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Yangtze is the first longest river in China and the third in the world, with its main channel length of 6,300 km and a drainage area of 1,800,000 km2. The Yangtze river basin includes large urban areas and significant croplands which play important and critical roles in China's economy and the health of the ecological environment. There are many notable projects associated with the Yangtze river basin, such as the Three-Gorge Dam project, and the water transferring project from south to north. Understanding of the natural terrestrial hydrological processes over the Yangtze river basin and the interactions between land surface and atmosphere, and the impact of the Three-gorge Dam project on its ecological environment is critical and challenging. As the first step in our effort of simulating the terrestrial hydrological process for the entire Yangtze river basin, a spatially distributed Three-Layer Variable Infiltration Capacity (VIC-3L) hydrological model is applied to a watershed called Baohe river watershed with a drainage area of 2500 km2 within the Yangtze river basin. Water fluxes of this watershed are simulated using VIC-3L at a spatial resolution of about 1 km. The soil properties and vegetation information from The Landuse and Landover Database of China at 1km Spatial Resolution for the study watershed are based on the spatial distribution patterns of vegetation, land cover, and soil type at 1km spatial resolutions. The meteorological information (i.e., precipitation, wind, air temperature) is obtained from meteorological measurement and is interpolated into each grid cell by Gauss weight method. The VIC-3L model is running on daily time step. A reservoir routing scheme together with river network routing is coupled with the VIC-3L model to simulate the streamflows. Simulation results are tested using daily streamflow measurements from the hydrologic station at the outlet of Baohe basin, Jinagkou in the Shaanxi province, China, from 1992 to 2001. Analyses of the water fluxes for the watershed will be discussed.

H11I MCC: 3024 Monday 1020h

Optimization for Model Calibration and Management in Water Resources II *(joint with NG)*

Presiding: **C A Shoemaker,** Cornell University**; S Sorooshian,** University of California, Irvine

H11I-01 1020h

A Self-Adaptive Hybrid Genetic Algorithm for Optimal Groundwater Remediation Design

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Identifying optimal designs for a groundwater remediation system is computationally intensive, especially for complex, nonlinear problems such as enhanced in situ bioremediation technology. To improve performance, we apply a hybrid genetic algorithm (HGA), which is a two-step solution method: a genetic algorithm (GA) for global search using the entire population and then a local search (LS) to improve search speed for only a few individuals in the population. The inclusion of local search helps to speed up the solution process and to make the solution technique more robust. The result of this research is a highly reliable numerical tool, the enhanced self-adaptive hybrid genetic algorithm (e-SAHGA) to more efficiently and effectively solve problems using simple genetic algorithms (SGAs). With this tool, the designer can evaluate different solution alternatives in a more timely fashion. The application of the eSAHGA algorithm to a hypothetical groundwater remediation design problem showed 90% reliability in identifying the solution faster than the SGA, with average savings of 64% across 100 runs with different random initial populations. Finally, e-SAHGA was tested on a field-scale remediation design problem, re-evaluation of the remediation system for Umatilla Army Depot, by means of a domain decomposition approach. In this approach, well locations are identified first and then pumping rates are identified subsequently in separate GA runs. The domain decomposition approach was shown to be much faster than the full solution approach with no loss in accuracy of the final solution for this problem, with computational savings between 30% and 60%.

H11I-02 1035h

Uncertainty-Based Multi-Objective Optimization of Groundwater Remediation Design

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Management of groundwater contamination is a cost-intensive undertaking filled with conflicting objectives and substantial uncertainty. A critical source of this uncertainty in groundwater remediation design problems comes from the hydraulic conductivity values for the aquifer, upon which the prediction of flow and transport of contaminants are dependent. For a remediation solution to be reliable in practice it is important that it is robust over the potential error in the model predictions. This work focuses on incorporating such uncertainty within a multi-objective optimization framework, to get reliable as well as Pareto optimal solutions. Previous research has shown that small amounts of sampling within a single-objective genetic algorithm can produce highly reliable solutions. However with multiple objectives the noise can interfere with the basic operations of a multi-objective solver, such as determining non-domination of individuals, diversity preservation, and elitism. This work proposes several approaches to improve the performance of noisy multi-objective solvers. These include a simple averaging approach, taking samples across the population (which we call extended averaging), and a stochastic optimization approach. All the approaches are tested on standard multi-objective benchmark problems and a hypothetical groundwater remediation case-study; the best-performing approach is then tested on a field-scale case at Umatilla Army Depot.

