

# **Groundwater Flow and Heat Transport in Wetlands: Transient Simulations and Frequency-Domain Analysis**

Hector R. Bravo, Associate Professor, Department of Civil Engineering and Mechanics,  
University of Wisconsin-Milwaukee

**Project I.D.:**  
UW-WRI #99-WLA-1

**Period of Contract:**  
July 1, 1998 to June 30, 2000

**Key Words:**  
Groundwater Modeling, Wetlands, Heat Transport, Time-Series Analysis

*This project was supported, in part, by General Purpose Revenue funds of the State of Wisconsin to the University of Wisconsin System for the performance of research on groundwater quality and quantity. Selection of projects was conducted on a competitive basis through a joint solicitation from the University and the Wisconsin Departments of Natural Resources; Agriculture, Trade and Consumer Protection; Commerce; and advice of the Wisconsin Groundwater Research Advisory Council and with the concurrence of the Wisconsin Groundwater Coordinating Council.*

**II. TABLE OF CONTENTS**

Groundwater Flow and Heat Transport in Wetlands: Transient Simulations and  
Frequency-Domain Analysis..... 1

II. TABLE OF CONTENTS..... 2

III. LIST OF FIGURES AND TABLES..... 3

IV. PROJECT SUMMARY ..... 4

    Title: Groundwater Flow and Heat Transport in Wetlands: Transient Simulations and  
    Frequency-Domain Analysis. .... 4

    Project I.D.: UW-WRI #99-WLA-1 ..... 4

    Investigators:..... 4

    Period of Contract: July 1, 1998 to June 30, 2000..... 4

    Background/Need: ..... 4

    Objectives: ..... 4

    Methods: ..... 4

    Results and Discussion: ..... 5

    Conclusions/Implications/Recommendations:..... 5

    Related Publications: ..... 5

    Key Words: Groundwater Modeling, Wetlands, Heat Transport, Time-Series Analysis..... 5

    Funding: UWS Groundwater Research Program..... 5

V. INTRODUCTION ..... 6

VI. PROCEDURES AND METHODS..... 8

    Groundwater Flow and Heat Transport Model..... 8

    Parameter Estimation Procedure..... 9

    Frequency Domain Analysis..... 9

VII. RESULTS AND DISCUSSION ..... 9

    Calibration of Synthetic Examples ..... 9

    Frequency domain analysis of field data and selection of modeling scenarios for transient  
    simulations ..... 11

    Steady flow and transient heat transport model of the Wilton wetlands ..... 13

VIII. CONCLUSIONS AND RECOMMENDATIONS ..... 14

IX. REFERENCES ..... 15

### III. LIST OF FIGURES AND TABLES

|   |    |
|---|----|
| Figure 1: Typical simulated flow and temperature fields in synthetic section model. Velocity vectors converge to the river and are perpendicular to contour lines of hydraulic head $h$ . Contour lines of temperature $T$ shows significant variation near the surface.....      | 7  |
| Figure 2. Hourly head data collected during the 1996 growing season in well F2 in the constructed wetland. ....   | 8  |
| Figure 3. Typical groundwater temperature measurements at site F2 showing evidence of an annual cycle component.....  | 8  |
| Figure 4. Contour lines of objective function $\phi$ versus $\log(K)$ and $\log(\text{flux})$ for single-layer model with noisy observations. a) Flow model with $h$ observations; b) Flow and heat transport model with $h$ and $T$ observations.....                            | 10 |
| Figure 5. a) Autocorrelation function of hourly water level data; b) autocorrelation function of hourly groundwater temperature at a depth of 1.2 ft.; c) spectral density of hourly water level; d) spectral density of hourly groundwater temperature at a depth of 1.2 ft..... | 12 |
| Table 1. Typical results of harmonic analysis of temperature data. ....   | 13 |
| Table 2. Wilton wetlands: parameter estimation results.....   | 14 |

#### IV. PROJECT SUMMARY

**Title:** Groundwater Flow and Heat Transport in Wetlands: Transient Simulations and Frequency-Domain Analysis.

**Project I.D.:** UW-WRI #99-WLA-1

**Investigators:**

Principal Investigator – Hector R. Bravo, Associate Professor, Department of Civil Engineering and Mechanics, University of Wisconsin-Milwaukee (UWM).

Research Assistant – Feng Jiang, Department of Civil Engineering and Mechanics, UWM.

**Period of Contract:** July 1, 1998 to June 30, 2000.

**Background/Need:**

Reliable estimates of inflows to a wetland and hydrogeologic parameters can be crucial for understanding wetland hydrology as well as the sustainability of constructed wetlands. Yet inflows are spatially heterogeneous and time-dependent, and their characterization is not trivial. Groundwater models are one method for scaling point measurements up to the site scale, but the information provided by measured heads is frequently insufficient to find unique parameter values. That insufficiency can be overcome by including flux data or by jointly inverting head and temperature measurements.

Including heat transport in the model could result in different time scales than are traditionally considered dominant in groundwater flow. Frequency analysis of head and temperature data can characterize these time scales and facilitate the model construction.

**Objectives:**

The objectives of this project were: 1) to use a set of synthetic models to demonstrate the utility of including temperature data with traditional head data to constrain estimation of parameters important for groundwater flow modeling, 2) to use frequency-domain analysis to characterize a head and temperature data set collected at a wetland in Wilton, Wisconsin, and relate this characterization to proper model construction, and, 3) to apply the approach to simulating flow and heat transport at the Wilton wetland.

**Methods:**

The procedure consists in an optimization component and a simulation component. In the optimization module the unknown parameters are the flux across the water table and hydraulic conductivity; the objective is the minimization of a weighted sum of squared differences between measured and predicted heads and temperatures; and the constraints are the governing equations and boundary conditions in the simulation component. In the simulation module the primary unknowns are pressure and temperature; the governing equations express flow and energy balance; the set of boundary conditions includes the flux across the water table. The procedure was developed using hypothetical models and applied to the Wilton wetlands. The hypothetical models included a one-dimensional steady flow and transient heat transport model, and two dimensional steady state section models. The Wilton model is a two dimensional steady flow and transient heat transport model.

