

Report as of FY2010 for 2009LA61B: "Bayesian Model Averaging for Saltwater Intrusion Management under Model Uncertainty"

Publications

Project 2009LA61B has resulted in no reported publications as of FY2010.

Report Follows

SYNOPSIS

Title: Bayesian Model Averaging for Saltwater Intrusion Management under Model Uncertainty

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Primary PI: Frank T.-C. Tsai

Problem and Research Objectives

Ground water is the primary source of drinking water for 61 percent of Louisiana's residents. Irrigation withdrawal is accounted for 37 percent of the total ground water withdrawal (Sargent, 2007). Ground water has been a significant factor to the continuation of Louisiana economic development. However, rapid growth in population and industry has increased ground water demand and resulted in saltwater intrusion to many freshwater aquifers (Tomaszewski, 1996). In addition, recent drought in Louisiana has escalated ground water withdrawal and accelerated the saltwater encroachment (Bohr, 2003). To protect the ground water, Louisiana legislature Act 446 (2001) declares: ground water resource is a matter of public interest. Ground water must be managed, protected, and regulated in the best interests of all the citizens of the state. Act 49 (2003) requires the ground water resource management program to meet the goal of long-term sustainability of the state's ground water aquifers and to sustain the economic welfare of the state's citizens.

For long-term economic growth, effective planning and management of ground water sustainability become an urgent task. Louisiana needs a scientific, systematic management plan to protect ground water from further saltwater intrusion without causing environmental detriment.

In this project, we propose a multimodel approach to study the groundwater head prediction under model uncertainty for the "1,500-foot" sand aquifer in the Baton Rouge area. The study area, shown in Figure 1, extends over about 300 km² and includes the major part of the Baton Rouge metropolitan area. Due to downthrow on the south side of the Baton Rouge Fault, the "1,500-foot" sand (north) connects to the "1,200-foot" sand (south). The fault acts as a conduit-barrier (Bense and Person, 2006) and allows ground water to cross the fault. South of the fault, the aquifer contains mostly saltwater, which comes from dissolved brine solution from two nearby salt domes, the St. Gabriel salt dome and Darrow salt dome (Bray and Hanor, 1990). North of the fault, the aquifers store excellent quality and quantity of water for the public and industry (Sargent, 2002). Heavy pumping has caused this aquifer to decline by as much as 90 m since the 1940s.

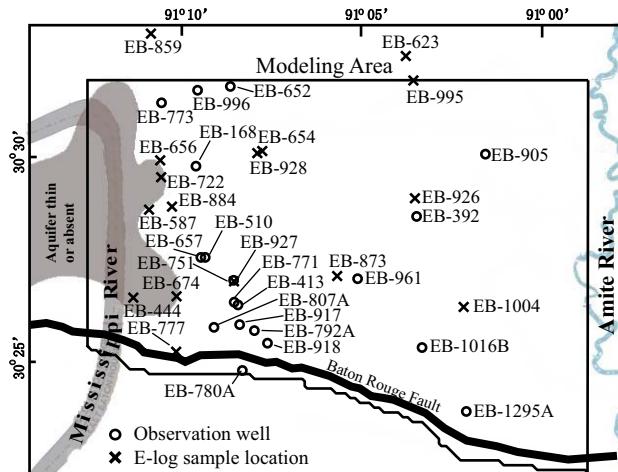


Figure 1: The “1500-foot” sand of the Baton Rouge area, Louisiana.

In the literature, the saltwater intrusion management model is commonly based on one parameterization method for distributed aquifer parameters in one simulation model. However, due to data scarcity and lack of hydrogeological information, the developed conceptual model and the chosen parameterization method are not unique. We are often overconfident in the management results from one method and one model, and neglect the impact of model uncertainty in the management decision. Detrimental results could be caused by overlooking the model uncertainty.

The goal of the project is to predict groundwater head distribution in the “1,500-foot” sand aquifer under the consideration of model uncertainty. Model uncertainty contains model structure uncertainty and model parameter uncertainty.

Objectives

To achieve the project goal, we propose the following specific objectives:

Objective 1 Develop a generalized parameterization method

The project will improve the hydraulic conductivity estimation by extending the generalized parameterization (GP) method (Tsai and Yeh, 2004; Tsai, 2006) to fuse different types of data. The GP method will be able to integrate different parameterization methods under the geostatistical framework. The conditional estimate and conditional variance of the GP method will be formulated to assess the uncertainty of the hydraulic conductivity estimation.

