analysis (SSA), has been a fruitful extension of the PCA technique. The common drawback of these classical methods is that only linear structures can be correctly extracted from the data. Since the late 1980s, neural network methods have become popular for performing nonlinear regression (NLR) and classification. More recently, multi-layer perceptron neural network methods have been extended to perform nonlinear PCA (NLPCA), nonlinear CCA (NLCCA) and nonlinear SSA (NLSSA). This paper presents a unified view of the NLPCA, NLCCA and NLSSA techniques, and their applications to various datasets of the atmosphere and the ocean, especially in the nonlinear study of the El Niño-Southern Oscillation (ENSO) phenomenon.

H11F-0911 0830h POSTER

Prediction of Fluid Velocity in Highly Heterogeneous Conductivity Fields Using a Genetic Algorithm-Designed Artificial Neural Network

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A genetic algorithm (GA) is used to select the operational parameters of artificial neural networks (ANN) which are trained to predict fluid velocity. Populations of three-layer, feedforward backpropagation ANN's with varying numbers of hidden nodes, types and slopes of activation functions, alpha and beta learning rates and initial distributions of weights for both the input and hidden layers are created by the GA. The GA- defined ANN's are trained with inputs-output pairs of hydraulic conductivity neighborhoods and resulting fluid velocities at certain points in the simulation domain. The hydraulic conductivity fields are highly heterogeneous with an ensemble log conductivity variance of 1.0. Results of the GA are defined and selected ANN velocity predictions are presented.

H11F-0912 0830h POSTER

Detection of Visual Events in Underwater Video Using a Neuromorphic Saliency-based Attention System

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The Monterey Bay Aquarium Research Institute (MBARI) uses high-resolution video equipment on remotely operated vehicles (ROV) to obtain quantitative data on the distribution and abundance of oceanic animals. High-quality video data supplants the traditional approach of assessing the kinds and numbers of animals in the oceanic water column through towing collection nets behind ships. Tow nets are limited in spatial resolution, and often destroy abundant gelatinous animals resulting in species undersampling. Video camera-based quantitative video transects (QVT) are taken through the ocean midwater, from 50m to 4000m, and provide high-resolution data at the scale of the individual animals and their natural aggregation patterns. However, the current manual method of analyzing QVT video by trained scientists is labor intensive and poses a serious limitation to the amount of information that can be analyzed from ROV dives. Presented here is an automated system for detecting marine animals (events) visible in the videos. Automated detection is difficult due to the low contrast of many translucent animals and due to debris ("marine snow") cluttering the scene. Video frames are processed with an artificial intelligence attention selection algorithm that has proven a robust means of target detection in a variety of natural terrestrial scenes. The candidate locations identified by the attention selection module are tracked across video frames using linear Kalman filters. Typically, the occurrence of visible animals in the video footage is sparse in space and time. A notion of "boring" video frames is developed by detecting whether or not there is an interesting candidate object for an animal present in a particular sequence of underwater video – video frames that do not contain any "interesting" events. If objects can be tracked successfully over several frames, they are stored as potentially "interesting" events. Based on low-level properties, interesting events are identified and marked in the video frames. Presented here is performance data that compare the automated detection method with that of human annotators. The system enhances the productivity of human video annotators and/or cues a subsequent object classification module by omitting "boring" frames and marking candidate objects.

URL: http://www.mbari.org

H11F-0913 0830h POSTER

A Hybrid Global MISR Cloud Mask using Support Vector Machines and Active Learning

