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146

DELINEATING A SPRING'S RECHARGE AREA USING NUMERICAL GROUNDWATER FLOW MODELING AND GEOCHEMICAL INVESTIGATION

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Executive Summary

The Pheasant Branch watershed is in an area expected to undergo significant development. There are concerns that this development will adversely effect the water resources of the area, including a large spring complex. This work was conducted as part of a larger three-year study that included an integrated groundwater-surface water modeling and data collection effort.

Initially, a previously developed county-wide scale MODFLOW model (regional model) was used to assess the efficacy of possible refinements in the vicinity of Pheasant Branch. A telescopic mesh refinement (TMR) model was constructed using layering and boundary conditions from the regional MODFLOW model, and further refined by adding nearby surface water features, updating the recharge array to reflect results of the surface water model, and increasing the vertical connection between the deep Mt. Simon aquifer and the upper Paleozoic bedrock in the area of the Frederic Springs. These changes resulted in an improved overall calibration. This TMR model was then formally optimized using the parameter estimation code UCODE. Using the head and flux targets from this work and the original regional model, initial parameter sensitivity analyses showed that only the horizontal hydraulic conductivity of the upper Paleozoic bedrock (layer 2) and lower Mt. Simon Cambrian sandstone (layer 3) were sensitive. Therefore, optimization was performed using these two parameters. During the optimization, the most emphasis was placed on the Pheasant Branch flux target at Highway 12 because it had the longest and most complete data set of the calibration targets.

The results of optimization demonstrated that the best fit was obtained by using a horizontal hydraulic conductivity 300 percent larger than the original regional model for layer 2 and 80 percent smaller for layer 3. While not hydrogeologically unreasonable, the project scope did not allow collection of data to discriminate between the optimized TMR values and the values that provided a best fit for the regional model. This uncertainty was formally considered, however, using a stochastic Monte Carlo approach. A large number of model runs (200) used randomly sampled horizontal hydraulic conductivity values between the range given by the TMR optimized values and the previously constructed regional model. Because there was no evidence for which values were more likely, a uniform distribution function was used that allowed all values within the range to be equally likely. This approach allowed calculation of a probability distribution of particles captured by the spring, or a "probabilistic capture zone". In addition to portions of the local surface watershed, the capture zone encompassed distant areas in the North Fork of the Pheasant Branch watershed and areas outside of the Pheasant Branch entirely – demonstrating that the groundwatershed and surface watershed do not align in this area.

In addition to numerical modeling, geochemical sampling of the Springs within the Pheasant Branch Marsh and a nearby municipal well identified large contrasts in chemistry, even when springs were within 50 feet of one another. The differences were stable in time, were present in both ion and isotope analyses, and showed a distinct gradation from high nitrate, high calcium, Ordovician carbonate dominated water in western spring vents to low nitrate, lower calcium, Cambrian sandstone-influenced water in eastern spring vents. The difference in chemistry was explained by different bedrock geology in the recharge area as demonstrated by overlaying the 50 percent probability capture zone over a bedrock geology map for the area. This finding gives additional confidence to the capture zone calculated by the groundwater flow model.

I. INTRODUCTION

This project was designed to provide scientific basis for evaluating changes to the water resources of the Pheasant Branch Creek (PBC) and Lake Mendota watersheds as the system responds to increasing changes in land use. The project used both field data collection and advanced numerical modeling to refine a groundwater flow model. The refined model was used to delineate recharge areas and assess the effects to groundwater resources as changes to groundwater recharge occurred.

The period of the project extended from October 1, 1998 through September 30, 1999. Funding was provided by the Wisconsin Department of Natural Resources. We would like to acknowledge the assistance of Teresa Mansor for her assistance in collecting field data. The City of Middleton and the Friends of Pheasant Branch are thanked for support for other portions of the project that were important for completion of this work.

II. BACKGROUND/NEED

A. Need for scientific basis for evaluating land use

As the city of Middleton and its surroundings continue to develop, the Pheasant Branch North Fork Basin is expected to undergo significant urbanization. For the downstream city of Middleton, headwater urbanization can mean increased flood peaks, increased water volume and increased pollutant loads. More subtly, it may also reduce groundwater recharge and adversely effect down-gradient ecosystems such as Pheasant Branch marsh. The relation of stormwater run-off, wetland loss, and reduced groundwater recharge is complex because the surface water system is coupled to the underlying groundwater system as in most parts of Wisconsin. In many cases there is movement of water from one system to the other that varies seasonally or daily depending on transient events. Therefore, it is difficult to reliably predict the effects of urbanization on stream baseflow and spring flows *a priori*. Moreover, mitigating the adverse effects after development is established can be expensive and administratively difficult. Overlying these concerns are issues such as land owner's rights – both of those developing their land and those whose land is affected by this development – the rights of the public, and stewardship of the resource. With these often-contradictory goals, a scientific basis for assessing effects and effectiveness of mitigation measures is crucial for effective decision making.

B. Lack of previous work in this area

Portions of the basin have been investigated previously by others, the work was either included in a larger regional study or focused solely on the stream itself. Krohelski et al. (in press) included the PBC basin in their larger groundwater flow model for Dane County, however the PBC system was coarsely gridded, and did not include many of the hydrologic features that are locally important (e.g., Frederick Spring, Dorn Creek). Grant and Goddard (1980) looked at channel erosion and sediment transport in the stream. Krug and Goddard (1986) evaluated the effects of urbanization on the stream system. Selbig (1996) characterized the Pheasant Branch Marsh and springs as part of a UW-Madison wetlands ecology course. Presently, the USGS, in conjunction with the City of Middleton and the Wisconsin Department of Natural Resources, have initiated an integrated study that focuses on both the groundwater and surface water systems of the Pheasant Branch watershed. This work – which includes the work described here – was started in 1996 and will be completed in September of 2000. Because the project is funded by multiple parties and is due to be completed in 2000, the findings presented here are an interim reporting of a portion of the overall project.

III. OBJECTIVES

A. Increasing the understanding of the Pheasant Branch hydrologic system

While many hydrologic studies focus only on one component of the groundwater-surface water continuum, the overall study includes all elements of the hydrologic cycle including rainfall, snowmelt, evapotranspiration, interflow, streamflow, baseflow, and groundwater flow. The entire system is characterized quantitatively; output from surface water modeling (recharge) is coupled to the groundwater model input. This allows more realistic scenarios (i.e., urbanization affects surface water storm flows and groundwater recharge) and allows an additional check for reasonableness. While both surface water and groundwater modeling is being performed as part of the overall project, this report will focus on the groundwater modeling aspects, and assessment of recharge rates dervied from the surface water model..

B. Identify the source of the spring feeding the Pheasant Branch Marsh

The spring system is an important water resource in the Pheasant Branch watershed, and an important source of water for a rare wild rice community in the Pheasant Branch Marsh. Identifying the source waters for the spring is the first step in ensuring its protection. In this study our objective is to use the groundwater model and geochemical information to identify areas that feed the springs.

IV. METHODS

A. Site Description

The Pheasant Branch watershed consists of 24 square miles located on the edge of the Driftless Area in Dane County (fig. 1). The geology of the area from base upward consists of an impermeable PreCambrian basement, an extensive Cambrian aquifer (the Mt. Simon), a shaly confining unit (the Eau Claire Shale), a Paleozoic bedrock unit, and an overlying unconsolidated sedimentary unit (Krohelski et al., in press). The shale confining unit is present in the western portions of the county, but is absent in eastern Dane County.

The watershed is composed of a south fork, a north fork and a lower system that flows into the Pheasant Branch Marsh (fig. 1). At the marsh, its flow combines with flows from the spring and groundwater discharged to the marsh; this combined flow ultimately discharges into Lake Mendota. During present conditions, these three components (stream flow, spring flow, and groundwater discharge to the marsh) are roughly equal (around 2 cfs each) during baseflow conditions (USGS, unpublished data).

The hydrology of the watershed has been significantly modified over the last 100 years. Prior to the turn of the century, the Pheasant Branch watershed above Highway 12 drained into a large wetland that occupied the flat-lying land that surrounds the present confluence of the North and South Forks (Maher, 1999). The watershed was closed in most years, but in extremely wet years may have spilled into the Black Earth Creek watershed to the west. At the turn of the century the wetland was drained to Lake Mendota. Most of the presently existing channels in the Pheasant Branch watershed formed after land in the watershed was converted to agricultural uses. The channel that extends from Highway 12 to the Pheasant Branch Marsh has a high gradient (90 feet drop over 2 miles) resulting in high erosion rates that threaten infrastructure such as bridges and sewer lines. The City of Middleton has spent approximately $500,000 in the last 30 years in an attempt to protect these structures from erosion.

The Pheasant Branch Marsh is a diverse wetland system that contains stands of native herbaceous and shrub-scrub vegetation near the spring area, reed canary grass and stinging nettles near the Pheasant Branch outlet, and wild rice and cattails near the confluence of the spring and Pheasant Branch Creek channel (Selbig, 1996). Originally the Pheasant Branch channel flowed north into the Pheasant Branch Marsh and discharged to the northwest portion of the wetland but during the 1950's the channel changed course and followed the southern boundary of the marsh (Grant and Goddard, 1980) as a result of dumping near the old outlet (D'Onofrio, 1973). By 1971 the stream was re-routed to the northwest outlet by the City of Middleton in an attempt to trap sediments and reduce the overall stream gradient. However, the stream system still conveys large amounts of sediment and associated phosphorus to the Lake Mendota system. For example, the Pheasant Branch system had the highest sediment load per unit area for all rural streams measured in Dane County (Lathrop and Johnson, 1979). Increased stormwater flows resulting from future development are expected to exacerbate erosion in the stream channel and sediment transport; these issues have become a topic of concern for the citizens of Middleton (e.g., North Fork Pheasant Branch Watershed Committee, 1999).

The lower Pheasant Branch connecting the Pheasant Branch Springs to Lake Mendota is dissimilar to the rest of the system in a number of ways. First, a channel connects a large spring complex (Springs) and has probably existed in this location for thousands of years. The Springs themselves have flows on the order of 2 cfs, additional groundwater discharge is captured as the stream flows to Lake Mendota. Secondly, the stream in this area has a flat gradient. Finally, whereas the rest of the stream is characterized by relative low groundwater discharge and high stormwater flows, the springs and associated channel have relatively high groundwater discharge components.

B. Numerical modeling – Refined TMR Model

The model approach consists of extracting an inset model (fig. 1) from the recently developed Dane County Regional Model (DCRM - Krohelski et al., in press) and modifying elements of model construction and model parameters (fig. 2). The DCRM grid was used to assign constant head boundary conditions along the perimeter of the inset model and the inset model grid was refined using a telescopic mesh refinement (TMR) approach following the methodology of Ward et al., 1987. The TMR routine was performed using Groundwater Vistas (Rumbaugh and Rumbaugh, 1996). The original grid spacing was 1,312.4 feet on a side; the refined grid is one-fourth the spacing, or 328.1 feet on a side. Thus every DCRM model node is represented by 16 nodes in the TMR model. As a result of the smaller grid spacing, surface water features and the hydraulic head distribution were represented more accurately in the TMR model. Therefore, stream-aquifer interactions and three-dimensional effects near the streams are simulated more accurately. A second refinement was converting all streams in the TMR model domain from the MODFLOW River package to the more sophisticated Stream Routing Package (Prudic, 1989). This allows accounting of streamflow in the streams, and limits the amount of water a stream can lose to the aquifer to the amount of water captured upstream. The final modification to the DCRM model construction was the refinement of the representation of the existing streams and the addition of additional streams (e.g., Dorn Creek northeast of the Springs – fig. 2) that were not critical for the regional model calibration but important for the TMR model calibration.

In addition to changes to model construction, model parameters were adjusted during the TMR model refinement. During the TMR routine the properties of the DCRM were directly translated; a subset of these parameters were modified during subsequent TMR model runs. One of the most important was recharge over the PBC basin. Recharge rates determined by surface water modeling (Steuer and Hunt, in preparation) were input into the groundwater flow model via the MODFLOW recharge array. The surface water model hydrologic response units (HRUs) were grouped such that hydrologic characteristics of an area (soil infiltration capacity, evapotranspiration, rainfall-runoff properties) were averaged into one representative value over the area; this grouping resulted in 21 recharge zones over the Pheasant Branch Watershed (fig. 3). Recharge rates ranged from a high of 9.5 in/yr to a low of 2.3 in/yr; the average recharge rate of the 21 zones was equal to 7.7 in/yr. This new recharge array corresponded to an average recharge over the Pheasant Branch watershed of 7.96 in/yr. It should be noted that this value is significantly higher than that used for the Pheasant Branch watershed in the regional Dane County Model (equal to 4.8 in/yr). The original recharge array was considered theoretical, however (Krohelski et al., in press; Swanson, 1996), and did not simulate baseflows for Pheasant Branch Creek very closely (see below).

Other significant changes to parameters included changes to horizontal hydraulic conductivity of the bedrock aquifers (layers 2 and 3), and the degree of vertical connection between the layers underneath the Spring. The refined model was calibrated to the heads and fluxes used in the DCRM, as well as additional data collected for the project. In particular, the calibration was aimed at more accurately simulating stream and spring discharge measurements while not significantly degrading head calibration.

It should be noted while the majority of this discussion focuses on the TMR model, many of the refinements discussed here were input into the DCRM before the TMR perimeter boundaries were extracted. In addition to giving insight into the type of modifications needed in the TMR model to adequately simulate the system, it ensured that the most appropriate perimeter boundary was specified. That is, the springs themselves are a regional feature (discharging more on a daily basis than any single municipal well in the county); thus the Spring could conceivably have measurable influence at a given TMR perimeter. Conceptual model refinements, albeit coarsely discretized, to the Dane County Regional Flow model before the model grid was refined helped ensure that boundary effects would be minimized.

C. Numerical Modeling – Parameter Estimation on TMR Model

The TMR model was calibrated using parameter estimation techniques. The use of parameter estimation, or "inverse" models, for calibration is a relatively new advancement for the science. There are numerous publications detailing the advantages of inverse models (e.g., Hill 1992, Poeter and Hill, 1997, Hill 1998). Briefly, the primary benefit of a properly constructed inverse model is its ability to automatically calculate parameter values (e.g., hydraulic conductivity) that are a quantified best fit between simulated model output and data measured in the real world (e.g., head, stream baseflow). Other benefits are also realized, such as the quantification of the quality of the calibration and a statistically rigorous measure of the uncertainty (i.e., confidence interval) of predictions made using the optimized model. In addition, parameter correlation (e.g., hydraulic conductivity and recharge) and parameter sensitivity can be quantified and assessed. In this work, the TMR model in the Pheasant Branch area was coupled to the inverse code UCODE (Poeter and Hill, 1998). The pre-processor Groundwater Vistas (Rumbaugh and Rumbaugh, 1996) was used to construct the files used by UCODE.

One of the most important operations in parameter estimation is the selection of observations and associated weight given to these observations. There can be subjective aspects to the assignment, where the ultimate goal is obtaining an optimization evaluation that reflects the modeler's judgment of goodness of fit. Some have proposed using only measurement error to assign observation weights, however, in practice the measured value has additional, less quantifiable, sources of error. Primarily, these errors relate to how representative the measurement is to the condition being modeled. In our case we are simulating steady state conditions when the system is rarely at steady state. For example, measured head values varied over tens of feet between years, and the location and elevation of the wells is often imprecisely known (especially for static well levels from well construction logs). Yet measurement error of head at a given well at a given time is roughly 0.01 feet. Given that our head calibration set is predominantly from well construction logs that span over 40 years of time clearly using only measurement error for assigning weights would give too much credence to the value of the data. In addition, stream flows that are point measures in time may have an "excellent" (±5%) measurement rating, but knowledge of how well this measurement represents average system conditions is unknown without a determination of flow duration. In addition, as shown in Figure 3 there are many more head targets (450) in the model domain than the number of flux targets (4). Therefore, in practice observation weights are not assigned using set criteria, but rather in such a way that trade-offs in optimization are similar to the decisions a modeler might make in trial-and-error calibration.

The TMR model described above was optimized using the following criteria for head and flux targets in the Pheasant Branch area:

1) The average flow (Q_{50}) at the gaging station at Pheasant Branch Creek at Highway 12 was the most highly weighted observation due to having the best flow duration information available for the study period. The weight reflects the site's long flow record (continuously monitored from July 1974 through the study period) used to determine the site's flow duration. The measured Q_{50} of 1.8 cfs for 1974-1998 was given a coefficient of variation = 0.01 (= 95% confidence interval that spans ±1% around the measured value). This value is more accurate than reported by Holmstrom et al. (1999) for the gage (fair, or ±15%) because the weight reflects its much higher quality on a relative scale to the other data used to optimize the model. That is, the weight represents the fact that we are willing to trade better results in other targets to have the optimization routine match this target well.

2) Flow data from Pheasant Branch Creek at Century Avenue and at Frederick Springs had a much smaller number of discharge measurements than the Highway 12 gaging station. Therefore, these targets were given an intermediate weight reflecting their shorter period of record and fewer measurements (coefficient of variation = 0.3 and 0.2, respectively).