A univariate frequency domain analysis of water level, groundwater temperature and land surface data was done to uncover relevant time scales in those variables. The relative importance of heat conduction and advection was investigated through a bivariate analysis of land surface and groundwater temperature data.

### **Results and Discussion:**

Synthetic and field models that did not converge to an optimal parameter set when only head data were used did converge when head and temperature data were used. The study demonstrated the viability of estimating groundwater inflows averaged over periods of the order of days by using average values of hydraulic head along with hourly temperature data. While the true values of the hydraulic conductivity and flux across the water table at the Wilton field site are unknown, the coupled inversion methodology produced estimates that were consistent with field measurements.

Harmonic analysis of groundwater temperature data showed that most of its variance is explained in terms of the annual cycle. That analysis showed consistency, at the yearly level, between land surface temperature and groundwater temperature at all depths. For frequency components other than the yearly cycle the significance of frequency relations decreases for records at deeper depths. In other words, the relative importance of heat conduction from and to the land surface decreases rapidly with depth.

### **Conclusions/Implications/Recommendations:**

Joint inversion of head and temperature data is an effective method to estimate simultaneously hydraulic conductivity and inflow to wetland systems. While the computational effort required for the procedure increases for analysis of transient flow, time- and-frequency-domain analyses of head and groundwater temperature data can limit modeling time periods to those that provide the best return in parameter estimation. The methodology should have wide applicability in areas where the groundwater-wetland interaction influences the temperature distribution of the shallow groundwater system and in areas where there is sufficient annual and/or daily temperature fluctuation. However, due to the larger data sets required, the reduced utility in multi-layer systems, and the additional uncertainty resulting from the additional thermal parameters needed to simulate the coupled system, these methods will complement rather than supersede calibration methods that use measured heads to estimate hydraulic conductivity and flux. They are expected to be of special use in systems where flux data are not readily available.

### **Related Publications:**

Bravo, H.R., F. Jiang and R.J. Hunt, 2001. Using groundwater temperature data to constrain parameter estimation in a groundwater flow model of a wetland system, submitted to *Water Resources Research*.

Bravo, H.R., F. Jiang and R.J. Hunt, 2001. Parameter estimation for a groundwater flow and heat transport model of a wetland system: Selection of time scales through frequency domain analysis, submitted to XXIX IAHR Congress, Beijing, China.

Bravo, H.R., F. Jiang and R.J. Hunt, 2000. Improving wetland simulations by coupling groundwater flow and heat transport modeling, Proc. of the 4th International Conference Hydro Informatics 2000, Theme EW1, Cedar Rapids, Iowa.

Bravo, H.R., F. Jiang and R.J. Hunt, 2000. Analisis de temperatura del agua subterranea en el dominio de frecuencia y estimacion del aporte a bañados, Proceedings of the XIX Latin American Congress on Hydraulics, p. 437-446, Cordoba, Argentina.

Jiang, F., 2000. Calibration of model for ground water flow and heat transport in wetlands, M.S. Thesis, University of Wisconsin-Milwaukee.

**Key Words:** Groundwater Modeling, Wetlands, Heat Transport, Time-Series Analysis.

**Funding:** UWS Groundwater Research Program.

## V. INTRODUCTION

Reliable estimates of groundwater inflow into a wetland (flux across the water table) and hydrogeologic parameters can be crucial for understanding wetland hydrology as well as the success and sustainability of constructed wetlands. Yet groundwater inflows are spatially heterogeneous and time-dependent, and their characterization and estimation is not trivial. Moreover, field measurements of the groundwater system are often limited to a number of point measurements, yet the project objective may require a larger scale characterization of the groundwater system.

Groundwater models are one method for scaling point measurements of the groundwater system up to the site scale. However, parameters used in groundwater flow modeling are non-unique. The information provided by measured heads is frequently insufficient to find unique values of inflows and parameters. It has been suggested that the inclusion of flux data can constrain a “best fit” estimate of the hydraulic conductivity and recharge, but in many cases a site may not be suitable for the collection of flux data (e.g., fens without clearly defined surface water outlets). Another way to overcome that insufficiency is to simulate jointly and invert the relevant head and temperature measurements. Several researchers have used flow and heat transport models to estimate model parameters in deep and shallow systems. Woodbury and Smith [1988] successfully simulated and inverted flow and heat transport data to investigate groundwater flow at spatial scales of the order of thousands of meters. Ronan et al. [1998] summarized previous work of shallow systems.