H11I-03 1050h

Identification of Spatially Distributed Soil Hydraulic Properties in Hydrologic Modeling Using Global Optimization

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In the past few years, computational capabilities have evolved to a point, where it is possible to use multi-dimensional physically based hydrologic models to study spatial and temporal patterns of water flow in the vadose zone. However, so far these models based on complex multi-dimensional governing equations have only received very limited attention, in particular because of their computational, distributed input and parameter estimation requirements. The aim of the present paper is to explore the usefulness and applicability of the inverse method to estimate spatially distributed soil hydraulic properties using the solution of a physically-based three-dimensional distributed model combined with spatially distributed measured tile drainage data from the 4000 ha BWD (BWD) in the San Joaquin Valley of California. The inverse problem is posed within a single criterion Bayesian framework and solved by means of the computerized Shuffled Complex Evolution Metropolis (SCEM-UA) global optimization algorithm. To study the benefits of using a complex spatially distributed three-dimensional vadose zone model, the results of the 3D model were compared with those obtained using a simple conceptual bucket model and a spatially-averaged one-dimensional unsaturated water flow model. District-wide results demonstrate that measured spatially distributed patterns of drainage data contain only limited information towards the identification of the vadose zone model parameters, and are particularly inadequate to identify the soil hydraulic properties. In contrast, the drain conductance, and a bypass coefficient were highly identifiable, indicating that the dominant hydrology of the BWD was determined by drain system properties and preferential flow. Despite the significant CPU time needed for model calibration, results indicate that there are advantages of using physically-based hydrologic models to study spatial and temporal patterns of water flow at the scale of a watershed, as these models not only generate consistent forecasts of spatially-distributed drainage data during the calibration and validation period, but also possess unbiased predictive capabilities of measured groundwater table depths not included in the calibration.

H11I-04 1105h

A Polygonal Cells Approach for Optimal Selection of Monitoring Wells

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This study concerns the concept, methodology, and application of an optimal strategy for groundwater contamination monitoring. The research objective is to develop a robust technique for accurately and quickly monitoring and locating the contaminant sources and plumes in a comparatively large contaminated area. The monitoring plan incorporates cycles of sampling. In each cycle the decision variables are wells selected for sampling, where the number of sampled wells at each cycle is the primary constraint. The proposed methodology approaches this optimization problem by dividing the site into area cells, and sampling a representing well within each cell, within each cycle. A Utility Function (UF) is defined for each point in the aquifer. The integral of the UF over a specific area results in a Density Utility Function (DUF) that quantifies the utility of sampling in that area. A Genetic Algorithm (GA) then divides the aquifer into area cells whose DUF's are uniformly distributed as much as possible, and whose number is equal to the number of samples available in each cycle. Exemplifying applications of the proposed methodology have shown to achieve smaller errors, which gradually decrease at each sampling cycle and thus higher efficiency of the well sampling is obtained, in comparison with other contamination monitoring algorithms.

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H11I-05 1120h

Inverse Problem and Management Applications in Groundwater Modeling: Equivalent Model Sets and Data Sufficiency Evaluation

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Inverse modeling is a powerful tool for calibrating complex distributed groundwater models. Traditionally, the inverse problem has been formulated as finding the parameter values that minimize a measure of the difference between model output and observed field data. Additionally, the process has been extended to include the influence of model structure error. A calibrated model, however, can be no better than the available data used in the parameter estimation process. Likewise, the fitness criteria adopted in model calibration can influence the decision of whether or not to accept a simulation model for management applications. This research aims at developing a methodology that combines management application and inverse modeling to assess the existence of a family or a set of equivalent groundwater flow simulation models. The definition of such a family is prescribed on uncertainty tolerance requirements applied in the parameter and management spaces. The parameter space is defined as the set of admissible parameter values, plus initial and boundary conditions. The management space is the set of management policies that is expected to satisfy a group of planning objectives. Multiobjective optimization and first-order approximation analysis are linked to evaluate the influence of parameter uncertainty over the set of non-inferior solutions that provides a starting point for decision-making in groundwater management.

