Appendix A. Introduction to Groundwater Flow Modeling

Scientists and engineers often cannot directly analyze natural systems because they are too complex or cumbersome, and instead must use models to describe and analyze the systems. The modeling process begins with the development of a conceptual model, which is a summary of the major components of the system and the processes that link them. The conceptual model of the aquifers of interest to this study identifies the aquifers and their extent, the associated surface-water bodies, the stresses of pumping and recharge, and the physical process of water moving through porous media. The conceptual model is quantified by a mathematical model, which is the set of equations representing the physics, properties, stresses, geometry, etc. of the system. The solution of the mathematical model yields the hydraulic heads and flow rates corresponding to the conceptual model, which can be used to simulate the aquifers' responses to projected stresses. Solving the many interrelated equations of a detailed mathematical model is a tedious task that is commonly addressed by programming a computer. Computer programs for modeling groundwater flow, or modeling codes, represent generic sets of physical properties that can be adapted to a specific system by assigning parameters that describe the system and its stresses. The modeling code and the input parameters for a specific groundwater system are collectively referred to as the model. That is, the code is written once, but the model is designed and built for each specific application (Anderson and Woessner, 2002).

A.1. Finite-Difference Groundwater Flow Modeling

Representing the irregular geometries and spatial variability of aquifers and surface-water bodies frequently results in a complex mathematical model whose solution requires special techniques. In this study, the mathematical model is solved using the finite-difference method, a technique that mathematicians classify as a numerical solution. The finite-difference method begins by superimposing a checkerboard-like grid on the modeled region and dividing the aquifers into a set of finite differences, or blocks. Each block represents an aquifer volume of homogeneous properties where the hydraulic head will be determined. The hydraulic head in each block is governed by classical equations for mass conservation and flow in porous media that depend on the aquifer properties and the hydraulic head in the surrounding blocks. To this are added mathematical constraints known as boundary conditions to represent sources, sinks, and aquifer limits (recharge, wells, rivers, etc.). Because the hydraulic head in each block depends on the head in the surrounding blocks, the equations for the block are an interrelated set that must be solved simultaneously. Various mathematical tricks are employed to solve the set of equations to yield a solution for the hydraulic head at each block center and the flow rates among all components of the modeled system. Changes in the system with time can be found by repeating the finite difference solution for a series of time steps for a so-called transient solution. In this instance, the hydraulic head in the blocks during each time step depends on changes in the boundary conditions (e.g., pumping rates), the amount of water released from storage, and the hydraulic heads of the previous time step. The computational burden increases dramatically with the number of blocks in the grid and the number of time steps in the transient simulation.

A.2. Data Requirements of Groundwater Flow Modeling

A detailed finite-difference model can faithfully represent the system and provide a highly resolved simulation of groundwater flow in the region of interest. But in addition to the computational burden, every block and time step require input parameters. For a site-specific modeling study, inferring these parameters requires data and information on surface hydrology, geology, and pumping history. Further, calibrating the model and building confidence in its results also require observations of hydraulic head and discharge to streams for comparison to model simulations. In short, an extensive, detailed model requires supporting databases and software to manage input parameters and interpret the results. While there are extensive databases available at the regional scale related to, for example, geology, hydrology, and topography, developing a groundwater model generally requires developing supporting databases for local details and pumping history.

Every finite-difference model requires defining the rows, columns, and layers of the grid. This grid definition is largely developed from the geologic model, with the top and bottom surfaces of hydrostratigraphic units used to define the grid layers, so that each block corresponds to a specific portion of the modeled system. Model grids generally have greater resolution in the area of interest (for increased precision) and near pumping wells (for increased accuracy). Grid resolution is decreased in areas of peripheral interest to reduce the computational burden.

Hydraulic properties must also be assigned to each block, including hydraulic conductivities, storage properties (specific storage and specific yield), and effective porosities. Because these can be highly variable and observations are sparse, hydraulic properties are inferred from the statistics of interpreted field tests, previous modeling studies, and from studies in neighboring regions. In this modeling study, and in many others, hydraulic properties are assigned using a zoned approach, with zone boundaries based on geology. For example, research may show that areas of bedrock-surface exposure of a model layer are more permeable as a consequence of weathering, so these areas of exposure are defined as a zone, and that zone is assigned a single value of hydraulic conductivity reflecting the increased permeability. Lithology can also be used as a basis for zone definition.