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The Multiangle Imaging SpectroRadiometer (MISR) onboard NASA's Terra EOS satellite provides unique sensing capabilities that promise potentially much better global cloud identification. A number of algorithms have been developed and implemented for detecting clouds in MISR data, some of which use MISR's unique multiangle sensing capability. All of these techniques are firmly grounded in the physics of remote sensing, but the accuracy of each method is highly dependent on different specific conditions. This presents a unique opportunity for soft computing methods. We are investigating techniques that use Support Vector Machines (SVMs) to combine the raw MISR data and the output of existing MISR cloud mask algorithms into a new and more robust global cloud mask. One of the main challenges in training a SVM (or any other supervised classifier) is that it is very expensive and time consuming to collect training data. To address this problem we have incorporated and are continuing to refine the relatively new technique known as active learning, in which the algorithm queries the human expert to supply training labels in regions that would be most beneficial for improving the model. We have developed an interactive application which utilizes SVMs and active learning to allow a scientist to quickly train a classifier for MISR data. In addition, we have performed a number of small-scale case studies and a global sampling study which compare the accuracy of the existing MISR cloud mask algorithms to our best SVM models.

H11F-0914 0830h POSTER

Using Decision Trees to Examine Relationships between Inter-Annual Vegetation Variability, Topographic Attributes, and Climate Signals

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The objective of this research is to develop KDD (knowledge discovery in databases) techniques for spatio-temporal geo-data, and use these techniques to examine inter-annual vegetation health signals. The underlying hypothesis of the research is that the signatures of inter-annual variability of climate on vegetation dynamics as represented by the statistical descriptors of vegetation index variations depend upon a variety of attributes related to the topography, hydrology, physiography, and climate. NDVI (normalized differential vegetation index) is enlisted to represent vegetation health and relationships between this index and topographic attributes such as elevation, slope, aspect, compound topographic index (CTI), and the proximity to a stream, are analyzed. Several scientific questions related to the identification and characterization of the inter-annual variability ensue as a consequence of our hypothesis. Investigations were performed using 13 years of 1-km resolution NDVI data from the AVHRR instrument on NOAA's POES (polar-orbiting operational environmental satellite) over the continental U.S. Various temporal change indices were used in order to identify anomalous inter-annual behavior in the NDVI index, including maximum absolute and relative deviations from the 13-year mean and positive and negative persistence indices (after Zhou et al., 2001). The KDD technique used in this research is the decision tree, which falls under the classification and prediction division of data mining techniques. The algorithm is similar to c4.5 and id3, but can handle continuous input and output values without binning and is optimized to determine the minimum error. Future work will incorporate clustering algorithms (both distance and density-based) and association rule algorithms (constraint-based) adapted for spatial-temporal data. Investigations will also be performed at smaller spatial scales, integrating higher resolution data. Throughout the growing season, elevation and slope are dominant factors associated with increased vegetation variability. From May to September slope prevails at high, rather than low elevations, although in the beginning and end of the growing season (April and October) this is not the case. This may possibly be due to the lack of vegetation at higher elevations at the fringes of the growing season. In general, the lower the slope, the greater the relative change in vegetation, thus linking zones of moisture convergence typically associated with low slopes to increased changes in vegetation over time. The relative change in vegetation is greater at mid-range elevations in April through June, high elevations in July through September, and low elevations in October. Zones of subsurface flow convergence, as captured by the CTI, play an important role in July through October; however, the influence alternates from low elevations in July to high elevations in August, reverting back to low elevations in September and October.

H11F-0915 0830h POSTER

A New Perspective on Modeling Groundwater-Driven Health Risk With Subjective Information

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Fuzzy rule-based systems provide an efficient environment for the modeling of expert information in the context of risk management for groundwater contamination problems. In general, their use in the form of conditional pieces of knowledge, has been either as a tool for synthesizing control laws from data (i.e., conjunction-based models), or in a knowledge representation and reasoning perspective in Artificial Intelligence (i.e., implication-based models), where only the latter may lead to coherence problems (e.g., input data that leads to logical inconsistency when added to the knowledge base). We implement a two-fold extension to an implication-based groundwater risk model (Ozbek and Pinder, 2002) including: 1) the implementation of sufficient conditions for a coherent knowledge base, and 2) the interpolation of expert statements to supplement gaps in knowledge. The original model assumes statements of public health professionals for the characterization of the exposed individual and the relation of dose and pattern of exposure to its carcinogenic effects. We demonstrate the utility of the extended model in that it: 1)identifies inconsistent statements and establishes coherence in the knowledge base, and 2) minimizes the burden of knowledge elicitation from the experts for utilizing existing knowledge in an optimal fashion.