By comparing the robustness of a given model in the observation space as well as in the management space, the need of additional data for calibration is assessed.

H11I-06 1135h

Hydrogeological characterization of sedimentary rocks with numerical inversion using steady-state hydraulic head data

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In the hydrogeological characterization of sedimentary rocks, hydraulic properties of fault and cap rock structures are important factors. Although, the certainty of a hydrogeological model depends on the amount of geological or hydrogeological data, mainly obtained from boreholes, it is indispensable to make a preliminary model from a small amount of data obtained in the early stage of field investigation, and improve the details of the model as the number of observations increases. In sedimentary rocks, several aquifers often have different hydraulic heads, caused by various reasons such as surface topography, long-term change of sea level, or cap rock structures that were not explicitly observed during geological investigations in boreholes. In this study, we used the steady-state hydraulic head distribution obtained in the pressure monitoring (or the water level monitoring) during the drilling of boreholes as the observed data, and applied numerical inversion code iTOUGH2 to construct alternative hydrogeological models for the Horonobe underground research laboratory site of Japan Nuclear Cycle Development Institute. We applied random sampling for the coverage of an assumed cap rock, and two models for the hydrogeological structure of faults in the study area. The following are the main results of this study. 1. It is necessary to assume a low permeability cap rock structure that was not clearly observed in boreholes, to reconstruct the deep high-pressure zone as a characteristic hydraulic feature in this site. 2. The numerical inversion with random sampling of cap rock shows that if the cap rock coverage is larger than 75%, the observed hydraulic head profile can be reproduced. 3. The hydrogeological structure of the fault dominates the vertical groundwater flow in the vicinity of the fault. 4. The hydraulic head profile of the deeper zone is controlled by the hydrogeological structure of a steep fault in this area. Thus, the increase of hydraulic head in the deeper zone, and numerical inversion can determine the hydrogeological structure of the fault. From these results, numerical inversion using the steady state head distribution has proven to be a useful method to construct a preliminary but quantitative hydrogeological model from a small amount of data obtained in the early investigation stage.

H11I-07 1150h

Parameter estimation via risk-based optimization

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Most hydrologic systems are inherently heterogeneous and are characterized by parameters that can be sampled at a few selected locations. Yet, numerical simulations of system behavior require that the system parameters be specified at every point of a computational domain. Traditionally, this is done by means of statistical interpolation schemes, such as kriging, that produce the system parameter fields that are much smoother than their true counterparts. This yields predictions of the system states that provide little, if any, insight into the likelihood of a system failure (the so-called rare events). This problem arises in a variety of applications that range from flood prediction, to contaminant transport in groundwater, to oil and gas extraction or water supply. To resolve this issue, we present a new paradigm for parameter estimation. It is based on risk-based optimization, thus providing decision-makers with best and worst case scenarios of the system behavior.

H11I-08 1205h

A Coupled Zonation-Kriging Method for Parameter Structure Identification in Groundwater Modeling: A Case Study of a Seawater Intrusion Problem, the Alamitos Barrier in Southern California Coastal Plain

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In this research, we propose a coupled zonation-kriging method for parameter heterogeneity characterization as well as parameter structure identification. With a set of distinct point measurements over a field, on one hand, a zonation structure for the field can be created based on a Voronoi tessellation method. Each Voronoi cell contains one sampled point and has the corresponding measured value. On the other hand, a kriging method can be used to characterize a continuous parameter distribution. In this study, we only use local information for the kriging method to estimate the parameter value at an unsampled site. First, we apply Voronoi tessellation and Delaunay triangulation to define a set of natural neighbors among the sampled points for an unsampled site. Each site has its unique natural neighbors. Then the kriging method uses the local information provided from these natural neighbors for the estimation. This is called the natural neighbor kriging (NNK) method. We combine the zonation method and the NNK method together as one parameterization method by introducing a set of weighting coefficients to the measurement points. The zonation-NNK method unifies zonation and kriging methods and generates a distribution between a pure zone structure and a continuous structure over a set of weighting coefficients. It shows greater flexibility in manipulating spatial distribution and spatial optimization. When a non-smooth field is investigated, the zonation-NNK outperforms all other parameterization schemes. For the inverse problem, we identify parameter heterogeneity with the zonation-NNK method by seeking the optimal weighting coefficients while minimizing the fitting residual of observations. We demonstrate the developed methodology by a case study of the Alamitos barrier for the seawater intrusion problem in Southern California Coastal Plain. The unknown distributed parameter is the hydraulic conductivity of five aquifers. We adopted the FEMWATER as a model to simulate the density-dependent coupled flow and transport in the coastal aquifers. For the given set of head and salinity concentration observations, we have identified the hydraulic conductivity field in three dimensions.

