[1]UFZ Centre for Environmental Research Leipzig-Halle in the Helmholtz Association, Department of Hydrogeology, Theodor-Lieser-Str. 4, Halle/Saale 06120, Germany

Groundwater aeration by discontinuous oxygen gas pulse injections appears to be a promising concept for enhanced natural attenuation of dissolved contaminants that are susceptible for oxygenase enzyme attacks. Oxygen amendments facilitate indigenous microbiota to catabolize groundwater pollutants, such as aromatics, that are considered to be recalcitrant in absence of dissolved oxygen. As a rule, natural attenuation of many pollutants under aerobic conditions is considerably faster than under anaerobic conditions. Thus, enhancing the dissolved oxygen level appears to be worthwhile. In situ aeration of groundwater has been accomplished by air sparging, H2O2-supply, or by utilization of oxygen release compounds. However, continuous aeration of previously anaerobic groundwater is not desirable for several reasons: (a) economic efforts too high, (b) pollutant dislocation towards surface (desired only in air sparging), (c) risk of aquifer clogging (gas clogging, oxidation of ferrous iron, formation of bioslimes). In contrast, discontinuous oxygen gas sparging provides only for periodical groundwater aeration which is followed by microaerobic and suboxic conditions. Microaerobic conditions can prevail spatially (e.g., at plume fringes or within biofilms) or temporarily (e.g., at discontinuous bioventing). They still allow adapted bacteria to transform environmental pollutants to less toxic compounds, e.g., aromatic ring cleavage after dioxygenasis attack. Ring cleavage products, on the other hand, may be degraded more easily by anaerobic consortia than the initial aromatic compounds, making oxygen depletion periods highly intriguing in regard to an initiation of natural attenuation processes at plume fringes. In our work we outline the effect of oxygen depletion conditions on biodegradation of monchlorobenzene (MCB) as they occur subsequently to temporary aeration periods. For microaerobic conditions, relative to the oxygen supply, a stoichiometric transformation of MCB to cis,cis-2-chloromuconate is demonstrated. In order to examine effects of enhanced natural attenuation, initiated by aeration, on geohydraulics, discontinuous oxygen gas injections were simulated in two flow-through systems. Design, processing, and first results of our ongoing research are presented for the automatized lab column system CAMERA and a pilot field reactor at a MCB polluted site at Bitterfeld, Germany. Bubble mediated oxygen gas transfer is briefly discussed in light of the model presented recently by Holocher (Environ. Sci. Technol., 2003. 37: p. 1337-1343).

### H11D-0893 0830h POSTER

### Natural attenuation of copper in the water table aquifer below an industrial site

Monika A.M. Kedziorek[1] (33 559 80 68 98; monika.kedziorek@univ-pau.fr)

Alain C.M. Bourg (33 559 80 68 99; alain.bourg@univ-pau.fr)

[1]Laboratory of Hydro-Geochemistry and Environment, Dept. Earth Sciences, Univ. of Pau, BP 1155, Pau Cedex 64013, France

The contamination of soils and aquifers by inorganic pollutants is so extensive in industrial sites that it hardly seems economically feasible to decontaminate the large areas or soil volumes involved. It is therefore worthwhile to investigate whether the local environment is capable of attenuating contamination. Natural attenuation by degradation seems realistic for many organic pollutants. We show that it can also occur for inorganic pollutants. The phreatic-fill aquifer underlying an industrial plant located on the banks of the Garonne River (Southwestern France) is contaminated by acidic water (pH down to 1) and high concentrations of sulfate (up to 50 g/L) and copper (up to 30 g/L). As acidic water, rich in Cu and sulfate, moves away from the contamination source, pH increases due to buffering of aquifer solids, dissolved Cu concentrations decrease by 6 orders of magnitude, while sulfate concentrations decrease little. The Cu disappearing from the water phase is found as solid in cores in the area of the site where pH increases to 5-6.

### H11D-0894 0830h POSTER

### Analytical Modeling of A By-product Transport in Chain Reactions

Yunwei Sun[1] (sun4@llnl.gov)

Kenrick Lee[1] (lee23@llnl.gov)

Thomas A Buscheck[1] (buscheck1@llnl.gov)

[1]Lawrence Livermore National Laboratory, PO Box 808 L-646, Livermore, CA 94550, United States