3) Flow duration data from Pheasant Branch Creek at the Lake Mendota Outlet has a relatively large record but was not collected contemporaneously with our study and being a downstream endpoint it integrates all upstream uncertainty. Moreover, this location is difficult to measure discharge accurately due to lake backwater effects (D. Graczyk, USGS, 1999, personal communication). Therefore, these measurements were given less weight (coefficient of variation = 0.5)

4) Head measurements in the TMR model domain were given a low weight (standard deviation = 10 feet, or ±20 feet around the measured value comprises the 95% confidence interval) due to the uncertainty regarding their representativeness for the conditions simulated during calibration. That is, these data are the sum of all measured water levels for the area were not collected contemporaneously, but span 40 years. In addition, these data are also less precisely located, both horizontally and vertically. Therefore, the resulting unfiltered head target data set often had multiple head values for a single node. Moreover, the measured head values for a single node might span over 100 feet. Clearly a finite difference model (e.g., one head value calculated per node) cannot simulate these data. The measured head data were filtered for use in the TMR model so that nodes with multiple measured values were replaced with an average value and only one value was entered for the node.

The parameters initially chosen for optimization included the hydraulic conductivity (6 zones in layer 1, 1 zone in layers 2 and 3), the hydraulic conductivity and leakance of nodes immediately beneath Frederick Spring, and the conductance of Lake Mendota littoral and deep lake sediments. Initial runs on parameter sensitivity showed the model was insensitive to changes in layer 1 hydraulic conductivity and lake bed conductance (fig. 4); that is, the measured observations used in the optimized calibration did not contain enough information to constrain these parameters. As a result, all subsequent runs were run using fixed values of for these parameters based on the Dane County Regional Model and optimizing the remaining sensitive parameters.

D. Numerical Modeling – Stochastic MODFLOW and MODPATH runs using TMR Model

The effect of parameter uncertainty can be more formally addressed using stochastic approaches. While detailed discussion of stochastic techniques is beyond the scope of this work, a brief discussion follows. A Monte Carlo approach was used as a means to obtain the probability distribution of the capture zone of the Springs. This approach allows calculation of the probability of a certain occurrence, in our case the probability that the Spring will capture water from different parts of the North Fork of the PBC basin, given the uncertainty that exists for a discrete set of parameters. In this approach, a large number of MODFLOW model runs using the TMR model were performed using Stochastic MODFLOW (Ruskauff et al., 1998) while randomly varying the horizontal hydraulic conductivity of the upper (layer 2) and lower (layer 3) Paleozoic bedrock over a reasonable range of values based on the results of UCODE optimization. In the case of layer 2, this range was uniformly distributed (all values are equally likely) between 1 and 15 ft/d; layer 3 was uniformly varied between 0.7 and 10 ft/d. Each run is called a "realization", and reflects one possible set of parameters for the model. Because combinations of reasonable parameter values may yield unrealistic results, the realizations were evaluated (or "conditioned") and unreasonable realizations were removed. Particle tracking using Stochastic MODPATH (Ruskauff et al., 1998) in the Pheasant Branch watershed. This code utilizes output from the Stochastic MODFLOW realizations to delineate the recharge area for Frederick's Spring using a probability distribution where 1 is contributing in 100% of the realizations, and 0 is contributing in 0% of the realizations.

E. Geochemical Sampling

Geochemical investigation focused on the Pheasant Branch Springs (Springs) and a nearby municipal well. The Springs area was divided up into 7 areas in the main Spring complex, one additional minor spring located 1300 feet west of the main Spring complex, and one ephemeral stream. Sampling included both ion and isotope chemical constituents. Major ions and nutrients were measured periodically from the Springs during March 1998 through April 1999. The municipal well was sampled once in August 1998. Springs and stream were sampled using a peristaltic pump; the municipal well was sampled from the pump well head. Unfiltered samples were used for field measurements of conductivity, temperature, dissolved oxygen, pH and lab measurements of alkalinity. Filtered samples (0.45 μm cellulose nitrate filter) were collected for determination of major ions, nitrate + nitrite (NO_3+NO_2), ammonia (NH_4), total N and Total dissolved inorganic phosphorus (DIP) analyses.

Because water and strontium isotope chemistry not widely used in hydrological investigations, a short description, taken from Hunt et al. (1998), is given here. Water isotopes (oxygen and deuterium) are ideal conservative tracers of water sources because they are part of the water molecule itself. Stable isotopes of water are conservative in aquifers at low temperature, but fractionate on the surface at less than 100 percent humidity (Gat, 1970). Because the vapor pressure of $H_2{}^{16}O$ is greater than $H_2{}^{18}O$, the residual liquid is characterized by a higher $H_2{}^{18}O$ content after evaporation. Hydrogen and deuterium also fractionate, but to a greater extent due to larger percent mass difference. Thus, characteristic $^{18}O/^{16}O$ and $^{2}H/^{1}H$

ratios can fingerprint water sources. Strontium-87 is produced from radioactive decay of rubidium-87. Assuming a given initial $^{87}Sr/^{86}Sr$, minerals that have high Rb/Sr concentration ratios will attain higher $^{87}Sr/^{86}Sr$ than minerals that have low Rb/Sr concentration ratios. Sr isotopes are not significantly fractionated by biological or low-temperature abiotic processes; the isotopic composition of Sr (unlike that of the lighter elements) is entirely controlled by the mixing of Sr from geologic regimes having different isotopic composition (Graustein, 1989). Sr isotopes, when considered together with ion chemistry, can thus distinguish weathering reactions from cation exchange processes. This ability makes them suitable for water-rock interaction investigations (e.g., Bailey et al., 1996; Bullen et al., 1996) and discerning sources of water from isotopically distinct source areas (Eastin and Faure, 1970; Fisher and Steuber, 1976).

The major ions (Ca, Mg, Na, K, SO_4), total P, nitrate+nitrite, NH_4, and total N were analyzed by the University of Wisconsin Soil and Plant Analysis Laboratory and State Laboratory of Hygiene during the periods March 1998 – October 1998 and November 1998 – April 1999, respectively . Alkalinity was analyzed by gran titration at the University of Wisconsin Water Chemistry Department. Chloride analyses were performed using liquid chromatography at the USGS, Middleton, WI. Analyses of water and strontium isotopes were performed at the US Geological Survey National Research Program Laboratory in Menlo Park, California. Oxygen-18 values were measured using CO_2-H_2O equilibration (Epstein and Mayeda, 1953) on a Finnigan-Mat 251 mass spectrometer. Oxygen-18 values are reported in standard delta notation relative to Vienna Standard Mean Ocean Water (VSMOW). Analytic error (2σ) is estimated at ±0.1 per mil. Strontium isotope analyses were performed using the methodology described by Hunt et al. (1998).

V. RESULTS AND DISCUSSION

A. Numerical Modeling

TMR Modifications

TMR modifications to the DCRM improved head and flux calibration for the Pheasant Branch Watershed. The inclusion and more accurate depiction of nearby surface water features (e.g., Brewery Creek, Dorn Creek, headwaters of Black Earth Creek) improved the DCRM head calibration in the area encompassed by the TMR model (Table 2). The TMR area of the DCRM domain was slightly better calibrated than the overall model (RMSD = 36.1 ft in TMR area, 37.4 ft for the overall domain – Krohelski et al., in press). More notably, the recharge rate derived by the surface water modeling significantly improved the flux calibration while only minimally degrading the head calibration (first TMR column versus last TMR column in Table 2). Given the uncertainty associated with the accuracy of some of the head targets (e.g., significantly different observed values reported for the same model node) and the significant improvement in simulated flux, the slight degradation in head calibration was considered to not invalidate the recharge array derived from the surface water modeling.

The basin recharge rate is considered relatively well known (based on the surface water modeling work), thus the recharge rate was fixed and horizontal hydraulic conductivity (Kh) became the driver for head calibration. The DCRM used a sedimentolgical based method for assigning conductivities (Swanson, 1996; Krohelski et al., in press) that resulted in a large number of Kh values to represent the conductivity field of layer 1. A large number of values is not suitable for parameter estimation because each value requires three model runs to perform sensitivity analysis or optimization, which in turn results in unacceptably long run times and time-intensive data handling. As a means to assess the effects of changes to hydraulic conductivity, the Kh values were grouped into eight Kh zones (Table 1). Differences between the original DCRM Kh field and the Kh field created from the zones were negligible (i.e., calibration statistics were identical to two significant figures). A sensitivity analysis was run on the eight Kh zones and demonstrated that only the zone representing the Kh of the upper and lower bedrock (layers 2 and 3) significantly affected the model results (fig. 4). This is not surprising in that much of layer 1 is dry in the Pheasant Branch basin, and all head targets are located in layers 2 and 3.

Parameter Estimation

The smaller number of Kh zones allowed investigation of the TMR model using the parameter estimation program UCODE. During the optimization process a significant difficulty was encountered. First, the automatic routines of UCODE that perturb parameters and run MODFLOW in batch mode have an unfortunate artifact – the perturbation required by UCODE can cause the stable base MODFLOW model to become unstable and not converge. This in turn will result in a failed UCODE run. If the modeler chooses to continue on without convergence (an option in Groundwater Vistas) the UCODE routine will successfully complete. However, there is a chance that the UCODE optimization evaluation included a non-converged model run that ended with an iteration that yields an unrealistic model (e.g., poor mass balance). Because the model is re-run and model output files overwritten, it can be difficult to discern if non-convergence occurred. We found in the TMR model runs that non-convergence was a particular problem caused by dry nodes in layer 1 and high conductance of stream nodes in the Stream Routing Package (STR). Higher values of Kh cause segments of headwater streams to dry sporadically and re-wet; high values of stream conductance effectively transmit the effects of the headwater stream nodes to the groundwater, which cause oscillations in the groundwater solution. The model solution at the end of the maximum number of iterations often had inaccurate simulated stream flows that were used by UCODE to formulate the new (poorly based) parameter values. We overcame the instability at higher Kh values by removing a small set of headwater STR nodes until the model was stable for the range of perturbed values. It should be noted that the issues would likely be worse if constant flux or general head boundary conditions are used instead of constant head nodes on the model perimeter because constant head boundary conditions fix the head at the perimeter thus dampening the oscillation throughout the model domain.

When only head targets were used to obtain the optimal calibration the head residual was minimized (fig. 5) but resulting Kh values were three times higher than the DCRM for layer 2, and over ten times lower for layer 3 (Table 2). As might be expected when flux targets are not considered, the measured Q_{50} fluxes are poorly simulated (fig. 5). When heads and flux targets are considered the optimization routine obtains a minimum in the residual sum of square error (fig. 5) but increases for the Kh of layer 2 is nearly twice the DCRM value, and decreases Kh of layer 3 to roughly one-fifth the DCRM value (Table 2). This yields the "optimal" solution for these targets and weights, but should be considered with the following caveats.

It is conceivable that in the PBC area the Kh of layer 2 and 3 is, in truth, similar to that estimated by UCODE. Layer 2 bedrock includes a carbonate aquifer that outcrops throughout the area and is characterized by extensive fracturing and dissolution; conductivities for Cambrian sandstones elsewhere in Wisconsin have also been on the order of that reported by the UCODE optimization (Young, 1992). However, it is also possible that the parameter optimization results were driven by biases in the head data used for calibration. There are few data in Layer 3, and they are dominated by water levels from high capacity wells. There are problems with representativeness of pumping wells (Driscoll, 1986) due to such confounding factors such as well loss effects. In addition, Layer 2 results could be overly influenced by biases in the head targets and how well they represent the regional water levels. This problem could be especially important for the TMR model in that the model domain contains a large extent of the near moraine and Driftless areas. These areas are expected to have more perched systems, and are likely responsible for the large range of water levels reported for a single model node (Krohelski et al., in press). In addition, these errors are always biased towards higher heads (i.e., perched water levels will always be above the regional water table). While not within the scope of this work, critically evaluating and filtering the head calibration targets is a subject of on-going work. Thus it can be argued that either set of parameters are reasonable; this parameter uncertainty can be addressed by stochastic modeling (described below).

Flux simulation was also refined in the TMR modeling. Preliminary investigation was performed using the DCRM and included both changes to the recharge array and the degree of vertical connection (leakance) between layers 2 and 3 near Frederick Springs. The use of the DCRM was advantageous because the Springs are a regional hydrologic feature, thus are suitable for the larger grid spacing of the DCRM. Any changes that were required could be first tested for efficacy and reasonableness without the concern of boundary violations and added work of translating all changes to the TMR model. Based on this work, modifications to recharge array based on the surface water model were deemed reasonable and simulated flows at the Highway 12 gaging station were much improved. Spring discharge was improved by the new recharge array although it was noted that Spring flows could not be simulated using only Layer 2 capture. We concluded that maintaining a tight confining unit between the Mt. Simon and upper Paleozoic aquifer in the area of the Spring could not yield sufficient water to simulate measured spring discharge given our present understanding of the recharge distribution. A change to the degree of vertical connection between the deep sandstone aquifer (layer 3) and the upper Paleozoic bedrock (layer 2) was investigated using the DCRM; this work indicated that a breach in the Eau Claire confining unit could explain high Spring discharge. Modifications to the degree of connection between layers 2 and 3 were further investigated using the TMR model.

Simulation of fluxes in the TMR model was significantly improved throughout the system from the unmodified DRCM (Table 2). Flux at the Highway 12 gaging station improved from being 60% under-simulated to within measurement error (11% under-simulated) in the optimized case. Spring discharge was improved by the new recharge array and modifications to the location of the Eau Claire Shale confining unit. The modifications to layer 2-3 leakance were restricted to nodes near the Spring (fig. 6) and include one TMR node immediately beneath the Spring that has much higher conductance (such as might be expected from a prominent fracture zone) and an area of leakance typical of the areas where the Eau Claire is absent (fig. 6). While the area modified is restricted to the size of one DCRM node (1312 ft by 1312 ft), the exact locations where the Eau Claire confining unit is absent is poorly understood in this area. Therefore, it is conceivable that this area extends from the Springs to the area near Lake Mendota where the Eau Claire was missing in the DCRM (fig. 6). This is a potential topic of for investigation, and may be addressed in future work in the Pheasant Branch.

Further improvement in simulated fluxes by UCODE optimization was limited by the parameters chosen for optimization. That is, recharge was not varied in the UCODE runs, and optimization proceeded by changing only hydraulic conductivity of layer 2 and 3. This approach is not as powerful as changing recharge rates, and global optimization is obtained by balancing the improved head calibration against degrading the flux calibration at Highway 12. Moreover, the simulated flux in the Spring complex could be more closely simulated by increasing the conductivity of layer 3 (Table 2) without degrading head calibration, but simulated flow at Highway 12 was notably worse. This case was not considered the optimal model because: 1) the flow duration record at the Highway 12 gaging station (24 years) was of better quality than the Spring discharge record (2 months), and 2) the surface water modeling work and resulting recharge array focused on the areas upstream of Highway 12; the Springs capture zone encompasses a significant area outside the area studied in the surface water modeling work (see below). These areas outside of the Pheasant Branch surface water basin were, by default, assigned the lower flux rates of the original DCRM recharge array.

Given the model results presented above, it is apparent that the existing data do not identify a single set of parameters that can best simulate all facets of the Pheasant Branch system. The regional DCRM had an acceptable calibration to head and flux over the entire county. Head calibration of the TMR indicates that layer 2 should have higher conductivity and layer 3 should have lower conductivity for the Pheasant Branch area than specified in the DCRM. Calibration to heads and fluxes suggests that the DCRM values should be altered less, but are still different than the DCRM. None of the values can be easily dismissed as unreasonable, and different parameter sets might be explained by differences in scale, preferential flowpaths/spatial heterogeneity of hydraulic conductivity, and uncertainty in the measured data (e.g., wide variety in measured head for a single node, short flow duration records from some flux targets). While such areas will be topics of future work, stochastic methods can be used with our present understanding to address the effects of this parameter uncertainty on predictions.

Stochastic Numerical Modeling

Stochastic methods are ideal for incorporating the uncertainty in Kh for layers 2 and 3 because they are designed around the concept of probability. Similar to flipping a coin a large number of times to obtain probability of heads versus tails, a large number of model simulations can be run varying Kh to assess the probability of different head and flow configurations. By analyzing the set of model results an assessment of the results and the uncertainty in predictions can be obtained. In our case layer 2 and layer 3 Kh was allowed to vary within the range specified by the UCODE optimization – between 5 and 15 ft/d for layer 2 and between 0.7 and 10 ft/d for layer 3. Because there are no data to suggest which of values are more likely, the simulations were set up such that all values within the range were equally likely (i.e., a uniform distribution). There are no set rules for the number of runs needed to adequately characterize the problem, however an analysis of changes to the absolute mean head difference showed that the problem had stabilized at 200 realizations (fig. 7a). A check of the model using 300 realizations and a different random number seed also confirmed that 200 realizations were sufficient. Examination of the variability in absolute mean head difference for 200 realizations, show the presence of outlier combinations that clearly do not yield a calibrated model (fig. 7b). These outliers point out the need for filtering the 200 runs such that only reasonable models are left for predictions.

