Hierarchical Modeling and Parameter Estimation for a Coupled Groundwater–Lake System

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Abstract: In this paper, a generalized hierarchical multiscale approach for modeling coupled groundwater and surface water systems is demonstrated. Groundwater–lake interactions are simulated by coupling the groundwater equations with the lake's continuity equation and by providing a two-way iterative feedback between models at multiple scales using specified head/flux boundary conditions. A hierarchical parameter estimation method that allows data and parameters at different scales to communicate between each other is also developed. These methods are applied to simulate a lake augmentation system for the Sister Lakes in southwest Michigan, which involves pumping a large amount of water from an irrigation well into the lakes. This problem requires resolution of time scales ranging from site-scale (hours) to local-scale (months) to watershed-scale (years) and spatial scales ranging from a few meters to a few kilometers. A hierarchical modeling framework consisting of five interlinked models was created, and model calibration was performed using drawdown data from a 72-h pumping test. The calibrated model was then used to simulate the entire lake augmentation system. The results indicate that the proposed modeling and parameter estimation approach can help improve the ability to model real-world complexities. **DOI:** 10.1061/(ASCE)HE.1943-5584.0001219. © 2015 American Society of Civil Engineers.

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Introduction

The so-called myth of groundwater budgets was addressed by Bredehoeft et al. (1982). They claimed that the magnitude of sustainable development (groundwater pumping) was not dependent on the amount of recharge that can be captured, but rather on the rate at which discharge from the system can be captured. From this perspective, consider the case of a groundwater pumping well near a lake system, i.e., a series of lakes. The critical question to ask in such a scenario is from where the water comes. During the initial period of pumping, water comes from aquifer storage. As time proceeds and the drawdown cone expands, lake stages fluctuate as water circulates from lake to lake in response to the new stress in the watershed. In particular, the lakes in close proximity lose water to the pumping well, but also establish lower hydraulic head to induce flow from lakes further from the pumping center. The challenge in describing this flow system lies in the different spatiotemporal scales at which that the movement of water occurs.

For the extreme climate scenario of zero recharge to the system, the lakes will go dry if pumping continues for a sufficient time. This does not happen in reality because recharge in Michigan is high and can offset the dropping lake levels. Circulation of flow between lakes does take place, but this phenomenon is hard to observe because of the following: (1) very small change in lake levels, (2) very long time-scale of the circulation, and (3) complex interplay between multiple sources and sinks (such as rainfall, evapotranspiration, base flow, and so on). However, it is possible to notice this effect on lakes using numerical simulations, where all other sources and sinks can be removed and only the effect of induced pumping can be observed.

Even by reducing the complexity of the model by removing real-world sources/sink, the flow system of a stressed groundwater–lake system is difficult to numerically model. This is due to the interplay of multiple spatial and temporal scales. At the watershed scale, there is a regional flow system with variability occurring across kilometers and years, whereas the site-scale dynamics near the pumping well exhibit variability of the order of meters and hours. Modeling a system with such disparity between scales is challenging in two aspects. as follows: (1) forward modeling, creating a multiscale modeling framework that can incorporate all the spatial and temporal scales and capture the significant dynamics of the system; and (2) inverse modeling, i.e., estimating parameters for a multiscale model that has data and parameters at multiple scales. Parameter estimation poses several questions, such as how to distinguish between the different scales of data or how to assimilate the various scales of data and parameters into one comprehensive framework. Addressing these challenges is the objective of this paper. A literature review of multiscale modeling and parameter estimation is presented next, which provides the basis for the adopted approach.

Multiscale Modeling

Multiscale modeling is appropriate whenever there is a need to understand both regional and local processes. Several approaches have been used for this purpose, including local analytical correction,

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global grid refinement, and local numerical correction (or nested grid modeling). The hierarchical patch dynamics paradigm (HPDP) was used within the *Interactive Groundwater* modeling environment (Li and Liu 2006a, b, 2008; Li et al. 2006) to simulate a complex groundwater remediation system (H. Liao et al., "Hierarchical modeling of a groundwater remediation capture system," Working Paper, Michigan State University, East Lansing, Michigan). This field application of HPDP revealed leaking contaminants through forward and reverse particle tracking. The algorithms for upscaling and downscaling between models at different spatial scales were provided as well as the discretization, numerical scheme, and grid layout in the various model levels. In the research reported in this paper, the algorithm development is extended for transient problems involving subtiming for flow and transport. Mathematical models for surface and groundwater interactions are also incorporated into HPDP. First, a review of nested grid model applications is provided.

Nested Grid Modeling

Over the last 40 years, many nested grid models have been applied in groundwater studies. Mrosovsky and Ridings (1974) used a three-dimensional (3D) orthogonal petroleum reservoir model with a well situated in one vertical column, which was discretized using a radial grid. The orthogonal grid provided flux boundary conditions (BCs) for the radial grid. Graham and Smart (1980) used a fine-grid model nested in a coarse-grid model for simulating a reservoir in communication with a large pressure-supporting aquifer. Townley and Wilson (1980) developed a finite element aquifer flow model, *AQUIFEM-1*, that used boundary conditions (both prescribed flux and prescribed head) for small-scale models from large-scale models. Heinemann et al. (1983) applied dynamic local grid refinement for a multiple application reservoir simulator. Ward et al. (1987) used telescopic mesh refinement (TMR) to create a series of nested models at regional, local, and site scales to model the contaminant transport at the Chem–Dyne hazardous waste site. However, coupling between the different scales was only one-way, i.e., from the large mesh to the small mesh. Fung et al. (1992) used a control-volume FEM using linear triangular elements to simulate thermal multiphase flow in porous media; so-called near-well resolution was achieved by local grid refinement. Leake et al. (1998) proposed different methods for assigning boundary conditions in small-scale groundwater models from large-scale, block-centered, finite-difference models such as *MODFLOW* (McDonald and Harbaugh 1988). Efendiev et al. (2000) presented coarse-scale numerical models of flow in heterogeneous porous media that incorporated subgrid effects. This method first upscales the deterministic fine-grid permeability description and then solves the pressure equation over a coarse grid to get coarse-scale velocities. Mehl and Hill (2002) use a so-called shared-node technique between the parent and child models to develop a new method of local grid refinement for two-dimensional (2D) block-centered finite-difference meshes. They used both interpolated heads and fluxes as boundary conditions at the interface between parent and child models, therefore creating an iteratively coupled feedback mechanism. de Tullio et al. (2007) solved the 3D preconditioned Navier–Stokes equation for compressible flows with an immersed boundary approach by using a flexible local grid refinement technique to achieve high resolution near the immersed body and in other high-flow-gradient regions.

Subtiming for Flow and Transport

Although all the techniques mentioned so far are applicable for both spatial and temporal grids, the literature cited so far has dealt mostly with spatial subgridding. Bhallamudi et al. (2003) describe a subtiming approach for flow and transport problems as a logical extension of spatial subgridding. This approach can be used for transient simulations that couple surface and subsurface flows or that resolve temporal dynamics close to a pumping well or a contaminant plume. This approach uses small time-step sizes in areas of so-called high activity and large time-steps elsewhere, which is highly suitable for situations where large portion of the domain are temporally overdiscretized. The subtime-step is selected such that it is an integral portion of the larger time-step. Park et al. (2008) used implicit subtime-stepping for simulating flow and transport in fractured porous media using the Galerkin finite-element formulation. This was applied to density-dependent flow and transport simulations in predominantly discrete, highly conductive fracture zones. In another study, Park et al. (2009) applied implicit subtime-stepping for numerical modeling of the nonlinear coupled surface–subsurface equation. This methodology was applied to enhance the computational efficiency of integrated flow simulation in the San Joaquin Valley, California.

Multiscale Parameter Estimation

In general, the goal of parameter estimation is to find model parameters (hydraulic conductivity, recharge, and so on) that minimize the objective function. Typically, the objective function is the sum of squared residuals between the observed data and the model's predictions. A key aspect of multiscale parameter estimation is determining how to construct the objective function. Should one objective function be used for each scale? Or should one objective function be computed by combining the data from all scales? Also, should one objective function be used for each kind of observation (hydraulic heads, stream flows, and so on), or should they be combined into one objective function? Hill and Tiedeman (2007) posed such questions and opined that since data is usually scarce, it is better to use a single objective function that considers all data simultaneously by assigning appropriate weights to data at different scales.

