

## H52B-0891 1330h POSTER

## Constant Capacitance Model Prediction of Boron Speciation for Varying Soil Water Content

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The aqueous speciation of boron and its partitioning to a tetrahedral surface species ( $\text{SH}_3\text{BO}_4^-$ ) were studied using the constant capacitance model. Aqueous B species were boric acid ( $\text{H}_3\text{BO}_3$ ) and the borate anion  $\text{B}(\text{OH})_4^-$ . Adsorption of B on clay minerals is pH-dependent with  $\text{SH}_3\text{BO}_4^-$  increasing with increasing pH in the range 7-9. Modeling of equilibrium among the B species in a drying soil thus requires that the pH be computed. We calculated equilibrium among major cations and anions for hypothetical soil solution chemistries using a matrix-based numerical solution that included cation exchange reactions and dissolution/precipitation of calcite. Numerical experiments were performed for 20 hypothetical soil textures with 10-60% clay content, generating a range of cation exchange capacities, and three soil solution compositions. The effective  $K_d$  ( $\text{SH}_3\text{BO}_4^-/\text{total solution B}$ ) decreased with gravimetric water content ( $\theta_g$ ) over the range  $\theta_g=1.5$  to 0.01. This was due to a calculated decrease in  $[\text{H}^+]$  concentration with decreasing  $\theta_g$  for all soil textures and fluid compositions. A decrease in  $\text{SH}_3\text{BO}_4^-$  is consistent with experimental work showing decreasing fractional adsorbed B with decreasing pH in the range 7-9. An application of this type of calculation would be prediction of adsorbed and solution B concentrations at field water content based on experimental determinations of adsorbed and solution B concentration for saturated paste extracts. Such predictions would be useful for generating initial conditions for solute transport modeling and for determining whether solution B concentrations at field water contents would be beneficial or harmful to plants.

## H52B-0892 1330h POSTER

## Heating Unsaturated Sediments Using Solar Energy to Enhance Passive Sediment Remediation Technologies

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Sediment heating has been shown to enhance passive sediment remediation technologies such as bioremediation and barometric pumping (passive soil venting). Sediment heating raises the slow remediation rates that often limit the widespread use of these technologies. In bioremediation applications, a 10 degree C increase in subsurface temperature is expected to double the microbial activity, and thus the remediation rate. The removal rate of tetrachloroethylene (PCE - a common subsurface contaminant) by passive soil vapor extraction is expected to nearly double in low-permeable sediments when the subsurface is heated 10 degree C from ambient temperatures due to an increased vapor pressure in the PCE. When the sediment is heated using renewable energy sources, these thermally enhanced remediation technologies can be environmentally benign alternatives to conventional remediation techniques that rely on large external energy inputs. The thermally enhanced passive technologies may be particularly useful for remediating unsaturated, low-permeable lenses that are troublesome to most conventional remediation technologies such as conventional soil vapor extraction and co-solvent flushes.

The main objective of this work was to quantify subsurface sediment heating using a solar powered heat injection well. To do this, a pilot sediment heating system was installed in Vermont and high resolution meteorological and sediment temperature data were collected using a stand-alone data acquisition system. Unsaturated, silty sediments were heated in-situ by converting the direct and indirect solar energy available at the surface to heat energy in the subsurface using stand-alone renewable energy sources and a resistive element heat injection well. The heat injection well was powered by a 600-W passively tracking photovoltaic (PV) array and a small 1.2-m swept area wind turbine. It is envisioned that the heat injection well would be placed directly into an area of high subsurface contamination to speed up remediation efforts at a contaminated site.

## H52C MCC: Hall C Friday 1330h

## Using Groundwater Models to Guide Field Data Collection II Posters

Presiding: C Tiedeman, U.S.

Geological Survey; B Wagner, U.S. Geological Survey

## H52C-0893 1330h POSTER

## Modeling the Transport of Dissolved Contaminants Originating From a Rectangular Prism-shaped Multicomponent NAPL Source in Groundwater

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A three-dimensional, semi-analytical model for simulating the transport of contaminants originating from a dissolving rectangular prism-shaped, multicomponent nonaqueous phase liquid (NAPL) source in groundwater is developed. The NAPL dissolution process for each component is envisioned to occur in a series of continuous short intervals. The equilibrium aqueous concentration and the source dimensions are assumed to remain constant for the duration of each short interval. Individual component aqueous phase concentrations resulting from each dissolution interval are determined by an existing single component analytical solution. A synthetic two-component NAPL mixture is used for model simulation. Results show that for a dissolving multicomponent NAPL mixture, downstream aqueous phase concentrations may not always reflect source characteristics. The model is useful for an understanding of field data in homogeneous saturated porous media and for interpretation of bench-scale laboratory experiments.