This filtering (or "conditioning" in Monte Carlo parlance) was performed using the absolute mean head difference. The UCODE results in Table 2 are considered reasonable model results – of those results the highest acceptable absolute mean difference (AMD) was 25.2 ft. Therefore, this was the cutoff value for conditioning; realizations with an AMD less than or equal to 25.2 were passed and included in the predictive runs. Of the original 200 realizations, 136 realizations met this criterion. The automated routine in Groundwater Vistas can only condition based on head results, therefore the reasonableness of these 136 realizations with respect to flux calibration was not assessed. However, this was not considered problematic because none of the simulated fluxes using the surface water-derived recharge array in Table 2 are grossly out of calibration, and the effects on simulated fluxes are expected to be less sensitive than if recharge rates were included in the stochastic runs.

The stochastic runs were summarized by performing statistics and particle tracking on the conditioned runs. Mean heads are the average heads in the 136 realizations; the standard deviation addresses the variability of simulated heads. These results show a reasonable distribution of head, with the largest variation in simulated heads away from surface water features or near pumping wells (figs. 8a and 8b, respectively). The conditioned heads and cell-by-cell flows can also be used to perform particle tracking with a stochastic version of the USGS program MODPATH. In this application the program computes the probability that specified particles are captured by a boundary condition of interest. In the stochastic code used here no MODPATH variables are considered uncertain and all uncertainty is assumed to occur in the MODFLOW results. In our case we calculated capture probability using particles placed near the top of layers 2 and 3 in the northern half of the model domain and a stream node representing Frederick Springs.

The Springs's recharge area is outside its immediate surface watershed (fig. 1, figs. 9a and 9b) demonstrating that the groundwatershed and surface watershed are not aligned. The majority of the Spring's recharge area is within the larger Pheasant Branch Creek watershed illustrating the strong connection between the North Fork of the Pheasant Branch and the Pheasant Branch Spring complex. The fact that the DCRM capture zone for layer 2 (fig. 1) approximates the TMR capture zone for layer 2 (fig. 9a) underscores the regional nature of problem. The longest travel times (from the farthest reaches of recharge area) are on the order of thousands of years. The stochastic results show that the uncertainty in Kh of layers 1 and 2 has relatively isolated effects on the north and west edges of the Spring's recharge area. Moreover, the layer 3 capture zone is larger than and encompasses all of the layer 2 capture zone demonstrating the reduced effects of competing water sinks (e.g., nearby streams) in the deeper layer.

The larger layer 3 capture zone can also be thought as a conservative estimate of the whole Spring capture for the following reasons. We did not include the global leakance between layer 2 and 3 in sensitivity, optimization and stochastic runs because of lack of data for the Eau Claire confining unit properties/occurrence and sparse head data in the deep sandstone aquifer (layer 3) that would be used to constrain the leakance parameter. As a result the TMR model used unmodified calibrated values from the DCRM. However, it is conceivable that there is a more conductive hydraulic connection between the layers. If this was the case, water could flow to the deeper layer instead of laterally flowing to a competing water sink in areas where there is capture in layer 3 but not layer 2; the layer 2 capture zone shown in Figure 9a would be more applicable if the connection between the layers 2 and 3 were tighter. Because the layer 3 capture zone encompasses the whole of the layer 2 capture zone, it encompasses the range of possible layer 2-3 leakance scenarios.

B. Geochemical Sampling

The water in the Pheasant Branch area is calcium-magnesium-bicarbonate type (table 3), the most common type in natural waters (Stumm and Morgan, 1981). Locally, other ions can be important (e.g., nitrate in Frederick Springs 1 and 2, table 3). As demonstrated by the small standard deviations reported in Table 3, the variation in water chemistry over time at a given location is relatively small. There are, however, notable differences in chemistry sampled at the Frederick Spring complex, the Gate Spring, and the Culvert Crossing surface water runoff location (fig. 10) that are described below.

One of the most notable findings of the geochemical sampling was the large spatial variability of the Fredrick Springs throughout the sampling period; there were large differences observed between the west (Frederick Springs 1 and 2) and east (Frederick Springs 5 and 6) portions of the Springs, even though the spring vents 1 and 6 are located within 50 feet of each other (table 3, figs. 11 through 14). The difference in spring chemistry is gradational such that Frederick Springs 3 and 4 are intermediary between the west and east spring water type. Moreover, this pattern holds for total dissolved solids as measured by specific conductance (fig. 11), major ions (e.g., fig. 12), as well as strontium (fig. 13) and oxygen-18 (fig. 14) isotopes. In most cases the variability within the Frederick Springs is larger than that between Frederick Springs and a spring that was sampled 1300 feet away (Gate Spring, table 3).

The water chemistry differences observed in the springs might be attributed to changes in location in the recharge area. Groundwater flow occurs in "flow tubes" that extend from the recharge areas to the discharge point. These tubes do not cross, and can be delineated using flow net analysis (Freeze and Cherry, 1979) or particle tracking in numerical modeling. Once a contributing area is defined, the relation between recharge area and discharge point chemistry (i.e., spring vent chemistry) can be made.

In the case of the Frederick Spring system, there is evidence for different conditions in the recharge areas influencing the water chemistry observed at the spring vent. The calcium distribution (fig. 12) and strontium isotope (fig. 13) plots can be combined to show a two-component mixing diagram where the two end members are Ordovician carbonate dominated water in the western spring vents (Frederick Springs 1, 2a and 2b in fig. 15) and water that was influenced by a Cambrian sandstone component in the eastern vents (Frederick Springs 5 and 6 in fig. 15). The two components identified can be used to provide additional evidence for the capture zone calculated by the stochastic particle tracking described above. When the 50 percent probability capture zone is plotted on the bedrock map for Dane County (Massie-Ferch et al., in review), the western spring vents coincide with the western portion of the capture zone that is capped by Ordovician carbonate (symbol OP in fig. 16). The northeastern portion of the capture zone feeds the east vents and are characterized by an absence of Ordovician carbonate, with the uppermost bedrock consisting of Cambrian sandstones (CT and CTC in fig. 16). The eastern spring vents also have similar chemistry to Municipal Well #4 (figs. 11, 12 and 14) – a well that is opened only to the Cambrian sandstone. The western area of Ordovician carbonate is larger than the northeastern area where it is missing, corresponding to the qualitative assessment that the flow from western spring vents was much larger than the flow from eastern spring vents.

The water isotope Oxygen-18 samples from the spring vents also showed a difference between the western and eastern vents (fig. 14). The western vents were characterized by lighter $^{18}O/^{16}O$ ratios (had more negative values); eastern vents had slightly heavier ratios. There are a number of mechanisms that could explain this difference including factors such as different ages of water thus different climate and associated meteoric water line during recharge, amount of arable land in the recharge area (e.g., Darling and Bath, 1988), or differing ratio of snowmelt to rain precipitation in recharge water (Clark and Fritz, 1997). One possibility is that the elevation of the recharge area of the western vents is higher than that of the eastern vents. Others have noted the relationship between increasing elevation and more depleted (or lighter, more negative) $^{18}O/^{16}O$ ratios; this has been observed even in areas of minor relief, with the amount of change ranging from –0.15 to –0.5 per mil for every 100 m (328 feet) of elevation increase (Clark and Fritz, 1997). A rough estimate of the average elevation of the recharge area was calculated using the 30 m (98 feet) digital elevation model (DEM) for the basin and the estimated capture zones for the western and eastern vents; this calculation showed that the western portion of the capture zone was about 40 feet higher than the eastern, on average. While this difference is not enough to explain observed differences, the discrepancy may be due to errors in the 30 m DEM or inaccuracies in the exact location of the capture zone for the east and west spring vents. Alternatively, the difference in elevation may only be one factor, and other controls such as age of recharge water, land use, or slope aspect may play a role in the composition of water isotopes measured in the spring vents.

Nutrient chemistry among the spring samples also was spatially variable. Dissolved nitrate+nitrite was significantly different between the western and eastern spring vents (fig. 17), likely reflecting the effects of different agricultural practices in the recharge area. Others (e.g., Gambrell et al., 1975) have noted that a comparison of dissolved nitrate to dissolved chloride can indicate if denitrification was occurring along the flowline from recharge area to discharge area; no evidence of denitrification was found during this study (fig. 18). Finally, as is true in most natural systems, only low concentrations of total dissolved phosphorus was observed in the groundwater. Surface water concentrations of total dissolved P measured in the ephemeral stream (Culvert Crossing in fig. 19), were much higher than that observed in groundwater. However, there is not enough data to discern if the temporally short but high concentration surface water input is a more important source of nutrients to the Pheasant Branch Marsh system than the longer duration, low concentration, groundwater inputs.

VI. SUMMARY AND CONCLUSIONS

The notable findings of this work can be summarized as follows:

- The linking of the groundwater modeling to the surface water model gave higher confidence in the results of both models than if either had been used independently. Values of recharge calculated with the surface water model improved flux calibration in the groundwater model. By linking the two approaches the entire water budget (precipitation, evapotranspiration, baseflow, stormflow and groundwater recharge) is encompassed; this helps ensure that reasonable values are used for all parameters.

- Parameter estimation sensitivity analyses on the groundwater flow model demonstrated that the calibration targets used in this study only supported changes in the upper Paleozoic bedrock model layer (layer 2) and the lower Mt. Simon bedrock unit (layer 3). Other potential parameter changes did not have significant effects on the calibration.

- Parameter estimation optimization of the groundwater flow model suggested that the horizontal hydraulic conductivity of the upper bedrock layer (layer 2 in the model) might be higher in the Pheasant Branch area than the global value that represented a best fit for the Dane County Regional Model (DCRM). The parameter estimation routine also suggests that the lower Mt. Simon sandstone (layer 3) may have lower horizontal hydraulic conductivity than the global value used in the DCRM. The range was not exceedingly large (5 to 15 ft/d for layer 2; 0.7 to 10 ft/d for layer 3); insight into which values best represent the bedrock in the Pheasant Branch area was not readily available, nor within the scope of the project.

- The uncertainty in the horizontal hydraulic conductivity identified in the parameter estimation optimization was formally addressed by stochastic Monte Carlo simulations using the groundwater flow model. In the Pheasant Branch model we allowed the Monte Carlo simulations to sample a range of horizontal hydraulic conductivity values spanning from 5 to 15 ft/d in layer 2 and 0.7 to 10 ft/d in layer 3. The ranges were specified using a uniform distribution thus all values between the endmembers were equally likely. This approach allowed calculation of a probability distribution of the capture zone for the Frederick Spring complex.

- The calculated capture zone for the Springs showed that the Springs are receiving water that was recharged from areas inside and outside of its immediate surface watershed. The capture zone encompassed the North Fork of Pheasant Branch basin, areas downstream of Highway 12 in the Pheasant Branch surface watershed, and an area outside of the Pheasant Branch watershed. This result underscored the need for linking the surface water model of the North Fork basin to the groundwater model of the Pheasant Branch Springs, even though the surface water systems are in different basins.

- Geochemical sampling of the Frederick Spring complex showed very large differences in chemistry between the Spring vents that were located within 50 feet of each other. The differences were stable in time, were present in both ion and isotope analyses, and showed a distinct gradation from high nitrate, high calcium, Ordovician carbonate dominated water in western spring vents to low nitrate, lower calcium, Cambrian sandstone-influenced water in eastern spring vents. The difference in chemistry was explained by different bedrock geology in the recharge area as demonstrated by overlaying the 50 percent probability capture zone over a bedrock geology map for the area. This result gives additional confidence to the capture zone calculated by the groundwater flow model.

VII. SUGGESTIONS FOR FUTURE WORK

As a result of the work presented here, a number of suggested future work elements were identified. They can be described in terms of 1) refining our knowledge of the physical system, and geochemical system, 2) expanding the approach to nearby surface watersheds that affect the Pheasant Branch watershed.

Our understanding of the physical system of the Pheasant Branch watershed could be improved by the following work elements. The conceptual model employed here used an enhanced hydrologic connection between the deeper Mt. Simon sandstone in layer 3 and the upper layers due to a simulated breach in the Eau Claire confining unit. This is an alternative conceptual model to that proposed for the Nine Springs system in central Dane County (high conductivity zone located within the Tunnel City member of the Cambrian sandstone, Swanson and Bahr, 1999). A piezometer nest installed near the Frederick Springs with monitoring points emplaced above and below the level where the Eau Claire should exist (based on Middleton Municipal Well #4) would verify the existence or absence of the confining unit, as well as document the degree of hydraulic connection by comparing the measured heads. Additional work on the permeabilities of the bedrock units in the Pheasant Branch area (e.g., flow logging, packer testing) would help narrow the range of uncertainty for the horizontal hydraulic conductivity values for the upper Paleozoic bedrock (layer 2) and the Mt. Simon sandstone (layer 3) identified by the parameter estimation in this work.

The model calibration could be improved by augmentation and increased quality of the calibration targets. More flux calibration targets that utilize long-term flow duration data would provide a better assessment of the recharge distribution calculated by the surface water modeling. Most notably, only a few flow measurements have been made at the Frederick Spring complex, and none that quantifies the flow from the various spring vents. This data set is critical to discern between different conceptual models for the origin of the spring waters and refine the contributing areas of the west and east vents, as well as to quantify and assess the effects of changing land use in the upgradient areas. Long-term data collection is required to allow statistically valid analysis of trends in the spring flow, and would be critical for providing scientifically valid data that could be used to protect the Springs. Flux targets from the surrounding stream systems (e.g., Dorn Creek, Six Mile Creek, upper Black Earth Creek) would help ensure that groundwater divides are simulated correctly. In addition, there are uncertainties in the head targets resulting from potential biases in head due to suspected perched systems and uncertain well locations and representativeness of the measured head. Filtering the head calibration targets or adding new wells in suspect areas would improve the conceptual and numerical model. Moreover, continuous water level measurements from new wells near the Frederick Springs coupled to continuous spring discharge measurements would allow a integrated representation of the groundwater and surface water systems, and an increased understanding of the importance of local and regional flow to the spring system.

Refinements to the numerical groundwater flow model would also improve our ability to simulate the Pheasant Branch groundwater system. The surface water model does have the ability to output monthly and daily recharge values in addition to the annual recharge values used here. This information, along with the flow duration record at Highway 12 and a small data set for the Springs measured by Selbig (1996), could be used to form the basis of a transient model calibration. However, a corresponding head data set would be needed to provide head targets for the transient model. Additional vertical discretization in the upper Paleozoic bedrock (layer 2) would improve representation of the bedrock in the Frederick Springs area. The scope of the modeling could be increased to include a larger emphasis on the Pheasant Branch Marsh as a whole. This would include simulation of the Frederick Springs, the Gate Spring complex, various seeps along the western bluff of the marsh, the unnamed tributary that enters the marsh from the northwest, and the groundwater-wetland interaction in the marsh itself. This increased scope would allow a more accurate assessment of site specific effects to the Pheasant Branch Marsh resulting from changes in the groundwatershed (e.g., change of pumping schedule, placement of additional wells). In addition, the Monte Carlo code used here did not allow conditioning based on flux targets, only heads targets. This additional criteria for conditioning might narrow the number of realistic realizations used to calculate the probability of capture.

Information regarding the shallow groundwater system chemistry in the Pheasant Branch watershed would also increase our understanding of the system. Sampling of the Frederick Springs has shown distinct water types feeding the west and east vents; these water types should be identifiable in the upgradient groundwater. Sampling of new and existing wells could further refine the recharge areas for the Frederick Springs, and improve the numerical model. Including additional strontium and water isotope analyses would provide additional evidence for the location of recharge areas. Finally, although in the Spring sampling conducted here spatial variability was much greater than temporal variability, there were temporal changes in ion and isotope chemistry. Additional temporal sampling of the Frederick Spring complex with corresponding sampling of the groundwater system would help quantify the transfer of solutes from the shallow subsurface to the springs, and the importance of local and regional flow. This information, in turn, will enhance our understanding of the time lags associated between changes in land use and measurable effects on the surface water resources. Information on the magnitude of time lags could be further augmented by field verification of time of travel using CFCs, tritium, or helium analyses to estimate the age of groundwater discharging from the springs.

The understanding of the Pheasant Branch system would also be improved by expanding the approaches used here to nearby surface watersheds that affect the Pheasant Branch watershed. The majority of the contributing area to the Frederick Springs encompassed areas not included in the surface water modeling (e.g., outside the basin to the north, the Pheasant Branch basin downstream of the Highway 12 gaging station). However, the groundwater flow model presented here was primarily optimized using the Highway 12 gaging station; this optimization resulted in the Frederick Spring flows to be undersimulated. Investigation of these areas not included in the surface water model would reveal if the undersimulation was the result of errors in the conceptual model of the springs, or if the recharge rates used in the areas not simulated in the surface water model (i.e., the areas that used the original Dane County Regional Model recharge array) were too low. This refinement would ensure that the entire hydrologic system that feeds the Pheasant Branch system – springs and stream channel – was accurately simulated.