Several researchers have performed multiobjective calibration for various reasons. Medina and Carrera (1996) coupled the parameter estimation of flow and solute transport parameters using both head and concentration data. Madsen (2008) calibrated a rainfall–runoff model using multiple objective functions that measured the following aspects of their hydrograph: (1) overall water balance, (2) overall shape of the hydrograph, (3) peak flows, and (4) low flows. Khu et al. (2008) performed parameter estimation on a hydrologic model using five objective functions. Separate objective functions were used for groundwater levels and runoff from catchments. Variables of the same type, but from different sites, were grouped together using data mining techniques, creating one objective function for each variable. Keating et al. (2003) used a coupled basin-scale and site-scale model to perform parameter estimation and found that the parameters estimated from the two models were not identical. They caution against the application of parameter estimates obtained from large-scale models to small-scale models and vice versa. In the research reported in this paper, while the basin-scale and site-scale models were hydrologically coupled, parameter estimation was performed by considering weighted residuals at different scales.

Motivation

A major drawback of implementing the nested model approach is that the interaction between the parent and local models, of which there can be many, depends on the offline analysis and processing of model modifications or simulation results from the parent model to obtain boundary conditions and initial conditions (ICs) for the local model. For example, once a simulation step is completed using the regional model, new boundary conditions and initial flows (and solute transport conditions, if applicable) are determined for each local model. Making modifications to models or processing simulation results for use in different scales of models can be time-consuming, especially when the flow field is unsteady or coupled with a solute transport simulation, or if a feedback loop is needed to account for potential significant two-way interaction between parent and nested submodels. The effort involved may become impractical when the offline conceptual changes must be made iteratively or in more than one model. Because of this laborious procedure, applications of the nested grid approach are limited, in most cases, to a very small number of submodels (e.g., one or two), and are implemented with little flexibility. This has severely limited the ability to take full advantage of the nested grid approach for solving complex groundwater problems, especially those that span multiple spatial scales.

No prior study has implemented parameter estimation for a multiscale model that allows communication between the different models, such that the large-scale calibration may benefit from the small-scale calibration and vice versa. In the research reported in this paper, we address both the challenges of forward modeling and inverse modeling by creating a framework that allows multiscale modeling and multiscale parameter estimation. The methodology that has been developed is presented in the next section, and then an illustrative example of a lake augmentation project in southwest Michigan.

Hierarchical Groundwater Modeling

In the research reported in this paper, HPDP is used to simulate a complex surface water–groundwater system. To do so, further development of HPDP was needed, including nested time-stepping, numerical coupling of surface water and groundwater, and hierarchical parameter estimation. These enhancements are described the subsequent subsections.

Nested Time-Stepping

In addition to resolving multiple spatial scales using the nested grid approach, a multiscale transient model should be applied to resolve multiple temporal scales. The basic principle is that a multitude of child models with smaller time-steps are nested in one larger time-step of their parent model. Temporal information propagation between upper and lower model levels is needed since the boundary conditions along the parent–child model interfaces are time-dependent. Therefore, in multiscale modeling, the nested time-stepping is implemented in an eight-step hierarchical manner, as follows:

1. The time-step, Δt^l, at each model level is different, but is the same in each patch (i.e., the so-called child) model for a given model level.
2. Downscaling starts from the main (i.e., the so-called parent) model and its initial conditions are needed to perform downscaling at $t = 0$ for all level's models such that ICs for every submodel become available. Otherwise, ICs for every submodel must be user-defined.
3. Advancing to the next time-step with known heads at the current time-step in nested time-stepping algorithm is vastly different from that of uniform time-stepping and is demonstrated in Fig. 1. The difference is that there are not only shared time nodes in the so-called time-grid system (solid lines in Fig. 1), but also nonshared nodes (dashed lines in Fig. 1). Thus, both spatial and temporal interpolation would be involved in this algorithm. Considering one time-step in the main model as one unit of the downscaling–upscaling loop in the nested time-stepping algorithm, the local information updating approach (LIUA) is presented in Fig. 1 with a four-level example, including the sequence of operations. The remaining steps describe the LIUA for one unit of downscaling-upscaling.
4. Given the head at the previous time level $n - 1$, H^0_{n-1}, (the initial conditions when $n = 1$), the head at the current time level n, H^0_n, is obtained for the main model by solving the transient equation. These heads, H^0_n and H^0_{n-1}, are used to interpolate heads on the parent–child model interface(s), forming the time-dependent boundary conditions for the nested time step in the child model(s). Temporal interpolation is necessary if time-step in child model is not the same as that of the main model, whereas there is no need for temporal interpolation when a so-called time node is shared by both child model and its parent model (solid lines in Fig. 1).
5. In general, boundary conditions for model level l are derived from model level $l - 1$, and the head distribution from the previous time step (referred to as ICs) is known. Then, transient equations are solved for the first time step, Δt^l. Temporal interpolation is performed to obtain BCs for model level $l + 1$ at nested time step Δt^{l+1} ($\Delta t^l > \Delta t^{l+1}$, and usually Δt^{l+1} can be designed to be a factor of Δt^l). At level $l + 1$, now with the necessary BCs and head distribution from the previous time-step, all transient equations are solved. Temporal interpolation is again used to obtain BCs for model level $l + 2$ at nested time step Δt^{l+2} ($\Delta t^{l+1} > \Delta t^{l+2}$, and Δt^{l+2} can be a factor of Δt^{l+1}). This procedure can be applied at each model level until the last child model is solved.
6. Once the transient equations for all nested time steps in the last child model are solved (completion of Sequence Operation 10 in Fig. 1), the heads at the nonshared time node and the downscaled BCs from its parent model (Sequence Operation 11) are used to solve the transient equation for the next time step in the last child model (Sequence Operation 12). This solution provides the BCs for the parent model (Sequence Operation 13) to advance to the parent model's calculations at the next time-step in the parent model level. Thw downscaling associated with Sequence Operation 14 is necessary to solve the transient equation for model level M^2 (Sequence Operation 15). With the resulting solution, temporal interpolation is possible (Sequence Operation 16) to provide BCs (Sequence Operation 17) for solving the next time-step in model level M^3 (Sequence Operation 18). This process of information exchange between child models and parent models is continued (Sequence Operations 19–43) until all solutions are obtained for all child models and the main model in this one time-stepping unit (i.e., one downscaling–upscaling unit).
7. If a shared so-called time node (at level l) is also shared with $l - 1$ time node, the upscaling of BCs will proceed upward until this shared time node path line ends.
8. Once convergence occurs in the previous downscaling–upscaling loop, heads in each model will be used as the ICs of the next time-stepping unit loop, and then Steps 5–8 are repeated until the total simulation time is reached.

Table 1 lists the number of times each algorithm operation is applied in one time-stepping loop. This includes partial differential equation (PDE) solving, temporal interpolation, and boundary condition interpolations.

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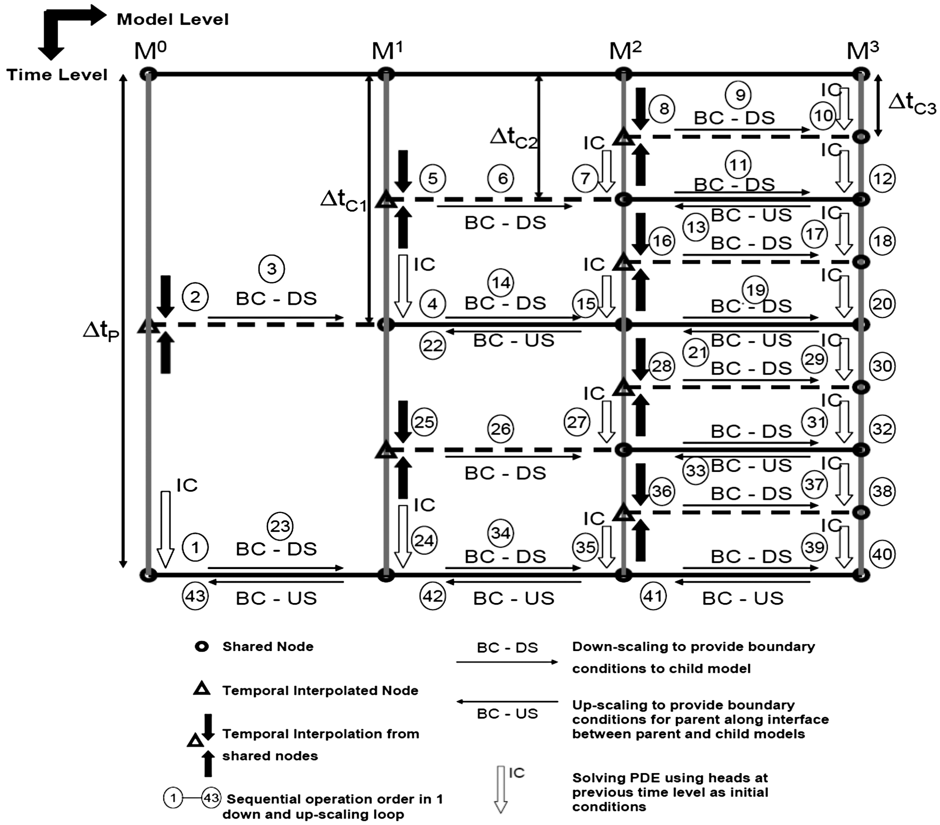

