Groundwater

Uncertainty Analysis of a Groundwater Flow Model in East-Central Florida

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Abstract

A groundwater flow model for east-central Florida has been developed to help water-resource managers assess the impact of increased groundwater withdrawals from the Floridan aquifer system on heads and spring flows originating from the Upper Floridan Aquifer. The model provides a probabilistic description of predictions of interest to water-resource managers, given the uncertainty associated with system heterogeneity, the large number of input parameters, and a nonunique groundwater flow solution. The uncertainty associated with these predictions can then be considered in decisions with which the model has been designed to assist. The "Null Space Monte Carlo" method is a stochastic probabilistic approach used to generate a suite of several hundred parameter field realizations, each maintaining the model in a calibrated state, and each considered to be hydrogeologically plausible. The results presented herein indicate that the model's capacity to predict changes in heads or spring flows that originate from increased groundwater withdrawals is considerably greater than its capacity to predict the absolute magnitudes of heads or spring flows. Furthermore, the capacity of the model to make predictions that are similar in location and in type to those in the calibration dataset exceeds its capacity to make predictions of different types at different locations. The quantification of these outcomes allows defensible use of the modeling process in support of future water-resources decisions. The model allows the decision-making process to recognize the uncertainties, and the spatial or temporal variability of uncertainties that are associated with predictions of future system behavior in a complex hydrogeological context.

Introduction

A population increase of nearly 70% from 1990 to 2010 in Lake, Orange, Osceola, Polk, and Seminole Counties in east-central Florida (Florida Office of Economic and Demographic Research 2012) has increased the demand for groundwater from the Floridan aquifer system (FAS), the primary source of water for potable, industrial, and agricultural purposes. In parts of Lake, Orange, Osceola, Polk, and Seminole Counties (Figure 1), declines in heads and spring flows, as well as increases in groundwater chloride concentrations, have occurred in the Upper Floridan Aquifer (UFA), the upper hydrogeologic unit of the FAS. The declines have been attributed to groundwater withdrawals and long-term below-average rainfall. To assist water-resource managers in assessing the effects of several proposed regional groundwater use scenarios on the potentiometric surfaces of the FAS and on spring flows that are of ecological and social importance, a groundwater flow model for east-central Florida was developed by Sepúlveda et al. (2012).

The regional hydrogeologic units in east-central Florida, in descending order, consist of the surficial aquifer system (SAS, Layer 1), the intermediate confining unit (ICU, Layer 2), and the units within the FAS. The FAS is composed of the UFA (Layers 3 to 5), the middle confining units I and II (MCU I/II, Layer 6), and the Lower Floridan Aquifer (LFA, Layer 7). The hydrogeologic units within the UFA include the Ocala permeable zone (OPZ, Layer 3), the Ocala low-permeable zone (OLPZ, Layer 4), and the Avon Park permeable zone (APPZ, Layer 5). Sepúlveda et al. (2012) provide a detailed analysis of the hydrogeology in east-central Florida and a description of the development and calibration of the transient groundwater flow in the SAS, ICU, and FAS that serves as the basis for this study.

The initial spatial distribution of aquifer hydraulic properties for the SAS, ICU, and FAS in the east-central Florida model area (Figure 1) was inferred from the analyses of data acquired from more than 100 aquifer performance tests conducted in all hydrogeologic units and from the interpretation of geologic data and potentiometric surface maps. A steady-state approximation of hydrologic conditions was assumed for 1999 and 2003 based on an estimated minimal change in aquifer storage

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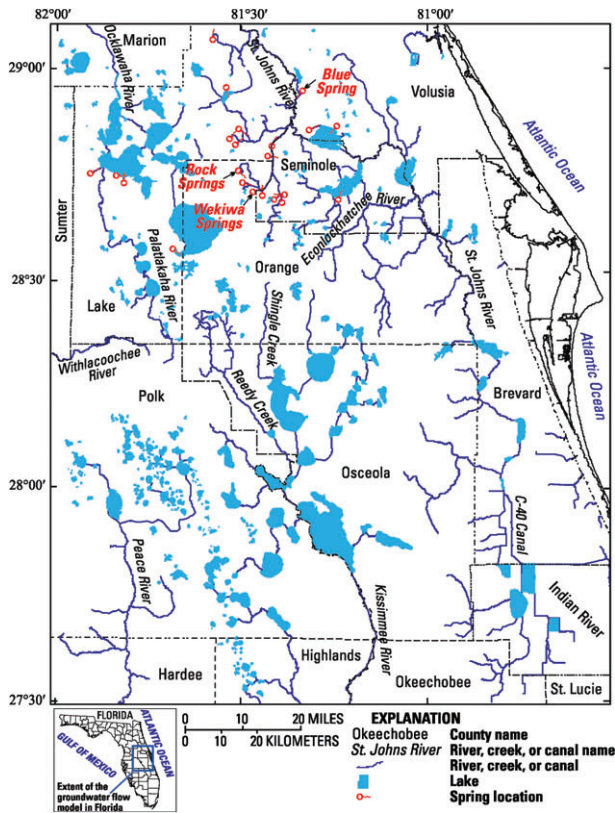
Figure 1. Areal extent of the calibrated groundwater flow model in east-central Florida.

over each of these 2 years. The data used for calibration of the steady-state model were heads and spring flows averaged separately over measurements spanning 1999 and 2003. Average annual recharge rates for 1999 and 2003 were simulated by routing infiltration through the unsaturated zone with the UZF1 package (Niswonger et al. 2006), a component of a calibrated transient 1995 to 2006 groundwater flow model (Sepúlveda et al. 2012). The final spatial distribution of aquifer properties was achieved by using the parameter estimation code PEST (Doherty 2013a, 2013b) for inverse modeling. Hydraulic properties throughout the model domain were represented using a combination of zones and pilot points.

The use of a model to predict heads and flows is normally accompanied by uncertainties associated with model conceptualization, use of a particular spatial parameterization scheme, and numerical issues associated with grid/temporal discretization. In addition to these, limitations in expert knowledge and a paucity of measurement data can lead to nonunique inference of parameter through model calibration. The latter factor in particular leads to uncertainty of hydraulic properties represented in the model. A result of this uncertainty is that the effects of projected pumping stresses on aquifer response can never be known precisely. Freeze et al. (1990) note that the innate uncertainty associated with predictions of future system states should be quantified by a model, and that this uncertainty can then be incorporated into the assessment of the risks associated with different proposed management scenarios. Risk can be defined generally as the probabilities associated with unwanted events multiplied by their cost. If risks are quantified, they can then be balanced against known benefits; costs can be associated with different management strategies to support a quantitative decision-making process that enables a choice to be made between the proposed management strategies while acknowledging the uncertainties associated with predictions of the future behavior of environmental systems.