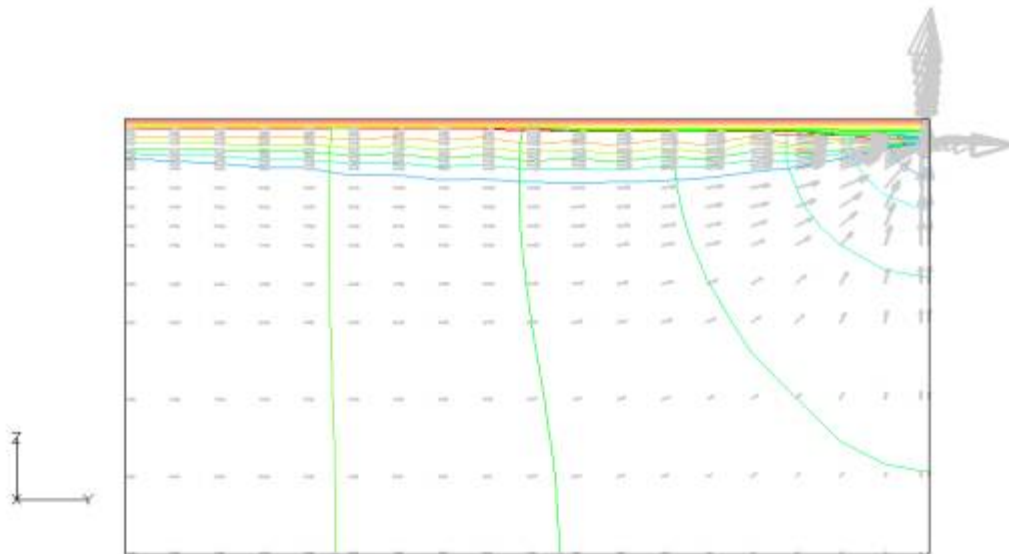
Including heat in groundwater flow models brings additional considerations with respect to time discretization. The appropriate conceptualization of transience in the system is becoming more recognized in groundwater modeling. It follows, therefore, that the addition of temperature stresses to the problem could result in different system time scales than are traditionally considered dominant in the groundwater flow system. Frequency analysis of water level and temperature data can be used to characterize these potentially disparate time scales and facilitate the most appropriate construction of a coupled heat-water transport model.

In this study we used hydraulic head and shallow water temperature data collected in a wetland located in a temperate climate, a coupled groundwater flow and heat transport model, and parameter estimation techniques to estimate simultaneously groundwater inflow into the wetland and aquifer hydraulic conductivity. The technique was applied to several synthetic examples for which we knew the true model structure in order to investigate the robustness of the approach. The temporal characteristics of the simulation scenarios were selected by analyzing the time-and-frequency-domain attributes of head and temperature data. The rationale behind this method is that frequency relationships reveal the time scales that are relevant for different physical processes and consequently allow choosing appropriate time discretizations for the simulations to best represent the important time periods. Frequency domain analysis was also used to investigate the effect of land surface temperature (as represented by air temperature) on groundwater temperature. While several previous works share some of the characteristics of the problem faced in this study, none of them tackled the estimation of parameters for shallow systems through inversion of unsteady flow and heat transport data and the use of frequency domain analysis to select appropriate time scales for the inversion.

Hunt et al. [1996], describe the natural and constructed wetlands near Wilton, located along the Kickapoo River in the unglaciated region of southwestern Wisconsin. The high topographic relief results in groundwater flow paths that extend from the highlands to the adjacent river

bottom. The high relief and incised drainage network result in a system characterized by downward hydraulic gradients in the highlands and upward gradients in the river bottom discharge areas. In the headwater regions of the driftless area, localized discharge promotes the formation of river bottom wetlands that receive groundwater inflow. The wetland considered here is characterized by a peat/fluvial sediment layer and a sandstone layer approximately 100 m thick, and a temperature field that varies seasonally and daily within a few meters below the land surface. Figure 1 illustrates the typical flow pattern in a synthetic model in a cross section of the system as calculated by the model with the flow converging to the Kickapoo River. The associated simulated temperature field is also shown. The field investigation of the Wilton wetlands included installing a closely spaced network of nested wells that were monitored for eight years for water level, groundwater temperature and other relevant variables. Figures 2 and 3, which show head and temperature data, illustrate the dynamic character of the system. Between 1990 and 1996 water level was measured at the Wilton wetlands with different sampling frequencies in more than 30 wells. Figure 2 shows hourly data collected in 1996 at site F2 in the constructed wetland [Hunt et al., 1996]. Similar hourly data were collected at sites F1 in the constructed wetland and at sites W1 and W2 in the natural wetland. Figure 3 shows hourly groundwater temperature data collected between May 1993 and December 1996 (with a gap in 1994-95) at site F2; similar data were collected at sites W1, W2 and F1.

Figure 1: Typical simulated flow and temperature fields in synthetic section model. Velocity vectors converge to the river and are perpendicular to contour lines of hydraulic head  $h$ . Contour lines of temperature  $T$  shows significant variation near the surface.



The specific objectives of this paper are: 1) to use a set of synthetic models to demonstrate the utility of including temperature data with traditional head data to constrain estimation of parameters important for groundwater flow modeling, 2) to use frequency-domain analysis to characterize a head and temperature data set collected at a wetland in Wilton, Wisconsin, and relate this characterization to proper model construction, and, 3) to apply the approach to simulating flow and heat transport at the Wilton wetland.

Figure 2. Hourly head data collected during the 1996 growing season in well F2 in the constructed wetland.