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Table 1 - Parameters used in TMR model

Hydraulic Conductivity (ft/d)

		TMR base	head optimized	head and flux optimized
Layer 1	zone 1	0.3	0.3	0.3
	zone 2	0.5	0.5	0.5
	zone 3	1	1	1
	zone 4	3	3	3
	zone 5	5	5	5
	zone 6	7	7	7
Layer 2		5	0.7	2.0
Layer 3		10	15.0	9.6

Nodal Recharge Rate (inches/yr)

Original DCRM	max	12.4
	min	0.0
	area weighted average	4.8
TMR model	max	9.5
	min	2.2
	area weighted average	8.0

Table 2 - Results of Pheasant Branch model calibration

	Original DCRM Dane46	TMR Model DCRM R and K UCOD20a	TMR Model New base UCOD20c	TMR Model Head Targets only UCOD 20d	TMR Model Head & Flux Targets UCOD20e
Sum of Squares	NA	5276	5659	5864	5249
Residual Mean	-1.08	4.46	0.96	5.06	3.26
Res. Std. Dev.	36.14	33.52	34.67	33.22	34.07
Head Abs. Res. Mean	26.50	23.61	25.20	23.28	24.43
Flux Abs. Res. Mean (cfs)	NA	99974	28842	62391	49132
Flux @ Hwy 12 (meas=1.8 cfs)	1.2	0.7	1.5	1.3	1.6
Residual Flux @ Hwy 12 (cfs)	0.6	1.1	0.3	0.5	0.2
Kx zone 7 (lay 3) ft/d	10.0	10.0	10.0	0.73	2.0
Kx zone 8 (lay 2) ft/d	5.0	5.0	5.0	15.0	9.6
Parmeters:	Orig DCRM streams DCRM Recharge array DCRM L2/L3 Kh	TMR modified STR pkg DCRM Recharge array DCRM L2/L3 Kh	TMR modified STR pkg PRMS Recharge array DCRM L2/L3 Kh	TMR modified STR pkg PRMS Recharge array UCODE L2/L3 Kh (heads targets only)	TMR modified STR pkg PRMS Recharge array UCODE L2/L3 Kh (head&Flux targets)
RJH 2/4/2000					

Table 3 -Results of geochemical sampling 1998-1999

	n		Temp. (C)	D.O. (mg/L)	Sat. (%)	Cond. (uS/cm)	pH	Ca mmol/L	Mg mmol/L	Na mmol/L	K mmol/L	Alkalinity mmol/L CO3	Cl mmol/L	SO4 mmol/L	NO3-N mmol/L	NH4-N mmol/L	Total N-N mmol/L	Tot Filt P umol/L
Gate Spring 1	8	average	9.6	4.9	43	714	7.1	1.98	1.62	0.45	0.04	3.14	0.87	0.20	0.44	0.004	0.46	0.61
		std dev	0.1	0.4	4	8	0.2	0.08	0.05	0.03	0.01	0.07	0.02	0.01	0.01	0.003	0.03	0.11
Fred. Spring 1	8	average	10.4	7.7	69	787	7.0	2.19	1.80	0.40	0.04	3.16	0.99	0.29	0.89	0.002	0.94	0.54
		std dev	0.8	0.4	4	8	0.2	0.11	0.08	0.02	0.01	0.07	0.02	0.00	0.09	0.002	0.06	0.04
Fred. Spring 2A	8	average	9.6	7.9	69	776	7.1	2.18	1.79	0.32	0.04	3.10	0.83	0.28	0.94	0.002	1.00	0.57
		std dev	0.1	0.2	1	8	0.2	0.10	0.07	0.02	0.01	0.07	0.01	0.00	0.09	0.002	0.18	0.05
Fred. Spring 2B	8	average	9.6	7.8	68	779	7.0	2.18	1.80	0.33	0.04	3.13	0.85	0.28	0.93	0.002	1.01	0.58
		std dev	0.1	0.3	3	7	0.2	0.07	0.07	0.02	0.01	0.03	0.02	0.00	0.08	0.002	0.08	0.07
Fred. Spring 3	8	average	9.7	8.0	70	687	7.1	1.96	1.62	0.32	0.05	3.04	0.64	0.23	0.57	0.003	0.68	0.56
		std dev	0.1	0.4	4	34	0.2	0.08	0.04	0.01	0.01	0.04	0.07	0.01	0.05	0.003	0.20	0.06
Fred. Spring 3C	6	average	10.1	8.2	72	636	7.1	1.80	1.50	0.26	0.06	3.00	0.45	0.20	0.31	0.003	0.32	0.60
		std dev	0.7	0.4	4	14	0.3	0.13	0.08	0.05	0.01	0.08	0.06	0.01	0.06	NA	0.21	0.07
Fred. Spring 4	8	average	10.1	7.6	68	565	7.2	1.65	1.39	0.20	0.04	2.91	0.23	0.12	0.17	0.003	0.31	0.48
		std dev	0.8	0.3	3	8	0.2	0.05	0.04	0.01	0.01	0.07	0.03	0.01	0.03	0.002	0.28	0.05
Fred. Spring 5	8	average	10.1	6.8	60	512	7.2	1.51	1.30	0.14	0.02	2.86	0.08	0.06	0.04	0.004	0.13	0.46
		std dev	1.1	0.3	3	8	0.2	0.04	0.05	0.01	0.01	0.05	0.01	0.00	0.02	0.002	0.15	0.20
Fred. Spring 6	8	average	10.0	6.7	59	548	7.2	1.62	1.36	0.20	0.03	2.88	0.22	0.09	0.15	0.003	0.13	0.42
		std dev	0.9	0.1	2	13	0.2	0.12	0.13	0.05	0.02	0.07	0.05	0.01	0.07	0.003	0.09	0.04
Culvert Crossing	2	average	14.1	4.8	44	475	7.5	0.61	0.61	0.44	2.21	1.10	0.80	0.06	0.01	1.086	1.36	36.2
		std dev	6.8	0.9	NA	200	0.0	0.38	0.40	0.33	1.28	NA	0.58	0.00	NA	NA	NA	NA

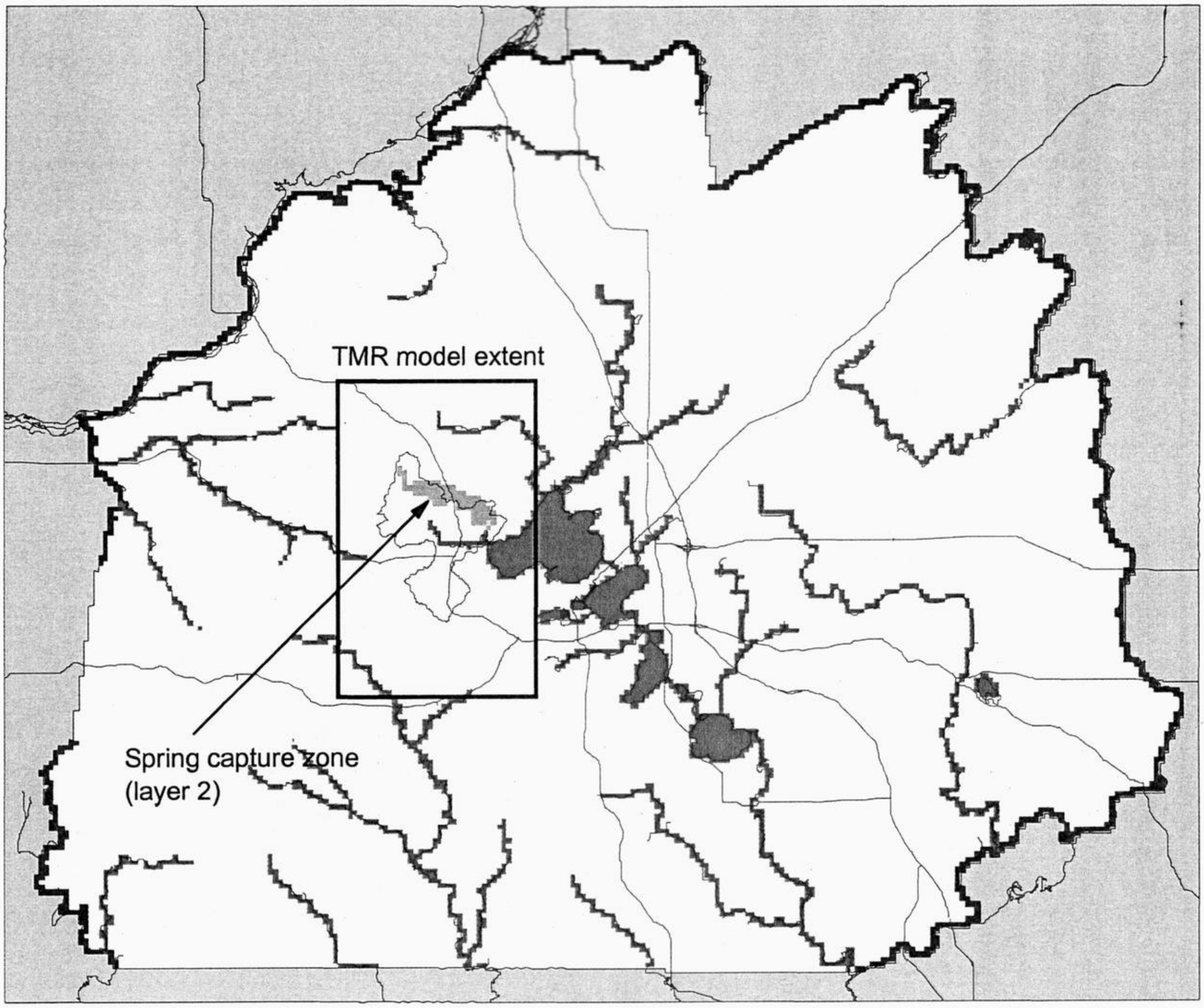


Figure 1 - The Dane County Regional Model (DCRM) is used to specify perimeter boundaries for the inset telescopic mesh refinement (TMR) model. Because the Spring is a regional feature the DCRM was also used to coarsely define the capture zone of the spring and to test the efficacy of possible changes for the TMR model.

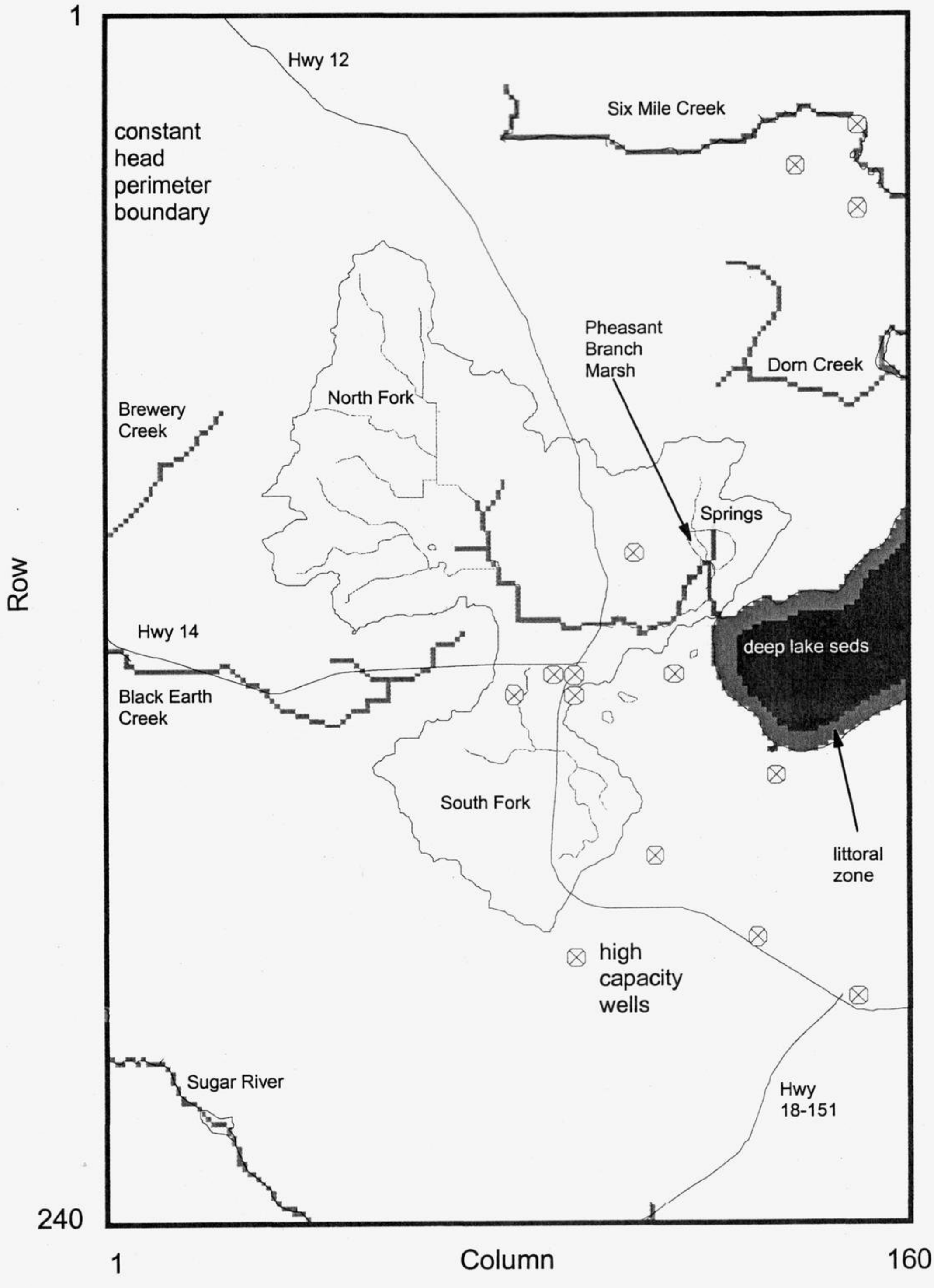


Figure 2 - Final TMR model configuration; note smaller grid size allows more accurate representation of surface water feature geometry and extent (e.g., Pheasant Branch Creek). Surface water features important for the PBC area are also added to the DCRM surface water features (e.g., Brewery Creek, Dorn Creek).

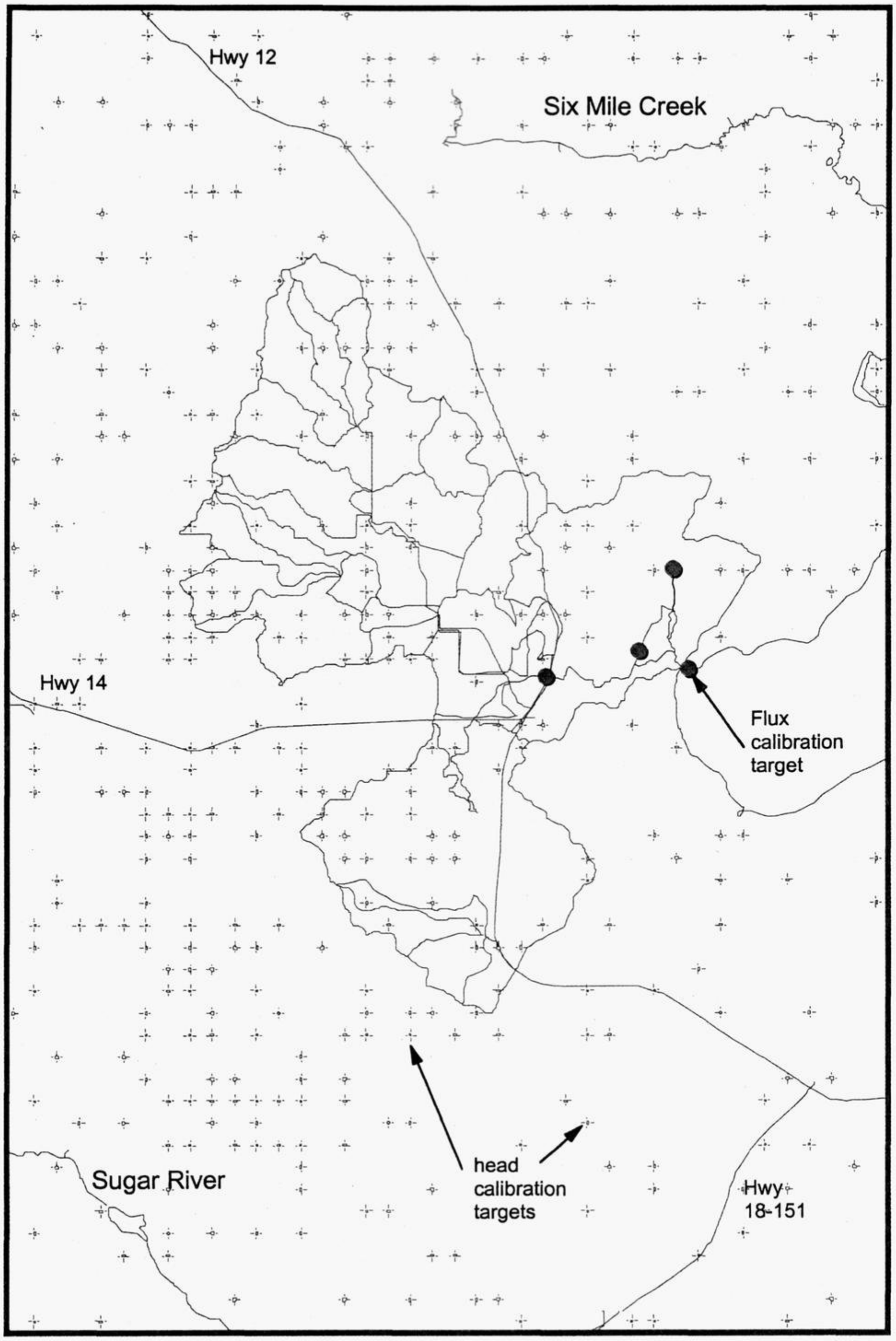


Figure 3 - Locations of the hydrologic response units (HRUs) used in the Pheasant Branch surface water modeling. Head and flux targets used in the TMR model calibration are also shown.