The analysis of the uncertainty associated with hydrologic models used by water-resource managers, for decision-making purposes, is presented in this paper by making predictions using many different parameter sets, all of which are considered to be hydrogeologically plausible, and all of which allow the model to replicate observations comprising the calibration dataset to a level considered acceptable. Acceptability of the calibration dataset must consider measurement errors, model approximations such as the steady-state assumption, and conceptual model imperfections. Each of the parameter field realizations the model employs in making predictions embodies a different realization of horizontal hydraulic conductivities within the SAS, OPZ, APPZ, and LFA, and vertical hydraulic conductivity within the ICU, OLPZ, and MCU. Each parameter field also employs a different realization of local conductances that affect flows in springs; each also introduces a different realization of a small amount of spatial recharge variability throughout the model domain. It is acknowledged that the collective uncertainties these parameter field realizations embody are unlikely to represent all sources of predictive uncertainty; however, these embody enough of the sources for the uncertainties revealed by their use to be calculated with a reasonable degree of reproducibility. Despite receiving considerable attention in the environmental modeling literature (Tonkin and Doherty 2009), quantification of predictive uncertainty is rare in everyday model-based decision making, notwithstanding the need for such quantification. As such, the modeling methodologies and strategies described herein are relevant to many other study areas, including environmental decision-making processes.

Management of water resources incorporating uncertainty has resulted in well-defined systematic strategies to implement adaptive management approaches. Adaptive management can thereby incorporate lessons learned from outcomes of previous actions (Pahl-Wostl et al. 2007; Rouse and Norton 2010). The assessment and characterization of uncertainty in environmental modeling using parameter estimation, predictive uncertainty, and Monte Carlo analysis has been delineated by Refsgaard et al. (2007). The concept of uncertainty has become increasingly acknowledged in water-resource management scientific literature. A case study where uncertainty analysis was taken into account during the operation and management of reservoirs was presented by Gómez-Beas et al. (2012). The implementation of climatic and hydrological uncertainty into water system planning and management was illustrated by Pallottino et al. (2005).

This paper describes (1) the generation of parameter field realizations representing different sets of hydraulic conductivities, spring flow conductances and recharge rates, each of which calibrate the model for the same set of observations; (2) the simulation of groundwater flow under projected groundwater withdrawals for 2035; (3) the simulation of drawdown and spring flow reductions between the steady-state conditions of 1999 and those assumed for 2035, due to projected groundwater withdrawals for 2035; and (4) the calculation of the associated uncertainty. The uncertainty of the 1999 and 2035 heads and flows are calculated and compared to the uncertainty of the differences between heads and flows for these 2 years.

Though the methodology through which calibration-constrained parameter fields are generated is not itself new, it is the authors' experience that application of this methodology in routine groundwater management practice is extremely rare. This paper attempts to demonstrate that such an analysis is not particularly difficult, and therefore there is little justification for failing to accompany model predictions with an estimate of their uncertainty. This study is designed to show that uncertainty analysis can separate predictions for which the uncertainty is relatively low from those for which it is relatively high. The paper suggests that if groundwater managers are armed with this information and other conclusions that may emerge from a routine analysis of the uncertainty associated with model predictions, the approaches that they take to everyday groundwater management may be considerably enhanced.

Generation of Parameter Field Realizations Using Null–Space Monte–Carlo Analysis

Methods

Parameter uncertainty is not the only source of predictive uncertainty because uncertainties in a model's conceptual basis may also contribute to its ultimate predictive uncertainty; however, parameter uncertainty is the main focus of this study. A calibration-constrained Monte-Carlo analysis was used to explore the uncertainty associated with model parameters, and with predictions made by the calibrated model as it depends on model parameter uncertainty. Model structural inadequacies and simplifications are taken into account through an acceptance of calibration misfits that exceed the statistics of measurement error alone, which is a conventional calibration practice. This acceptance promulgates greater variability between parameter field realizations generated in the manner described below.

The purpose of calibration-constrained Monte-Carlo analysis is to generate a suite of parameter field realizations that express the potential for hydraulic property spatial variability throughout a model domain; a result derived from the application of measured heads and flows, the thicknesses of the hydrogeologic units, and the initial distribution of hydraulic properties derived from aquifer

performance tests. The prior knowledge of these system characteristics is referred in this paper as "expert knowledge." Each of these parameter field realizations must respect the constraint that dependent model outputs used in the calibration process provide an acceptable match with their observed counterparts.

Calibration-constrained parameter field generation was implemented using the Null Space Monte Carlo (NSMC) method described by Tonkin and Doherty (2009) and Doherty et al. (2011), and implemented in PEST (Doherty 2013a, 2013b). The method is able to achieve a relatively high level of numerical efficiency in enforcing calibration constraints on random parameter fields by decomposing these fields into two components. One of these components is composed of parameter combinations that have little impact on model outputs corresponding to data used in the calibration process (and hence belongs to the so-called null space as far as the calibration dataset is concerned). The other component is composed of parameter combinations that are uniquely estimable on the basis of the calibration dataset. The latter combinations are estimated through calibration. Implementation of the NSMC method concentrates on varying the former parameter combinations subject to limitations imposed by expert knowledge, though the latter combinations are varied to some degree as they inherent uncertainty from model-to-measurement misfit arising from measurement error and model structural imperfections. Implementation of the NSMC method requires the following six steps.

1. Initially, a model is calibrated. An appropriate Tikhonov regularization methodology is employed to pursue a minimum error variance solution to the nonunique inverse problem of model calibration, and to ensure that model-to-measurement misfit is maintained at a level that prevents the emergence of unrealistic parameter values through so-called "over-fitting"; see Doherty (2003) for details. Nonuniqueness follows from the fact that many parameters are employed in this process. These parameters can thus represent the potential for spatial variability of hydraulic properties throughout the model domain. The fact that these hydraulic properties cannot be uniquely estimated is a major source of predictive uncertainty; a suitable number of parameters to represent the potential spatial variability is required if this contribution to predictive uncertainty is to be properly represented.
2. Random realizations of model parameter values are generated based on an appropriate stochastic characterization of their variability and spatial correlation. The random realizations are centered on the calibrated parameter field achieved in Step 1.
3. Each random parameter field is subjected to projection onto both the solution and null subspaces of the linearized model operator. The latter is represented by the observation-weighted Jacobian matrix of sensitivities of model outputs used in the calibration process to parameters that are subject to adjustment using that process.