Fig. 1. One unit of local information updating approach to resolve multiple temporal scales

In the nested time-stepping algorithm, temporal interpolation is needed to obtain heads along the boundary of the child models that utilize a smaller step-size. Temporal interpolation is not only applied to heads along the interfaces of parent–child models, but also over the whole computational domain of a child model. The ICs for the nested time steps is provided by the parent model in which the time step is larger than that of the child model. If a so-called shared time nodes scheme is used in designing the nested time step system, i.e., the nested time step is a factor of parent model's time step ($n = \Delta t_P/\Delta t_C$), then the head values at shared time nodes and nonshared nodes can be easily calculated as done for the spatial grid layout where nodes are shared.

Initial Conditions

The initial conditions (or previous time-step head distribution) for every advancing time step in a child model are the heads at the previous time-step in the same model. For the parent model, initial conditions are obtained from the heads at the previous time-step by directly solving the PDE. The heads in the area that is common to the parent and child models are updated from the child model by means of upscaling.

Table 1. Total Number of Operations in One Downscaling–Upscaling Loop

Operation	Main model M^0	Level 1 M^1	Level 2 M^2	Level 3 M^3
Solving PDE	1	2	4	8
Temporal interpolation	1	2	4	—
Boundary conditions for downscaling	2	4	8	—
Boundary conditions for upscaling	—	1	2	4

Boundary Conditions

In the case of updating BCs along the path of so-called share time nodes, both the parent and child models are at the same time level and it is not necessary to perform any temporal interpolation. Spatial interpolation will be required to define updated boundary conditions from either the parent or child model.

As seen in Fig. 1, dashed lines are actually the extensions of those solid lines that miss so-called current information from their parent model. The function of the downscaling along the dashed lines is to provide missing current information from a parent model at the nonshared (so-called broken) nested time-step of a child model, such that calculation in child models can advance to the next nested time-step. For example, assume that time-step in a parent model is Δt_P, and Δt_C is the time-step in the child model. Let there be three nested time-steps in one Δt_P, or $\Delta t_P = 3\Delta t_C$. The transient equation is solved in the child model at time level $t + \Delta t_C$ with boundary conditions temporally interpolated from heads at time levels t and $t + \Delta t_P$ in the parent model. A similar procedure is used to derive boundary conditions at time level $t + 2\Delta t_C$. If a linear interpolation is applied, then boundary conditions (prescribed head) assigned to the child model at time levels $t + \Delta t_C$ and $t + 2\Delta t_C$ can be expressed as

$$H_C(t + \Delta t_C) = \frac{2}{3} H_P(t) + \frac{1}{3} H_P(t + \Delta t_P) \tag{1a}$$

$$H_C(t + 2\Delta t_C) = \frac{1}{3} H_P(t) + \frac{2}{3} H_P(t + \Delta t_P) \tag{1b}$$

where H_C = head for child model; H_P = head for the parent model.

Generally, if the number of nested time-steps in a child model is n, then their boundary conditions can be derived from the parent model in the form

$$H_C(t + i\Delta t_C) = \frac{n-i}{n} H_P(t) + \frac{i}{n} H_P(t + \Delta t_P); \quad i = 1, (n-1) \tag{2}$$

Coupling between Groundwater and Surface Water

The mathematical model for interaction between surface and groundwater is described by a system of two partial differential equations. These two governing equations must be coupled and solved simultaneously since the simulated system involves interaction terms between groundwater and surface water; in this case, lakes, wetlands, and reservoirs. The groundwater flow is governed by

$$\mathrm{S_s} \frac{\partial H^{GW}}{\partial t} = \nabla(\mathbf{K} \cdot \nabla H^{GW}) - q_{GW} + q_{SW} \tag{3}$$

where $\mathrm{S_s}$ = specific storage coefficient; H^{GW} = groundwater head (L), t = time; $\mathbf{K}$ = saturated hydraulic conductivity tensor; q_{GW} (L/T) = groundwater source/sink terms; and q_{SW} (L/T) = incoming or outgoing discharge from the surface water body. The source/sink term can be discretized as

$$q_{SW} = \sum_i^N (H_i^{SW} - H_i^{GW}) L_i \tag{4a}$$

$$H_i^{GW} = \begin{matrix} H_i^{SW} & \text{if } H_i^{SW} > Elev_b \\ Elev_b & \text{if } H_i^{SW} < Elev_b \end{matrix} \tag{4b}$$

where H_i^{GW} (L) = groundwater head in the ith cell that has interaction with surface water; H_i^{SW} (L) = surface water head corresponding to its counterpart of groundwater head H_i^{GW}; $L_i(\mathrm{T}^{-1})$ = leakance of the interactive cell; $Elev_b$ (L) = bed elevation of the surface water body (which could be spatially variable); and N = total number of surface water cells.

The surface water bodies' water level, H^{SW}, is governed by the subsequent continuity equations

$$\frac{\partial V_{SW}}{\partial t} = Q_{SW} - Q_{GW} \tag{5a}$$

$$\frac{\partial V_{SW}}{\partial t} = S_{SW} \frac{\partial H^{SW}}{\partial t} + H^{SW} \frac{\partial S_{SW}}{\partial t} \tag{5b}$$

where V_{SW} = storage volume of the water body (L^3); $Q_{SW}(\mathrm{L}^3/\mathrm{T})$ = incoming discharge; Q_{GW} (L^3/T) = incoming or outgoing discharges from groundwater; S_{SW} = surface water area (L^2); and H^{GW} = surface water level (L). Assuming S_{SW} does not vary with time, the governing set of coupled equations for the groundwater–lake system is

$$S_{SW} \frac{\partial H^{SW}}{\partial t} = Q_{SW} - Q_{GW} \tag{6a}$$

$$Q_{GW} = \sum_i^N (H_i^{SW} - H_i^{GW}) L_i A_i \tag{6b}$$

$$H_i^{GW} = \begin{matrix} H_i^{SW} & \text{if } H_i^{SW} > Elev_b \\ Elev_b & \text{if } H_i^{SW} < Elev_b \end{matrix} \tag{6c}$$

where A_i = area of the ith interactive cell (L^2), which could be a function of time and of water elevation. Interaction of surface water and groundwater will be implemented through constantly updating the coupling terms q_{SW} in Eq. (3) and Q_{GW} in Eqs. (5a) and (5b) in a nonlinear fashion. Numerical schemes to approximate Eq. (3) have already been described previously. The surface water head is approximated by applying backward difference scheme to the time derivative and an explicit scheme to the coupling terms in the right-hand side (RHS) of Eqs. (5a) and (5b)

$$H^{SW(n+1)} = H^{SW(n)} + \frac{\Delta t}{S_{SW}} \left[Q_{SW}^{(n+1)} - \sum_i^N (H_i^{SW(n)} - H_i^{GW(n)}) L_i A_i \right] \tag{7}$$

where n and $n+1$ denote previous and current time levels, respectively; and Δt = time-step.

Hierarchical Parameter Estimation

In multiscale modeling, both the model parameters and the observed data can be at multiple scales, making the parameter estimation more difficult. For example, calibration of a regional model involves data measurements at multiple scales, such as drawdown results from an aquifer test, which are mostly at site scale, and static water levels at the regional scale. If this model were to be calibrated without distinguishing between site-scale and regional-scale data, oftentimes the problem may tend to become ill-posed because the relatively large grid sizes used for a regional model cannot accurately characterize site-scale drawdown. Therefore, it is necessary to have a series of nested models that can capture the different scales of variability and to calibrate these models. Nested modeling can thus integrate information from different scales appropriately, which can enhance the predictive abilities of multiscale groundwater studies (Yeh et al. 2008).