Hydrologic data are taken from various sources to develop the groundwater model. Boundary conditions representing surface-water bodies and their elevations are taken from digital maps. Streamflow statistics are used to determine plausible ranges of base flow for use in calibrating the models. Maps of low-flow characteristics are used to identify streams to be represented as drains that go dry under conditions of low recharge or high pumping. Hydraulic head measurements in wells (water level measurements) are interpreted to create the potentiometric surface maps used in developing the conceptual model and initial conditions. Estimates of groundwater recharge are developed from streamflow statistics, rainfall data, and watershed characteristics. Recharge estimates are difficult to come by, and the estimation techniques are an area of active research (National Research Council, 2004). Water level measurements are also used directly in calibrating and verifying groundwater flow models. Ideally, such hydrologic data are available for each stream and aquifer at a high level of resolution in space and time. Groundwater salinity and temperature are used indirectly to adjust the hydraulic conductivity at great depth, and to evaluate the effect of unmodeled movement of salinity.

Drained areas are challenging to characterize in general, because their locations are rarely mapped and difficult to detect. Locations are typically inferred from soil maps and topography, and drain elevations, based on typical practices in Illinois, are assumed to be below the depth of freezing (that is, about 3 ft). The drain leakance is typically calibrated to maintain base flow, balance recharge, and imitate natural wetlands.

Wells can have an enormous affect on the model results, and require several types of data. This includes the location of the well and aquifers from which it withdraws water (the open, or screened, interval). The operating interval and rate need to be taken from owner surveys or inferred from population data. The same information set is required for any hypothesized wells to be simulated in projections into the future.

A.3. Nested Models and Telescopic Mesh Refinement

The design of the finite-difference grid for a model must balance the needs for accuracy and precision with the need to include regional flow patterns in the model. Satisfying both of these objectives would result in an extensive, detailed model grid with the associated burdens of slow computational times, large memory requirements, extensive datasets, and cumbersome data processing tasks. An alternative strategy is to first simulate the regional flow pattern with a coarse-grid model, then create a second, local-scale model with a finely spaced grid for the area of interest. The models are joined, or nested, by taking simulated flows or heads from the regional model and applying these along the edges of the local model as boundary conditions. This strategy, known as *telescopic mesh refinement* (TMR), reduces the computational burden while providing the necessary detail in the area of interest (Ward et al., 1987). The challenge of TMR is to design the local model grid such that the local model boundaries need not be updated to reflect transient effects or changed scenarios. In practice, this can be achieved by positioning the edges of the local model at natural boundaries (e.g., low permeability strata, rivers) and maintaining a buffer zone between the area of interest and the edges of the local model. TMR boundaries can be assembled from regional model simulations using a model post-processor such as Groundwater Vistas (Environmental Simulations Inc., 2005) or using spreadsheets and GIS as necessary. Regardless of the time step of the regional model used for TMR or the data processing approach, the analyst must verify that TMR boundaries accurately transfer the regional conditions to the local model and that only trivial changes occur along the TMR boundary as the local model simulates transient conditions or pumping changes (Anderson and Woessner, 2002).

A.4. Model Calibration

Calibration is the process of adjusting the components and input parameters of the model so that values simulated by the model match the equivalent values measured in the field. Calibration is necessary in groundwater modeling because the modeled process is complex and the simulated values of hydraulic head and flow are more easily measured than the input parameters of hydraulic conductivity, storage parameters, recharge, and leakage (Hill, 1998). Although one perspective is that calibration is only the so-called inverse problem (given the model results and some target observations of head and flow, find the set of input parameters) (Anderson and Woessner, 2002), this report uses model calibration to refer to the following:

- checking data discrepancies (for example, missing records, aquifer assignment errors, etc.);
- managing strata that are discontinuous;
- choosing approaches for representing desaturating aquifers;
- refining parameter zones;
- fine-tuning the numerical algorithms for a stable solution;

- assigning weights to target observations;
- calculating the sensitivity of the results to the input parameters;
- adjusting input parameters to match model-simulated values to observed values (the inverse solution);
- assessing the plausibility and uncertainty of input parameters;
- testing alternative models (e.g., zonation of parameters, weighting schemes);
- examining model errors;
- transient verification; and
- assessing the sensitivity of model projections to uncertain input parameters.