Many chemical reactions of contaminants in the subsurface involve complex reaction pathways and networks. As one of those reaction networks, chain-reactions can be found in radionuclide decay, denitrification, biodegradation of chlorinated solvents, etc. For example, this reaction pattern can be illustrated by the biodegrdation of tetrachloroethylene (PCE) and trichloroethylene (TCE). PCE reacts to produce TCE and TCE reacts to form dichloroethylene (DCE). DCE will further reacts to form vinyl chloride (VC) and finally VC reacts to produce thylene (ETH). During the chain reactions, by-products, such as chloride in PCE reaction chain, can be produced in groundwater. For this reason, by-prodcut concentrations in the contaminant plumes are elevated relatively to ambient concentrations. Because of the neutral chemical behavior of some by-products, they can be treated as indicators to identify the sources of contaminants and to estimate reaction rates. Often, a single by-prodcut is produced from multiple steps in a reaction chain. Then, the partial differential equation for by-product mass balance is coupled by multiple reactants. This makes it difficult, if not impossible, to derive analytical solutions using integral transforms. Instead, we conduct singular value decomposition (SVD) analytically and develop a closed-form solution of a by-product transport in multiple chain reactions. In achieving the analytical solution, all reactions are assumed to be first-order and the system is assumed to be homogeneous and isotropic.

## H11E MCC: Level 2 Monday 0830h

## Moving Beyond the Model Development Stage: Groundwater Model Validation, Postaudits, and Long-Term Monitoring Posters

*Presiding:* **T D Scheibe,** Pacific Northwest National Laboratory**; A E Hassan,** Desert Research Institute**; B S Minsker,** University of Illinois

### H11E-0895 0830h INVITED POSTER

### Validation of Groundwater Models: Meaningful or Meaningless?

Leonard F Konikow (703-648-5878; lkonikow@usgs.gov)

U.S. Geological Survey, 431 National Center, Reston, VA 20192

Although numerical simulation models are valuable tools for analyzing groundwater systems, their predictive accuracy is limited. People who apply groundwater flow or solute-transport models, as well as those who make decisions based on model results, naturally want assurance that a model is "valid." To many people, model validation implies some authentication of the truth or accuracy of the model. History matching is often presented as the basis for model validation. Although such model calibration is a necessary modeling step, it is simply insufficient for model validation. Because of parameter uncertainty and solution non-uniqueness, declarations of validation (or verification) of a model are not meaningful. Post-audits represent a useful means to assess the predictive accuracy of a site-specific model, but they require the existence of long-term monitoring data. Model testing may yield invalidation, but that is an opportunity to learn and to improve the conceptual and numerical models. Examples of post-audits and of the application of a solute-transport model to a radioactive waste disposal site illustrate deficiencies in model calibration, prediction, and validation.

### H11E-0896 0830h INVITED POSTER

### Development of an Integrated Ground-Water Monitoring Strategy for Supporting Performance Assessments of Nuclear Facilities

Thomas J. Nicholson[1] (1-301-415-6268; TJN@NRC.GOV)

Van Price[2] (1-803-951-8470; vprice@advenvsoln.com)

[1]Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission, MS T-9F31, Washington, DC 20555, United States

[2]Advanced Environmental Solutions, 899 Sycamore Drive, Aiken, SC 29803, United States

The U.S. NRC is funding research to develop an integrated ground-water monitoring strategy to support performance assessments (PA) of nuclear waste and decommissioning sites. These PAs provide the scientific and regulatory bases for a risk-informed decision as to the long-term safety of waste disposal and decommissioning sites. The strategy will assist in NRC staff reviews of predicted consequences related to potential radionuclide releases from licensed nuclear facilities. The strategy couples site characterization and PA through identification and monitoring of hydrogeologic system performance indicators such as distributions of water content in the unsaturated zone and ground-water potential in the saturated zone, as well as radionuclide concentrations. The strategy considers the need to monitor for a range of alternative conceptual groundwater models, and to quantify parameter and model uncertainties. The strategy will be tested using real-time monitoring datasets. Recognizing that each site has its unique set of features, events and processes, the strategy will focus on methods for designing monitoring systems to detect both current conditions and changes in the system's behavior relevant to radionuclide leaching and transport. Beyond identifying and mapping contaminant plumes, the monitoring goals are to: identify the presence or potential for preferential transport pathways; assess the effectiveness of contaminant isolation systems; identify and support alternative conceptual flow and transport models; and communicate the monitored performance indicators through effective data management, analysis and visualization techniques for decision makers and stakeholders. Progress to date involves the review and harmonization of monitoring programs, strategies and guidance presently used to evaluate both radioactive and toxic waste facilities.