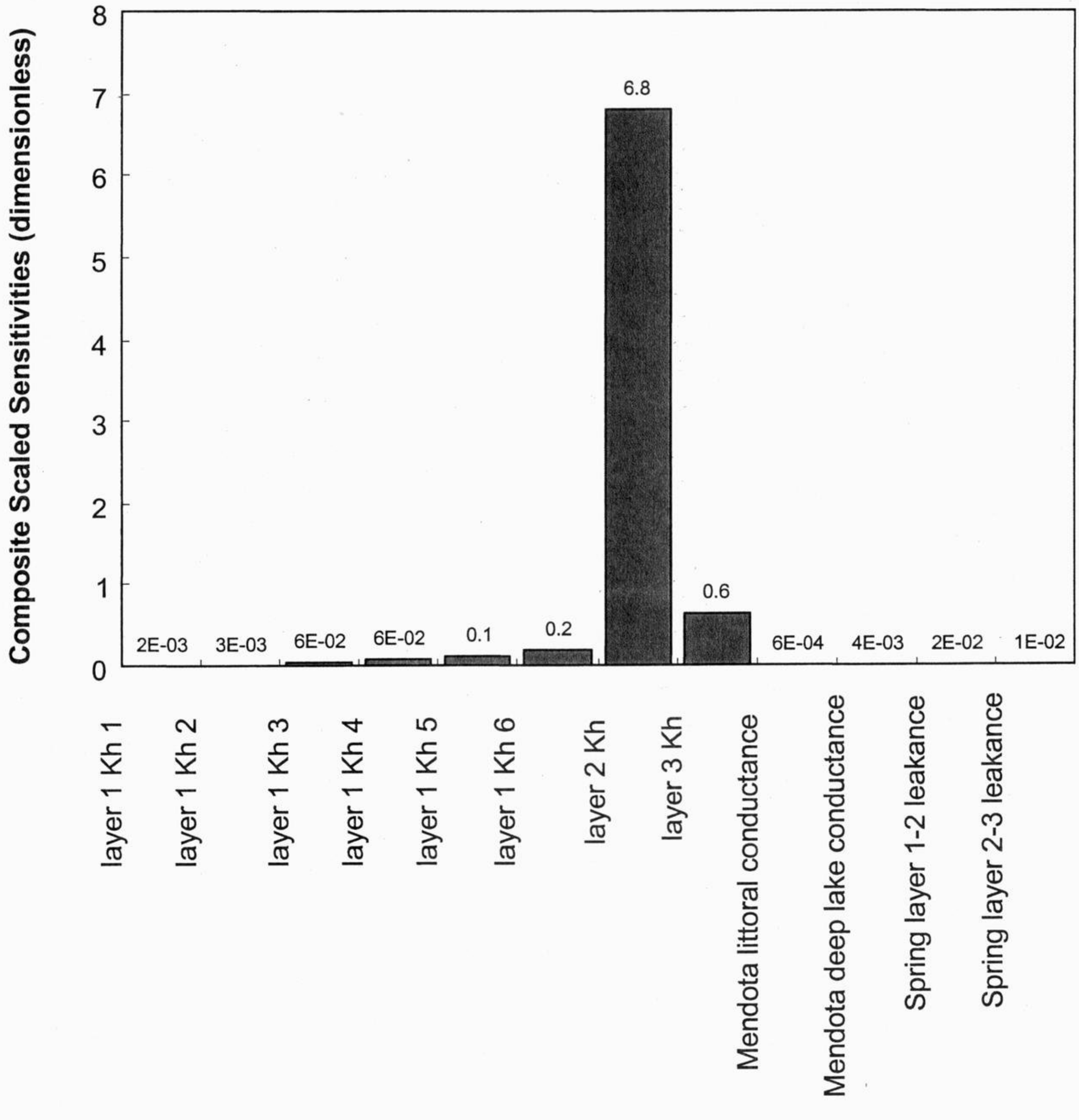


Figure 4 - Plot of parameter sensitivity from UCODE Phase 22 run. Horizontal hydraulic conductivity zones representing layer 2, and to a lesser extent layer 3, were the most sensitive parameters. Additional work with optimization and stochastic runs was restricted to modifications to these two parameters.

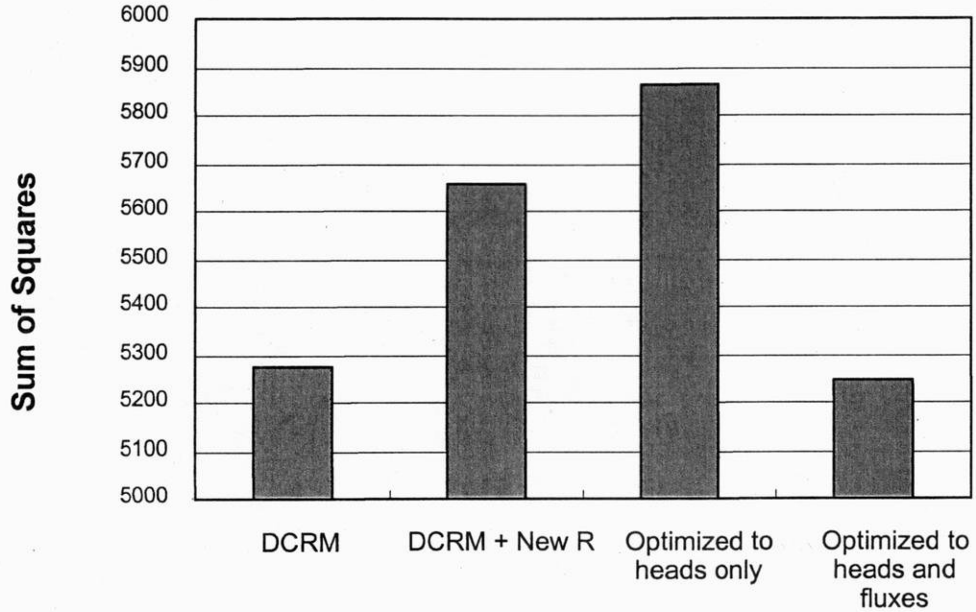


Figure 5a - Plot of sum of squares residual for UCODE optimization. Note that although there are many more head targets than flux targets the weight assigned the flux target at Highway 12 results in an overall worse fit when only head targets are considered.

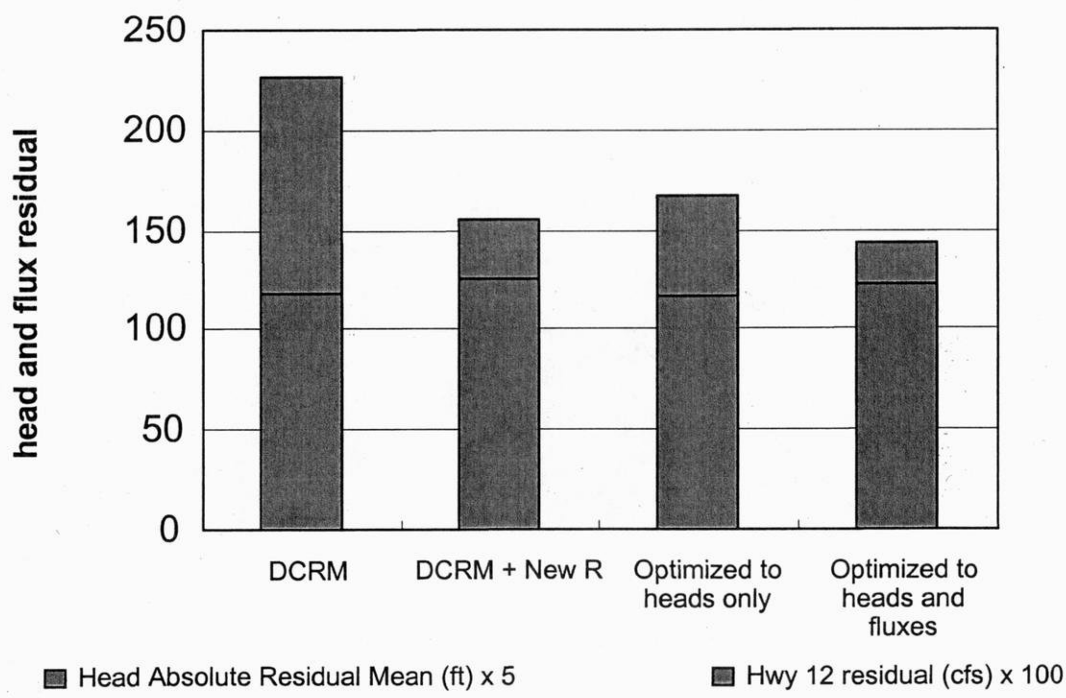


Figure 5b - Plot of residuals from all head calibration targets and the flux residual at PBC at Highway 12.

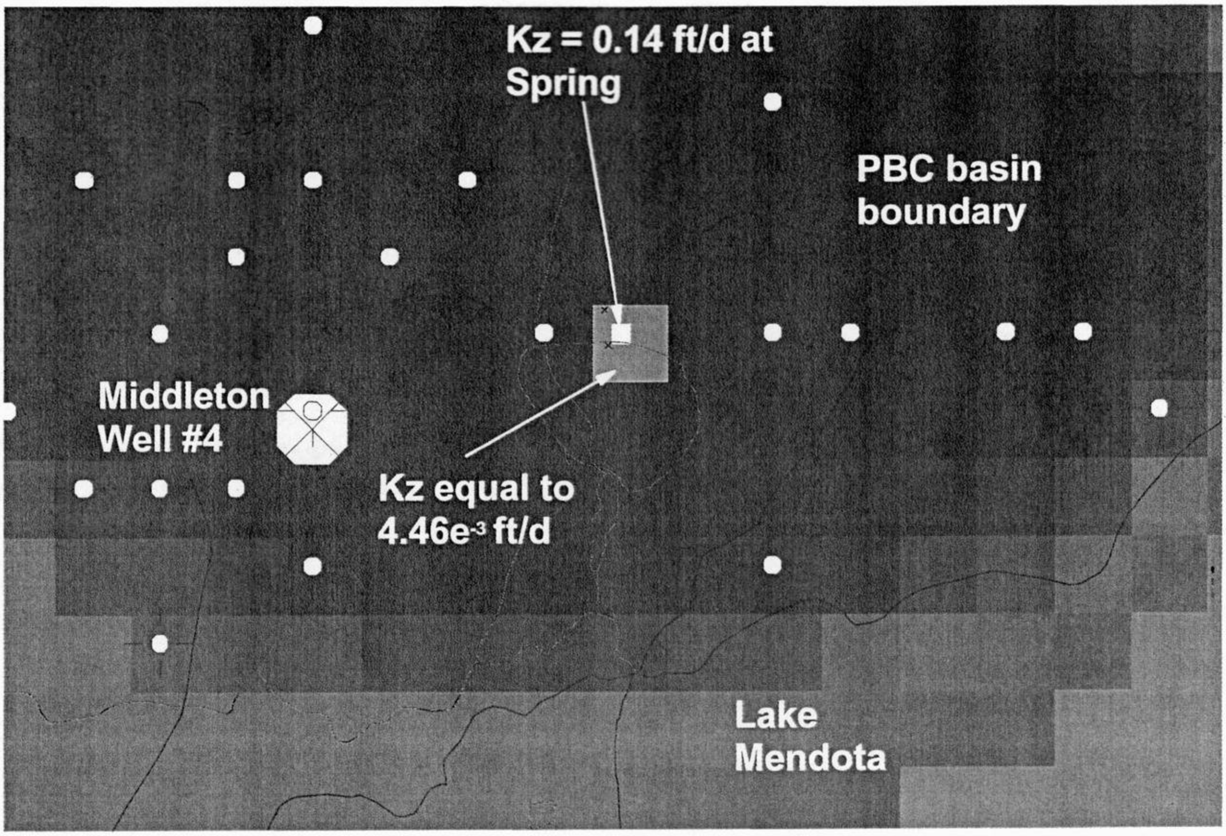


Figure 6 - Areas where the connection between layers 2 and 3 were modified from the original DCRM are shown above. The area where Kz = 4.46e-3 ft/d represents one DCRM node with leakance equal to areas where the Eau Claire confining unit is absent (e.g., Lake Mendota). The area where Kz = 0.14 ft/d corresponds to one TMR node that represents a possible fracture conduit enhanced by dissolution.

Figure 7a - Cumulative absolute mean difference (AMD) for 200 realizations of Stochastic MODFLOW. Random number seed equal 988, Kh of layers 2 and 3 varied between 5 and 15 ft/d and 0.7 and 10 ft/d, respectively.

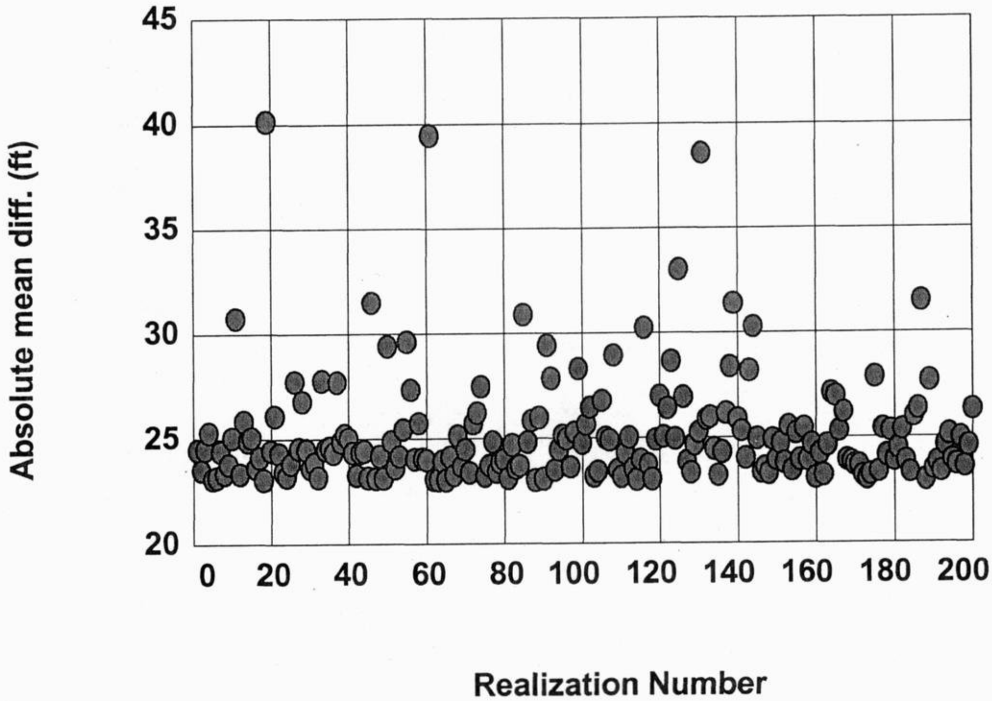


Figure 7b - Scatter plot of absolute mean difference (AMD) for each of the 200 realizations of Stochastic MODFLOW. Random number seed equal 988, Kh of layers 2 and 3 varied between 5 and 15 ft/d and 0.7 and 10 ft/d, respectively. The plot illustrates the presence of outlier combinations of Kh that result in a uncalibrated model.

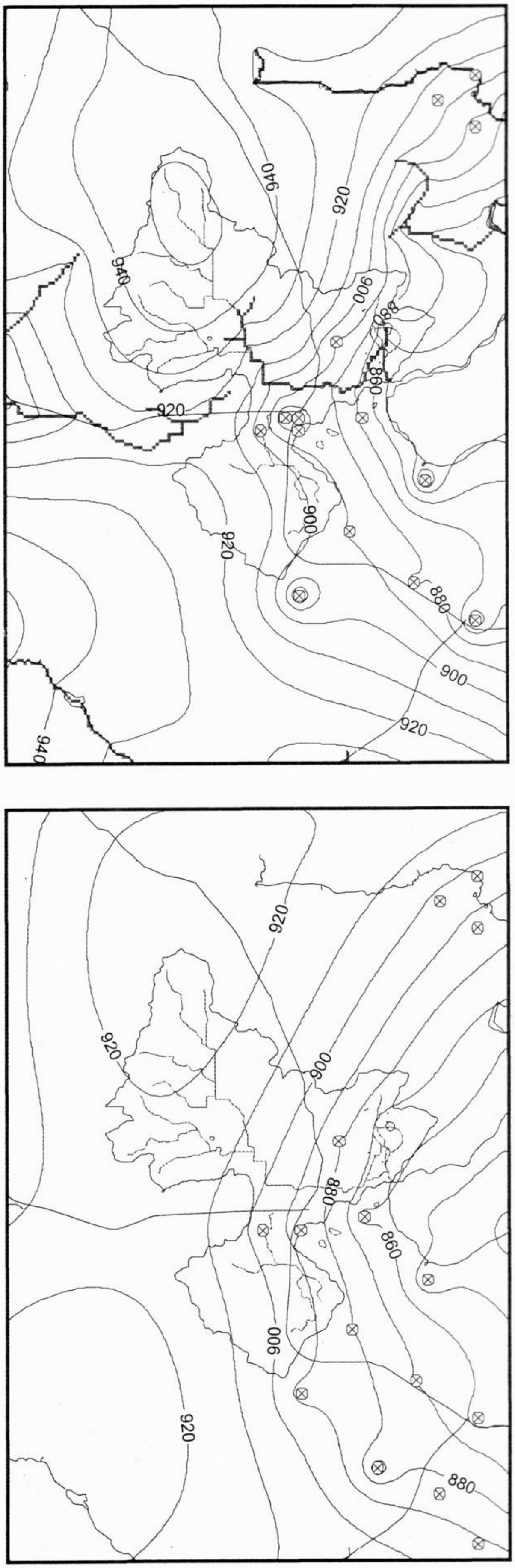


Figure 8a - Results of conditioned stochastic MODFLOW runs for the Upper Paleozoic bedrock aquifer (top figure, model layer 2) and the deeper Mt. Simon aquifer (bottom figure, model layer 3). The figures show mean heads for the 136 realizations; the absolute mean difference equals 23.78 ft. Contour interval equal 10 feet.