A key consideration is how to assign model parameters in the main and nested models. Imagine a hierarchical model with one parent and one child model, and let there be observations of hydraulic head for both the parent and child models. If these models were calibrated, the value of hydraulic conductivity that best fits the parent model's observations need not necessarily be the same as the value that best fits the child model's observations. Thus, the model parameters should have different values at different scales.

The procedure for hierarchical parameter estimation is similar to traditional parameter estimation, except that there are many models and each has its own calibration targets and calibration parameters. Instead of optimizing each model individually, all models are optimized together by computing one objective function that combines residuals from all the models, while assigning an appropriate statistical weight for parameters from a given model level. For example, a site-scale model may have residuals of the order of centimeters (inches) while the regional model may have residuals of the order of meters (feet). Both residuals cannot be assigned equal importance in the calibration.

This process of combining the residuals from different models ensures that a change in the regional model can influence the site-scale model (and vice versa). This parameter estimation approach also benefits from the two-way iterative head/flux coupling between the models; every model can influence the calibration of other models in the hierarchy. Computer software *UCODE* (Poeter and Hill 1999; Hill and Tiedeman 2007) was used to perform the hierarchical parameter estimation.

Assume there are models at N different scales, each with some unknown model parameters $\vec{\mathbf{a}}_1, \vec{\mathbf{a}}_2, \ldots, \vec{\mathbf{a}}_N$ which have to

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be estimated. Let each scale have a set of observations $\vec{\mathbf{Y}}_1, \vec{\mathbf{Y}}_2, \ldots, \vec{\mathbf{Y}}_N$. The residuals are defined as

$$\vec{\mathbf{r}}_i(\vec{\mathbf{a}}_i, \vec{\mathbf{x}}) = \vec{\mathbf{Y}}_i - \vec{\mathbf{Y}}_i^*(\vec{\mathbf{a}}_i, \vec{\mathbf{x}}) \qquad i = 1,2, \ldots, N \tag{8}$$

where $\vec{\mathbf{Y}}_i^*(\vec{\mathbf{a}}_i, \vec{\mathbf{x}})$ = simulated values at the corresponding observation in space and time. Each residual is a vector depending on the number of observations at each scale. The objective function for the ith scale can be expressed as

$$s_i = \sum \left(\sqrt{w_j^{SC-i}} r_j^{SC-i}\right)^2 \qquad j = 1,2, \ldots, N^{SC-i} \tag{9}$$

where w_j^{SC-i} = weighting for the jth observation; r_j^{SC-i} = residuals for the jth observation; and N^{SC-i} = total number of observations, all at ith scale (i.e., all patches).

The weights in this context may be assigned to account for the different types of observations, i.e., heads and flows. Since the magnitude of the residuals for these observations are different, assigning appropriate weights to them (see the subsequent text) ensures that all types of observations have equal importance within each submodel. The final objective function for the whole system is taken as the weighted sum of the weighted residual of each scale as

$$S = \sum w_i^s s_i \tag{10}$$

where w_i^s = weighting for the ith model scale.

To optimize the objective function an iterative procedure that equates the first derivative to zero is used, and thus obtains the new value of parameters for the next iteration until the mathematical convergence criterion is met as shown next

$$\mathbf{J}^{\mathrm{T}}(\vec{\mathbf{a}})\mathbf{W}\vec{\mathbf{r}}(\vec{\mathbf{a}}) = 0 \tag{11}$$

where $\mathbf{J}$ is the Jacobian matrix with $J_{ij} = \partial r_i / \partial a_j$; and $\mathbf{W}$ is the weight matrix. Eq. (11) can be rewritten as

$$\sum_m^M \sqrt{w_m} r_m \frac{\partial[\sqrt{w_i} \sum r_m]}{\partial \vec{\mathbf{a}}_i} = 0 \qquad i = 1, \ldots, N_P \tag{12}$$

where $M = N^{SC-1} + N^{SC-2} + \ldots + N^{SC-i}$ = total number of observations; $N_P = N_{P1} + N_{P2} + N_{PN}$ = total number of parameters; and w_m = composite weighting computed as

$$w_m = w_i^s w_m^{SC-i} \tag{13}$$

where w_m^{SC-i} = weighting for the mth observation at scale i. Eq. (11) can be solved by the modified Guass–Newton method.

The weights in Eq. (10) are for the different scales and can be fixed by a process of trial-and-error. In general, the weights for the smaller scales are larger than the weights assigned at larger scales. This is evident because the residuals and objective functions for the smaller scales will be, in general, smaller in magnitude than those for the larger scales. A commonly adopted value for the weight is $(\sigma^2)^{-1}$, i.e., the reciprocal of the variance for the parameter of interest.

With the appropriate weights assigned, the objective function is then minimized to obtain the model parameters that best fit the observations at all the different scales. The Jacobian matrix for this case will be a composite, comprising all the residuals and all parameters from all scales. Thus, if there are n observations and m parameters in the entire modeling hierarchy, the Jacobian matrix will have dimensions $n \times m$.

If the hierarchical model is a transient model with both downscaling and upscaling, the parameter estimation process will consist of the following six steps:

1. Make an initial guess of model parameters,
2. Run the hierarchical model for entire simulation length with the downscaling–upscaling iteration performed for every time step,
3. Compute residuals for entire simulation length,
4. Recompute model parameters,
5. Check convergence criterion (if satisfied, go to Step 6; otherwise, go to Step 2), and
6. Stop.

Illustrative Examples

In order to illustrate the hierarchical parameter estimation approach two examples are presented, as follows: (1) a synthetic example that shows that even for a relatively simple scenario, the traditional approach of parameter estimation results in nonunique solutions, which was overcome by using the hierarchical approach; and (2) a real-world application of hierarchical modeling and parameter estimation, for a coupled surface-water-groundwater system.

Synthetic Example

Problem Statement

The goal is to estimate hydraulic conductivity (K) and recharge (ε) within the study area (Fig. 2), consisting of a fairly homogeneous sandy aquifer ($3{,}000 \times 3{,}000$ m) with unknown K and some localized heterogeneity (clay zones). The hydrologic features in this area include four perfectly connected water bodies (small lakes and a river), and a uniform but unknown recharge. A pumping well ($2{,}500\ \mathrm{m^3/day}$) is situated near a lake and a known clay layer. A monitoring well is located about 20 m away from the pumping well. The western edge of the study area has a constant head boundary (river), while the other edges are no-flow boundaries.

Problem Design

The study area is simulated at a fine resolution, both spatially (10 m) and temporally (10 s), using $\mathrm{K} = 100$ m/day and $\varepsilon = 25$ cm/year. This model is treated as the so-called truth and is then sampled at random locations and also at various times at the monitoring well location to create a time series. Then, and attempt is made to calibrate the model using only the sampled data in order to verify if the parameter estimation approach can reproduce the original parameter values. In this parameter estimation problem the only unknowns are the parameters themselves, since the conceptual model (sources/sinks, boundary conditions, and geologic framework) is identical to the one used to generate the data. The specific steps that were used in this process are given, as follows:

- Create a single steady-state model of the study area with the pumping well turned off.
- Sample the steady-state model at a few scattered points to create synthetic head data. These data represent the regional-scale processes.
- Create a transient model at the same resolution to simulate the dynamics created by turning the pumping well on. The steady-state model heads provide initial conditions to the transient model. Due to high K and the presence of a lake nearby, the transient model quickly reaches steady-state (~7 min). The time-step used in this model is 10 s.