## H52C-0894 1330h POSTER

## Salt Distribution in a Coastal Aquifer Determined From Geoelectric Soundings and From Numerical Groundwater Modeling

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To understand the interaction between salty sea water and non-salty groundwater it is essential to compare investigations of the salt content in the groundwater using numerical process modeling. The interaction of salt- and freshwater results in a 3D spatial pattern of the salt distribution in the aquifer. The paper discusses comparisons between geoelectric measurements and numerical calculations for a coastal aquifer in northern Germany. The large scale geoelectric model is based on a wide set of DC-soundings. The comparison uses results from medium scale numerical simulations of the density-influenced groundwater dynamics.

The area under investigation is situated between the estuaries of the rivers Elbe and Weser on the German North Sea coast. It covers an area of more than 1,000 square kilometres (400 square miles). The spatial pattern of the salt water distribution in the aquifers is investigated. The goal is to arrive at a characterization of the dynamics between salty and non-salty water to improve sustainable management of the groundwater resource. Numerical simulation is a tool suitable for management and forecasting purposes. The modeling must take into consideration the effect of salt on the density of water. Reliable simulations require extensive data to allow comparison of the numerical results with reality as well as providing a basis for good calibration of the numerical groundwater model.

Geoelectric soundings offers the possibility of establishing a closely meshed network of data on groundwater salinity. Our data base consists of over 1,000 soundings. Most reach a depth of 150 to 200 m (500 to 650 ft), sometimes more. Down to this depth we can determine the salt water distribution in the investigation area and build up a 3D spatial salinity model. The spatial interpretation of salinity is buttressed by salinity measurements at boreholes and pumping wells, by petrographic data and interpretations of high resolution AEM. In subregions of the investigation area, the resulting model is compared with numerical simulations of groundwater dynamics.

The results underline the applicability of comparisons between salt water distribution determined from geoelectric soundings and numerical groundwater simulations. This method is therefore suitable as a control

of numerical simulations over the entire investigation area.

## H52C-0895 1330h POSTER

## Optimal Experimental Design for Inverse Problem in Groundwater Modeling

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This research investigates experimental design in conjunction with the inverse problem of parameter structure identification in groundwater modeling. Despite the importance of model calibration, there exists only a few published works that systematically consider experimental design, model structure complexity and model application reliability. In this research, experimental design for parameter structure identification is formulated as a mixed integer nonlinear programming problem. To link the inverse problem with model application, the data sufficiency of a design is judged by solving a generalized inverse problem. The generalized inverse problem seeks to find the simplest parameter structure and its associated parameter values that satisfy the accuracy requirement in model application. To solve the inverse problem, it requires the calculation of sensitivity coefficients of state variables with respect to model parameters.

In this research, we use the adjoint state method to compute the sensitivity coefficients for all computation nodes. This method is superior because it only requires running the simulation model (L+1) times, where L is the number of observation wells. We use MODFLOW to simulate groundwater flow. Additionally, the developed adjoint state equations are solved by MODFLOW.

Since experimental design is predicated on the parameter values, which themselves are to be estimated before performing the experiments, prior information is combined with Monte-Carlo simulation to assess the reliability of data sufficiency. A global/local optimization method is used to solve the generalized inverse problem. Finally, a genetic algorithm solves the optimal experimental design problem.