URL: http://www.ISCMEM.Org

### H11E-0897 0830h POSTER

### Linking the Model Validation Process and Long-Term Monitoring Design for Central Nevada Test Area

Ahmed E. Hassan[1,2] (702 862 5465; hassan@dri.edu)

[1]Desert Research Institute, 755 E. Flamingo Road, Las Vegas, NV 89119, United States

[2]Irrigation and Hydraulics Dept., Cairo University , Gamaa Street, Giza 12613, Egypt

A multi-staged approach for development of the long-term monitoring well network for the Central Nevada Test Area (CNTA) is proposed. This multi-staged approach will proceed in parallel with the validation efforts for the groundwater flow and transport model of CNTA. The first stage of the plan is to use the hydrogeologic insight combined with the simulation and probability-based approaches to select the first set of monitoring wells that will serve two purposes or objectives. The first high-priority objective is the collection of data for the initial evaluation of the groundwater flow and transport model. The selection criteria will thus be tailored more toward meeting this objective and facilitating the collection of the most relevant data from the most important locations for evaluating the different model components. The second objective, which has a lower priority, is to place this set of wells in locations likely to encounter fast migration pathways, and thus benefiting from the wells in the long-term &a

### H11E-0898 0830h POSTER

### Analysis of Measurement Error and Estimator Shape in Three-Point Hydraulic Gradient Estimators

Sean A McKenna[1] (505 844 2450; samcken@sandia.gov)

Arun K Wahi[2]

[1]Sandia National Laboratories, Geohydrology Department, PO Box 5800 MS0735, Albuquerque, NM 87185-0735, United States

[2]University of Arizona, Department of Hydrology and Water Resources,1133 E North Campus Drive, Tucson, AZ 85721, United States

Three spatially separated measurements of head provide a means of estimating the magnitude and orientation of the hydraulic gradient. Previous work with three-point estimators has focused on the effect of the size (area) of the three-point estimator and measurement error on the final estimates of the gradient magnitude and orientation in laboratory and field studies (Mizell, 1980; Silliman and Frost, 1995; Silliman and Mantz, 2000; Ruskauff and Rumbaugh, 1996). However, a systematic analysis of the combined effects of measurement error, estimator shape and estimator orientation relative to the gradient orientation has not previously been conducted. Monte Carlo simulation with an underlying assumption of a homogeneous transmissivity field is used to examine the effects of uncorrelated measurement error on a series of eleven different three-point estimators having the same size but different shapes as a function of the orientation of the true gradient. Results show that the variance in the estimate of both the magnitude and the orientation increase linearly with the increase in measurement error in agreement with the results of stochastic theory for estimators that are small relative to the correlation length of transmissivity (Mizell, 1980). Three-point estimator shapes with base to height ratios between 0.5 and 5.0 provide accurate estimates of magnitude and

orientation across all orientations of the true gradient. As an example, these results are applied to data collected from a monitoring network of 25 wells at the WIPP site during two different time periods. The simulation results are used to reduce the set of all possible combinations of three wells to those combinations with acceptable measurement errors relative to the amount of head drop across the estimator and base to height ratios between 0.5 and 5.0. These limitations reduce the set of all possible well combinations by 98 percent and show that size alone as defined by triangle area is not a valid discriminator of whether or not the estimator provides accurate estimates of the gradient magnitude and orientation. This research was funded by WIPP programs administered by the U.S Department of Energy. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

### H11E-0899 0830h INVITED POSTER

### Post-audits of Three Groundwater Models for Evaluating Plume Containment

Peter F. Andersen (1-770-642-1000; pandersen@geotransinc.com)

GeoTrans, Inc., 1080 Holcomb Bridge Road Building 100, Suite 190, Roswell, GA 30076, United States

Groundwater extraction systems were designed using numerical models at three sites within a U.S. Army Ammunition Plant in Tennessee. Each site, and hence model, has unique qualities such as boundary conditions, extensiveness of the contaminant plume, and quantity and quality of hydrogeologic data. Performance of each of these extraction systems has been evaluated throughout their operation, providing an opportunity to perform post-audits on the accuracy of the groundwater models that were used in their design. Areas of comparison between the models and the observed response in the natural systems include hydraulic head, drawdown, horizontal and vertical gradients, and extent of capture zones. The results of the post-audits show the importance of using all available data in the construction and calibration of the models, the importance of having sufficient data, and the critical nature of an accurate conceptual model. The post-audits also show that although it may be possible to assess the accuracy of the model predictions, it is often not possible to explain the reasons for discrepancies between predicted and observed results. From a practical perspective, parameter uncertainty is important to account for in the development of the models and subsequent design of the extraction systems.