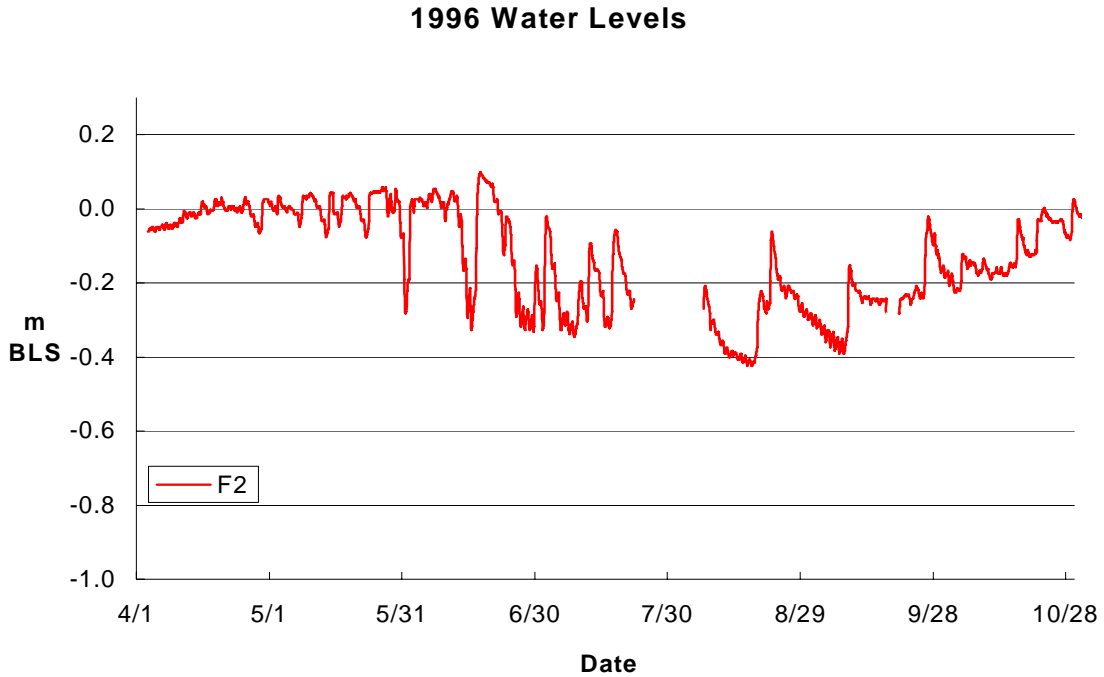
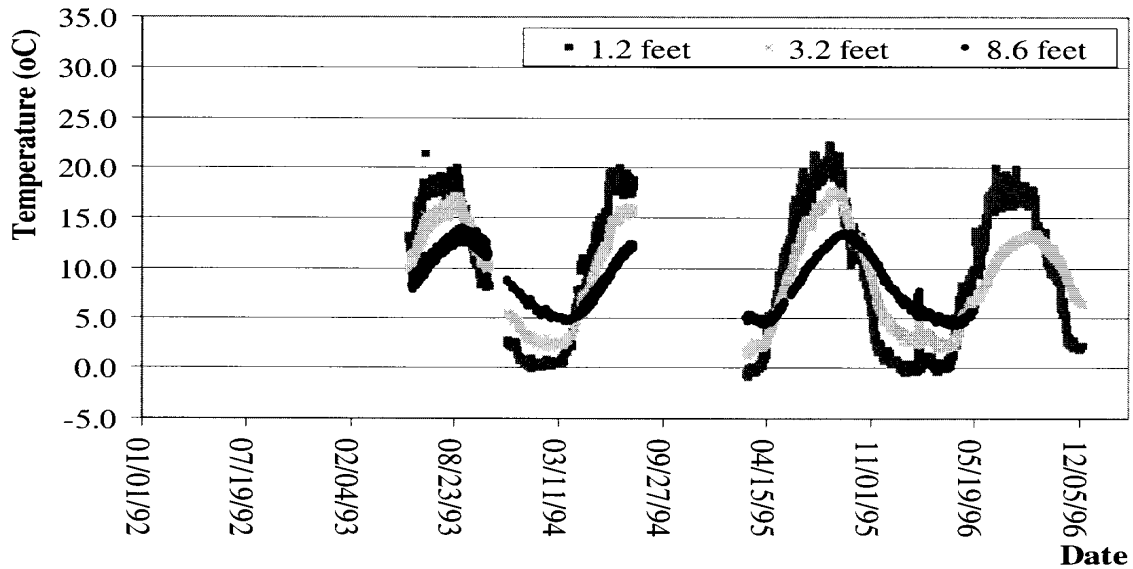


Figure 3. Typical groundwater temperature measurements at site F2 showing evidence of an annual cycle component.



## VI. PROCEDURES AND METHODS

### Groundwater Flow and Heat Transport Model

The simulator HST3D [Kipp, 1987] was used to solve the coupled flow and heat transport equations. HST3D uses finite-difference techniques to discretize the governing equations and can handle several types of boundary conditions, including specified pressure and/or



temperature, specified fluid and/or heat flux, and an unconfined aquifer, free surface boundary condition. A limitation of HST3D is that it cannot simultaneously simulate free surface (unconfined or water table) conditions and heat transport. The models were therefore set up in two steps with iteration, 1) a free-surface flow model and 2) a fixed-region flow and heat transport model. Iteration between the free-surface and the fixed-region models, including change in size and shape of the saturated region, was necessary when the boundary conditions produced significant change in the water table geometry; increases in the level of flow unsteadiness increases the number of water table configurations needed to represent the problem, which in turn increases the number of iterative steps. The first iterative step calculates the free surface geometry. The calculated water table surface is then discretized to represent the top of the modeling region in the second step. To ensure that the same vertical flux across the water table is used in both steps, the velocity and pressure fields from the two steps were compared, and iteration was performed until agreement was reached.

### **Parameter Estimation Procedure**

Calibration of the flow and heat transport model brings together the flux across the water table and its associated temperature, lateral boundary condition resulting from the far-field flow, as well as system parameters (e.g., hydraulic conductivity and thermal diffusivity). The goodness-of-fit is evaluated using field observations of hydraulic head and groundwater temperature. Parameter estimation determines a set of model parameters for which the model-simulated results are as close as possible to a set of measured observations in the least-square sense. The approach was tested using synthetic examples where, prior to parameter estimation, the true values were solved for using the model in a forward mode. A subset of those results was used as ‘observations’ in parameter estimation. A field site in Wilton, Wisconsin was also modeled to assess the approach’s applicability to a real world hydrologic setting. The parameter estimation code PEST [Doherty, 1998] was used to automatically calibrate the synthetic and Wilton models used in this study. PEST is a nonlinear parameter estimation code that finds parameters that minimize the weighted least squares objective function  $\phi$ .

### **Frequency Domain Analysis**

Water level and temperature fluctuations may have different time scales. While HST3D can encompass a range of transience in both groundwater flow and heat transport, the problem should be posed such that the world of possible stress periods is distilled so that only transient characteristics that improve our understanding of the system behavior are simulated. Frequency domain analysis is one method for characterizing the temporal nature of the observations used for calibration. A univariate analysis of water level, groundwater temperature data and land surface data was done to uncover relevant time scales in those variables. The relative importance of heat conduction and advection was investigated through a bivariate analysis of land surface and groundwater temperature data.