4. Solution space random parameter projections are replaced by solution space projections of parameters inferred through the model calibration process. Null space parameter projections have little effect on model outputs under calibration conditions, and their retention in random parameter field realizations degrades the level of model-to-measurement fit achieved through the calibration process to a relatively small extent. The fact that there is any degradation of model-to-measurement fit at all is a result of (a) model nonlinearity and (b) demarcation of the boundary between the solution and null spaces at low rather than zero singular values, thus preventing amplification of measurement noise in estimating values for parameters as a result of what is popularly referred to as "over-fitting"; see Moore and Doherty (2005) for details.

5. Solution space parameter components are adjusted to ensure that the level of model-to-measurement fit is in accordance with user specifications. Such adjustment of solution space parameter components allows representation of parameter variability that is inherited from measurement error, and from the contributions made to model-to-measurement misfit by model structural defects.

6. The resulting parameter field realizations are manually scrutinized to eliminate any that are not considered plausible, or that lead to model outputs at noncalibration sites that are considered to be irreconcilable with local expert knowledge.

The NSMC method is not strictly Bayesian. In fact, mathematically, NSMC explores the potential for error in the calibrated parameter field of minimum error variance rather than posterior parameter uncertainty. However, NSMC can be implemented with far greater numerical efficiency in highly parameterized contexts than Bayesian methods such as Markov chain Monte Carlo (Tonkin and Doherty 2009) and leads to estimates of post-calibration predictive variability that are commensurate with those obtained by Bayesian methods (see, e.g., Keating et al. 2010).

Parameterization

Model construction details, including parameterization of the model domain, are described in Sepúlveda et al. (2012). The discussion herein of model parameterization is brief, because the purpose of this paper is to focus on some of the outcomes of predictive uncertainty analysis rather than on the details of its implementation.

The FAS model, the focus of this study, employs pilot points to represent spatial variability of horizontal hydraulic conductivity in Layers 1, 2, 3, 5, and 7, and vertical hydraulic conductivity in Layer 2. Zones are employed to represent spatial variation of vertical hydraulic conductivity in Layers 1 and 6; parameter spatial uniformity is assumed for other layers. Conductances calculated from calibrated hydraulic conductivity at 22 individual grid cells, used in the DRAIN package of MODFLOW-2005 (Harbaugh 2005) to simulate spring outflow, also are awarded parameter status. As for other parameters, these parameters undergo solution and null space projection in accordance with the NSMC methodology; random realizations of these parameters are thus generated and subjected to NSMC analysis.

Pilot point parameterization of the model domain takes place at two levels. Regional pilot points are distributed uniformly, with a separation distance of 31,250 feet (9525 m). These regional pilot points are supplemented with suites of pilot points with relatively high spatial density introduced in the vicinities of springs in Layers 3 to 5. The supplemental pilot points act as multipliers on parameter field realizations interpolated from regional pilot points. The separation distance between these pilot points averages 1250 feet (381 m).

A suite of regional pilot points that was not used in the model calibration process was introduced for the purpose of NSMC analysis. These points represent possible spatial variability of recharge rates other than those derived from modeling based on the application of the Green-Ampt infiltration equations (Chow et al. 1988) and unsaturated zone flow routing (Niswonger et al. 2006) to different land-use and vegetation types occurring throughout the model domain. The parameters associated with these pilot points act as multipliers on steady state recharge rates obtained by averaging of time-varying recharge rates calculated in this fashion; see Sepúlveda et al. (2012) for details.

For the purpose of random parameter field generation, the log of each parameter was assigned a spatially varying upper and lower bound based on expert knowledge and, where pertinent, aquifer test interpretations. The difference between upper and lower bounds was divided by four to obtain the standard deviation for each log parameter. Under the normality assumption, the bounds of each parameter are thus assumed to define its 95% confidence interval. A standard deviation between 0.1 and 0.3 was thereby assigned to the $\log_{10}$ of hydraulic conductivities, while a standard deviation of 0.021 was assigned to the log of recharge multipliers, which corresponds to a recharge factor of 1.05. Spatial correlation was not assumed for pilot points associated with hydraulic conductivity in Layers 1 and 2, and for recharge multiplier pilot points, because the distance between them was judged to be commensurate with that of parameter spatial variability. An exponential correlation and a distance factor exponent (roughly equivalent to a third of the variogram range) of 15,000 feet (4572 m) was assumed for pilot points assigned to other layers (Sepúlveda et al. 2012). For near-spring pilot point hydraulic conductivity multipliers, isotropic exponential correlation with a distance exponent factor of 1100 feet (335 m) was employed. No correlation was assumed between spring conductance parameters; log standard deviations ranging from 0.03 to 0.08 were assumed for these latter parameters. Realizations of a total of 2508 parameters were generated and adjusted during NSMC analysis.

Observations

The calibration dataset was composed of head and spring flow measurements for two 12-month periods (1999 and 2003) when the mean heads and flows were calculated to approximate steady state conditions. Regional groundwater withdrawal and recharge rates were different during these two periods; each of these periods was included in a joint calibration exercise encompassing both of them. A total of 445 and 505 head measurements were available from 1999 and 2003, respectively, supplemented by 22 spring flow measurements in each year. Weights assigned to the observations for use in the inversion process reflected credibility of these measurements; credibility is mainly a function of repeatability of measurement during each of the 2 years. Lateral boundary conditions for the flow model were calculated from potentiometric surface maps generated using monthly average heads. Annual average heads were specified at the lateral boundary cells for 1999 and 2003, as well as for the 2035 predictive period.