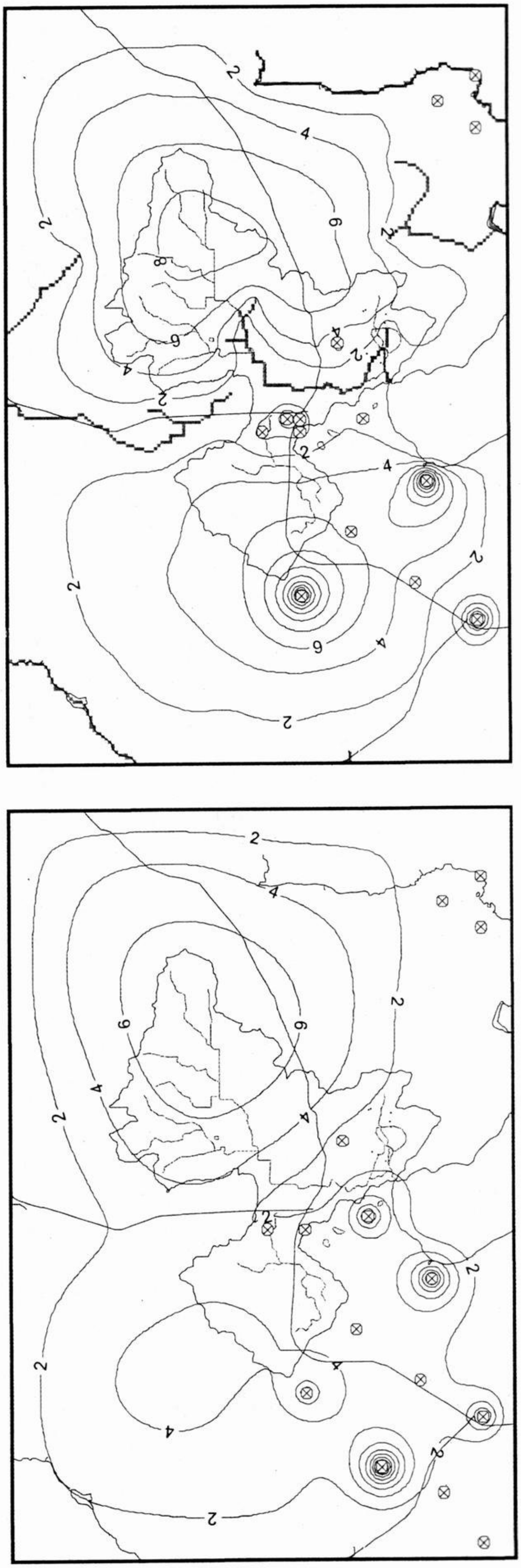


Figure 8b - Results of conditioned stochastic MODFLOW runs for the Upper Paleozoic bedrock aquifer (top figure, model layer 2) and the deeper Mt. Simon aquifer (bottom figure, model layer 3). The figures show standard deviation contours for the head distribution shown in Figure 8a. The largest variations in heads is near pumping wells and away from the surface water features. Contour interval equal 2 feet.

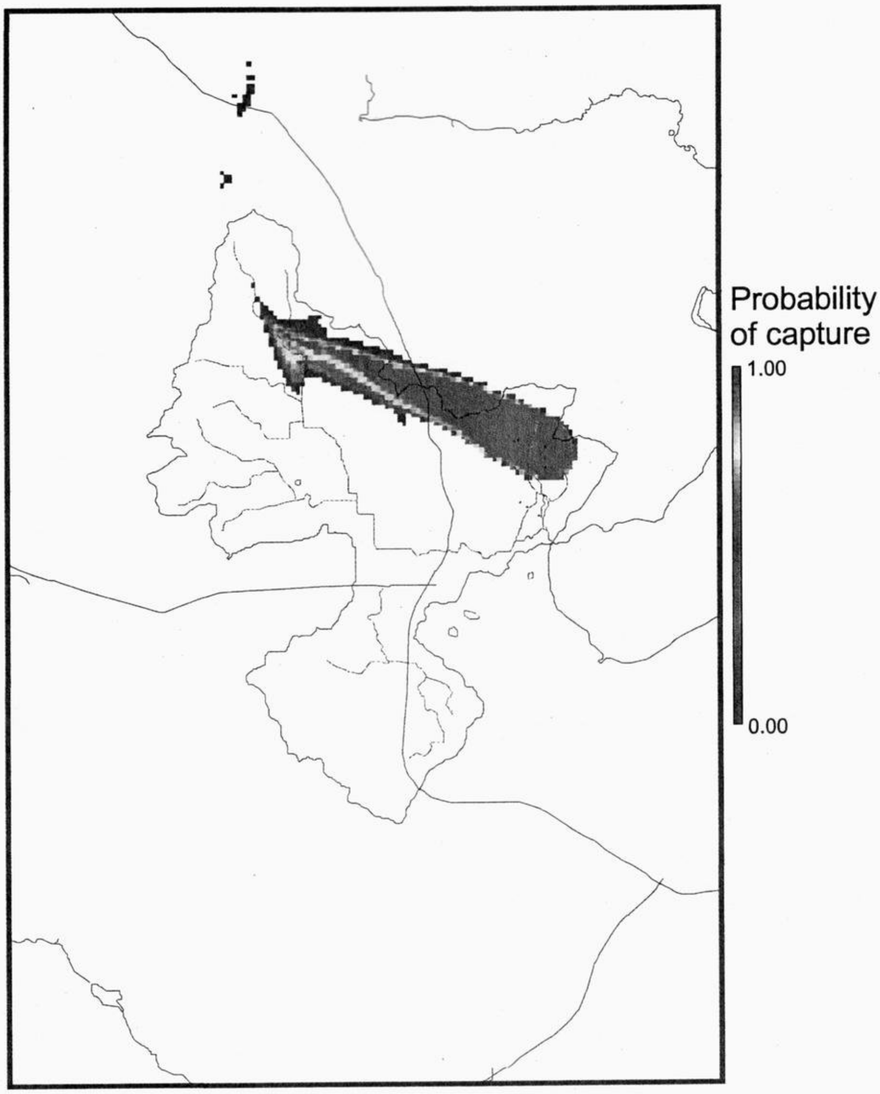


Figure 9a - Results of conditioned stochastic MODPATH runs for the Upper Paleozoic bedrock aquifer (layer 2). The probabilistic capture zone for the Frederick Springs area is calculated by tracking particles placed near the top of layer 2 and determining capture by the simulated spring. A value of 1 represents capture in 100% of runs. The capture zone is smaller than Figure 9b due to stronger effects of competing hydrologic sinks (e.g., other surface water features) in layer 2 than in the deeper layer 3. In addition, the TMR model compares well to the capture zone delineated by the DCRM in Figure 1.

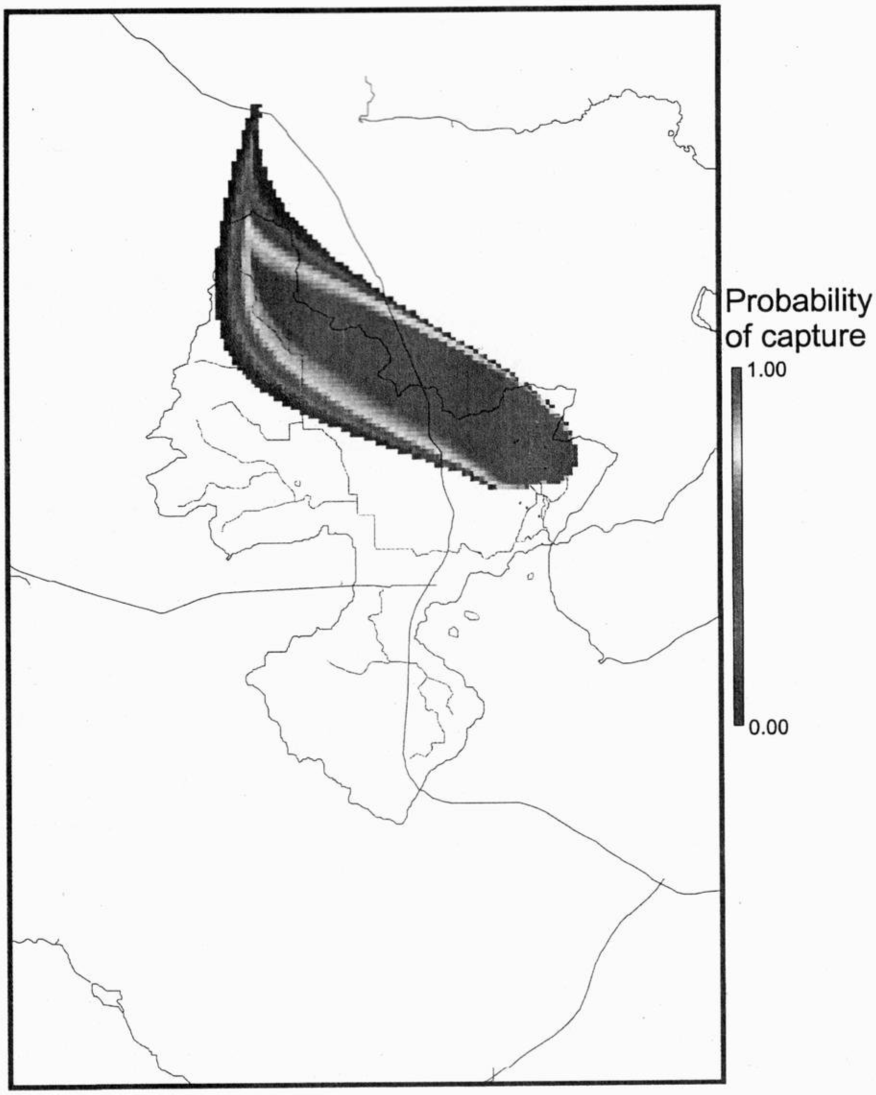


Figure 9b - Results of conditioned stochastic MODPATH runs for the Mt. Simon aquifer (layer 3). The probabilistic capture zone for the Frederick Springs area is calculated by tracking particles placed near the top of layer 3 and determining capture by the simulated spring. A value of 1 represents capture in 100% of runs.

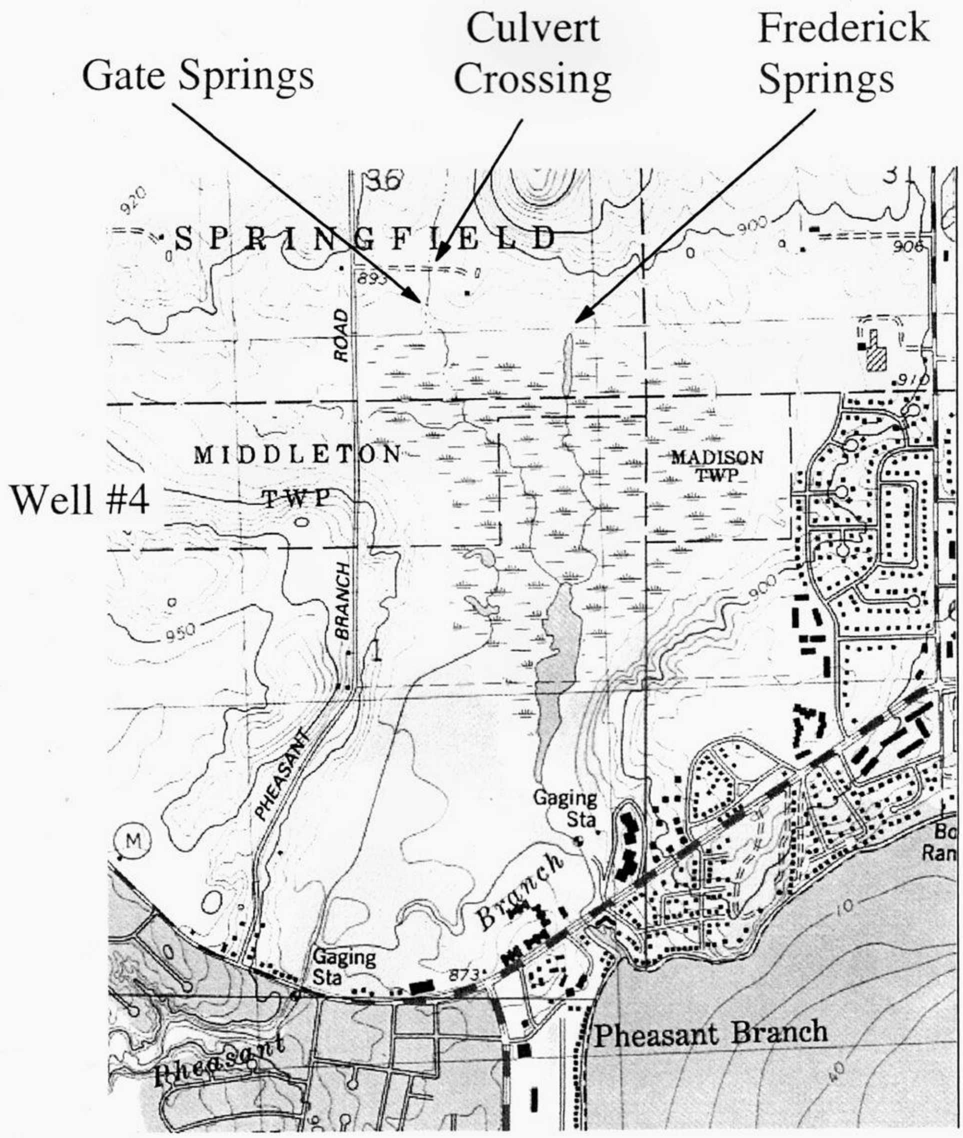


Figure 10 - Location of geochemical sampling sites. The Frederick Spring complex consists of eight spring vents located in a 50 foot by 50 foot area. The spring vents are numbered clockwise starting from the western edge (the largest boiling spring).

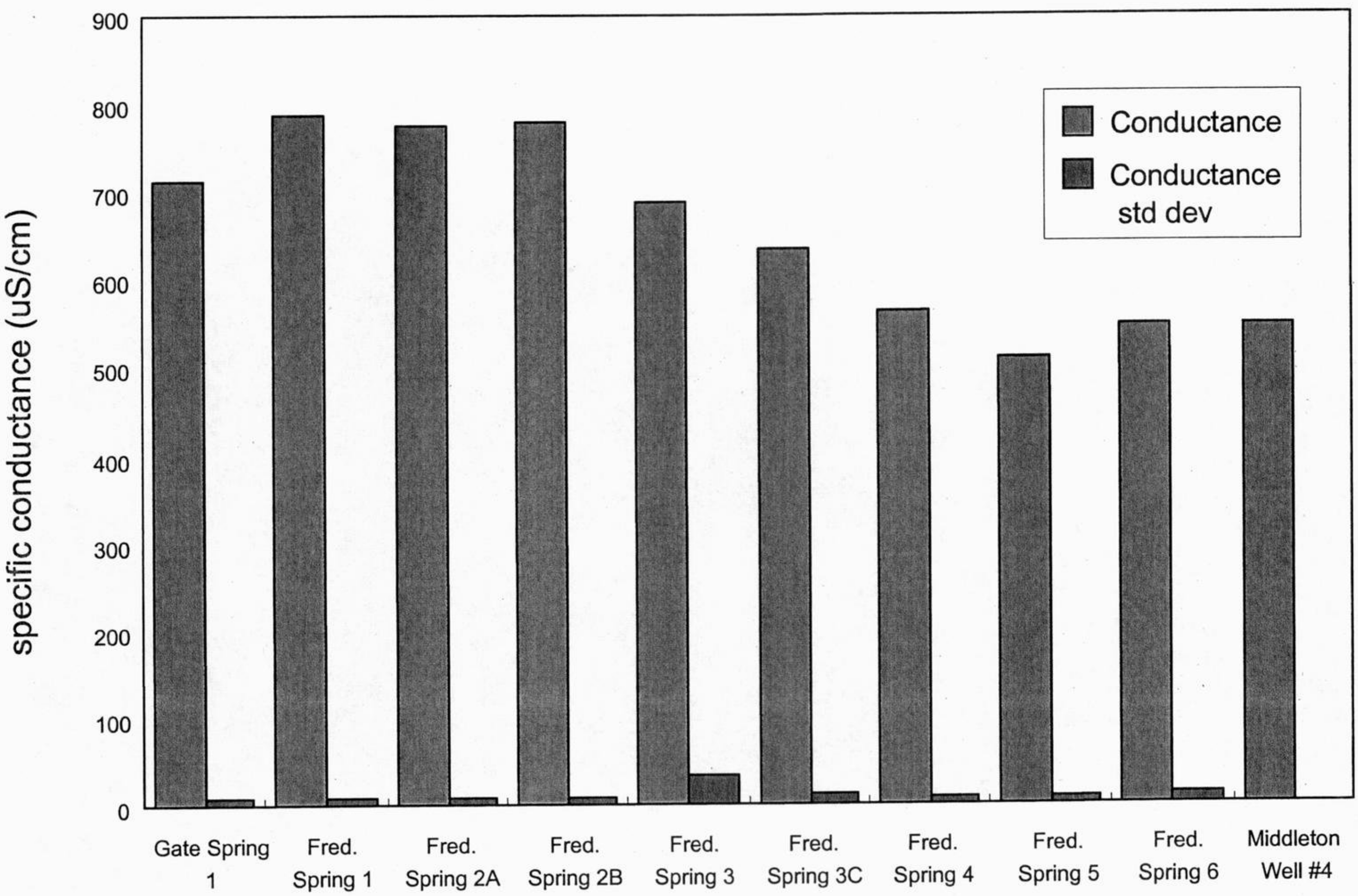


Figure 11 - Average specific conductance measurements for the period 1998-1999. The largest standard deviation is observed in Frederick Spring 3, an intermediate spring between the two dominant water types; this observation suggests that the source of water to this spring may vary as transient stresses are affecting the system. It is notable that this is occurring in a regional discharge area.