## **VII. RESULTS AND DISCUSSION**

### **Calibration of Synthetic Examples**

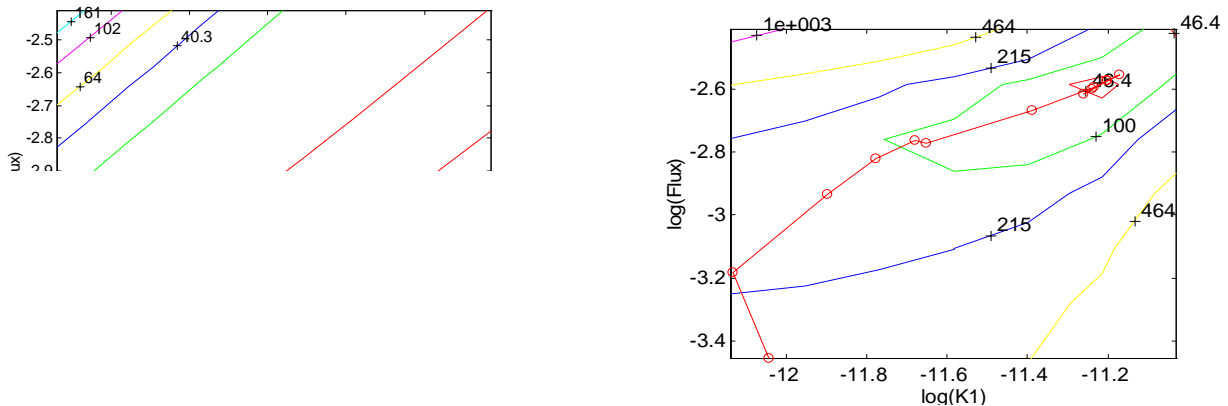
Synthetic models were developed to examine the ability of these procedures to constrain parameter estimation. The first set of models used “observations” calculated using known values of the parameters. The procedure and the quality of its results were evaluated by comparing simulated values to these “observations”. In a second set of tests, the computer-generated

observations were corrupted with Gaussian random noise, and the model misfits were compared with the known noise level; both concepts are defined below. The hypothetical models include a one-dimensional steady flow and transient heat transport model, and two dimensional steady state section models. The Wilton model is a two dimensional steady flow and transient heat transport model.

The present estimation procedure was applied to simulate and invert steady flow and time-dependent heat transport data in an isotropic, homogeneous medium that had known values of hydraulic conductivity, effective porosity, fluid density, density of the solid phase, heat capacity of the fluid phase at constant pressure, heat capacity of the solid phase at constant pressure, thermal conductivity of the fluid phase, and thermal conductivity of the solid phase. The top face boundary condition was a steady vertical flux across the water table, with an associated temperature that varied sinusoidally with a one-year period. At the model bottom the temperature was set constant. The computer-generated observations included monthly values of hydraulic head at 4 different depths and temperature at 2 depths. The calibration procedure was used to estimate the hydraulic conductivity and the vertical flux. The procedure was run numerous times, starting with initial parameter values that differed up to two orders of magnitude from their true values. In all runs the procedure converged to the exact, known parameter values.

The first cross sectional flow model was designed to estimate the hydraulic conductivity of the single aquifer that interacts with the wetland. The calibration procedure easily estimated the exact value of  $K$  when the flux across the water table is specified rather than estimated. In a second single-layer flow model that was intended to estimate the hydraulic conductivity and flux across the water table, however, the model failed to converge on the true values because of parameter correlation, as described later for noisy-observation models. The single-layer model was then modified to simulate heat transport. The inversion of the fixed-region flow and heat transport model consistently found the exact values of  $K$  and flux. This demonstrates that unsteady temperature data can be used to constrain groundwater flow system parameters in a problem that is otherwise non-unique.

Figure 4. Contour lines of objective function  $\phi$  versus  $\log(K)$  and  $\log(\text{flux})$  for single-layer model with noisy observations. a) Flow model with  $h$  observations; b) Flow and heat transport model with  $h$  and  $T$  observations.