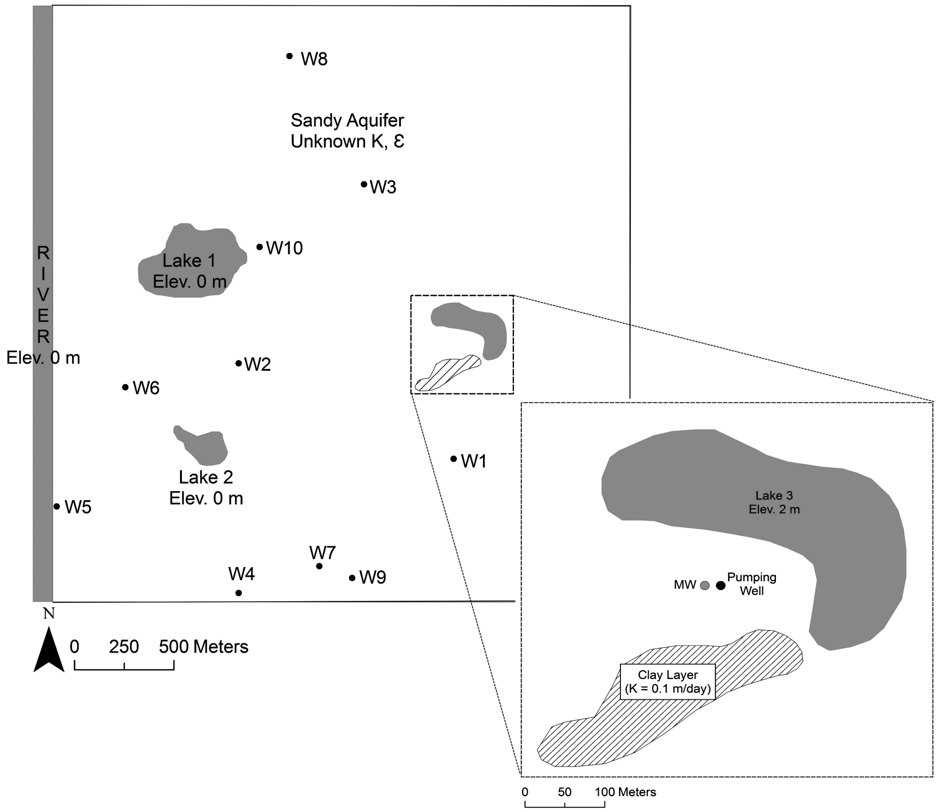

Fig. 2. Study area showing regional and submodel areas, sources and sinks, heterogeneity, and locations of monitoring wells

- Sample heads at the monitoring well at multiple times to capture the drawdown curve. These data represent the local-scale processes.
- Use the generated synthetic data to perform parameter estimation assuming K and ε are unknown. The synthetic data locations are shown in Fig. 2 and data values are listed in Table 2.

Parameter Estimation

Given the information about the study area and the data available for calibration, a few different approaches can be used to estimate K and ε. The first, and relatively simplest, approach is to simulate and calibrate a coarse regional model. The drawback of this approach is that it can use only the regional static water level data for calibration, because the regional model lacks the spatial or temporal resolution to resolve the local transient dynamics. The synthetic example demonstrates that when such a model is calibrated it can result in nonunique solutions. Another approach would be to use a local model around the pumping well to simulate the transient dynamics. This model cannot use the available regional head data, and moreover, would require boundary conditions from a regional model, which as described previously produced nonunique solutions. Yet another approach would be to use a single high-resolution model with a uniform grid that captures both the regional and local dynamics simultaneously. This approach is computationally very intensive and may be impractical for parameter estimation. Such dilemmas are very commonly faced in practical groundwater modeling and are not particular to this synthetic example. An effective way to tackle such issues is to use a hierarchical approach, which simulates the regional and local dynamics simultaneously. This approach has the advantage of making full use of existing data while still being computationally feasible.

Table 2. Synthetic Data

Steady-state data		Transient data (Monitoring well)	
Location	Head (m)	Time (s)	Head (m)
W1	1.338	10	1.928
W2	0.295	20	1.764
W3	0.991	40	1.695
W4	0.434	60	1.67
W5	0.008	80	1.655
W6	0.048	100	1.646
W7	0.739	150	1.634
W8	0.696	200	1.629
W9	0.871	300	1.626
W10	0.234	400	1.624

The goal of parameter estimation is to vary the parameters such that the objective function is minimized. In order to demonstrate the improved ability of the hierarchical approach, objective function w is computed for a range of values of the calibration parameters and compared it to a conventional regional model's objective function that ignored local data. In the hierarchical approach, the regional and local model's residuals (difference between simulated and observed values) were first computed [Eq. (8)]. The objective function for each scale was then computed as the weighted sum of the squared residuals [Eq. (9)]. In general, the weights are assigned to reflect the different types of data. In this case since the data were of the same type (heads), the weights were all equal. The overall objective function was then calculated as the weighted sum of the objective functions at each scale [Eq. (10)]. In this example, equal weights were assigned for the different scales.

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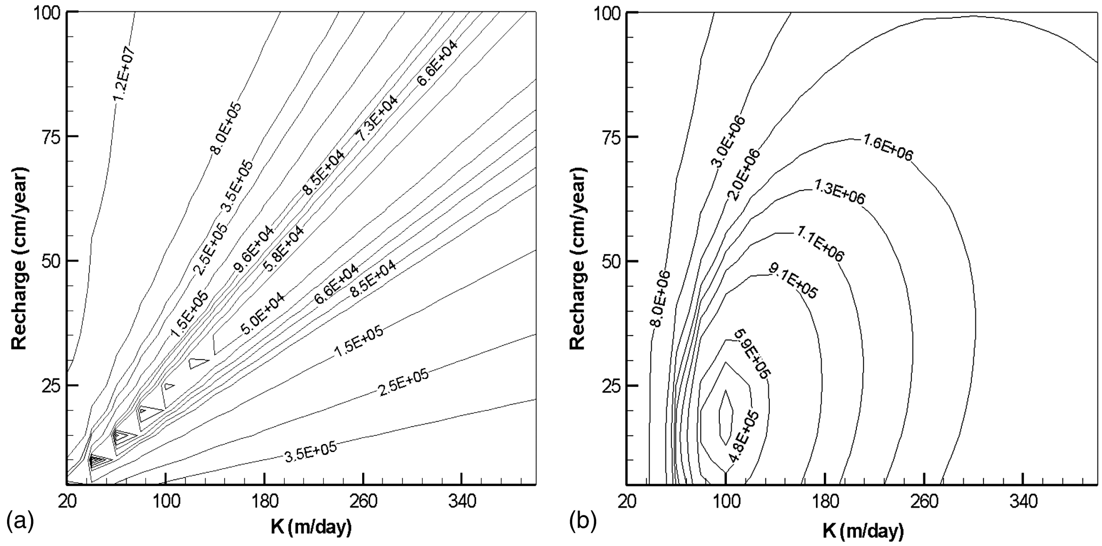

Fig. 3. Comparison of objective functions for the following: (a) regional model calibrated with regional data; (b) hierarchical model calibrated with both regional and local data

Results and Discussion

The objective functions for a single regional model and the hierarchical model are shown in Fig. 3. Such plots are very useful as they can easily identify the parameter values that minimize the objective function. It can also clearly indicate if the solution is nonunique or not, i.e., if more than one combination of parameter values can minimize the objective function. The regional calibration shows that the objective function is minimized for multiple combinations of K and ε, and therefore the parameter estimation problem is ill-posed, in the sense that the solution is nonunique. This is because when K and ε are increased/decreased proportionally, there is no effect on the heads. If additional data (e.g., time-series head data, flux data, and so on) are added, then the calibration may become more unique. Hierarchical calibration, on the other hand, produces a clear global minimum for the objective function that optimizes both the regional and local model simultaneously. The parameters obtained from the hierarchical calibration are $K = 100$ m/day, and $\varepsilon = 20$ cm/year, which are very similar to the true solution. The reason inability to recover the exact solution ($K = 100$ m/day and $\varepsilon = 25$ cm/year) is because the so-called true model used a finer grid than the hierarchical model. From this simple synthetic example it is clear that failing to use all available data for calibration can result in ill-posed problems. This synthetic example clearly illustrates that the hierarchical approach offers the flexibility of using all available data for calibration and also that it can improve the ability to uniquely estimate model parameters. This is important because in real-world situations many more parameters may need to be calibrated and available data are rarely enough to uniquely constrain the calibration.

Real-World Example

The hierarchical modeling and parameter estimation process is illustrated through its application to a model used for predicting the feasibility of augmentation of the Sister Lakes in southwest Michigan. Sister Lakes consist of three interconnected lakes, as follows: (1) Round Lake, (2) Big Crooked Lake, and (3) Little Crooked Lake. There are three other nearby surface bodies [(1) Cable Lake, (2) Dewey Lake, and (3) Magician Lake]. Lake augmentation for the Sister Lakes was planned such that water would be pumped from the irrigation well (IW) and discharged to the Sister Lakes to increase the lakes' water level. Fig. 4 shows a plan view of the entire modeling domain, including the location of the irrigation well and two observation wells (OWs), i.e., (1) OW-1, and (2) OW-2.