Predictions

The model was used to predict heads and spring flows that will prevail in 2035 based on projected groundwater withdrawals from the projected population increase in east-central Florida, anticipated changes in water use, (including changes in agricultural practices and public water-supply requirements), and a range of recharge rates for 2035 to simulate dry to wet conditions. Randomly generated factors between 0.75 and 1.50 were used to multiply the average recharge rates from 1995 to 2006 to generate the projected 2035 recharge rates. These bounds were chosen because the period 1995 to 2006 was considered to have below average rainfall (W. Jin, St. Johns River Water Management District, written communication, 2012). Predictions of drawdown in the FAS relative to 1999 heads were made using both the "calibrated parameter set" on which NSMC realizations were centered, and 204 parameter field realizations generated using the NSMC process described previously. These 204 parameter field realizations were retained from an original set of 500 NSMC-generated parameter fields after close inspection of all of these fields in accordance with Step 6 of the Methods section discussed above. Model predictions indicate that the largest 2035 drawdown, compared to 1999 levels, are likely to occur in the APPZ and LFA aquifers, or model Layers 5 and 7, because the largest groundwater withdrawal rate increases are projected to occur in these two layers (Table 1). The large hydraulic connection between the less permeable OPZ and the more permeable APPZ (Sepúlveda et al. 2012) causes large drawdown in the OPZ. Spatially, the largest groundwater withdrawal rate increases are predicted in parts of south Seminole, west and central Orange, southeast Lake, north and central Osceola, and southwest Polk Counties (Figures 1 and 2). These areas have the largest projected population increases in east-central Florida. The UFA, composed of model Layers 3 to 5, has a projected 37% increase in groundwater withdrawals in 2035 compared

Table 1
Total Groundwater Withdrawal Rates by Layer for 1999 and Projected Rates for 2035

Model Layer	Q1999	Q2035
1. SAS	36.17	10.78
2. ICU	−14.02	−33.16
3. OPZ	−951.03	−883.04
4. OLPZ	−50.78	−83.03
5. APPZ	−278.59	−784.42
6. MCU I/II	−4.56	−7.52
7. LFA	−207.73	−370.04
Total	−1470.54	−2150.43

Notes: Q1999, Q2035: total 1999 and 2035 groundwater withdrawal rates in cubic feet per second; negative rates indicate withdrawals; positive rates indicate injections such as rapid infiltration basins in the SAS.

to 1999 withdrawals. Overall, the model-wide projected groundwater withdrawals for 2035 represent an increase of 46% above 1999 rates, constituting a total of 2150 ft^3/s (60.9 m^3/s, Table 1). Notwithstanding this overall increase in extraction, decreases in groundwater withdrawals are projected for some parts of central Brevard, Lake, and Polk Counties (Figure 2). The projected changes in groundwater withdrawals are a result of the projected water-use changes calculated by the water utilities in Central Florida.
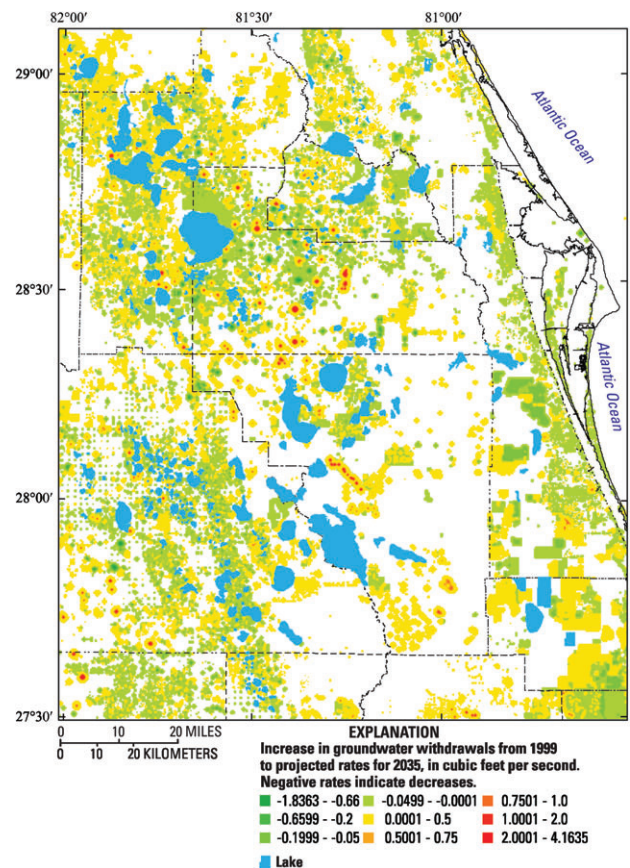

Figure 2. Changes in total groundwater withdrawals from all layers, from 1999 average rates to projected rates in 2035.
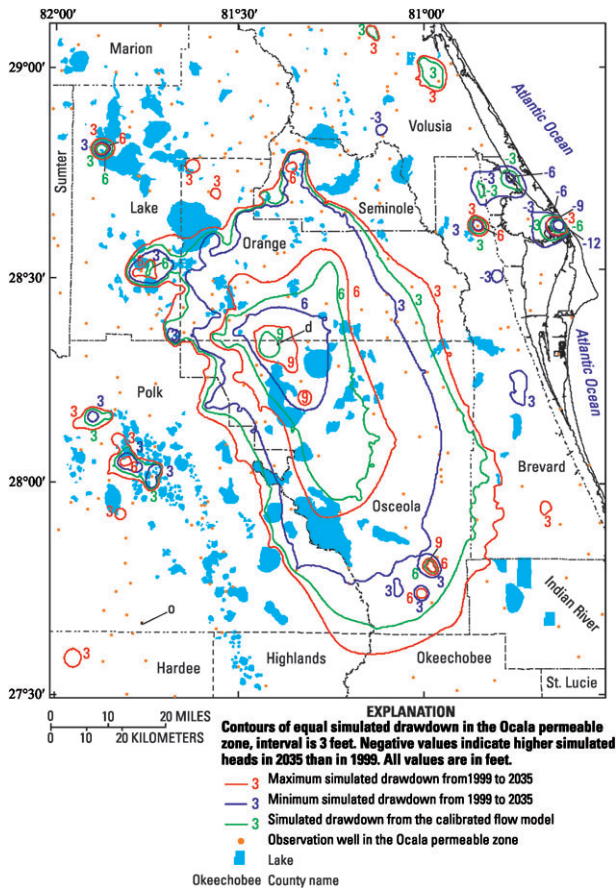
Figure 3. Simulated maximum and minimum drawdown in the Ocala permeable zone due to changes in groundwater withdrawals from 1999 to 2035. Predictions made by using the "calibration parameter field" are also shown.