## H52C-0896 1330h POSTER

## Modeling Well-Bore Skin Effects at Pumping and Observation Wells Under Variable Pumping Rate

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Well-bore skin effects have been recognized as a hydraulic influence at pumping wells during fully penetrating pumping tests with multiple observation wells conducted in the unconfined fluvial aquifer at the Boise Hydrogeophysical Research Site (BHRS). Because each well was constructed and completed in the same manner, skin effects are expected in both the pumping and the observation wells. Quantifying the effects of well-bore skin is important for accurate analysis and estimation of aquifer properties at the BHRS. For example, determinations of hydraulic parameters from fully penetrating pumping tests, tracer test injection behavior, and electromagnetic borehole flow-meter profiles are all sensitive to well-bore skin. Several lines of evidence indicate that well-bore skin effects at the BHRS are largely due to the presence of sand grains trapped in screen slots, with some fine material possibly left after cleaning. After construction, each well was cleaned to dissolve synthetic drilling mud and check for fine material. Pumping tests and geophysical logging were conducted before and after each cleaning to observe changes in skin effects and near-well physical properties. Video logging, laboratory tests, and modeling provide additional evidence that the skin effects are primarily caused by sand in the screen.

Well-bore skin is modeled here using modifications to the analytical model WTAQ of Moech (1997). We added capabilities to include the effects of well-bore skin at observation wells and also variable flow rate. In practice, analysis of well-bore skin effects may be complicated if the pumping rate takes some seconds to stabilize because skin effects occur at early time. With this in mind, we used a high-frequency measurement system in the field to collect flowrate and drawdown data during this period of variable flow rate. WTAQ and the parameter-estimation code UCODE were used

to invert for aquifer parameters and for well-bore skin. Data from three tests were inverted separately and jointly, including pumping and recovery data from a pumping test using well B6, and data from a pumping test using well B3. Eight wells, (including the pumping wells), were monitored, and pumping rates were approximately equal for the B6 and B3 tests. Well-bore skin estimates are consistent and within the 95% linear confidence intervals of each inversion for most tests.

URL: <http://cgiss.boisestate.edu/~billc/BHRS/bhrs.html>

#### H52C-0897 1330h POSTER

##### Modeling and Estimation of Bank Storage in a Gaining Reach of the San Pedro River, Arizona

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MODFLOW is a groundwater flow model that has been used to model flow in the San Pedro River basin. The San Pedro flows into Arizona from northern Sonora, Mexico, and is the largest undammed river in the southwest US. A portion of it - the San Pedro Riparian National Conservation Area - is federally protected in recognition of the ecosystem's importance to several threatened and endangered species, and because it is an important migratory flyway between the Americas.

Within the basin, expansion of groundwater pumping has caused many to question the impact of groundwater removal on the well-being of the river. Groundwater flow models have been central to debates about the area's water budget. Among several concerns is that MODFLOW does not consider bank storage, water that is temporarily stored in the river's banks following a high-flow event. Bank storage is a difficult phenomenon to monitor and quantify, but is potentially a substantial contributor to the river basin's water budget. If this is the case, various components of the San Pedro Basin water budget could be poorly estimated by MODFLOW.

To address these concerns, a transect of monitoring equipment was installed adjacent to and in a gaining reach of the San Pedro River. Soil moisture, soil tension, groundwater and stream levels were monitored over an 8-month period in 1998-1999. These data were subsequently used as input to HYDRUS 2-D, an unsaturated flow model, in order to monitor the behavior of bank storage, and provide an estimate of its contribution to the water budget.

While the bank storage estimate indicated a negligible contribution to the basin's water budget, it had a critical impact on the near-river hydrodynamics. While the bank storage volume per se was relatively small, its presence in the banks of the gaining river reach caused considerable back up of baseflow. This "baseflow backup" may be critical to prolong the seasonal water supply for the riparian vegetation, but has minimal effect on MODFLOW estimates of the basin's water budget. In addition, the monitoring of bank storage showed that most numerical descriptions of base flow do not accurately describe the behavior of bank storage for gaining river reaches.

#### H52C-0898 1330h POSTER

##### The Sensitivity Coefficient Approach: A Tool for the Analysis of the Influence of Heterogeneous Parameter Distributions on Hydraulic Tests