Objective 2 Develop a multimodel approach

The project will adopt a Bayesian model averaging (BMA) method (Draper, 1995; Hoeting et al., 1999) to integrate multiple groundwater flow models and multiple parameterization methods for prediction of groundwater head. Specifically, we will consider multiple GP methods for parameterizing the hydraulic conductivity field. We will also consider the uncertainty in boundary conditions to develop a number of ground water models.

Methodology

(1) Generalized Parameterization (GP)

A generalized parameterization (GP) method is proposed to estimate hydraulic conductivity:

$$\pi_{GP}(\mathbf{x}_0 | \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m) = \sum_{\substack{j=1 \\ j \neq k(\mathbf{x}_0)}}^m \phi_j (\pi_j - \pi_{k(\mathbf{x}_0)}) \beta_j + \pi_{k(\mathbf{x}_0)} \quad (1)$$

where β_j are the data weighting coefficients bounded between 0 and 1. The GP integrates an interpolation method and a zonation method honoring the sampled data. Consider that π is a random field in a region (Ω), the sampled data π_j are taken at locations \mathbf{x}_j , $j=1, 2, \dots, m$. The sample data π_j can be any form of hydraulic conductivity values, e.g., logarithmic values of hydraulic conductivity. Using the GP methods in equation (1), one can obtain an estimate of a zonal structure $\pi_{\text{Zonation}}(\mathbf{x}_0 | \mathbf{x}_k) = \{\pi_k | \mathbf{x}_0 \in \Omega_k\}$, a smooth distribution using an interpolation method $\pi_{\text{Interpolation}}(\mathbf{x}_0 | \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m) = \sum_{j=1}^m \phi_j \pi_j$, or a conditional estimate of a mixed distribution by considering different values of data weighting coefficients $\boldsymbol{\beta}_m = \{\beta_1, \beta_2, \dots, \beta_m\}$ to the m sample sites. In this way, the GP method greatly improves parameterization flexibility.

(2) Hydraulic Conductivity Estimation and Uncertainty using GP and Bayesian Model Averaging (BMA)

If a set of possible zonal structures $\boldsymbol{\Omega} = \{\Omega^{(1)}, \Omega^{(2)}, \dots\}$ and a set of interpolation methods $\mathbf{F} = \{\phi^{(1)}, \phi^{(2)}, \dots\}$ are considered for estimating hydraulic conductivity, combinations of many zonal structures and interpolation methods pose a multi-parameterization (multimethod) problem that involves many GP methods $\boldsymbol{\Theta} = \boldsymbol{\Omega} \times \mathbf{F} = \{\theta^{(p)}; p=1, 2, \dots\}$ to describe the hydraulic conductivity for the region. To cope with the multimethod problem, a Bayesian model averaging (BMA) approach is adopted to analyze the multiple GP methods. BMA uses the Bayes rule to assess prediction uncertainty using a set of models (Draper, 1995; Hoeting et al., 1999). Let $\Pr(\boldsymbol{\pi} | D, \boldsymbol{\Theta})$ be the conditional probability of the hydraulic conductivity given data and multiple parameterization methods. The Bayes rule (Draper, 1995) has

$$\Pr(\boldsymbol{\pi} | D, \boldsymbol{\Theta}) = \sum_p \Pr(\boldsymbol{\pi} | D, \theta^{(p)}) \Pr(\theta^{(p)} | D) \quad (2)$$

$\Pr(\boldsymbol{\pi} | D, \theta^{(p)})$ represents the conditional probability of hydraulic conductivity given data and a GP method. $\Pr(\theta^{(p)} | D)$ is the posterior probability of a GP method. According to the Bayes rule, $\Pr(\theta^{(p)} | D)$ is

$$\Pr(\theta^{(p)} | D) = \Pr(D | \theta^{(p)}) \Pr(\theta^{(p)}) / \sum_p \Pr(D | \theta^{(p)}) \Pr(\theta^{(p)}) \quad (3)$$