Simulated Drawdown Based on Monte–Carlo Realizations and the Calibrated Flow Model

Simulated 1999 and 2035 heads using all 204 realizations were calculated throughout the model domain and the parameter field constituting the "calibrated model" on which NSMC parameter field generation was centered (see Step 1 in section "Methods"). Cell-by-cell drawdown between 1999 and 2035 was calculated by subtracting the 2035 simulated heads from the 1999 simulated heads for all NSMC parameter field realizations and for the calibrated flow model. A positive drawdown corresponds to a decrease in head in 2035 relative to 1999 caused by increased groundwater withdrawals relative to 1999 rates. Conversely, a negative drawdown in 2035 compared to 1999 reflects an increase in head caused by a reduction in groundwater withdrawal rates. For brevity, drawdown for the OPZ layer only is shown herein. The maximum and minimum drawdown for all NSMC realizations were calculated for each model cell and the data were contoured (Figure 3). For the given development scenario, the range of predicted drawdowns that is compatible with information contained in expert knowledge and in historical measurements of system state is thereby shown in every cell of this model layer. Predictions made using

the "calibrated parameter field" (the parameter field of minimized error variance obtained through regularized inversion prior to undertaking NSMC analysis) are also shown. Similar results were obtained for the APPZ and LFA layers.

On the basis of the calibrated parameter field, the predicted 1999 to 2003 drawdown in the OPZ ranges from −12 feet (−3.66 m) in eastern Brevard County (a head recovery), to 9 feet (2.74 m) in south-central Orange and north-central Osceola County (Figures 1 and 3). For any cell, the "uncertainty range" of a head or drawdown prediction is characterized herein as the difference between maximum and minimum head or drawdown in that cell calculated using all of the 204 NSMC parameter field realizations. The "uncertainty standard deviation" is characterized as the standard deviation of the predicted head or drawdown values calculated with these same parameter field realizations. The outcomes of these calculations are exemplified for the cell labeled "o" (Figure 3), a cell with an observation well used during calibration, and for a second cell, labeled "d" (Figure 3), distant from observation wells used during calibration. Cell "d" is inside the 9-feet (2.74 m) contour of maximum drawdown (Figure 3).

At cell "o" (in southwest Polk County, Figure 3), the 1999 head residual (the difference between observed and simulated head at the observation well in this cell) simulated by the calibrated model is −3.71 feet (1.13 m). The uncertainty in calculated head at this well over all NSMC parameter fields realizations in 1999 and 2035 are 2.82 feet (0.86 m) and 3.43 feet (1.05 m), respectively (Figure 4A and 4B); corresponding uncertainty standard deviations of NSMC head are 0.51 and 0.53 feet (0.155 and 0.162 m). The range and standard deviation of head uncertainty for the drawdown incurred between 1999 and 2035 are 1.6 feet (0.49 m) and 0.33 feet (0.10 m), respectively (Figure 4). The head uncertainty in 1999 is comparable to the head model-to-measurement misfit achieved through the calibration process (as expected). The 2035 predicted head uncertainty at this same location is slightly greater. Note, however, that the uncertainty in the predicted 1999 to 2035 drawdown is considerably smaller than that of the predicted head in both of these years.

The uncertainty of the 1999 and 2035 heads, calculated at cell "d" (Figure 3) from the 204 NSMC realizations, are 2.85 feet (0.87 m) and 4.1 feet (1.25 m), respectively (Figure 5). The uncertainty of the 1999 to 2035 drawdown at this cell is 2.48 feet (0.76 m), which is less than the uncertainties of the 1999 and 2035 heads (Figure 5).

Uncertainty errors, using the NSMC realizations, were calculated for the simulated heads for 1999, 2035, and the simulated drawdown from 1999 to 2035, at all cells with observation wells used for model calibration. The uncertainty error of the drawdown, at each layer and at each cell with an observation well, was lower than either the uncertainty error of the simulated heads for 1999 or that for 2035. The average uncertainty error of the drawdown was lower than that for the absolute average
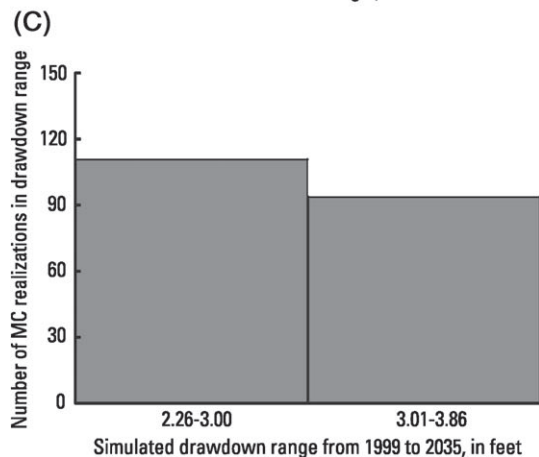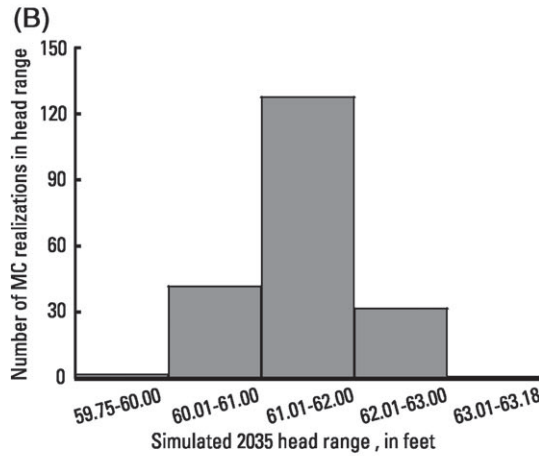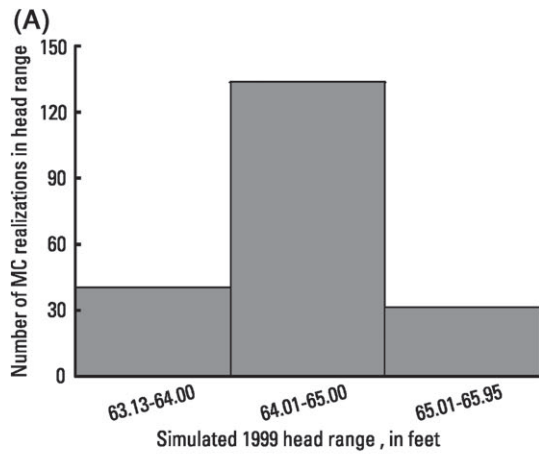
Figure 4. Histogram-based variability of simulated heads for (A) 1999, (B) 2035, and the (C) drawdown at cell "o" in Figure 3, which includes an observation well used for model calibration.

Figure 5. Histogram-based variability of simulated heads for (A) 1999, (B) 2035, and the (C) drawdown at cell "d" in Figure 3, distant from observation wells used for calibration.

for the simulated 1999 residuals from the calibrated model (Table 2). The standard deviation of the drawdown from 1999 to 2035 was also smaller than that for the 1999 or 2035 heads, suggesting that the prediction of drawdown between 1999 and 2035 can be made with greater accuracy than the prediction of heads in either 1999 or 2035.