H11G MCC: Level 2 Monday 0830h

Numerical Simulations of Flow and Transport in Heterogeneous Subsurface Systems Posters

Presiding: **Y Zhang,** University of Iowa

H11G-0916 0830h POSTER

Evaluation of the Effects of Potash Mining in the Region of the Waste Isolation Pilot Plant, Carlsbad, New Mexico

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The Waste Isolation Pilot Plant (WIPP) in southeast New Mexico has been developed for underground disposal of transuranic waste in halite beds of the Permian Salado Formation. Managed by the Department of Energy (DOE), the WIPP has been operational since March 1999. Regulatory requirements call for

the DOE to submit a Compliance Recertification Application (CRA) every five years, the first of which is due to the Environmental Protection Agency in 2004. In support of the CRA, performance assessment (PA) analysis is being conducted. PA is a series of linked models that make probabilistic assessments of possible future states of the WIPP and its performance under each of those states. One possible future state involves human intrusion into the repository creating pathways for upward migration of radionuclides into the Culebra dolomite aquifer. The Culebra is about 200 m below ground surface and 400 m above the repository. Current and future potash mining in the upper Salado Formation, within and outside the WIPP boundary, will likely cause subsidence of the Culebra, resulting in higher transmissivities that may change regional groundwater flow patterns. This analysis evaluates the impact of potash mining on the Culebra flow patterns and the resulting influence on repository performance. The impacts are modeled by creating 100 calibrated transmissivity (T) fields through stochastic inverse modeling using the parameter estimation code, PEST. Transmissivities in each field are then scaled in areas deemed to contain extractable potash by a random mining factor between 1 and 1000. Two mining scenarios are modeled: mining in all extractable areas within the WIPP boundary and across the entire region and mining everywhere except within the WIPP boundary. Three random mining factors are applied to each calibrated T-field for both mining scenarios, creating 600 instances of modified T-fields. Steady-state flow models are run for each instance and particle tracking is used to determine the flow path and travel time from the center of the WIPP to the site boundary. Cumulative probability distribution functions of travel time are produced for each mining scenario and compared to the undisturbed case. Particle pathways are also examined. Results show that the median travel times for the mining cases are 2.3 to 2.5 times longer than for the undisturbed case. This is due to increased transmissivity in the mining zones creating preferential flow routes around most of the WIPP site. Flow path changes are also apparent between the mining and undisturbed cases. No correlation is found between the travel times and the random mining factor, meaning small values of this factor are enough to shift the flow field from a non-mining pattern to a mining pattern.

H11G-0917 0830h POSTER

Numerical modeling of laboratory permeability upscaling experiments

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Aquifer/reservoir characterization and the subsequent integration of acquired spatial information into predictive flow and transport models face two basic limitations. First, the quantity of porous media observed and/or sampled is generally a minute fraction of the site under investigation. This gives rise to the need for models to predict material characteristics at unsampled locations. Secondly, technological constraints limit the measurement of material properties to sample supports (volume of porous media sampled) that are much smaller than those that can be accommodated in current predictive models. The linkage of these two limitations becomes the global problem of upscaling measurement data to the domain of interest. As part of the evolution of addressing this problem, laboratory experiments have been performed to physically explore permeability upscaling. The experiments make use of a gas permeameter that has been specially adapted for acquiring permeability measurements over a range of discrete sample supports subject to consistent flow and boundary conditions. Thousands of permeability measurements were made at four discrete sample supports for various rock samples. At each scale, two-dimensional maps of permeability across the surface of each rock sample were constructed. The experimental results exhibited strong, consistent trends in the mean, variance, and semivariogram of the permeability as a function of sample support. These distinct trends provide physical evidence of upscaling and insight into the factors that influence this behavior. To extend the value of the experimental results, this work uses a numerical model to reproduce the experimental data. The use of a numerical model allows for the creation of functional relationships between instrumentation, sample size, and other variables to measured permeability, while eliminating experimental and measurement error. These numerical experiments explore the relationship between tip-seal size, sample support, and rock sample size. In addition, Monte Carlo analysis on multiple heterogeneous fields at various sample supports attempts to recreate the experimental trends in mean, variance, and semivariogram measured on the different rock samples. The importance of this effort is two fold: first is it provides a means of interpreting the experimental results and secondly, it provides a foundation and means for future work in the investigation of the relationship between heterogeneity, scale and instrumentation for a broader suite of geologic materials and measurement tools.