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In the last few decades, numerous efforts have been spent to improve the understanding of effects on hydraulic tests due to variations in the distribution of the governing hydraulic parameters. However, up to recent times there is still a lack in the exact spatial physical understanding of potential changes with respect to parameter variations, such as heterogeneity or anisotropy. For example, an exact assignment of parameter estimates derived from conventional pumping tests is still uncertain. Therefore, concepts have

to be utilized which can contribute to the understanding of effects of heterogeneities to the observation during hydraulic tests. For this purpose the Sensitivity Coefficient Approach (SCA) is a useful tool allowing the analysis and evaluation of potential measurements providing an understanding of the influence of heterogeneities. In this approach, sensitivity coefficients relate changes in parameter distributions directly to a particular change in the observed hydraulic head and are therefore a measure of the effect of a deviation in the parameter distribution on the measured quantity. In this presentation, the theory of sensitivity coefficients is introduced which allows the analysis and evaluation of potential measurements incorporating the influence of heterogeneities on the observation during hydraulic tests. Furthermore, effects on hydraulic tests resulting from heterogeneity and anisotropy are evaluated based on the SCA. A numerical implementation of the SCA is used in order to give an assessment of how discrete parameter deviations affect hydraulic tests in homogeneous, anisotropic, and heterogeneous aquifers.

#### H52D MCC: Hall C Friday 1330h Linking Hydrology and Biogeochemistry II Posters (joint with B, GC)

**Presiding:** M Gooseff, Oregon State University; B Newman, Los Alamos National Laboratory; D DeWalle, Pennsylvania State University; J McDonnell, Oregon State University

#### H52D-0899 1330h POSTER

##### Evapotranspiration in the Nebraska Sand Hills

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The Nebraska Sand Hills cover over 50,000 square kilometers and are the largest stabilized sand dune field in the world. While this fragile ecosystem exists in a semi-arid climate (450 to 500 mm annual rainfall), there exists within it, several different sub-systems, representing a wide range of moisture regimes. These can range from wetlands and small, shallow lakes to dry dunal uplands. Soils in this ecosystem are mostly eolian sands and support a thin vegetation cover that is responsible for holding the dunes in place. Despite this seeming fragility, the region is home to a thriving free-range cattle industry and it's associated haying and grazing. To help in understanding this complex ecosystem, we have instituted a program of evapotranspiration measurements in areas that are instrumented with logging wells. In this poster, we will report on our results to date from two seemingly different valley ecosystems.

#### H52D-0900 1330h POSTER

##### Spatial distribution of the denitrification zone in a forested headwater catchment in central Japan: Influences of hydrologic conditions

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The spatial distribution of the denitrification process was investigated in tandem with hydrometric and chemical groundwater monitoring in a temperate forest catchment in Japan, to determine the effect of hydrologic conditions on the pathways of nitrogen loss from the catchment and streamwater chemistry, especially the temporal and spatial changes in  $\text{NO}_3^-$  concentrations in soil and ground water. Field investigations were conducted in an unchanneled headwater catchment (0.59 ha) in the Kiryu Experimental Watershed (KEW), which is covered by mixed stands of secondary broad-leaved deciduous trees and planted coniferous trees. The input-output analysis of nitrogen in the catchment found that approximately  $6 \text{ kg ha}^{-1} \text{ yr}^{-1}$  (average 1995-2001) of inorganic nitrogen was discharged through the stream system, and the amount of denitrified nitrogen was estimated at  $4-7 \text{ kg ha}^{-1} \text{ yr}^{-1}$ , suggesting that a significant portion of the nitrogen loss from the catchment was by denitrification. A previous study of the denitrification characteristics in the riparian zone of this catchment showed that denitrification occurred intermittently, corresponding to fluctuations in the groundwater level. The intensity of denitrification depended strongly on the saturation of the near-surface soil. The present investigation showed that the dissolved  $\text{N}_2\text{O}$  concentration, which is an indicator of denitrification intensity, was consistently higher in the shallower portion of the groundwater body than in the deeper portion. Correspondingly, the  $\text{NO}_3^-$  concentration decreased with depth in the groundwater body.  $\text{N}_2\text{O}$  generated in the shallower portion of the groundwater body was transported by lateral movement of the groundwater, and then released to the atmosphere at the exit point. Therefore, intense, consistent  $\text{N}_2\text{O}$  emissions occurred in the area surrounding the exit point, while emissions were intermittent in the riparian zone. In addition, in the hillside part of the catchment, which was covered by relatively dry forest soils, no  $\text{N}_2\text{O}$  emissions were detected, although the mineralization and nitrification potential were higher than in the riparian zone. These observations indicate that complete saturation by water is one of the critical factors determining the denitrification zone in this catchment.

#### H52D-0901 1330h POSTER

##### Investigating stream longitudinal geomorphic variability and hyporheic exchange residence time distribution using a groundwater flow model

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