The standard deviation was calculated from the simulated heads of the NSMC realizations for each cell in the OPZ layer, for 1999, 2035, and for their difference. The standard deviation of simulated heads in 1999 from
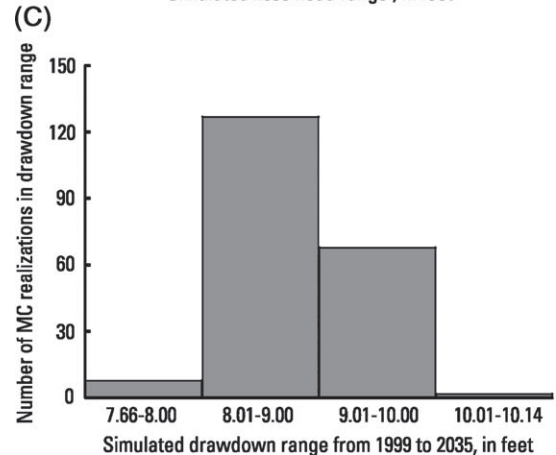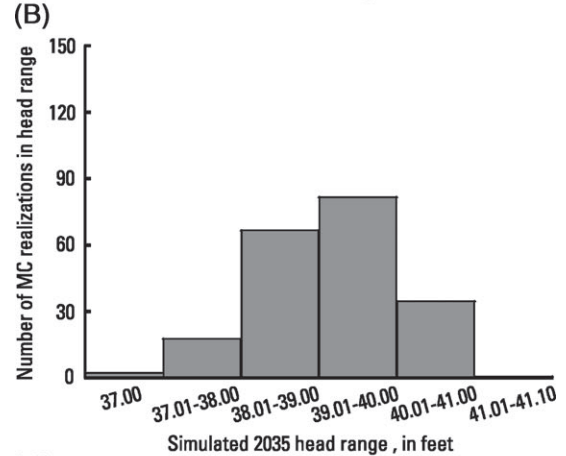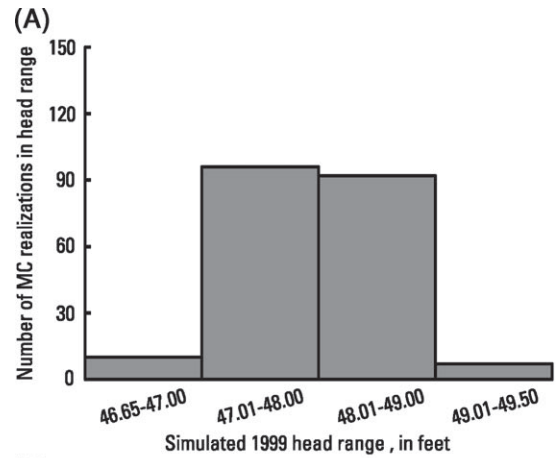
the NSMC realizations ranged from 1.5 feet (0.46 m) to 0.5 feet (0.15 m) throughout much of the model area (Figure 6A); nonzero contours extend throughout the western half of the model area. Although the spatial distribution of the standard deviation for the predicted heads in 2035 from the NSMC realizations is slightly different from that for 1999 (Figure 6A and 6B), the two sets of standard deviations have similar magnitudes. The calculation of the standard deviation of the head differences between 1999 and 2035 indicates that the deviation from the mean of these differences is clearly

Table 2

**Average Uncertainty Error and Standard
Deviation per Model Layer, Calculated from the
NSMC Realizations over Cells with 1999
Observation Wells Used for Model Calibration**

Layer	Nw	Au99	Au35	Aud	A99r	Sd99	Sd35	Sdd
1. SAS	128	5.50	5.52	0.27	1.89	0.731	0.771	0.096
2. ICU	44	3.75	3.81	0.51	2.47	0.586	0.614	0.113
3. OPZ	209	3.40	3.50	0.81	1.83	0.469	0.524	0.209
4. OLPZ	7	2.42	2.66	0.86	2.30	0.477	0.511	0.195
5. APPZ	38	2.35	2.49	0.83	2.37	0.445	0.479	0.176
6. MCU I/II	6	1.39	1.56	0.70	2.27	0.266	0.290	0.141
7. LFA	13	2.19	2.31	0.94	1.89	0.430	0.440	0.189
Total/Average	445	3.87	3.95	0.63	1.97	0.563	0.607	0.171

Notes: Nw: number of 1999 observation wells per layer used in the simulations; Au99, Au35, Aud, and A99r: average uncertainty of simulated 1999 heads, predicted heads for 2035, predicted drawdown from 1999 to 2035, and average absolute value of differences between simulated and average measured heads (residuals) at observation wells used for 1999, respectively, in feet; Sd99, Sd35, and Sdd: standard deviations calculated from NSMC realizations using 1999 simulated heads, predicted heads for 2035, and predicted drawdown from 1999 to 2035, respectively, in feet.

smaller than the standard deviation for 1999 or 2035 (Figure 6C). These findings on the standard deviation for the differences in simulated 1999 and 2035 heads confirm the previous results of smaller uncertainty in the simulated head differences.

Simulated Spring Flows

Spring flows were simulated for the average 1999 hydrologic conditions and for the projected 2035 groundwater withdrawals, using both the NSMC realizations and the calibrated flow model. For brevity, only results for Rock Springs (Figure 1) are described but similar uncertainties were obtained for Wekiwa and Blue Springs (Figure 1). The average 1999 measured spring flow for Rock Springs was $51.9\,\mathrm{ft^3/s}$ ($1.47\,\mathrm{m^3/s}$). The flow for Rock Springs simulated by the calibrated model was $49.6\,\mathrm{ft^3/s}$ ($1.40\,\mathrm{m^3/s}$). Relative to the measured flows, these simulated flows for Rock Springs were 4% lower.