The inverse solution itself can be a trial-and-error manual adjustment of input parameters, or an automatic process of multivariate nonlinear weighted regression. The calibration process ensures that the model is as accurate as the observations, provides an independent verification, and quantifies the effects of known uncertainties on the model predictions.

A.5. Applications of Groundwater Flow Modeling

Groundwater flow models have various uses in research and engineering. As interpretive tools, models are useful for error-checking and assimilating field data. Such interpretive models also evaluate the adequacy of the conceptual model, determine the sensitivity of model results to input parameters, and quantify the flow between various components of the hydrologic system. Model sensitivity analyses can assess the worth of additional data and thus help design field studies to improve the understanding of the modeled system. Interpretive models can be further developed into predictive models that assess the consequences of changing pumping schemes or recharge. For example, a predictive groundwater model can simulate changes in hydraulic head and groundwater discharge to streams that correspond to changes in groundwater withdrawal strategies. Regional and local-scale groundwater flow models also provide a starting point for site-scale detailed models of well fields or of subsurface contamination. There are also a variety of uses for groundwater models in the analysis of generic research problems.

A.6. Uncertainty

Uncertainty in models of natural systems arises from our inability to understand, measure, or completely represent all the features of the true systems (Gorelick, 1997). Uncertainties in groundwater models may be categorized as either *parameter uncertainty* or *conceptual uncertainty* (Neuman and Wierenga, 2003). *Parameter uncertainties* reflect our imperfect knowledge of both the input parameters of the model (hydraulic conductivity, recharge, pumping rates, aquifer geometry, etc.) and the variables the model simulates (hydraulic heads and flow rates). For example, field studies yield estimates of the hydraulic conductivity, but hydraulic conductivity varies by location such that a complete characterization is impossible. Further, field studies of hydraulic conductivity are plagued by scale effects and simple measurement errors. Calibrating model results to field observations can reduce the uncertainty of the input hydraulic conductivity, but the observations themselves also include errors such that the calibrated values retain uncertainty. That is, input parameters for the model can only be known within a range of values justified by field studies and calibration. *Conceptual uncertainties* arise from our imperfect knowledge of the processes governing the modeled system, which forces us to make assumptions regarding what processes to include in the model. In practice, conceptual models are based on expert judgment and can be evaluated to quantify the possible impact of conceptual uncertainties. For example, this study assumes that the dominant groundwater flow processes for this system are saturated, isothermal flow, driven by hydraulic gradients at relatively low velocities. The effects of salinity, temperature, and flow through unsaturated zones are not included because these processes are generally believed to have minor influences on the aquifers of this system (Feinstein et al., 2005a; Feinstein et al., 2005b; Mandle and Kontis, 1992). The impact of these conceptual uncertainties on the model can be quantified by ancillary calculations, but evaluating conceptual model uncertainty is an area of ongoing research (Neuman and Wierenga, 2003). It is important to note that both categories of uncertainty are present in the models of this study, and cannot be avoided; in short, "With any model, we get uncertainty for free" (Gorelick, 1997).

The groundwater flow models developed for this study embody the conceptual models developed from expert judgment and use the sets of calibrated model parameters, thus they represent the best understanding of the system. However, the conceptual and parameter uncertainties imply that reasonable variations of the expected-case model will yield a range of plausible predictions rather than a single prediction. The formal approach to uncertainty analysis would be to determine the probabilities of these predictions and summarize their range using, for example, confidence intervals. Such estimates could then be used by decision-makers to assess the reliability of model predictions and rationally evaluate the risks associated with management alternatives (Pappenberger and Beven, 2006). Unfortunately, the current technology for assigning probabilities to detailed groundwater models requires repeating the simulation many times (a so-called Monte Carlo analysis), an exercise that is beyond the scope of the current study. An alternative is to create a limited set of simulations that bound the range of plausible predictions using the most sensitive parameters and assumptions (Walker et al., 2003). Although probabilities cannot be assigned to these bounds, they do qualitatively express the reliability of model predictions for use in evaluating management alternatives (Wittman, personal communication, 2007). This study uses the parameter sensitivities calculated during model calibration to select the most sensitive parameters and then repeats the predictive simulations to estimate the range of model predictions.

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