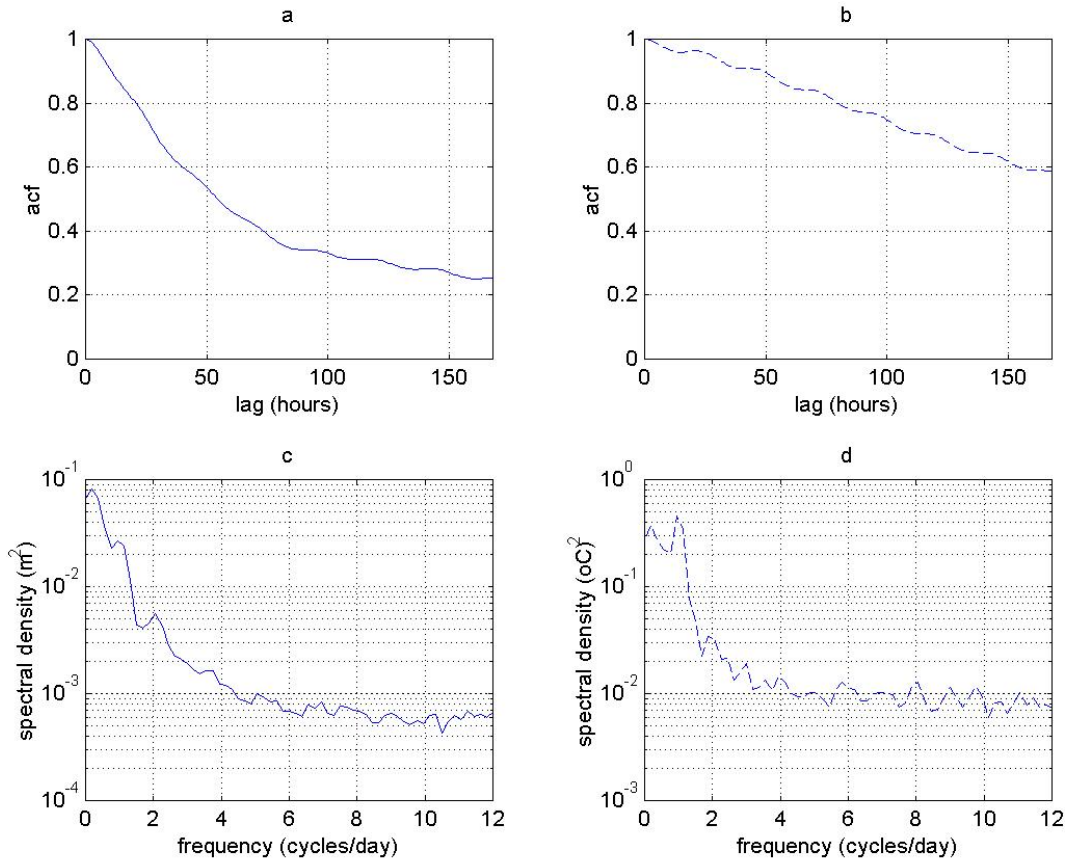
The noisy-observations flow model was used to estimate the hydraulic conductivity of a single stratigraphic unit when the flux across the water table is specified. Similar to the noise-

free case, the model converged on the correct K values. The model found a value of K close to its true value, and calculated very small values of its standard deviation,  $\sigma_K$  and model head misfit,  $S_{\hat{h}}$ . A second noisy-observations flow model was then implemented to estimate both K and the flux across the water table. That model was unsatisfactory because it under-estimated K and the flux, and produced relatively large values of flux standard deviation,  $\sigma_{\text{flux}}$ , and  $S_{\hat{h}}$ . Further tests of this model showed that its results were sensitive to the initial guess of parameter values – clear evidence that the problem is improperly posed. Figure 4.a shows a plot of contour lines of the objective function  $\phi$  that reveals a strong correlation between K and the flux. Hydraulic conductivity and flux were then estimated using a flow and heat transport model. That model estimated K and the flux very closely, and yielded relatively small values of  $\sigma_K$ ,  $\sigma_{\text{flux}}$ ,  $S_{\hat{h}}$ , and model temperature misfit,  $S_{\hat{T}}$ . The contour lines of the objective function  $\phi$  versus K and flux shown in Figure 4.b show convex shapes for this latter model.

### **Frequency domain analysis of field data and selection of modeling scenarios for transient simulations**

The only water level data collected with constant sampling frequency was the 1996 hourly record. This record is not long enough to quantify an annual cycle but contains enough information about smaller-period cycles, such as a daily cycle. Those records were inspected for periods of continuous and simultaneous water level and groundwater temperature measurements. One such period was identified between May 22, 1996 and July 22, 1996. Inspection of water level data in Figure 3 reveals a hint of a growing-season cycle pattern, a daily cycle that includes evapotranspiration effects, and six rainfall events in the 61-day period of interest. Furthermore, one can find periods when the water table is nearly steady. There are no clearly visible “steady” periods in the temperature record (Figure 3). The May 22, 1996 to July 22, 1996 water level and groundwater temperature records were used to calculate the autocorrelation functions and their Fourier transforms, the spectral density. Figure 5.a shows the autocorrelation function of water level and Figure 5.c shows the matching estimated spectral density. Figures 5.b and 5.d show the corresponding results for groundwater temperature at a depth of 1.2 ft. The autocorrelation function (acf) of groundwater temperature is broader than that of water table level. For lags of 24 and 120 hours (1 day and 5 days) the values of the acf of groundwater temperature are 0.96 and 0.70, respectively, while the corresponding values for water table data are 0.77 and 0.31. It is known that the widths of the acf and of the spectral density are inversely related. The spectral density of groundwater temperature (Fig. 5.d) shows a clear peak at 1 cycle/day and decays quickly for higher frequencies. The spectral density of water table level decreases more gradually and shows no clear peak at 1 cycle/day. This finding that the daily cycle is relatively more important for groundwater temperature than for water table level was used to select model settings for transient simulations. If the daily cycle of heat transport is important throughout the year while the daily groundwater flow cycle may be unimportant during certain periods, then there is reason to believe that a few daily cycles of temperature data (while the water table remains nearly steady) may contain enough information to constrain the calibration problem at hand. Furthermore, the observation that there are periods when the water table remains nearly steady while the temperature varies significantly gives justification to the implementation of steady state flow and unsteady heat transport models, greatly simplifying the work required by the two-step modeling approach.

Figure 5. a) Autocorrelation function of hourly water level data; b) autocorrelation function of hourly groundwater temperature at a depth of 1.2 ft.; c) spectral density of hourly water level; d) spectral density of hourly groundwater temperature at a depth of 1.2 ft.



Quantification of the yearly cycle in groundwater temperature was done using the hourly data collected between March 7, 1995 and December 15, 1996. Daily average groundwater temperatures for that 648-day period were calculated from the hourly records. Physical reasoning tells us that the yearly cycle of groundwater temperature is related to that of land surface temperature. Daily air temperature at a nearby weather station located in Cashton, Wisconsin, was used to represent the land surface temperature, for the same 648-day period. Calculated autocorrelation functions for land surface temperature and groundwater temperature showed strong evidence of the relevance of the yearly cycle in both data series. The mentioned data set was therefore used to carry out an harmonic analysis for the land surface temperature and for groundwater temperature at site F2, at depths of 0.2 ft, 1.2 ft, 2.2 ft, 3.2 ft, 5.5 ft, and 8.6 ft below the land surface. Let us reiterate that the available data set was insufficient to carry out a similar harmonic analysis of water level.