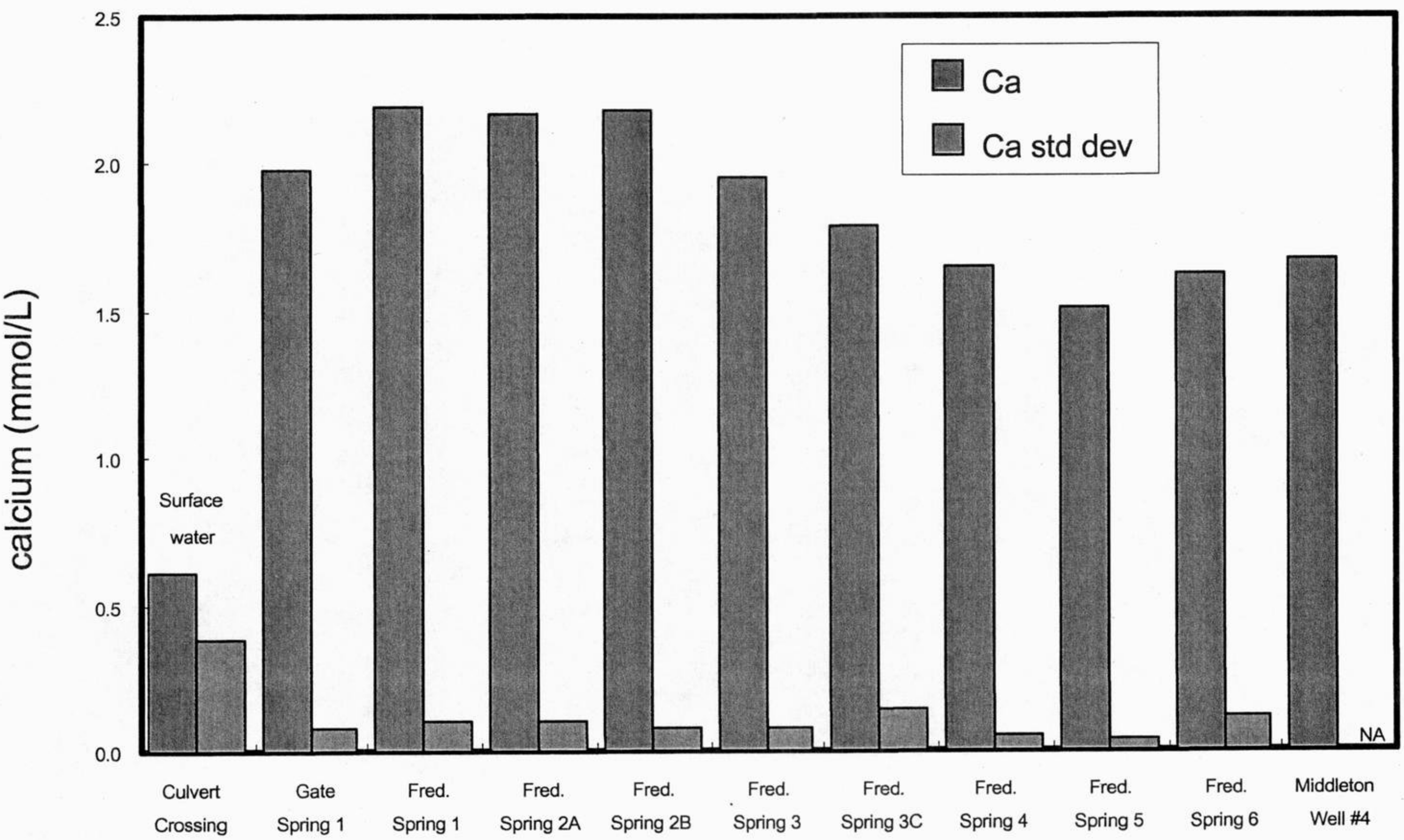


Figure 12 - Average calcium concentrations for the period 1998-1999. The distribution of high calcium agrees well with the distribution of high specific conductance show in fig. 11.

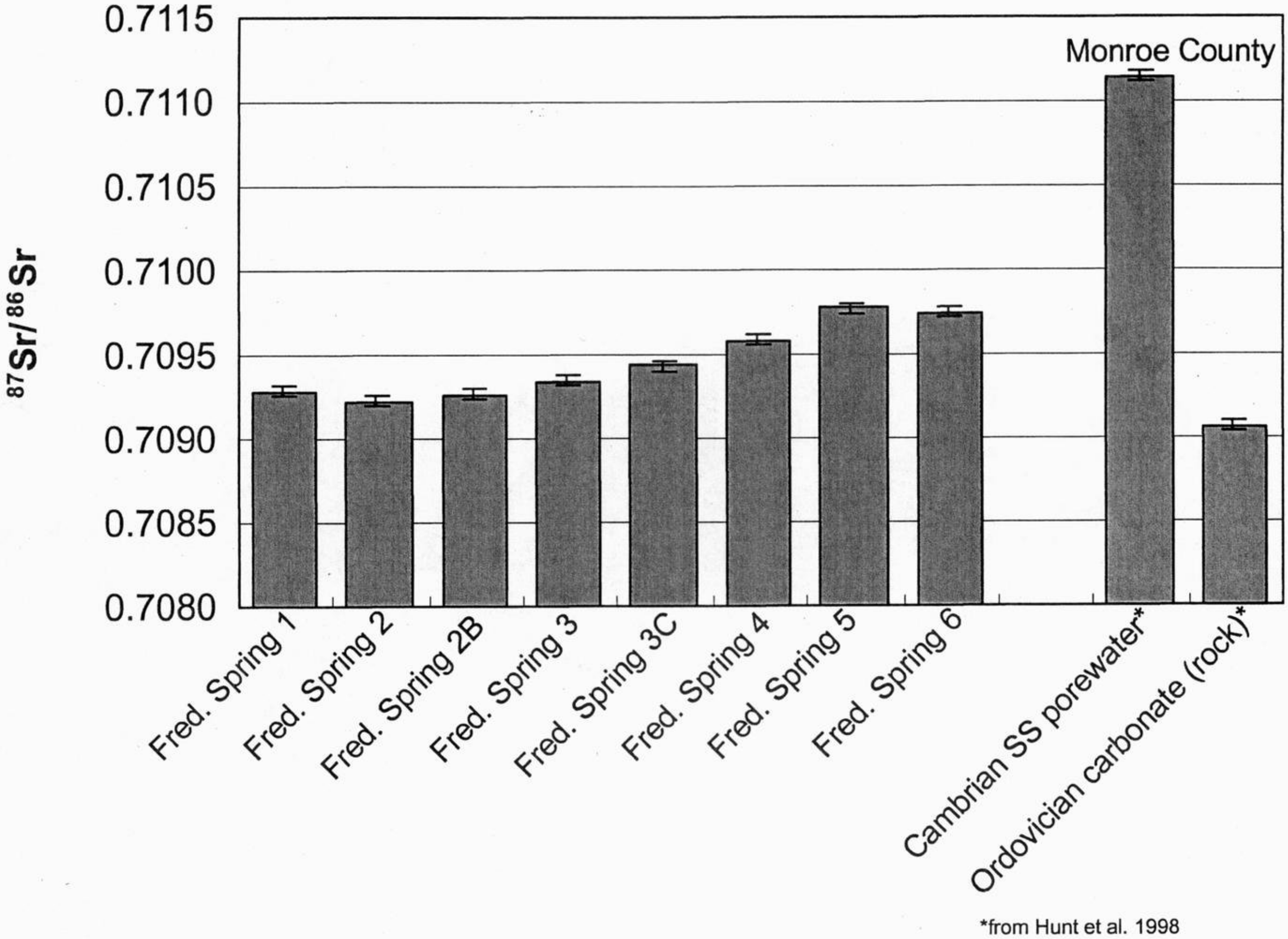


Figure 13 - Average strontium isotope ratios for the March 1998 and September 1998 sampling. Error bars reflect reported laboratory precision. Ratios obtained from a whole rock digestion of the Ordovician carbonate and porewater sampled from the Cambrian sandstone in Monroe County, Wisconsin, are also shown. Samples from the Gate Spring and the municipal well were not submitted for strontium isotope analysis.

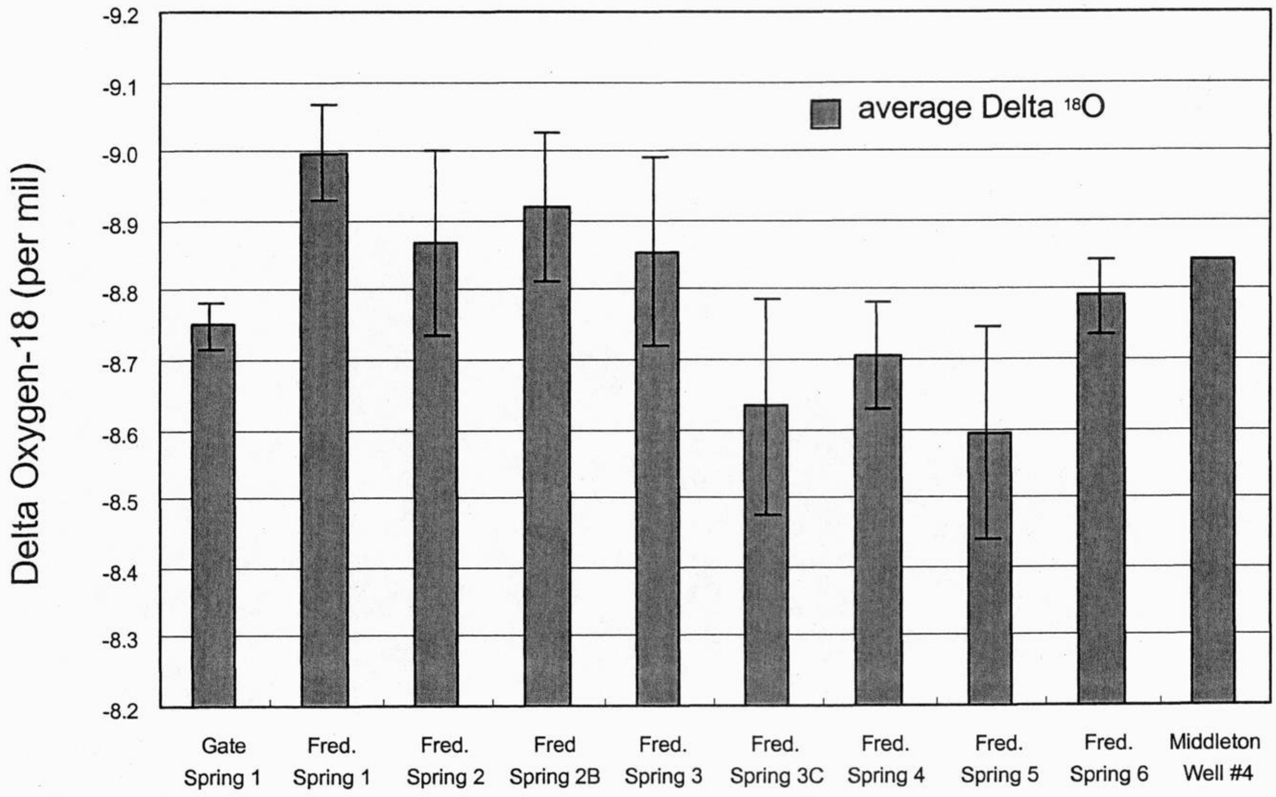


Figure 14 - Delta ^{18}O for the period 1998-1999. Error bars represent 1 standard deviation for all samples measured. The municipal well was sampled only once in August 1998 therefore no error bar can be calculated. Measurement precision is plus or minus 0.1 per mil.

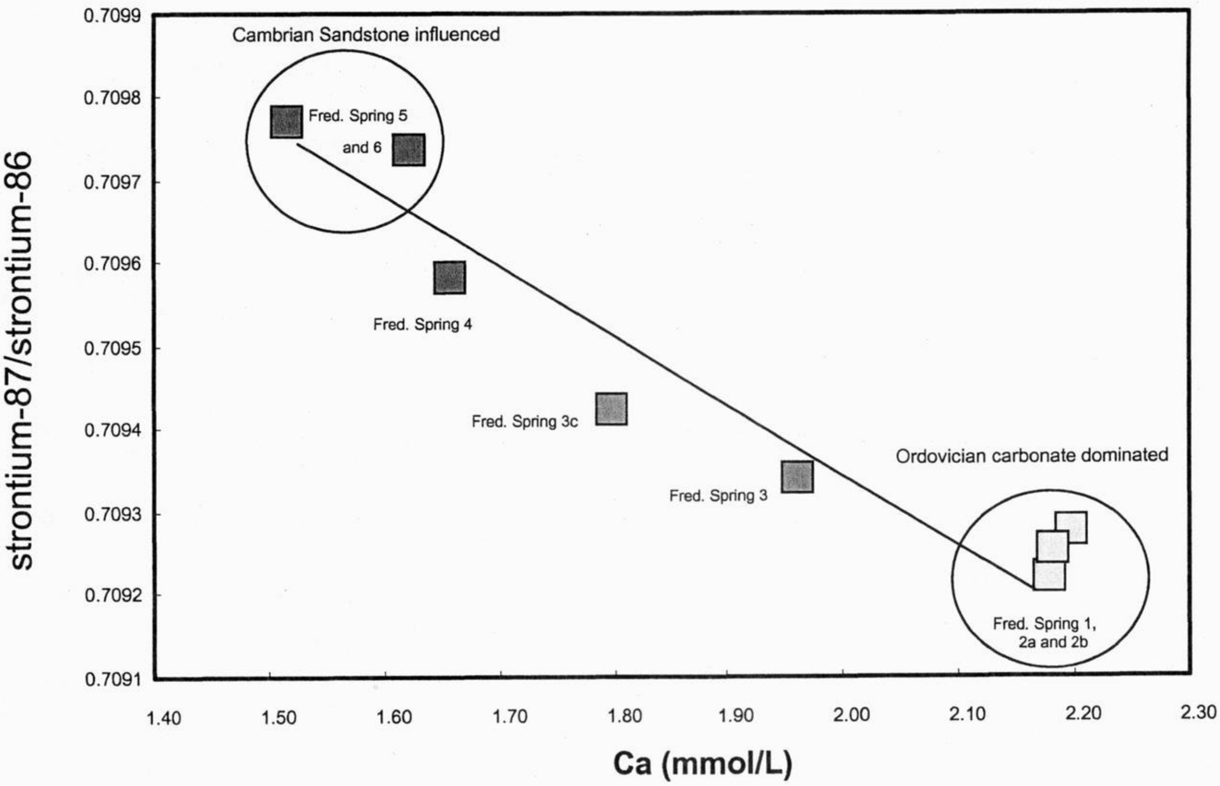
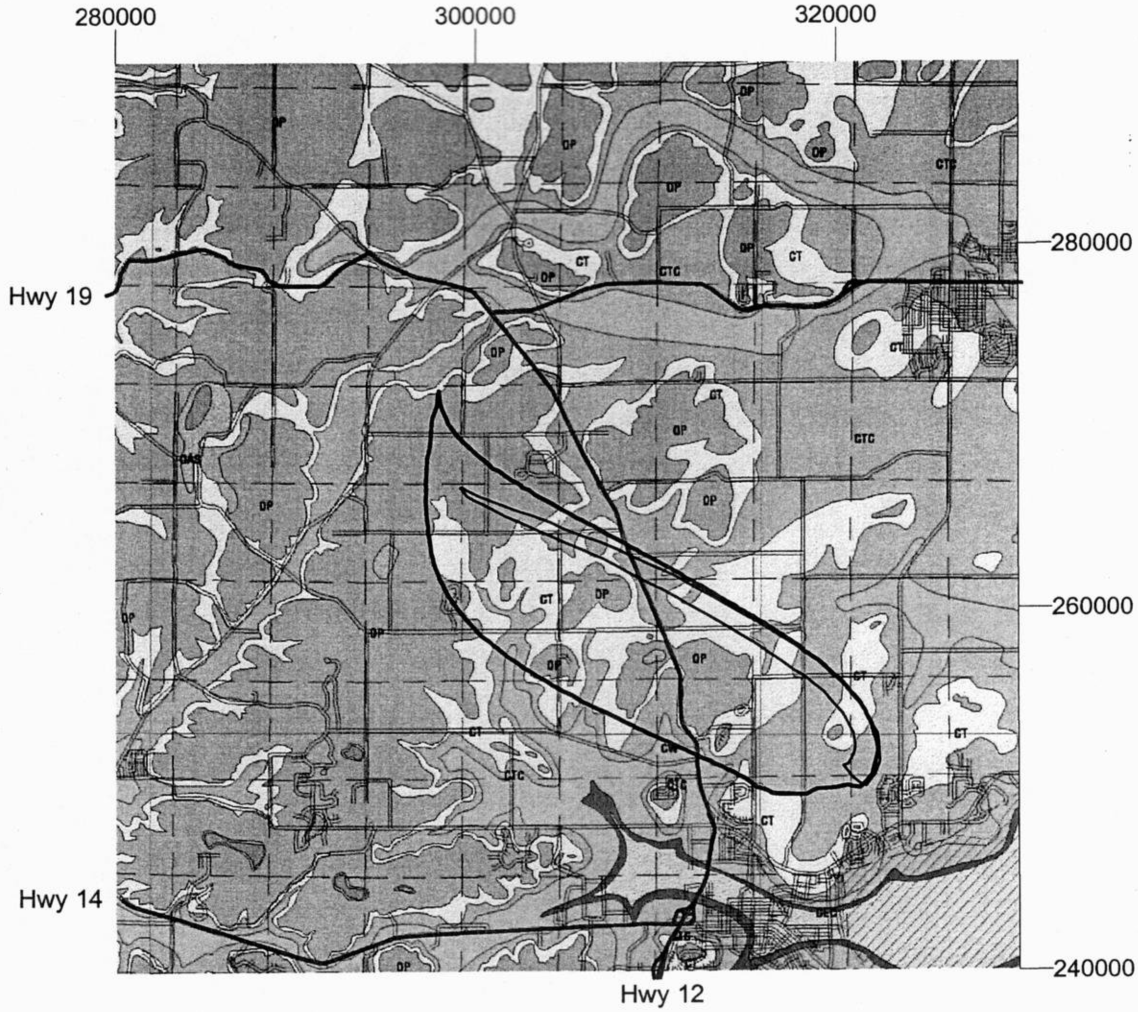


