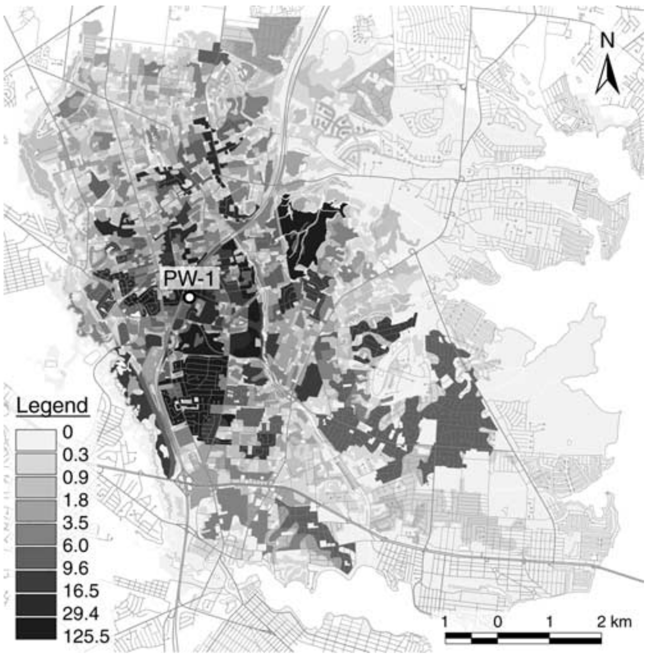

Figure 5. Marginal sensitivity of head at the well with respect to the recharge rate in each elementary unit.

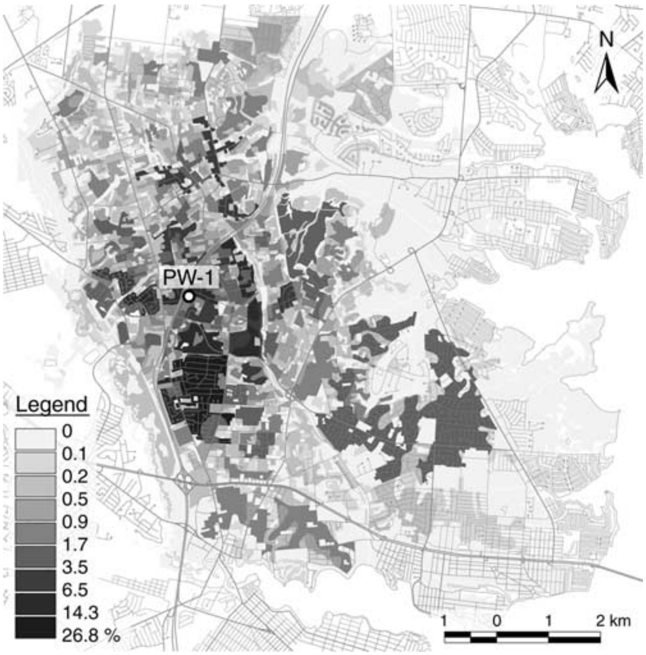

Figure 6. Percent difference in recharge between the mean and failure conditions (for $\tilde{h}_P = -0.5$ m and COV = 0.3).

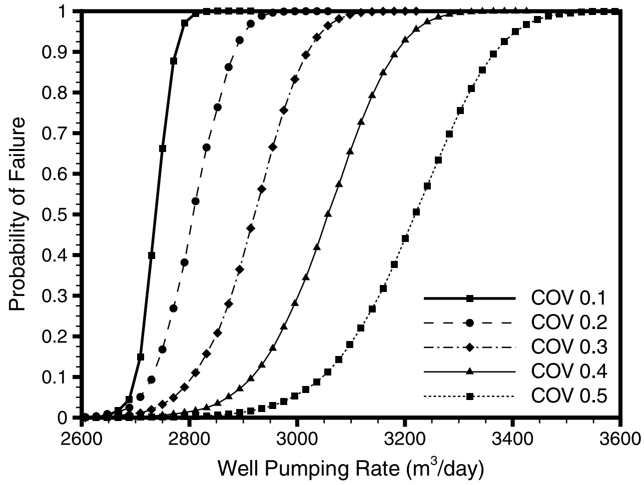

Figure 8. Probability of failure with respect to the pumping rate at the well.

subjected to a lesser change (lighter areas in Figure 5). As shown in Figure 6, the recharge rates were reduced by up to 27% in certain areas in order to drop the head in the well by 0.5 m. The estimated probability of failure using (9), that is, the probability associated with the 0.5 m drawdown at the well given the assumed uncertainty in the recharge distribution, was equal to 3.54×10^{-2}.

[51] The cumulative distribution function for the probability of failure at the well, shown in Figure 7, can be constructed by repeating the reliability analysis for various COVs and target head levels. As indicated, the probability of failure increases with the assumed uncertainty in the estimated recharge distribution. For example, for COV of 0.5 there is an 89% probability that the head at the well is greater than or equal to 0.5 m below the mean level (i.e., the drawdown at the well exceeds 0.5 m), while the probability is 53% for COV of 0.4. Increasing the confidence in the estimated recharge distribution will therefore decrease the probability of failure (or increase the reliability) of the simulated head at the well.