In an area where high pumping rates are applied, the effect of pumping is highly localized and changes rapidly with time. This water is pumped back into the lake and causes a sudden increase in water level in the lake. As the effect of pumping reaches the other lakes, they start providing water to the pumping well, causing a reduction in their water levels. At the same time, the increased water level in the Sister Lakes will induce flow from the Sister Lakes towards the other lakes. To simulate this complex flow system, it is necessary to create models at multiple scales that can capture the spatial and temporal dynamics and to capture the complex groundwater–surface water interactions. These multiscale models also need to be calibrated. Therefore, the hierarchical modeling and parameter estimation detailed previously is appropriate for the Sister Lakes site.

Conceptual Representation

The modeling area was the entire watershed shown in Fig. 4, even though the Sister Lakes and all observations needed for calibration were far from the no-flow watershed boundaries. The model was created using the perturbation approach, i.e., the initial condition of the model was of no flow input throughout the model domain. This ensures that the effect of other sources of water, such as recharge, are not taken into account and only the effect of pumping on lake levels is studied. Therefore, the changes in head (drawdown) caused by pumping are used for calibration instead of absolute head values.

Because the change in head was simulated, the absolute values of the aquifer elevations were not needed; the aquifer top elevation and thickness were assigned at a constant value of 1 and 80 m, respectively. The irrigation well was set to pump at 4,360 m^3/day, and this water is then pumped back into the Sister Lakes. The initial heads in the aquifer and all the lakes was set to 0 m. The

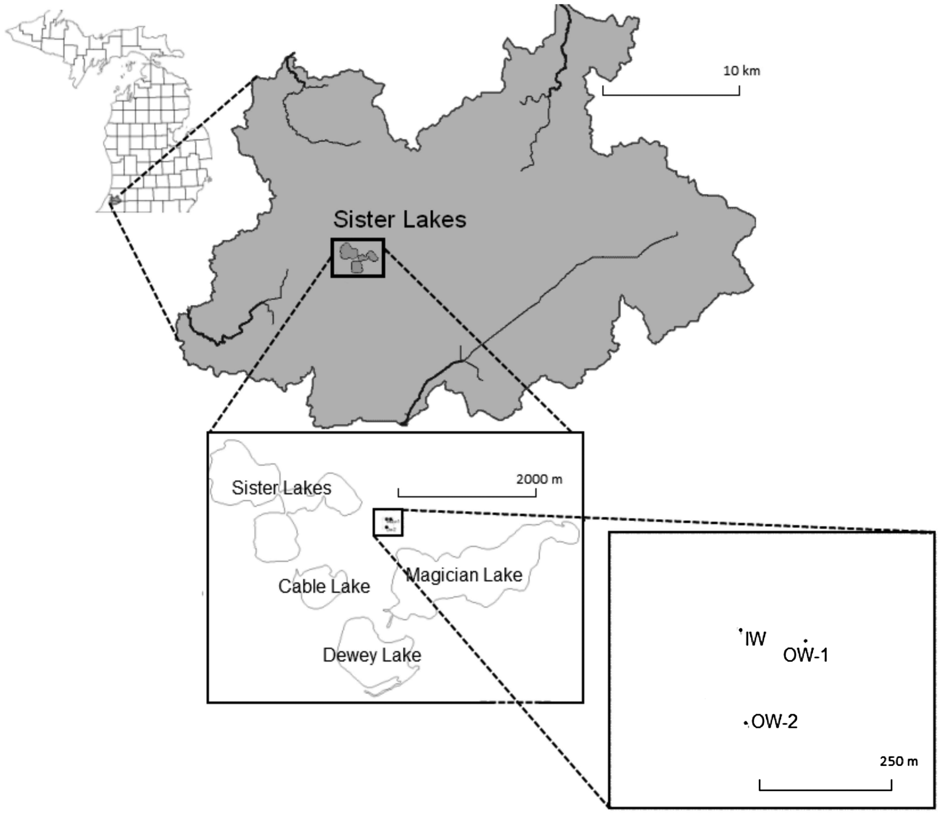

Fig. 4. Plan view of model site

hierarchical model parameters and the time-stepping information are defined in Tables 3 and 4, respectively. The models were run with a two-way head-coupling, i.e., hydraulic head was used for both downscaling and upscaling. In addition, the interaction between the lakes and the aquifer was modeled as a coupled process. In the hierarchical modeling framework, the child models were spatially nested, but no temporal nesting was applied. Therefore, the entire modeling framework utilized a time-step such that the smallest child model could sufficiently capture the temporal drawdown dynamics. The domain and grid size for each model level were chosen such that the fine-scale (submeter) drawdown effects at the lowest submodel level were adequately captured. The general principle in nested modeling is to create as many model levels as necessary while limiting the model grids to sizes that can be easily handled using the computer available (Afshari et al. 2008).

Transient Calibration and Modeling

Before running the entire simulation length of the model, it was calibrated using the transient data from a 72-h onsite pumping test

Table 3. Hierarchical Model Parameters

Model level	Model name	Domain size (km × km)	Grid	Grid size (m)
0	Main model	37 × 27	120 × 88	311
1	Submodel 1	6.8 × 4.7	111 × 76	62
2	Submodel 2	0.56 × 0.50	73 × 65	8
3	Submodel 3	0.186 × 0.195	97 × 101	2
4	Submodel 4	0.011 × 0.008	49 × 33	0.2

Table 4. Time-Stepping Information

Duration (day)	Time-step Δt (day)
$0 < t \leq 0.1$	0.002
$0.1 < t \leq 0.5$	0.01
$t > 0.5$	0.05

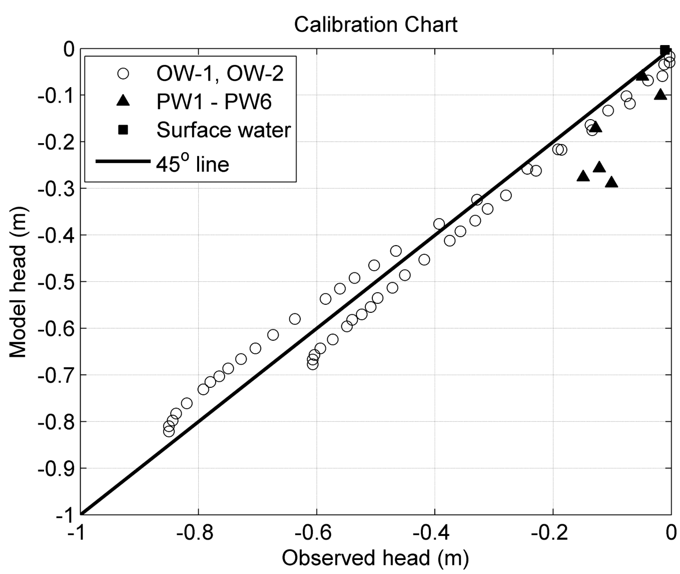

Fig. 5. Comparison of simulated an observed heads at Observation Well 1 (i.e., OW-1) and Observation Well 2 (i.e., OW-2), six private wells, and a surface water feature

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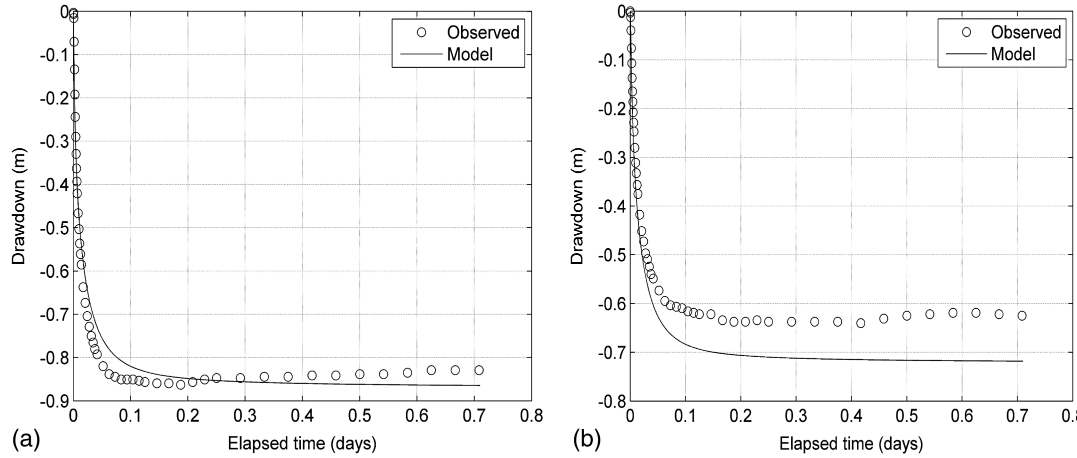