The simulated flows at Rock Springs, under average 1999 hydrologic conditions, using the NSMC realizations, ranged from 46.6 to $58.2\,\mathrm{ft^3/s}$ (1.32 to $1.65\,\mathrm{m^3/s}$, Figure 7A), with an uncertainty range of $11.6\,\mathrm{ft^3/s}$ ($0.33\,\mathrm{m^3/s}$). The simulated spring flow at Rock Springs, under the projected 2035 water use, ranged from 40.3 to $51.5\,\mathrm{ft^3/s}$ (1.14 to $1.46\,\mathrm{m^3/s}$, Figure 7B), with an uncertainty of $11.2\,\mathrm{ft^3/s}$ ($0.32\,\mathrm{m^3/s}$), or 22% of the average measured flow at Rock Springs for 1999. The average simulated flow from the NSMC realizations at Rock Springs for 1999 was $50.88\,\mathrm{ft^3/s}$ ($1.44\,\mathrm{m^3/s}$), and for 2035 was $44.35\,\mathrm{ft^3/s}$ ($1.26\,\mathrm{m^3/s}$), indicating that projected increases in groundwater withdrawals result in a projected decrease in flow of 13%. The uncertainty in predicting the flow reduction at Rock Springs from 1999 to 2035 was $1.9\,\mathrm{ft^3/s}$ ($0.05\,\mathrm{m^3/s}$, Figure 7C), far smaller than that for 1999 or 2035 simulations, or for the average measurement error, estimated to be 15% or $7.78\,\mathrm{ft^3/s}$ ($0.22\,\mathrm{m^3/s}$). The standard deviations of the simulated flows at Rock Springs,
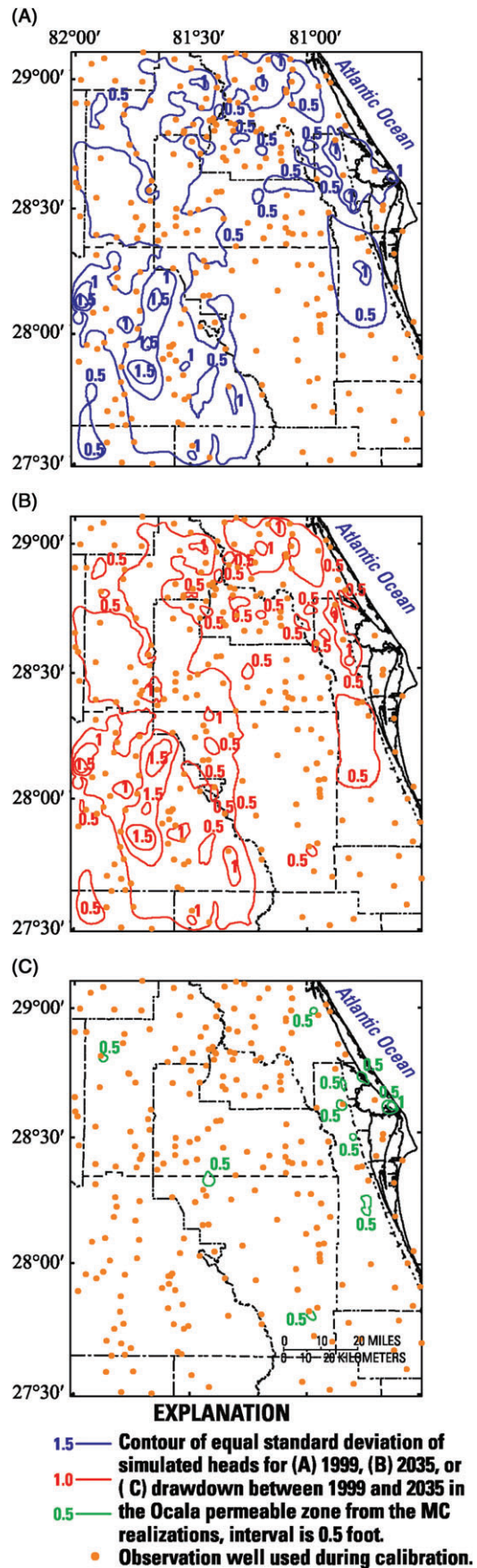

Figure 6. Standard deviation of simulated heads in (A) 1999, (B) 2035, and (C) drawdown between 1999 and 2035, calculated from the NSMC realizations.
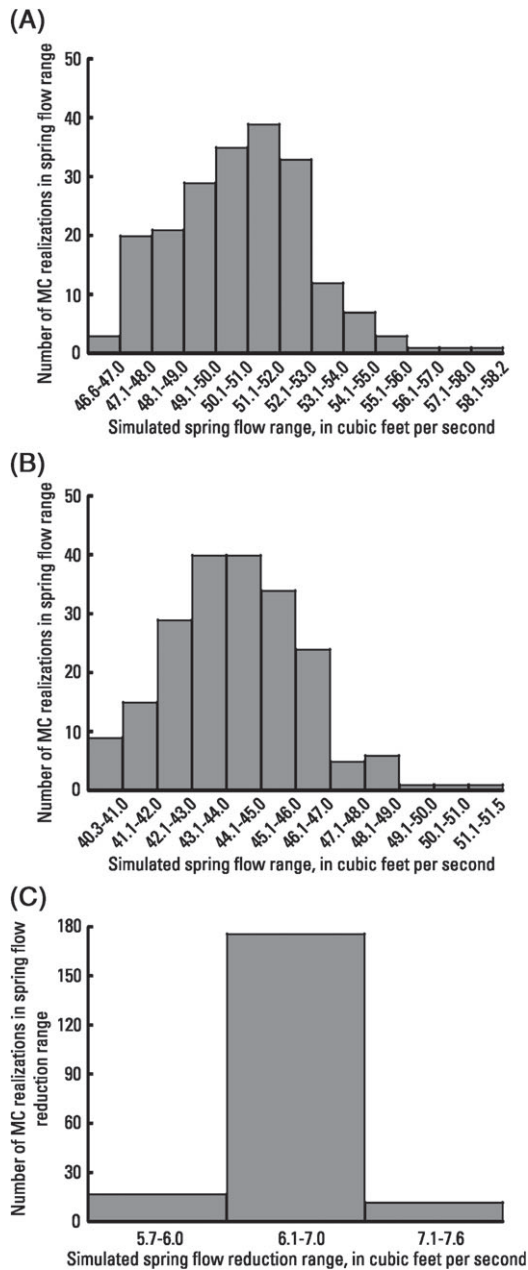
(A)

(B)

(C)

Figure 7. Histogram-based variability of simulated spring flow at Rock Springs for (A) 1999, (B) projected 2035 withdrawals, and (C) spring flow reduction from 1999 to 2035.

from the NSMC realizations, for 1999, 2035, and their differences were 2.12, 1.97, and 0.35 ft³/s (0.06, 0.05, and 0.01 m³/s), respectively, indicating the 1999 to 2035 simulated flow difference deviates considerably less from its mean value than the deviations of the simulated flow from either year to its corresponding mean value. In summary, the uncertainty of the simulated flows for each year is larger than the uncertainty of the predicted flow difference.

