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Model Structure Identification in Three Dimensions and Observation Design in Groundwater Modeling

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13. ABSTRACT (Maximum 200 words)

We have developed a methodology for optimal observation network design for parameter structure identification in groundwater modeling. The design objective is to minimize experimental cost subject to data sufficiency requirement. By incorporating the data sufficiency requirement as a constraint in the optimization model, the methodology quantitatively unifies observation network design, model structure identification and model application reliability. We use a geostatistical simulation method to generate realizations for the real parameter field according to the available prior information. For each realization, we search for the minimum cost design that satisfies the data sufficiency requirement. After solving the design problems for each of the realizations, we then analyze the overall results. Additionally, we combine the adjoint state method with MODFLOW for calculating sensitivity coefficients. For the remainder of the project, we will explore the possibility of generalizing the adjoint method for MODFLOW.

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Final Progress Report

1. Statement of the Problem Studied

The major objectives of this project are: (1) to develop a generalized parameterization method in three dimensions for the generalized inverse problem, (2) to build the theoretical basis for model structure identifiability, and (3) to develop a new methodology for observation network design that unifies model structure complexity, parameter identifiability and model application reliability.

2. Summary of the most important results

We have developed two global-local optimization methods for three-dimensional parameter structure identification in groundwater modeling. Parameter structure identification is formulated in terms of solving a generalized inverse problem (GIP), which allows for a determination of an appropriate level of parameter structure complexity, and the identification of its pattern and the associated parameter values. The structure complexity is determined by calculating the parameter structure error measured in the prediction space or management space, while the structure pattern and the associated parameter values are identified simultaneously by minimizing the fitting residual measured in the observation space. The former requires solving a continuous max-min optimization problem, and the latter requires solving a combinatorial optimization problem. The validity and applicability of the proposed methodology are demonstrated by numerical experiments. We have shown that the choice of an objective function in model application impacts the determination of the parameter structure complexity.

Additionally, we have developed a methodology for optimal observation network design for parameter structure identification in groundwater modeling. The design objective is to find the minimum cost design that can provide sufficient information for parameter structure identification. By incorporating the sufficiency requirement as a constraint in the optimization model, the proposed methodology quantitatively unifies observation network design, model structure identification and model application reliability. We use sequential Gaussian simulation to generate a large set of realizations which are used to represent the true parameter field. For each realization, we search for the minimum cost design that satisfies the data sufficiency requirement. After solving the design problems for each of the realizations, we analyze the overall results. We calculate the average model application errors for different parameter structures, the probability that the model application error takes on a value that is less than the specified accuracy requirement, the minimum number of wells required for the specified parameter structure, and the priority of the well locations. We also analyze the reliability of providing sufficient data for each given cost. The proposed methodology provides stochastic solutions for the decision-makers as a reference for the observation design. The decision-makers can specify different accuracy and reliability requirements and find the trade-off between the requirements and the design cost. The proposed methodology can provide a more

flexible and robust solution than the traditional design methods.

3. List of Publications

a. Journal Papers

Sun, N-Z., "Modeling Biodegradation Process in Porous Media by the Finite Cell Method," *Water Resources Research*, 38 (3): Art. No. 1029, 2002. (Joint funding with NSF)

Tsai, F. T-C., N-Z. Sun, and W. W-G. Yeh, "Global-Local Optimization for Parameter Structure Identification in Three-Dimensional Groundwater Modeling," *Water Resources Research,* 39(2), 1043, doi:10.1029/2001 WR001135, 2003. (Joint funding with NSF)

Tsai, F. T-C., N-Z. Sun and W. W-G. Yeh, "A Combinatorial Optimization Scheme for Parameter Structure Identification in Ground-Water Modeling," *Ground Water*, 41(2): 156-169, 2003. (Joint funding with NSF)

Tsai, F. T-C. and W. W-G. Yeh, "Characterization and Identification of Aquifer Heterogeneity with Generalized Parameterization and Bayesian Estimation," to appear in *Water Resources Research*, 2004. (Joint funding with NSF)

b. Conference Proceeding Papers

Tsai, F. T-C., N-Z. Sun, and W. W-G. Yeh, "A Combinatorial Optimization Scheme for Parameter Structure Identification in Ground-Water Modeling," *MODFLOW 2001 and Other Modeling Odysseys Conference Proceedings*, Vol.(I), 123-129, Golden, Colorado, Sep.11-14, 2001. (Joint funding with NSF)

Sun, N-Z., F. T-C. Tsai, and W. W-G. Yeh, "Parameter Structure Identifiability and Experimental Design in Groundwater Modeling", *Proceedings of the 4th International Conference on Inverse Problems in Engineering*, Angra dos Reis, Rio de Janeiro, Brazil, May 2002, pp. 37-48. (Joint funding with NSF)

Tsai, F.T-C., N-Z. Sun, and W.W-G. Yeh, "Parameter Structure Identification in Groundwater Modeling: A Universal Parameterization Method", *Proceedings of the EWRI World Water & Environmental Resources Congress*, Philadelphia, Pennsylvania, June 23-26, 2003, 10 pgs (CD-Rom). (Joint funding with NSF)

c. Conference Presentations

Yeh, W. W-G., "The Future of the Utility of Groundwater Models for Water Resources Management," An Invited Frontier Lecture, Presented at the *American Geophysical Union, Fall Meeting*, San Francisco, CA, December 8-12, 2003. (Joint funding with NSF)

Chang L-F., N-Z. Sun, and W. W-G. Yeh, "Optimal Observation Network Design for Parameter Structure Identification in Groundwater Modeling," *American Geophysical Union, Fall Meeting*, San Francisco, CA, December 8-12, 2003. (Joint funding with NSF)

d. Manuscript Submitted

Tsai, F. T-C., N-Z. Sun and W. W-G. Yeh, "Geophysical Parameterization and Parameter Structure Identification Using Natural Neighbors in Groundwater Inverse Problems," submitted to *Journal of Hydrology*, 2003. (Joint funding with NSF)

Chang, L-F., N-Z. Sun and W. W-G. Yeh, "Optimal Observation Network Design for Parameter Structure Identification in Groundwater Modeling," submitted to *Water Resources Research*, 2004. (Joint funding with NSF)

4. List of Participating Scientific Personnel

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