H12A MCC: Level 2 Monday 1330h

Model Calibration, Parameter Nonuniqueness, and Predictive Uncertainty Associated With Flow and Transport in Variably Saturated Media Posters

Presiding: **J A Tindall,** U.S. Geological Survey; **M J Friedel,** U.S. Geological Survey

H12A-0957 1330h POSTER

Inverse Calibration of the Dual-Permeability Model MACRO: Theoretical Analysis and Application to Microlysimeter Experiments.

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Macropore flow is a key factor for determining chemical transport in unsaturated soils, but the description of the complex processes involved in macropore flow requires several parameters that cannot be easily measured. Inverse modeling procedures are increasingly used for model calibration, because they are objective and reproducible. But this is only true when the problem is well-posed: an ill-posed problem leads to parameter nonuniqueness, and thus contributes to poor model performance, like error and/or uncertainty in model predictions. Factors linked to nonuniqueness are most often related to sensitivity issues and/or correlation among two or several parameters. This study focused on the use of inverse techniques to estimate parameters controlling macropore flow, transport, and transformation processes in the dual porosity/dual-permeability model of water flow and solute transport MACRO. MACRO was used together with the inverse modeling package SUFI. The Bayesian (global) approach followed by SUFI is stable, converging, and robust. Moreover, the procedure also predicts a posterior uncertainty domain for the estimated parameters. A theoretical study was carried out to test the inverse modeling tool SUFI/MACRO. Generated "dummy" data set were used for this purpose, representing transient leaching experiment for tracers and reactive solutes in small soil columns (20 cm height). General issues related to inverse modeling such as internal correlation and sensitivity were investigated, with the help of response surface analysis, as well as the influence of the choice of the goal function used in the inverse procedure. Attention was also focused on the most appropriate experimental design necessary for a reliable parameter estimation. The procedure was then applied to real data, obtained from tracer leaching experiments carried out on microlysimeters. Based on calculated model efficiencies, MACRO/SUFI gave good predictions of water movement and tracer transport. This is an encouraging first step prior to application against real data on reactive transport.

H12A-0958 1330h POSTER

Multiscale Heterogeneity and Solute Transport Model Parameter Uncertainty Study for a Fractured Low-Level Nuclear Waste Disposal Site in the Eastern United States

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The objective of this research is to determine multiscale fluid and solute transport parameters in support of a site characterization effort at the Waste Area Grouping 5 (WAG 5) at ORNL (Oak Ridge National Laboratory) in eastern Tennessee, USA. The study site is located within the top 10 m of the subsurface, in which groundwater flow dynamics is influenced by both infiltration and recharge events. The soil and rock formations are macroporous and/or highly fractured at WAG 5. A natural gradient, multiple tracer injection experiment (bromide, helium and neon), was conducted to quantify the solute transport and mass transfer processes in the highly fractured shale bedrock. The field site is intensively instrumented with arrays of drive point and multi-level sampling wells. Field observations of hydraulic head and bromide solute movement dynamics are used in this study to calibrate a two-pore-domain, fracture-matrix flow and non-reactive solute transport model. We use a nested Latin hypercube (NLH) sampling technique to determine the near-optimal combinations of model parameters. As a result of the sampling technique, empirical probability distributions of model parameters are derived. Heterogeneity in two scales, field and matrix block, are quantified in terms of field scale distribution of hydraulic and solute transport properties and fracture spacing between matrix blocks. Uncertainties arising from tracer source density effect are also addressed through model prediction uncertainty analysis. It is also concluded that NLH is a relatively effective optimization technique, often capable of locating the near-optimal combination of model parameters in a few iterations.

H12A-0959 1330h POSTER

Soil Hydraulic Property Uniqueness as Determined From Inverse Modeling Using Surface Temperature : the Role of Soil Type

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