Fig. 6. Calibration hydrograph for the following: (a) OW-1; (b) OW-2

with a pumping rate of 4,360 m^3/day applied at the irrigation well location. The calibration targets were the transient hydrographs and drawdown at two groundwater observation wells and the drawdown observed at six private wells 72 h after pumping began. A staff gage that measured the change in water level in Big Crooked Lake after 72 h of pumping was also used. The calibration parameters were the hydraulic conductivity and specific yield of the aquifer and the lakes' leakance values. However, instead of estimating the parameters themselves, their multipliers were selected for calibration

$$K = F_K K_r \tag{14a}$$

$$S_y = F_S S_{y0} \tag{14b}$$

$$L = F_L L_0 \tag{14c}$$

where K = hydraulic conductivity of the aquifer (LT^{-1}); F_K = multiplier for conductivity; and K_r = spatially explicit, interpolated

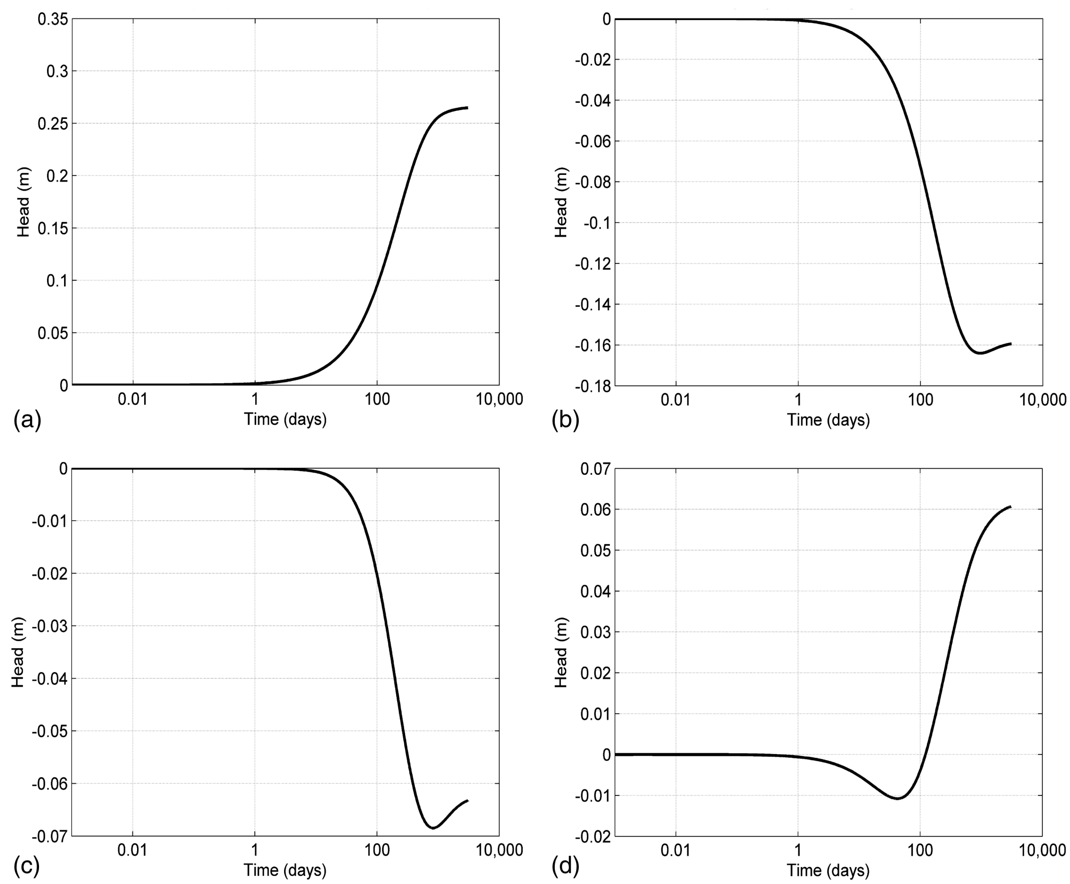

Fig. 7. (a) Head hydrograph at Sister Lake, L (R, D); (b) head hydrograph at Magician Lake, L (M); (c) head hydrograph at Dewey Lake; (d) head hydrograph at Cable Lake

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conductivity from the Wellogic database (MDEQ 2006). Similarly, S_y is the specific yield of the aquifer, F_S is its multiplier, S_{y0} is a given specific yield (constant over the domain), L is the lake leakance (T^{-1}), F_L its multiplier, and L_0 the given lake leakance (the same for all lakes). The initial estimates for F_K, F_S, and F_L were 0.4, 1.0, and 1.0, respectively, which were then calibrated. The values for S_{y0} and L_0 were 0.0005 and 1.0 day^{-1}, respectively. Values of S_{y0} and L_0 are constant in the entire hierarchy of models; thus, there are only three parameters to be estimated. The weights for the different scales were set to a value of 1, because change in head was used and not the absolute head values to calibrate the models. Therefore, the observations at different scales were all equally important. Using the parameters obtained from the transient calibration, the model was run for its entire simulation length of 3,000 days. This longer-period simulation is for the conditions under consideration and is not a real prediction of future conditions which may require more detailed information (e.g., climate conditions, future land use and land cover, and so on). The results from the simulation are discussed in the subsequent subsection.

Results and Discussion

The simulation was completed after about 24 h with a 3.2-GHz CPU with 4 GB of random-access memory (RAM). The results of the transient hierarchical parameter estimation are shown in Figs. 5 and 6. The calibration was satisfactory because the model was able to capture the transient dynamics in the hydrographs for both observation wells. The multipliers F_K, F_S, and F_L obtained from calibration were 0.4989, 200, and 0.77495, respectively. The resulting specific yield was 0.0003875 and lake leakance was 61 day^{-1}.

Fig. 7(a) shows the hydrograph for Sister Lakes, which shows a steady increase in water level reaching steady state at ~0.25 m after approximately 1,500 days. Similarly, Figs. 7(b and c) show the hydrographs of Magician Lake and Dewey Lake, respectively, revealing a gradual decline in water level and then recovery of a small portion to reach a steady-state towards the end of the simulation. Fig. 7(d) shows Cable Lake's hydrograph, which varies from all the others in that it shows a slight decrease in water level in the