where $\Pr(D | \theta^{(p)})$ is the likelihood probability of a GP method. $\Pr(\theta^{(p)})$ is the prior probability of a GP method and $\sum_p \Pr(\theta^{(p)}) = 1$. One can evaluate estimation uncertainty by looking at the conditional expectation of the parameter heterogeneity $(\boldsymbol{\pi} | D, \boldsymbol{\Theta})$ (Schweppe, 1973)

$$\mathbb{E}[\boldsymbol{\pi} | D, \boldsymbol{\Theta}] = \sum_p \mathbb{E}[\boldsymbol{\pi} | D, \theta^{(p)}] \Pr(\theta^{(p)} | D) \quad (4)$$

and the conditional covariance of the parameter heterogeneity $(\boldsymbol{\pi} | D, \boldsymbol{\Theta})$

$$\begin{aligned} \text{Cov}[\boldsymbol{\pi} | D, \boldsymbol{\Theta}] &= \sum_p \text{Cov}[\boldsymbol{\pi} | D, \theta^{(p)}] \Pr(\theta^{(p)} | D) \\ &+ \sum_p \left\{ \left(\mathbb{E}[\boldsymbol{\pi} | D, \theta^{(p)}] - \mathbb{E}[\boldsymbol{\pi} | D, \boldsymbol{\Theta}] \right) \left(\mathbb{E}[\boldsymbol{\pi} | D, \theta^{(p)}] - \mathbb{E}[\boldsymbol{\pi} | D, \boldsymbol{\Theta}] \right)^T \right\} \Pr(\theta^{(p)} | D) \end{aligned} \quad (5)$$

$\mathbb{E}[\boldsymbol{\pi} | D, \theta^{(p)}]$ and $\text{Cov}[\boldsymbol{\pi} | D, \theta^{(p)}]$ are the conditional expectation and conditional covariance of hydraulic conductivity given a GP method, respectively.

(3) Groundwater Head Prediction and Uncertainty using GP and BMA

Similarly, one can determine a set of groundwater models $\mathbf{M} = \{M^{(q)}; q = 1, 2, \dots\}$ (multimodel) from limited data to interpret groundwater flow process. However, each groundwater flow model embeds uncertain hydraulic conductivity estimates, which is described by multiple GP methods. The project extends the BMA to interpret the probability of groundwater head prediction, $\Pr(\mathbf{u} | D, \boldsymbol{\Theta}, \mathbf{M})$, with multiple simulation models and multiple GP methods:

$$\Pr(\mathbf{u} | D, \boldsymbol{\Theta}, \mathbf{M}) = \sum_q \sum_p \Pr(\mathbf{u} | D, M^{(q)}, \theta^{(p)}) \Pr(\theta^{(p)} | D, M^{(q)}) \Pr(M^{(q)} | D) \quad (6)$$

$\Pr(\mathbf{u} | D, M^{(q)}, \theta^{(p)})$ is the conditional probability of groundwater head prediction given data, a simulation model and a GP method. $\Pr(\theta^{(p)} | D, M^{(q)})$ is the posterior model probability based on data and a model. By the Bayes theorem, we have

$$\Pr(\theta^{(p)} | D, M^{(q)}) = \Pr(D | \theta^{(p)}, M^{(q)}) \Pr(\theta^{(p)} | M^{(q)}) / \sum_q \Pr(D | \theta^{(p)}, M^{(q)}) \Pr(\theta^{(p)} | M^{(q)}) \quad (7)$$

where $\Pr(D | \theta^{(p)}, M^{(q)})$ is the likelihood probability of a GP method given data and a simulation model. $\Pr(\theta^{(p)} | M^{(q)})$ is the prior method probability. A prior probability subjectively depends on the modelers' belief. A method should receive higher likelihood probability $\Pr(D | \theta^{(p)}, M^{(q)})$ if it produces better results given a simulation model.