Discussion

This study indicates that greater reliance should be placed on comparative outcomes of models, rather than

absolutes, because the former may often be made with less uncertainty than the latter. A model's capacity to predict differences is superior to its capacity to predict absolutes. This capacity has been demonstrated for differences in predicted heads and spring flows under different regional recharge and pumping rates. It may apply to other types of model predictive differences, such as the differences between heads and/or spring flows predicted for one management scenario from those predicted for another. It may then be possible to demonstrate that the outcome of one management strategy is superior to another despite the inability of a model to predict the outcome of either with great certainty, which has important implications for the way a model is used to support the decision-making process, and for the types of predictions that decision-makers should seek from models.

The suggestion that a model is better at predicting differences than absolutes can be at least intuitively comprehended through an inspection of the equation that expresses the variance of the difference between two random quantities. If these variances are identified as "1" and "2" then the equation can be written as $\sigma_{1-2}^2 = \sigma_1^2 + \sigma_2^2 - 2\sigma_{12}$, where σ^2 indicates variance and σ_{12} is the correlation between quantities 1 and 2 (Tonkin and Doherty 2009). If these are model outputs of similar type, but pertain to different times or locations, then the degree of correlation between them may be high. In some instances, particularly where outputs at different times are affected by the same model structural defects, the third term in the above equation may be as high as the sum of the other two, thus resulting in near-cancellation of the effects of these defects when computing predictive differences.

The incorporation of predictive uncertainty into the decision-making process is slowly becoming more common in water-resource management. The derivation of a threshold head Y or spring flow Z from a calibrated flow model that does not consider uncertainty of the simulated number could result in the implementation of an ineffective water-resource management strategy. If the economic cost of an ineffective decision is high, a threshold value of head Y that lacks certainty is not ideal but a range of values might be acceptable. However, if only a discrete number is tolerable to a resource manager, then perhaps an alternative number may be presented, for example that a spring flow Z will be maintained under a proposed management strategy with a 95% confidence level. The number Z may be far more relevant to responsible management of a goal that has high societal or ecological value than the number Y predicted by "a calibrated model," especially if the difference between Y and Z is likely to be large.

Uncertainty inevitably surrounds predictions of the environmental consequences that may result from a proposed management strategy. This does not make model-based environmental management impossible but may necessitate an acknowledgement of the inherent uncertainty associated with model predictions. The implementation strategy may benefit by identification of

the level of confidence that an unwanted environmental occurrence will not follow from a certain proposed action. The implementation strategy may also require that certain management actions are permissible but that an appropriate monitoring network be put in place to monitor their effects. Management can then be "adaptive" if a stakeholder can demonstrate that management responses to the exceeding of certain monitoring thresholds can preclude an unwanted environmental outcome at a certain level of confidence. This strategy and many other types of innovative and scientifically based management strategies can be developed if models become devices not only for encapsulating what is known about a system, but also for quantifying what is not yet known, and the management consequences thereof.

The NSMC analysis documented herein allows the modeler to quantify the uncertainties associated with predictions of future system behavior, and to establish the magnitude of these uncertainties, especially where they are likely to be large because they involve model outputs at locations different from those employed for calibration purposes. The method is readily extended to assessment of uncertainty associated with predictions that are of different types altogether from those used for calibration. Such predictions may include processed model outputs, such as areal and/or temporal averages of predicted heads, frequency/duration statistics associated with heads or spring flows, and/or other statistically based hydrological indicators of system status. A prediction of interest to water-resource managers can be made using each of the NSMC parameter field realizations, establishing the uncertainty associated with that prediction on the basis of variability of the prediction between the fields.

Conclusions

The approach of refining hydraulic properties using highly parameterized inversion in conjunction with a regularization method that guides the solution of the inverse problem of model calibration toward a parameter field of minimum error variance has gained acceptance as a standard modeling practice. However, using additional parameter field realizations to quantify the uncertainty in model results is not common. Parameter field realizations were generated, and calibration constraints were consistently implemented, using the NSMC method available in the PEST suite. In contrast to the calibrated parameter field, regularization was not employed in the NSMC process to suppress parameter heterogeneity that is not supported by the calibration dataset. Instead, these fields were generated stochastically to ensure that parameter heterogeneity was maximized. At the same time, hydrogeological feasibility of the parameter field realizations was assured by (a) characterizing parameter values probabilistically in a way that reflects expert knowledge as it prevails within the study area (through the expected values, spatial correlation structure, and limits on parameter variability implied by pertinent probability density functions), as well as gaps in expert knowledge

(through the fact that parameters are free to vary within the limits set by these probability density functions), and (b) manually inspecting each parameter field, and the values of model outputs calculated on the basis of such fields, and rejecting those considered questionable.

The calibrated parameter field, an outcome of regularized inversion, provides the modeler with only enough hydraulic property heterogeneity as that which is required to simulate observations of past system behavior. In doing so, it provides the heterogeneity that *must* exist if the model is to replicate historical head and spring observations. The suite of NSMC-generated parameter field realizations provides the modeler with many realizations of the hydraulic property heterogeneity that *may* exist. These realizations are all constrained by the necessity to respect expert knowledge and the need to allow the model to replicate observed system behavior. Neither the calibrated parameter field nor any of the NSMC-generated parameter field realizations are likely to constitute a representation of "real" hydraulic properties within the model domain. However, by making predictions of interest to water-resource managers with all of these fields, the uncertainty associated with these predictions can be estimated. Decisions regarding future management of the groundwater resources within the study area can then be made with knowledge of the uncertainty associated with predictions of outcomes of any particular future management scenario.

The calibration-constrained parameter field realizations generated in this study were used to explore the uncertainty associated with model predictions under stresses that prevailed during the calibration period, and under aquifer stresses that will prevail in the future if a particular management strategy is followed. Not surprisingly, the uncertainty associated with predictions that correspond to model outputs used in the calibration process is nearly the same as model-to-measurement misfit experienced in that process. In contrast, predictive uncertainty is greatest at locations within the model domain where measurements were not available for calibration. This type of prediction is equivalent to spatial interpolation. When predictions are made under stresses that are different from those experienced during the calibration process, uncertainties are generally higher than they are under calibration conditions. However, uncertainties in predictions made at the same locations as those where measurements are included in the calibration dataset are smaller than those at other locations.

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