### H11E-0900 0830h POSTER

### Simulation Of Groundwater Flow And Reactive Transport In A Tidally Influenced Estuarine Aquifer

Xiaomin Mao[1] (44-07876387651; xmao@ed.ac.uk)

David Andrew Barry[1] (D.A.barry@ed.ac.uk)

Patricia Enot[1] (patricia.enot@ed.ac.uk)

Ling Li[2] (L.li@uq.edu.au)

[1]Institute for Infrastructure and Environment School of Engineering and Electronics The University of Edinburgh, Crew Building King's Buildings Edinburgh EH9 3JN United Kingdom, Edinburgh EH9 3JN, United Kingdom

[2]School of Engineering The University of Queensland, Brisbane, QLD 4072 Australia, Brisbane QLD 4072, Australia

Existing groundwater monitoring data from an estuarine sandy aquifer situated below an old industrial landfill (Scotland) showed that (1) leaching from sulphurous waste located in the landfill has generated an acidic plume; (2) associated with the low pH, metal contaminants within the acidic plume are slowly migrating towards the estuary; and (3) the groundwater fluctuations are influenced by the tidal oscillations of the estuary. In order to test the possible influence of rainfall/precipitation, tidal fluctuation and salt water intrusion on the groundwater flow and reactive chemical transport, a model for multi-component reactive transport with density dependent flow was developed and applied to the site. The groundwater flow and chemical transport in this coastal aquifer were simulated. Both the field observations and numerical simulations showed that the tidal influence on the groundwater table fluctuations was great even far inland. This influence could not be explained by standard analytical solutions. It is expected that the local morphology and hydro-geological conditions cause this behaviour. The simulation performed with a conservative tracer showed that it took much less time to reach the estuary than the acidic plume originating from the landfill, with the rate of movement influenced by recharge and tidal oscillations. Due to buffering reactions occurring in the geochemical system during the migration of the contaminants (ion exchange, mineral precipitation/dissolution and oxidation/reduction), the movement of the acidic plume and associated metals is strongly retarded. Sharp differences are apparent in chemical concentrations, pH and pe, between the plume location and unaffected areas.

### H11E-0901 0830h POSTER

### An Intermediate-Scale Groundwater Contamination Experiment

Xinyu Wei[1] (8026567789; xwei@emba.uvm.edu)

George F Pinder[1] (8026568697; pinder@emba.uvm.edu)

[1]Research center for groundwater remediation design, 213 Votey Building University of Vermont, Burlington, VT 05405, United States

Intermediate-scale experiments fill the gap between bench and field-scale experiments. They compensate for the missing subsurface heterogeneity in bench-scale experiments and the lack of environmental control and insuffcient sampling in field-scale experiments. A 4.22 by 2.74 by 2.13m intermediate-scale indoor facility that mimics a heterogeneous subsurface environment was constructed. To characterize the facility and to obtain a 3D subsurface contamination dataset, a 20-day point source continuous-injection experiment was conducted. Using 63 Time Domain Reflectometry(TDR) sensors, a salt concentration dataset was collected at a frequency of 20 minutes per measurement per sensor. The experiment data were compared with a finite element model - Princeton Transport Code(PTC) simulation. In the horizontal plain, which contains a point source, the PTC simulation were consistent with the TDR data. At other sampling locations, vertical to this plain, there were siginificant deviations between the PTC simulation and the TDR data.

## H11F MCC: Level 2 Monday 0830h

### Use of Artificial Intelligence Methods in Geosciences Posters *(joint with A, NG)*

***Presiding:*** **M Morissey,** Oklahoma University**; S Postawko,** University of Oklahoma

### H11F-0902 0830h POSTER

### Comparison of Data-Driven Takagi–Sugeno Models of Rainfall-Discharge Dynamics

Hilde Vernieuwe[1] (hilde.vernieuwe@ugent.be); Olga Georgieva[2] (ogeorgieva@icsr.bas.bg); Niko E.C. Verhoest[3] (niko.verhoest@ugent.be); Valentijn R.N. Pauwels[3] (Valentijn.Pauwels@ugent.be); Bernard De Baets[1] (bernard.debaets@ugent.be); François P. De Troch[3] (francois.detroch@ugent.be)

[1]Department of Applied Mathematics, Biometrics and Process Control, Coupure links 653, Gent B-9000, Belgium

[2]Institute of Control and System Research, Bulgarian Academy of Sciences, P.O. Box 79, Sofia 1113, Bulgaria

[3]Laboratory of Hydrology and Water Management, Coupure links 653, Gent B-9000, Belgium

Three different methods for constructing fuzzy rule-based models of the Takagi–Sugeno type relating rainfall to catchment discharge are tested on the Zwalm catchment in Belgium. They correspond to the grid partitioning (GP), subtractive clustering (SC), and Gustafson–Kessel clustering (GK) identification methods. The data set used to parametrize and validate the models consists of hourly precipitation and discharge records. The models are parametrized using a one-year identification data set and are then applied to a four-year data set. All models are found to have a low computation cost. Although the models show a similar performance, the best results are obtained for the GK method. A real-time flood forecasting algorithm is then developed, in which discharge measurements are assimilated into the model at either an hourly or a daily time step. The results suggest that the GK method can potentially be used as an operational flood forecasting tool.