One can obtain the conditional expectation and covariance of the model output with respect to multimodel and multimethod as follows:

$$\mathbb{E}(\mathbf{u} | D, \boldsymbol{\Theta}, \mathbf{M}) = \sum_q \sum_p \mathbb{E}(\mathbf{u} | D, M^{(q)}, \theta^{(p)}) \Pr(\theta^{(p)} | D, M^{(q)}) \Pr(M^{(q)} | \theta^{(p)}) \quad (8)$$

$$\begin{aligned} \text{Cov}(\mathbf{u} | D, \boldsymbol{\Theta}, \mathbf{M}) &= \mathbb{E}_M \left\{ \mathbb{E}_\theta \left[\text{Cov}[\mathbf{u} | D, M^{(q)}, \theta^{(p)}] \right] + \text{Cov}_\theta \left[\mathbb{E}[\mathbf{u} | D, M^{(q)}, \theta^{(p)}] \right] \right\} \\ &+ \text{Cov}_M \left\{ \mathbb{E}_\theta \left[\mathbb{E}[\mathbf{u} | D, M^{(q)}, \theta^{(p)}] \right] - \mathbb{E}(\mathbf{u} | D, \boldsymbol{\Theta}, \mathbf{M}) \right\} \end{aligned} \quad (9)$$

Principal Findings and Significance (derived from Li and Tsai, WRR, 45, W09403, 2009)

(1) Head Predictions in the “1,500-foot” sand of the Baton Rouge area, Louisiana

The proposed methodology was applied to predict the groundwater heads of the “1,500-foot” sand of the Baton Rouge area in Louisiana. The “1,500-foot” sand belongs to the Evangeline equivalent aquifer system, which is part of the Southern Hills aquifer system (Griffith, 2003). It is one of the ten freshwater aquifers that were originally named according to their general depth

in the Baton Rouge industrial district (Meyer and Turcan, 1955). Precipitation originated in Mississippi is the primary source of recharge of freshwater to the aquifer system.

The study area shown in Figure 1 extends about 300 km² and includes a major part of the Baton Rouge metropolitan area. Due to throw-down at the south side of the Baton Rouge fault, the “1,500-foot” sand (north) connects to the “1,200-foot” sand (south). The Baton Rouge fault restricts northward flow of groundwater from the south of the fault; 706 observed groundwater heads were obtained from 18 head boreholes, and electrical resistivity was measured at 20 electrical logs. The pumping rates from 16 pumping wells were recorded from January 1, 1990 to December 31, 2004. Previous studies reported small variation in specific storage (Huntzinger et al., 1985; Griffith, 2003). A constant specific storage, 2.2×10^{-5} m⁻¹ is considered for the “1,500-foot” sand. A time-varied constant head boundary condition was applied to all boundaries of the study area (Figure 1). This study adopted the groundwater model developed by Tsai and Li (2008). The head variances range between 0.2126 and 237 m².

The Baton Rouge fault is rarely surveyed in this area and it can form pathways that connect aquifers at different depths due to the orientation and mode of fractures (Anderson and Fairley, 2008). Hydraulic anisotropy in the fault can result from a variety of mechanisms, including clay-smearing, drag of sand, grain re-orientation, and vertical segmentation of the fault plane (Bense and Person, 2006). Many studies (Chester et al., 1993; Bredehoeft, 1997; Salve and Oldenburg, 2001; Fairley et al., 2003) have been conducted to understand permeability in and near the fault zone and have shown that determination of the fault permeability still remains a formidable task. For the purpose of methodology implementation, the Baton Rouge fault is considered to be isotropic and homogeneous, where the hydraulic characteristic of the Baton Rouge fault was estimated to be 5.19×10^{-4} /day (Tsai and Li, 2008). Because the true HC value of the Baton Rouge fault is unknown, we consider three groundwater model structures: the impermeable-fault model M⁽¹⁾ with HC=0/day, the low-permeable-fault model M⁽²⁾ with HC= 5.19×10^{-4} /day, and the no-fault model M⁽³⁾ with HC= 9×10^5 /day. The very high HC value ensures no influence on flows crossing the horizontal flow barriers for the no-fault model.

To estimate the hydraulic conductivity distribution from the 20 resistivity data, the Archie law (Archie 1942) was adopted to interpret the formation factor into porosity. Typically, the pore geometry coefficient varies between 0.62 and 2.45, and the value of cementation factor has a range between 1.08 and 2.15, depending on the formation. By fitting to the observation data, the pore geometry coefficient and the cementation factor for the “1,500-foot” sand were estimated at 0.8 and 2.04, respectively. The effective grain size is 0.22 mm (Meyer and Turcan, 1955) and the groundwater temperature is 30^oC. The same seven grain-size based methods in Tsai and Li (2008) were used to convert porosity into hydraulic conductivity. The generalized parameterization (GP) that combines the Voronoi tessellation (VT) and the ordinary kriging (OK) was adopted to obtain the hydraulic conductivity distribution. A variance window with a scaling factor $\alpha = 0.08$ was applied, where $s_1 = 6$, $s_2 = 2$, and $\sigma_D = 37.6$.