[52] The results of the reliability analysis can also be related to the pumping rate at the well by substituting the pump curve into the limit state equation. The steady state or mean pumping rate of the well was equal to 2715 m^3/day. The cumulative distribution function with respect to pumping is shown in Figure 8. In this case, failure means the probability that the well could be pumped at a certain rate without changing the simulated head at the well from the mean condition (i.e., no additional drawdown). For example, as shown in Figure 8, there is an 8% probability that there would be an increase in drawdown, that is, head less than the mean value, if the well was pumped at 2800 m^3/day for COV of 0.3. Or in terms of reliability $(1 - P_f)$, for the same assumed uncertainty in the estimated recharge distribution, there is a 92% probability that the well could be pumped at 2800 m^3/day without changing the simulated head at the well.

[53] Figures 7 and 8 can therefore be used to determine the reliability of the head at the pumping well due to uncertainties in the estimated groundwater recharge rates. Because of the large number of random variables, estimation of the probability distributions using other methods, such as Monte Carlo simulation, would require considerably longer computation times.

[54] The unit gamma sensitivities, shown in Figure 9, describe the relative importance of each of the input parameters, that is, individual recharge rates, on the probabilistic outcome. The steady state capture zone for the pumping well determined under mean conditions is also included in Figure 9. As indicated by equation (10), the unit gamma sensitivity is scaled by the standard deviations and measures the sensitivity of the reliability index with respect to equally likely changes in the random variables, that is, the recharge rates. The negative signs in Figure 9 indicate an inverse relationship, that is, increasing the recharge rates will result in a decrease in the probability of failure. In other

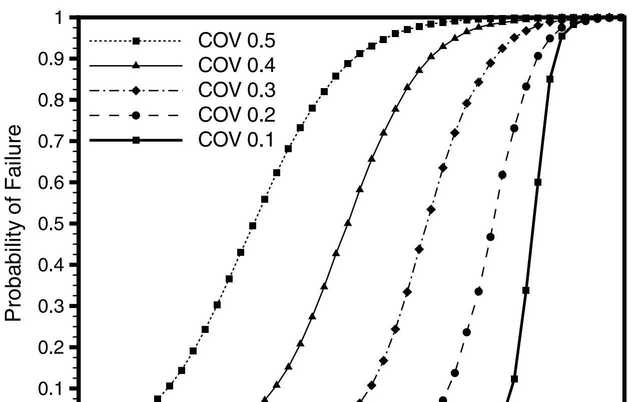

Figure 7. Probability of failure with respect to the target head at the well.

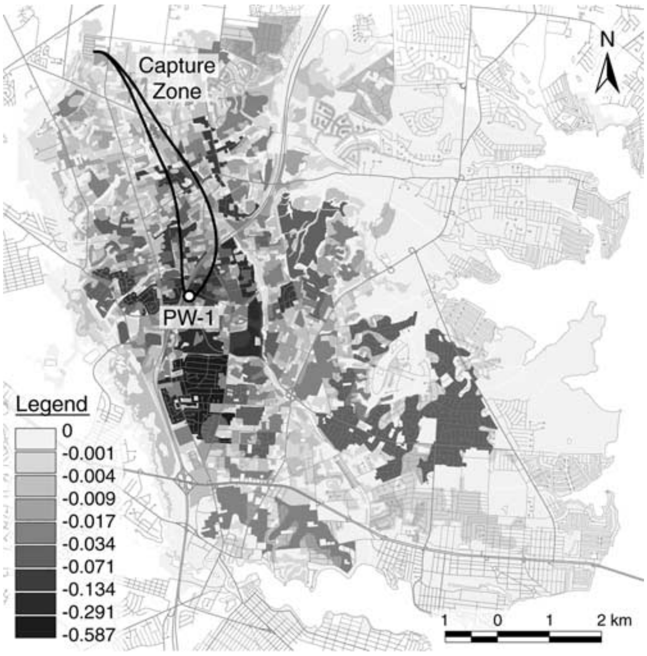

Figure 9. Unit gamma sensitivity.

words, increasing recharge will increase the reliability of head at the well.

[55] The most important feature of Figure 9 is that it readily identifies land use areas that have the highest impact on the probability of failure (or reliability) at the well. It is evident that the recharge rate in areas that are quite distant from the pumping well (and also downgradient and outside the steady state well capture zone) can have a significant impact on the head at the well (recall Figures 4 and 5). From a land use management perspective therefore Figure 9 identifies the most important land use areas that should be protected in order to maintain the head and hence production at the pumping well. This concept is generally neglected by wellhead protection programs which base their land use planning and management decisions purely on water quality criteria (i.e., the area bounded by the well capture zone).