Table 1 summarizes the results of the harmonic analysis. One can see in Table 1 that, as the depth increases, the amplitude  $R$  decreases in an exponential fashion while the phase (or lag)  $\phi$  increases. The yearly cycle of temperature at the 1.2 ft depth lags the air temperature cycle by 12 days, and the 3.2 ft depth temperature is lagged an additional 17 days. The values of  $r^2$  (0.835, 0.956, 0.963 and 0.966 at depths of 0, 1.2, 3.2 and 5.5 ft, respectively) indicate that most of the

total variance is explained by the first harmonic (or yearly) component. The relevance of the yearly cycle is very clear from these results.

Table 1. Typical results of harmonic analysis of temperature data.

| Depth (ft) | Amplitude R (°C) | Sample mean $\mu$ (°C) | Phase $\phi$ (day of the year) | Sample variance $S_T$ (°C) <sup>2</sup> | $r^2$ |
|------------|------------------|------------------------|--------------------------------|---|-------|
| 0.         | 15.87            | 6.79                   | 110                            | 150.73                                  | 0.835 |
| 1.2        | 10.21            | 8.15                   | 122                            | 54.54                                   | 0.956 |
| 3.2        | 6.90             | 8.22                   | 139                            | 24.73                                   | 0.963 |
| 5.5        | 5.76             | 8.48                   | 146                            | 17.20                                   | 0.966 |

### Steady flow and transient heat transport model of the Wilton wetlands

The joint inversion procedure was applied to the Wilton wetlands. A cross sectional model at  $x = 180$  m [Jiang, 2000] was constructed using data from six wells with hourly head observations and one well (F2) with hourly temperature measurements near that section. Figures 2 and 3 illustrate the type of data used. This data set is a relatively large one for a field application, but is obviously smaller than those used in the hypothetical models (17 head observations and 16 temperature observations).

A steady state flow period was identified between September 27 and October 18, 1996. Records showed rainfall trace on October 4, a steady water table level and a downward gradient, indicating a period of groundwater recharge. Groundwater temperature was, however, unsteady during that period. October 6, 1996 was the chosen one-day test period and the surficial temperature varied in the 9.4 °C - 14.6 °C range. Temperature observations every 4 hours at depths of 0.2 ft, 1.2 ft, 3.2 ft and 5.5 ft deep below the ground surface were used in the calibration. The temperature observed at 0.2 ft below the land surface was used to specify the temperature associated with the flux across the water table. Measured temperatures, averaged for one week before the test period were used to specify the temperature at the upstream boundary.

A single-hydrostratigraphic unit model was constructed to estimate hydraulic conductivity and recharge flux. The procedure started with a flow model calibrated against head data. The flow model was later coupled to the heat transport model in HST3D. The calculated flow field and temperature field patterns resembled those shown in Figure 1 for a hypothetical section model, for a case where the fluid flux across the water table was warmer than the average groundwater temperature. In that case the isotherms are depressed by recharge because of the downward flow of warmer water and were elevated near the river because of the upward flow of cooler water. The standard deviation of the temperature and head residuals remained within 0.25 °C and 0.3 m, respectively.

Because the true values of the parameters are unknown, the noise level and model misfit cannot be computed in field applications. However, the experience gained from the hypothetical models was transferred to the Wilton model. The hypothetical models were used to determine appropriate weights (in relation with the estimated measurement errors) for head and temperature observations, and to verify that the procedure resulted in model misfits smaller than the noise levels when the model was well-posed model and its structure was known. Those same weights were used in the Wilton model, and the spread in estimation results allowed us to assess the sufficiency of the field database to resolve the model parameters. Table 2 shows the summary results of numerous calibration runs that started with widely different initial parameter values, and includes estimated ranges and mean values of K and the flux, and their standard deviations. The spread in estimated parameter values reflects some data insufficiency to resolve these

parameters adequately, but the inverse simulation still obtains satisfactory results. Detailed inspection of the PEST run record files revealed that the temperature components of the residuals in the objective function were more persistent than the head components. This suggests that accuracy in temperature measurements is more important than accuracy in head measurement. Table 2 shows that the hydraulic conductivity and flux values estimated with the free surface flow model (i.e., no temperature simulation) vary by nearly one order of magnitude. On the contrary, the hydraulic conductivity and flux values estimated by the coupled flow and heat transport model range within factors of less than two. In addition, the standard deviations  $\sigma_K$  and  $\sigma_{flux}$ , are much smaller for the coupled model.

Table 2. Wilton wetlands: parameter estimation results.

|            | Free-surface flow model                                |  |  |  | Fixed-region flow and heat transport model             |  |  |  |
|------------|--|--|--|--|--|--|--|--|
|            | K (m/s)  | $\sigma_K$ (m/s)                                       | flux * (m/s)   | $\sigma_{flux}$ (m/s)                                  | K (m/s)  | $\sigma_K$ (m/s)                                       | flux * (m/s)   | $\sigma_{flux}$ (m/s)                                  |
| range      | 1.3 x 10 <sup>-6</sup><br>to<br>8.8 x 10 <sup>-5</sup> | 4.3 x 10 <sup>-6</sup><br>to<br>1.2 x 10 <sup>-4</sup> | 2.8 x 10 <sup>-8</sup><br>to<br>9.8 x 10 <sup>-7</sup> | 2.3 x 10 <sup>-7</sup><br>to<br>1.2 x 10 <sup>-6</sup> | 2.7 x 10 <sup>-5</sup><br>to<br>3.9 x 10 <sup>-5</sup> | 9.5 x 10 <sup>-6</sup><br>to<br>1.7 x 10 <sup>-5</sup> | 7.7 x 10 <sup>-8</sup><br>to<br>1.1 x 10 <sup>-7</sup> | 2.7 x 10 <sup>-8</sup><br>to<br>8.3 x 10 <sup>-8</sup> |
| mean value | 3.4 x 10 <sup>-5</sup>                                 | 5.0 x 10 <sup>-5</sup>                                 | 3.4 x 10 <sup>-7</sup>                                 | 6.4 x 10 <sup>-7</sup>                                 | 3.2 x 10 <sup>-5</sup>                                 | 1.3 x 10 <sup>-5</sup>                                 | 9.7 x 10 <sup>-8</sup>                                 | 4.4 x 10 <sup>-8</sup>                                 |

\* Calculated for October 6, 1996.