### H11F-0903 0830h POSTER

### Precipitation Estimation from Remotely Sensed Information using ANN-Cloud Classification System

Yang Hong[1] (5202417874; yhong@hwr.arizona.edu)

Kuolin Hsu[2] (kuolinh@uci.edu)

Soroosh Sorooshian[2] (soroosh@hwr.arizona.edu)

[1]Dept. of Hydrology and Water Resources, University of Arizona, Tucson, 1Dept. of Hydrology and Water Resources, The University of Arizona, Tucson, AZ, 85721, Tucson, AZ 85721

[2]2. Dept. of Civil and Environmental Engineering, University of California, Irvine, 2 Dept. of Civil and Environmental Engineering, University of California, Irvine, CA, 92697, Irvine, CA 92697

Abstract Artificial Neural Network (ANN) models, which contain flexible architectures and are capable of discerning the underlying functional relationships from data, are recognized as very useful tools in geophysical applications. In this study, we demonstrate a hybrid ANN modeling system to estimate surface rainfall from satellite infrared imagery. The proposed network, Precipitation Estimation from Remotely Sensed Information using ANN-Cloud Classification System (PERSIANN-CCS), includes several components: (1) cloud image segmentation, (2) cloud patch feature selection, (3) patch feature classification using a self-organizing feature map network, and (4) patch-based rainfall estimates from a group of multiple nonlinear cloud top temperature and rainfall functions. The PERSIANN-CCS model was first calibrated using observations from Geostationary Operational Environmental Satellite (GOES) infrared imagery and the Next Generation Radar (NEXRAD) rainfall network. To further extend PERSIANN-CCS rainfall estimates over the remote regions, Tropical Rainfall Measurement Mission (TRMM) microwave rainfall estimates (TMI product 2A12) were used to adjust PERSIANN-CCS model parameters. The calibrated nonlinear cloud top temperature and rainfall (Tb-R) functions of classified cloud patches show highly variability, reflecting the complexity of dominant cloud-precipitation processes over various regions. Case studies show that PERSIANN-CCS captures the variability in rain rate at 12kmx12km grid and 3-hour resolutions, with a standard error of 3.0mm/hr and a correlation coefficient around 0.65. Additional insights into the cloud evolution and precipitation process from the classified PERSIANN-CCS cloud patch features and rainfall distributions are discussed.

### H11F-0904 0830h POSTER

### Use of artificial neural networks in prediction of subsurface hydrological processes

A. W. Warrick[1] (aww@ag.arizona.edu)

Alex Furman[2] (alex@hwr.arizona.edu)

Dawit Zerihun[1]

Charles A. Sanchez[3]

[1]Soil, Water, and Environmental Sciences, Univ. of Arizona, Tucson, AZ 85721, United States

[2]Hydrology and Water Resources, Univ. of Arizona, Tucson, AZ 85721, United States

[3]Spoil, Water, and Environmental Sciences, Yuma Agricultural Center, Univ. of Arizona, Yuma, AZ 85364, United States

Modeling of surface runoff for hydrological or agricultural purposes typically makes use of empirical or semi-empirical infiltration functions such as those by Horton or Kostiakov. The alternative of detailed numerical solution of the Richards equation is generally limited to research purposes because of greater complexity than the empirical forms and the need for a greater effort in order to obtain results. A major drawback of the use of empirical functions with regard to the subsurface is that boundary and initial conditions are not explicitly taken into consideration and the details of water distribution are not calculated. This limits the accuracy of the surface models to be site and event specific. In addition, it limits the applicability of surface models for studying recharge. We present here a new alternative to the detailed numerical solution of the Richards equation which is based on artificial neural networks (ANN). The methodology relies on extensive numerical solutions for various soil properties and geometries, building a large training set for the ANN. A dimensionless form of the numerical increases the efficiency of the database generation. At a second stage, the ANN in its recall mode can replace the numerical solution to obtain a dramatically faster solution, while retaining acceptable accuracy for both infiltration rates and water content distributions. The methodology is presented for several case studies with an emphasis on infiltration from trenches and furrows.