Figure 15 - Average $^{87}Sr/^{86}Sr$ ratio versus average calcium concentration for the period 1998-1999. The samples represent a gradation between a two-component mixing where the end members include a high calcium water with a strontium isotope ratio near that measured in Ordovician carbonate and a lower calcium water with a strontium isotope ratio that suggests a larger contribution from Cambrian sandstones.



Draft Bedrock map: 1:100,000 Bedrock Geology of Dane County, Wisconsin by K.M. Massie-Ferch, R.M. Peters, and B.A. Brown, in review, WGNHS

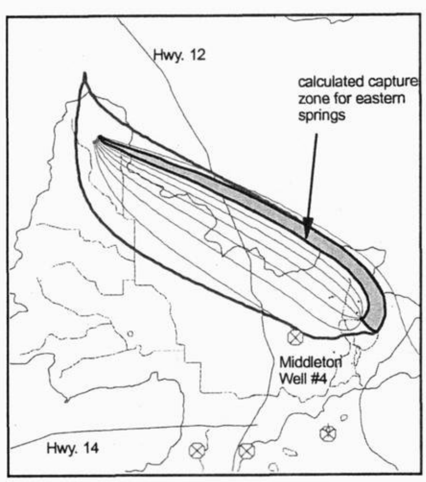


Figure 16 - Inset shows capture zone for eastern springs using the optimized model; this flow tube and the 50% probability capture zone using all conditioned realizations can be overlain on a bedrock map of the Pheasant Branch vicinity. Areas where the Ordovician carbonate is absent (northeast areas of the capture zone) have Cambrian sandstone bedrock in the recharge areas that feed the eastern spring vents at Frederick Springs. The southwestern areas of the capture zones are characterized by Ordovician carbonates (OP) and are the areas that feed the western spring vents.

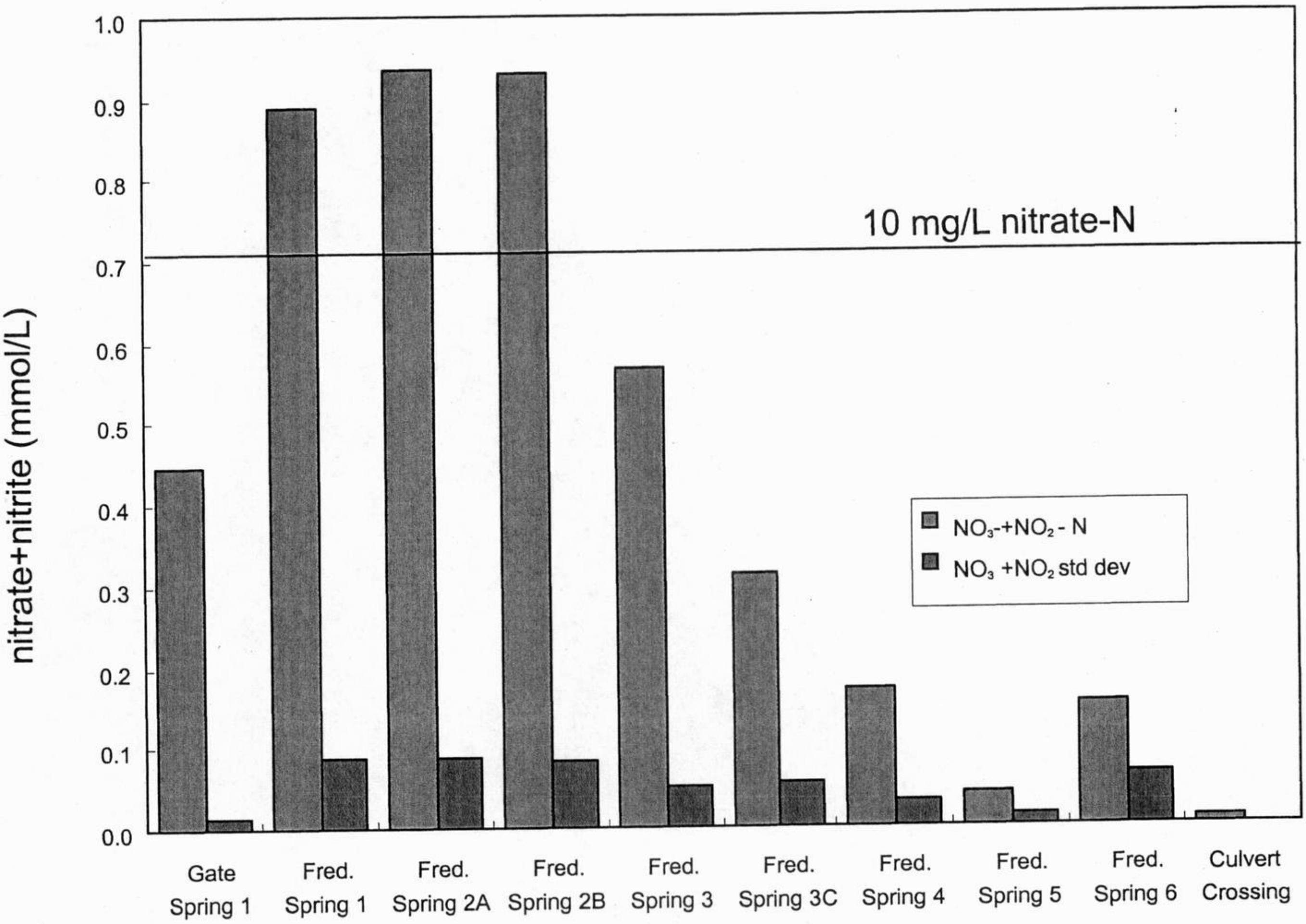


Figure 17 -Average nitrate+nitrite and standard deviations for the Pheasant Branch sampling 1998-1999. The 10 mg/L nitrate-N drinking water standard is shown for reference.

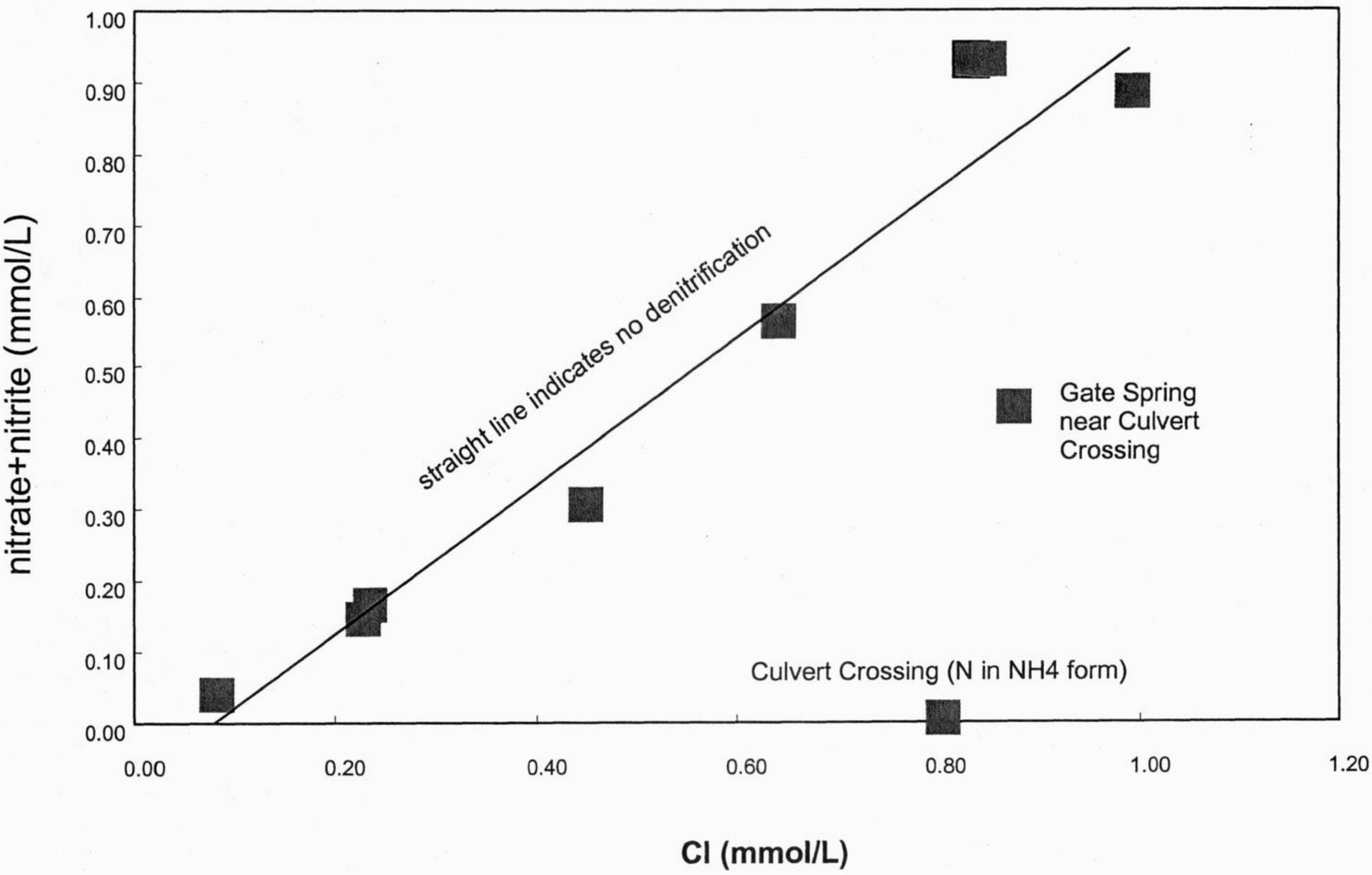


Figure 18 - Average nitrate+nitrite versus average chloride concentrations for the Pheasant Branch sampling 1998-1999. The straight line indicates that denitrification (which removes nitrogen but not chloride) is not occurring. The Gate Spring sample and the Culvert Crossing surface water sampling site is located 1300 feet west of the Frederick Springs complex and may reflect a different source of nitrogen.

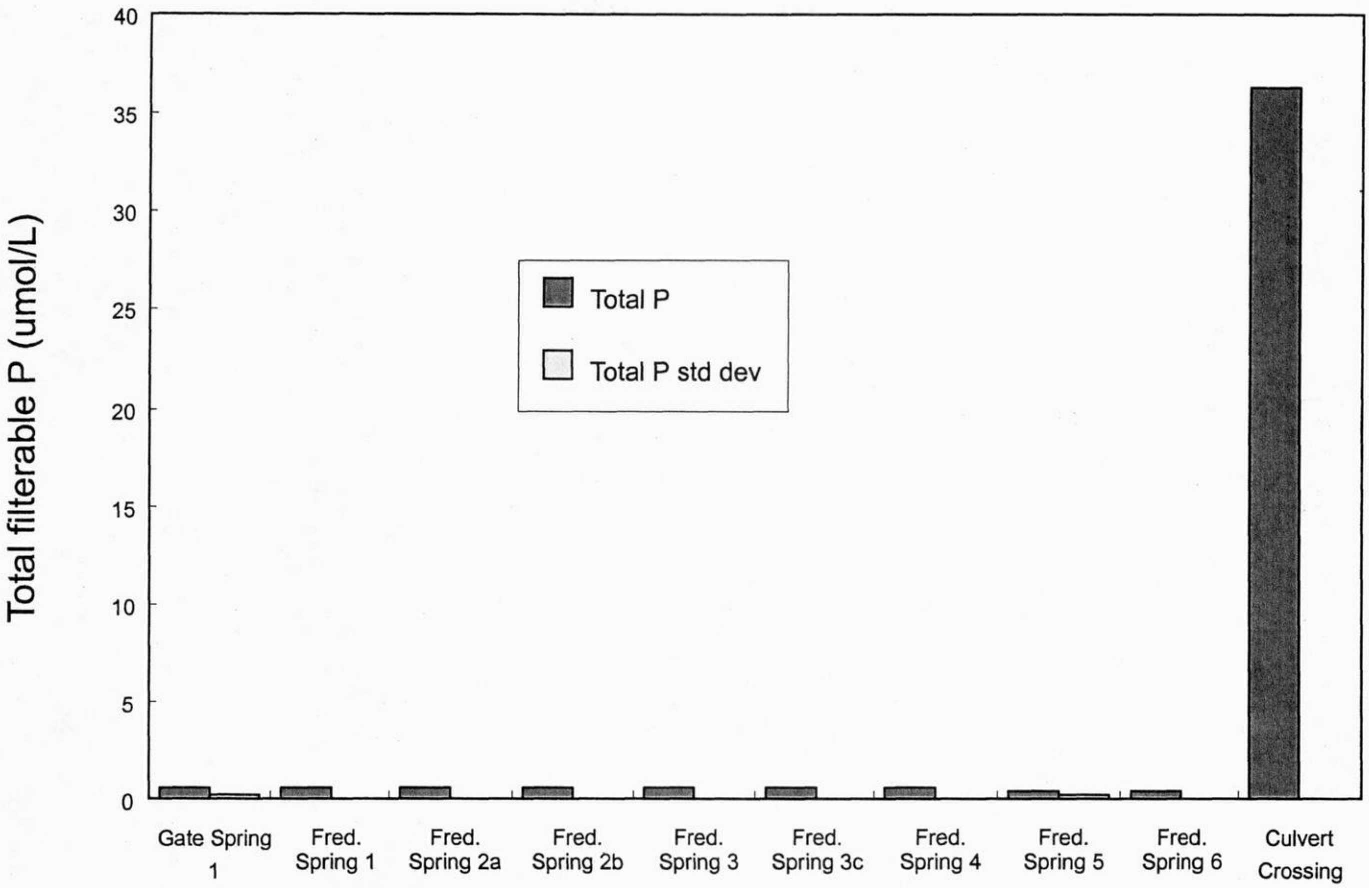


Figure 19 - Average total filterable phosphorus for the Pheasant Branch sampling 1998-1999. As is true in most natural systems, phosphorus is more efficiently transported in the surface water (Culvert Crossing). The Culvert Crossing surface water sampling site was only wet during the spring runoff event thus it is unclear if it is more important than the groundwater contribution on an annual scale.