(2) BMA Results

The BMA was applied to each groundwater model, where the averaged head values over the seven estimation methods were obtained. The datum of the groundwater heads is NGVD 29. The

regression coefficient of the low-permeable-fault model ($R^2=0.9033$) is slightly better than that of impermeable-fault model ($R^2=0.8916$). The no-fault model ($R^2=0.2038$) does not fit the observed data well. The no-fault model should not be considered because it cannot produce groundwater heads close to the observed heads. Using the variance window, the impermeable-fault model has a weight of 32.99% and the low-permeable-fault model has a weight of 67.01%. This indicates that the fault permeability is low. Both models favor the Kozeny-Carman method and the Sauerbrei method. The best combination is the Kozeny-Carman method with the low-permeable-fault model, which has a combined weight of 38.20%. The Kruger method and the Zunker method gain very small weights in the impermeable-fault model (1.61% and 1.51%, respectively) and slightly higher weights in the low-permeable fault model (6.29% and 7.38%, respectively). The Slichter method, the Terzaghi method, and the Zamarin method gain zero weight in both groundwater models.

Comparisons of calculated heads against the observed heads at EB-918, using the seven methods and BMA over methods in the low-permeable-fault model, are made. The Slichter method, the Terzaghi method, and the Zamarin method are far from one standard deviation from the BMA estimation. This demonstrates that the variance window is a valid model selection criterion for the purpose of BMA. Head uncertainty using the BMA is higher than individual methods for EB-918 at the observation space. This is because the BMA additionally considers the between-method variance and between-model variances. Using a single method may underestimate uncertainty. We also want to emphasize that due to intrinsic characteristics in individual methods, the best method may not necessarily have the smallest estimated head standard deviations. The Slichter method has a zero method weight, but has lower head standard deviations than the Kozeny-Carman method. Our point is that the estimated head standard deviation is a measure of uncertainty based on the selected method, but is not a measure of estimation accuracy for the method. Moreover, the head standard deviations increase over time because the parameter uncertainty propagates and accumulates to increase the head uncertainty.

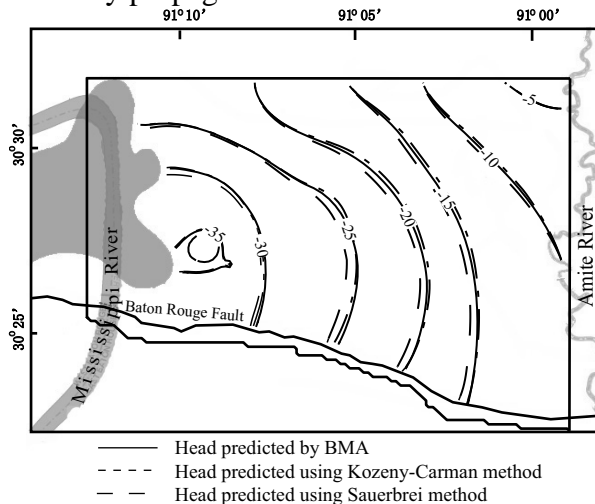


Figure 2: Comparisons of head prediction on 31 December 2019 by the BMA over models and methods and by the low-permeable-fault model with the Kozeny-Carman method and the Sauerbrei method.

Without the BMA analysis, one may conclude that the head uncertainty based on a wide range of methods is much larger than that from individual methods. This confirms the observation in Carrera and Neuman (1986) that the uncertainty from estimation method selection is much larger

than the uncertainty from parameter estimation. However, with the BMA analysis, the head uncertainty due to method uncertainty is similar to that of individual methods.

(3) Head Predictions and Uncertainty with Multimodel and Multimethod

The groundwater heads for the next 15 years (from 1/1/2005 to 12/31/2019) were predicted by keeping the same head boundary conditions at the last stress period (December 2004). The time-varied monthly pumping rates were fixed to the average pumping rates of the last three years (2002-2004). Figure 2 shows the head prediction on 12/31/2019 using the BMA with the variance window against the head predictions using the low-permeable model with the Kozeny-Carman method and with the Sauerbrei method.