The coupled modeling approach also more closely represents the conductivity and fluxes measured in the field. The estimated hydraulic conductivity from our modeling ranged between 2.7 x 10<sup>-5</sup> and 3.9 x 10<sup>-5</sup> m/s (230 to 340 cm/d), and the flux ranged between 7.7 x 10<sup>-8</sup> and 1.1 x 10<sup>-7</sup> m/s (0.66 to 0.95 cm/d). The conductivity values compare well to slug test results for the sandstone layer at well F2 (2.5 x 10<sup>-5</sup> m/s) reported by Hunt et al. [1996], and values reported in the literature for Cambrian sandstone. The period used to calculate flux across the water table simulated here does not coincide with that used by Hunt et al. [1996], therefore a comparison between flux estimates cannot be made. However, Lott [1997] collected precipitation and evapotranspiration data during this period, giving an independent estimate of the flux. During the period September 24 through October 15, 1996 the measured net flux across the water table equaled 0.92 cm/d (based on an average daily rainfall of 1.1 cm/d and an average evapotranspiration of 0.18 cm/d), which compares well with the range of simulated flux (0.66 to 0.95 cm/d).

## VIII. CONCLUSIONS AND RECOMMENDATIONS

Joint inversion of head and temperature data is an effective method to estimate simultaneously hydraulic conductivity and inflow to wetland systems. Synthetic and field models that did not converge to an optimal parameter set when only head data were used did converge when head and temperature data were used. While the computational effort required for the iterative two-step modeling procedure increases for analysis of transient flow, time-and-frequency-domain analyses of water level and groundwater temperature data series can limit modeling time periods to those that provide the best return in the process of parameter estimation.

Frequency domain analysis showed that, for the Wilton wetlands, frequencies of the order of days are less significant in the water table data series than in groundwater temperature data. This study demonstrated, therefore, the viability of estimating groundwater inflows averaged over

periods of the order of days by using average values of hydraulic head (which include the effect of evapotranspiration and rainfall) along with time-varying (say, hourly) temperature data.

Harmonic analysis of groundwater temperature data showed that most of its variance is explained in terms of the annual cycle. That analysis showed consistency, at the yearly cycle level, between land surface temperature and groundwater temperature at all depths. For frequency components other than the yearly cycle the significance of frequency relations decreases as one considers temperature records at deeper depths. In other words, the relative importance of heat conduction from and to the land surface decreases rapidly with depth.

The method's utility was demonstrated at the Wilton, Wisconsin field site. While the true values of the hydraulic conductivity and flux across the water table are unknown, the coupled water and heat transport inversion methodology produced estimates of hydraulic conductivity and flux that were consistent with field measurements. This resulted in an improvement over an earlier model calibrated by trial and error that did not include heat transport, because in that earlier model the flux was specified *a priori*, and resulting estimates of K were appreciably higher than values measured in the field.

The methodology should have wide applicability in areas where groundwater-wetland interaction is of sufficient magnitude to influence the temperature distribution of the shallow groundwater system and in areas where there is sufficient annual and/or daily temperature fluctuation. However, due to the larger data sets required, the reduced utility in multi-layer systems, and the additional uncertainty resulting from the additional thermal parameters needed to simulate the coupled system, these methods will complement rather than supersede multi-objective function calibration that uses measured heads to estimate hydraulic conductivity and flux. They are expected to be of special use in systems where flux data are not readily available.

## IX. REFERENCES

- Bravo, H.R., F. Jiang and R.J. Hunt, 2000. Using groundwater temperature data to constrain parameter estimation in a groundwater flow model of a wetland system, submitted to *Water Resources Research*.
- Doherty, J., PEST Model-Independent Parameter Estimation, Watermark Computing, Australia, 1998.
- Hunt, R.J., D.P. Krabbenhoft, and M.P. Anderson, Groundwater inflow measurements in wetland systems, *Water Resources Res.*, 32 (3), 495-507, 1996.
- Jiang, F., Calibration of model for ground water flow and heat transport in wetlands, M.S. Thesis, Univ. of Wisconsin-Milwaukee, 2000.
- Kipp, K.L., Jr., HST3D: A Computer Code for Simulation of Heat and Solute Transport in Three-Dimensional Ground Water Systems, USGS Water Resources Investigation Report 86-4095, 1987 and 97-4157, 1997.
- Lott, R.B., Estimating Evapotranspiration in Natural and constructed Groundwater Dominated Wetlands: Traditional and Geochemical Approaches, M.S. Thesis, University of Wisconsin, Madison, Wisconsin, 1997.
- Ronan, A.D., D.E. Prudick, C.E. Thodal, and J. Constantz, Field study and simulation of diurnal temperature effects on infiltration and variably saturated flow beneath an ephemeral stream, *Water Resources Research*, 34(9), 2137-2153, 1998.
- The Numerical Algorithms Group Ltd, "Computer-based documentation for the NAG Library", Oxford UK, 1999.
- Woodbury, A.D. and L. Smith, Simultaneous Inversion of Hydrogeologic and Thermal Data - 2. Incorporation of Thermal Data, *Water Resources Res.*, 24 (3), 356-372, 1988.