4.3. Assumptions and Limitations

[56] Besides the underlying limitations and assumptions of using FORM as opposed to using a higher-order approximation method such as SORM, one of the key assumptions in the analysis is the exclusion of the second term in the left hand side of the adjoint problem (24). This assumption is necessary in order to efficiently and easily implement the adjoint method in MODFLOW without serious and extensive modifications to the actual code.

[57] For confirmation, the results from the adjoint method were compared to perturbation analysis of selected grid blocks across the domain. A total of 175 grid blocks of various sizes and distances from the well were used in the analysis. Both central and forward finite difference approximations were used to estimate the sensitivity of the head at the well to the recharge rate at the selected grid blocks. The results from the analysis are shown in Figure 10. As indicated by Figure 10, the estimated adjoint sensitivities match quite well with the perturbation approach indicating that the nonlinear term in (24) has a negligible impact on the solution in this particular study.

[58] It should be added that some numerical instabilities related to the magnitude of the perturbation were encountered in the analysis; therefore various levels of perturbation were applied for each grid block. The head distribution simulated by MODFLOW is highly unstable and subject to the choice of equation solvers and their various control parameters and convergence criteria. Both input and output parameters are also specified and reported using single precision resulting in potential round off errors. Perturbing the recharge rate in a single grid block may consequently result in a completely unrealistic change in head at the location of interest (or even no change at all!). Therefore great care should be taken when using MODFLOW for calculating head-dependent perturbation marginal sensitivities.

5. Summary and Conclusions

[59] The first-order reliability method (FORM) was integrated with MODFLOW to study the influence of recharge on the groundwater flow system. The performance function was formulated in terms of head and flow rate at a pumping well, while the spatially varying steady state or mean recharge distribution was derived from a separate physically based hydrologic model utilizing detailed soil and land use information. All model parameters were considered deterministic except for the statistically described recharge rates which were assumed to be lognormally distributed. The coefficient of variation (COV) was used to reflect uncertainty in the estimates.

[60] The heavy computational burden of calculating the gradient sensitivity vector in the reliability analysis was overcome by implementing the adjoint method in MODFLOW. Consequently, the sensitivity of the performance function to recharge in all the boundary grid blocks

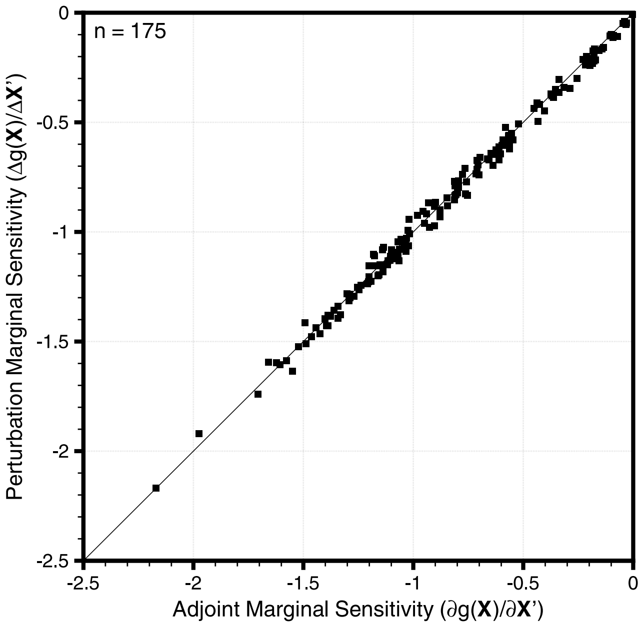

Figure 10. Perturbation versus adjoint marginal sensitivities for selected MODFLOW boundary grid blocks. Root-mean-square (RMS) error is equal to 6.25×10^{-2}.

could be computed in a single model run with only minor changes to the original MODFLOW code. The influence of the original physically based recharge distribution on the performance function was furthermore obtained using the grid block marginal sensitivities. This allowed the assessment of the impact of recharge on the groundwater flow system independent of the groundwater model discretization.

[61] The method was applied to a study area in New Jersey to estimate the sensitivity and uncertainty in flow and head at a selected pumping well due to uncertainties in the estimated recharge distribution. The results from the adjoint sensitivity analysis demonstrated how the sensitivity of head at the well with respect to the recharge boundary condition was only dependent on the importance function and the grid block areas. The gradients were therefore insensitive to the estimated recharge fluxes, thereby revealing the arbitrary nature and central weakness of the traditional approach of recharge calibration in a handful of subjective areas or zones.

[62] The first-order reliability analysis not only quantified the reliability of the head at the well in terms of uncertainties in the recharge distribution, but, through the normalized gamma sensitivity coefficient, also delineated areas of recharge that had the highest impact on the head and flow rate at the well. The results clearly demonstrated how distant land use areas that were completely outside and downgradient from the steady state well capture zone could have the greatest impact on the head at the well. Therefore land use planning and management decisions, as dictated by the traditional wellhead protection programs, need to extend beyond the well capture zones in order to ensure the protection of both the quality and quantity of our undergroundwater supplies.

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