The BMA prediction variance of heads includes the within variance (Figure 3a), the between-method variance (Figure 3b), and the between-model variance (Figure 3c). The total BMA variance shown in Figure 3d is the sum of these three variances. Although calculated heads can be significantly different when using different simulation models and estimation methods, the between-method and between-model head prediction variances are fairly small, and the within variance dominates the total BMA prediction variance. The small between-method variance arises from the high method weight of the Kozeny-Carman method, which has a weight of 73.48% in the impermeable-fault model and 57.01% in the low-permeable-fault model. However, the low-permeable fault model, with 67.01% of the total model weight, does not dominate. Hence, the small between-model variance indicates similar head predictions by the two groundwater models.

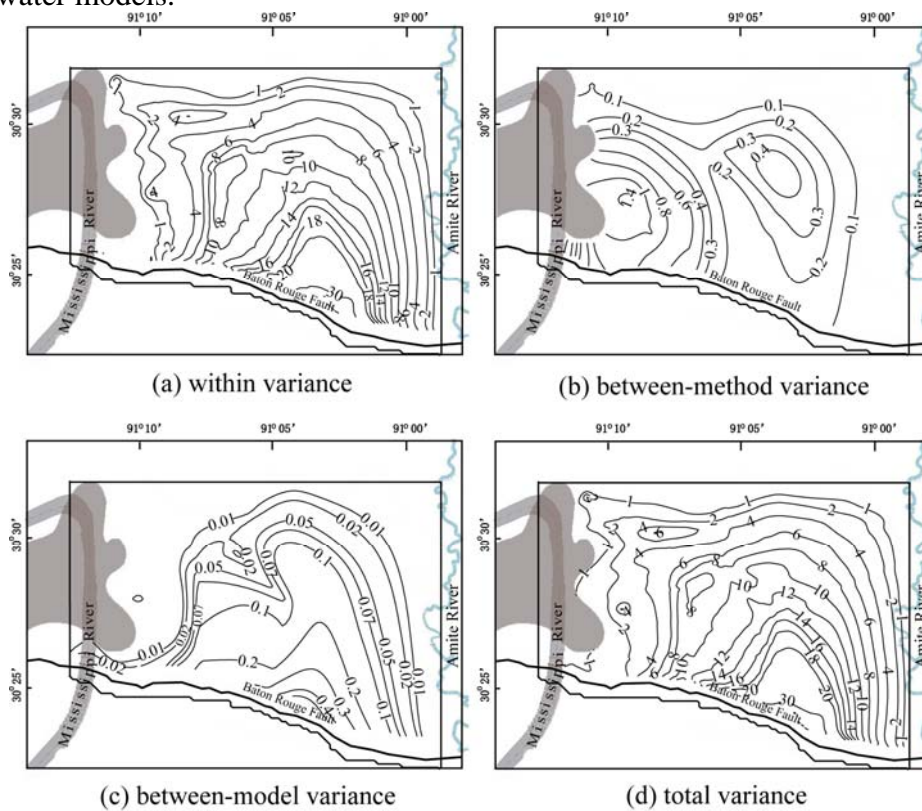


Figure 3: Head prediction variance (m^2) distributions: (a) within variance, (b) between-method variance, (3) between-model variance, and (d) total variance.

We note that small between-model variance does not suggest unimportance of the hydraulic characteristic of the fault to head predictions. It cannot be used to judge the sensitivity of faults to groundwater heads. Small between-model variance simply indicates that good models produce similar predictions close to the expectation of the BMA predictions. Bad models have very little influence on the head prediction because their model weights are very small while head predictions of bad models are far from the expectation of the BMA predictions. There is no direct implication that the hydraulic characteristic of the fault is relatively unimportant to head predictions.

The within variance overwhelms the between-model and between-method variances, indicating large uncertainty propagation from hydraulic conductivity estimation to head prediction. Specially, the head prediction variance at the southeast area is large because of less hydraulic conductivity samples and head observation data. To reduce head prediction uncertainty, future sampling on hydraulic conductivity and groundwater head in these areas is necessary. Moreover, large head prediction variance near the fault indicates the need for a better understanding of the fault characteristics.