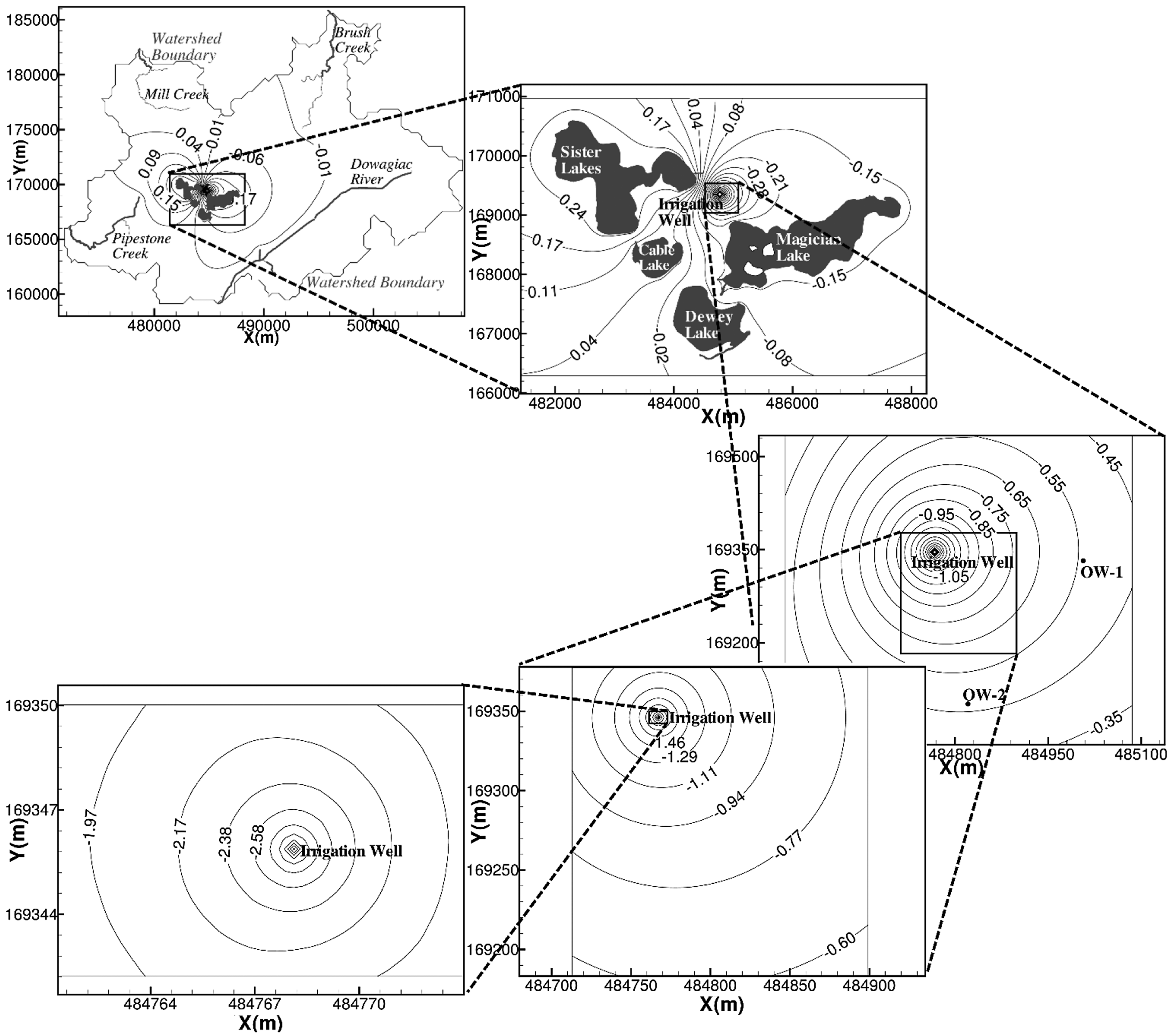

Fig. 8. Head contours (meters) from all model levels after $t = 3{,}000$ days

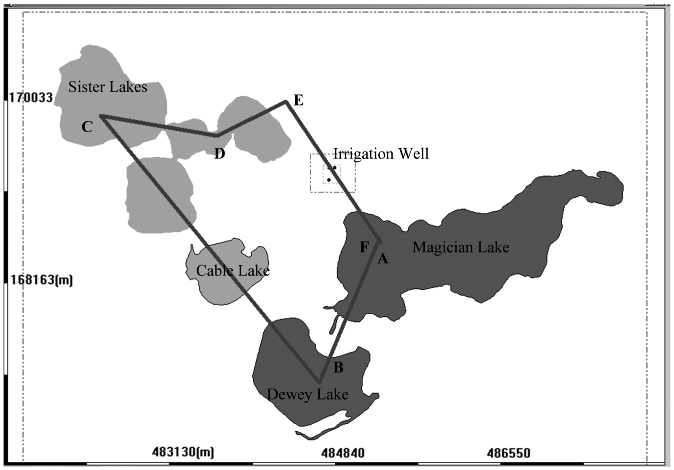

Fig. 9. Location of cross section A–E on the site

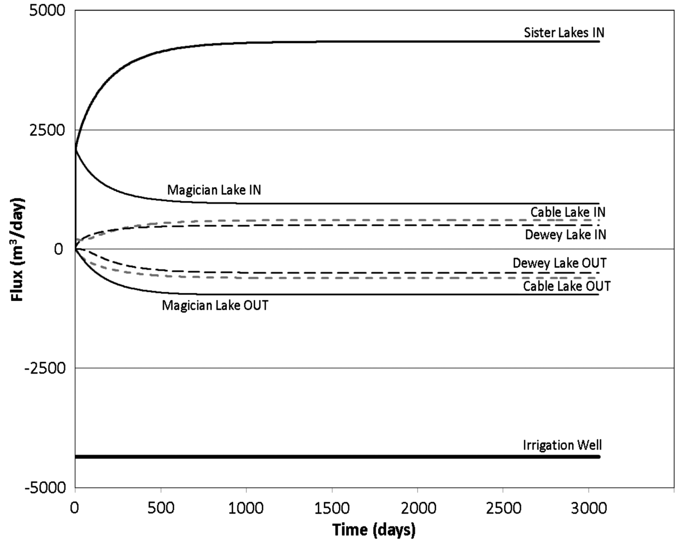

Fig. 11. Transient mass balance for the major sources and sinks

initial days of pumping, and then recovers at later times to an increased water level relative to its initial condition. Fig. 8 shows the head contours and the flow field created from the simulation of 3,000 days.

Fig. 9 shows a cross section that passes through all the lakes in the model. The change in head along this cross section is shown in Fig. 10, and indicates that the Sister Lakes saw the greatest increase in water level of approximately 0.3 m. Although Cable Lake did not directly have water pumped into it from the irrigation well, its water level increased by about 0.06 m (in spite of an initial decline in water level). Magician Lake, which is the largest and the lake closest to the pumping well, saw the greatest decline in water level at 0.16 m.

The transient mass balance is shown in Fig. 11. A close inspection of the mass balance shows that after 1 day of pumping, the outflow from Sister Lakes is ~46% of the pumping rate, and continues increasing to ~49% after 4 days of pumping. Eventually, the outflow from Sister Lakes is equal to all the water being pumped. However, the head contours suggest that not all the water goes directly to the pumping well. Some of this water flows into the nearby lakes, Cable Lake and Dewey Lake. The outflow from Cable Lake is ~5% of the pumping rate after 0.5 days. Subsequently, this outflow decreases steadily as a result of increasing inflow from Sister Lakes. This inflow continues to increase and eventually a steady-state is established. Examining the head contours reveals that some of the outflow from Cable Lake goes to the pumping well and the rest flows to Dewey Lake, and possibly to Magician Lake.

The effect of pumping takes almost 0.025 days to reach Dewey Lake, after which the outflows from Dewey Lake gradually increase. After more than 20 days of pumping, it starts receiving inflows from the other lakes. By the end of the simulation, Dewey Lake reaches steady-state. In addition, the head contours suggest that the entire outflow from Dewey Lake goes to Magician Lake. The outflow from Magician Lake, similar to that from Sister Lakes, is approximately 46% of the pumping rate after 1 day of pumping. This increases to ~47% after 4 days of pumping, and then starts decreasing. This decrease in outflow is accompanied by an increase in inflow from the other lakes, eventually causing Magician Lake to reach a steady-state configuration. Unlike the other lakes, the entire outflow from Magician Lake has to necessarily go to the pumping well, in order to close the loop, so to speak. This is evident both from the head contours and the cross-sectional view, which show that the only area with lower heads than Magician Lake is the pumping well.

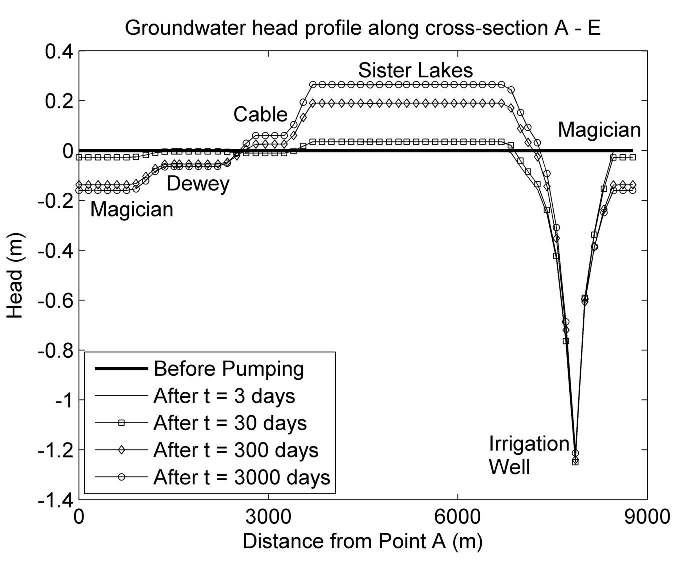

Fig. 10. Head profile along cross section A–E

Conclusions

A hierarchical modeling approach for complex flow systems having multiple spatial and temporal scales of variability was developed. A nested temporal grid layout was established that allows local models to take multiple small time steps within one large time step of the regional model. This approach is especially suited for simulating the interactions between groundwater and surface water (lakes and wetlands). A hierarchical parameter estimation that could include both data and parameters at multiple scales was developed and illustrated through the use of a synthetic example. The hierarchical modeling methodology was applied to a lake augmentation system for the Sister Lakes in southwest Michigan. A hierarchical framework consisting of five interlinked models was created with two-way communication between the models. The model was calibrated using drawdown data from a 72-h pumping test. The calibrated model was then used to run the entire simulation of lake augmentation. This field example indicates that

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hierarchical modeling and parameter estimation approach was able to satisfactorily model real-world complexities.

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