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Publications

1. Articles in Refereed Scientific Journals

- Tubbs, K. R., and F. T.-C. Tsai. (2010). GPU Accelerated Lattice Boltzmann Model for Shallow Water Flow and Mass Transport, *International Journal for Numerical Methods in Engineering*, DOI: 10.1002/nme.3066.
- Tsai, F. T.-C. and X. Li. (2010). Reply to Comment on "Inverse Groundwater Modeling for Hydraulic Conductivity Estimation Using Bayesian Model Averaging and Variance Window" by Ye, M., D. Liu, S.P. Neuman, and P.D. Meyer, *Water Resources Research*. doi:10.1029/2009WR008591.
- Servan-Camas, B., and F. T.-C. Tsai. (2010). Two-Relaxation-Time Lattice Boltzmann Method for Anisotropic Dispersive Henry Problem. *Water Resources Research*. doi:10.1029/2009WR007837.
- Tubbs, K. R., and F. T.-C. Tsai (2009). Multilayer Shallow Water Flow using Lattice Boltzmann Model with High Performance Computing. *Advances in Water Resources*, 32(11), 1767-1776.
- Li, X., and F. T.-C. Tsai.(2009). Bayesian Model Averaging for Groundwater Head Prediction and Uncertainty Analysis Using Multimodel and Multimethod. *Water Resources Research*, 45, W09403. doi:10.1029/2008WR007488.

2. Book Chapter

- Tsai, F. T.-C. and W. W-G. Yeh. (2010). Chapter 7: Model Calibration and Parameter Structure Identification in Characterization of Ground Water Systems, in Ground Water Management Manual (M. Aral and S. Taylor ed.) American Society of Civil Engineers. Accepted.

3. Dissertations

- Kevin R. Tubbs, 2010, Ph.D. Dissertation “Lattice Boltzmann Modeling for Shallow Water Equations Using High Performance Computing, Engineering Science Program, College of Engineering, Louisiana State University, Baton Rouge, Louisiana, 128 pages.

4. Water Resources Research Institute Reports

- Frank Tsai, 2009, Saltwater Intrusion Management with Conjunctive Use of Surface Water and Ground Water, Louisiana Water Resources Research Institute, Louisiana State University, Baton Rouge, Louisiana, 10 pages. (USGS 104G)
- Frank Tsai, 2009, Electrical Resistivity Tomography (ERT) Laboratory Experiments on Saltwater Encroachment Tracking and Modeling in Saturated Heterogeneous Sediment, Louisiana Water Resources Research Institute, Louisiana State University, Baton Rouge, Louisiana, 10 pages. (USGS 104B)

5. Conference Proceedings

- Tsai, F. T.-C. (2010). A Co-Generalized Parameterization Method for Hydraulic Conductivity Estimation, World Water & Environmental Resources Congress, Providence, Rhode Island, May 16-20, 2010.
- Tsai, F. T.-C. (2010). Multimodel Approach for Groundwater Model Calibration, Prediction, and Application, World Water & Environmental Resources Congress, Providence, Rhode Island, May 16-20, 2010. (invited)

6. Other Publications (Abstract/Presentations)

- Tsai, F. T.-C. (2010). Data Fusion using Co-Generalized Parameterization: Hydraulic Conductivity Estimation, 2010 Western Pacific Geophysics Meeting, 22–25 June 2010, Taipei, Taiwan
- Tsai, F. T.-C. (2010). Hierarchical Bayesian Model Averaging for Groundwater Multimodel Prediction and Management under Uncertainty, 2010 Western Pacific Geophysics Meeting, 22–25 June 2010, Taipei, Taiwan
- Tsai, F. T.-C. (2010). A Co-Generalized Parameterization Method for Hydraulic Conductivity Estimation, World Water & Environmental Resources Congress, Providence, Rhode Island, May 16-20, 2010.
- Tsai, F. T.-C. (2010). Multimodel Approach for Groundwater Model Calibration, Prediction, and Application, World Water & Environmental Resources Congress, Providence, Rhode Island, May 16-20, 2010. (invited)

7. Student Support

- Kevin R. Tubbs, PhD, Spring 2010 (Graduated)