H11G-0918 0830h POSTER

Impact of Mineral Fouling on the Long-Term Performance of Permeable Reactive Barriers

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A modeling study was conducted to investigate the impact of mineral fouling on the long-term performance of permeable reactive barriers (PRBs) using zero-valent iron. MODFLOW was used to simulate flow in an aquifer containing a PRB. RT3D was used to simulate geochemical reactions and to predict mineral fouling in the PRB. A geochemical algorithm including kinetic expressions of oxidation-reduction and mineral precipitation-dissolution was developed for RT3D. Predictions made with the model after calibration were in general agreement with field measurements reported for PRBs at Moffett Field, CA and Elizabeth City, NC. Mineral precipitation and related porosity reductions were simulated for different scenarios. Porosity reduction in PRB is found to be spatially variable as a result of flow heterogeneity. The largest porosity reductions occur between the entrance face and the mid-plane. Carbonate minerals precipitate in this region, and the amount of precipitated carbonates is closely related to the Darcy velocities. The relationship between mineral precipitation and Darcy velocity reflects the balance between the rate of mass transport and the geochemical reaction rates. Porosity reductions decrease and then level out as carbonates precipitates in front half of the PRB. Porosity reductions in the rear half of the PRB are primarily due to precipitation of ferrous hydroxide, and are not related to the Darcy velocity. The analysis shows that reduction of hydraulic conductivity and porosity by mineral fouling causes seepage velocities through the PRB to increase over time, which reduces the residence time. Shorter residence times make a PRB less effective because less time is available for contaminants to be treated. When precipitation in the reactive medium is so extensive that very large reductions in hydraulic conductivity occur in the PRB, changes in the flow paths occur, along with flow bypassing. Both the reduction in residence times caused by mineral fouling and bypassing may have a significant impact on the long-term effectiveness of PRBs.

H11G-0919 0830h POSTER

Multi-dimensional Numerical Simulation of Hydrothermal Fluid Flow and Mass Transport with Application to the Formation of Mineral Deposits

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Numerical modeling has proven an efficient predictive tool for testing, comparing and contrasting different geological hypotheses. Computer models simulating fluid flow and mass transport in complex hydrothermal systems can provide considerable insight into how these systems operate to produce economic concentration of metals. This paper presents a finite element algorithm that fully couples transient, multi-dimensional fluid flow, heat and mass (solute) transport in discretely fractured porous media. The numerical method employs non-orthogonal quadrilateral meshes and their geometry, size and orientation can be adjusted freely to best fit complex earth structures in reality, such as uneven surface topography, arbitrarily-shaped geological units, and free-oriented fractures and faults. The McArthur basin hosting the HYC deposit in northern Australia is used as a field example. Its salinity conditions are first considered, followed by other scenarios simulating the Irish-type and the US gulf coast-type salinity conditions. Numerical results indicate that salinity plays an important role in controlling hydrothermal ore-forming fluid migration. High salinity at basin floor (evaporitic conditions) strengthens the thermally-induced buoyancy force and hence promotes free convection of basinal solutions; whereas high salinity at bottom (sedimentary brines) counteracts the thermal function and thus suppresses the development of hydrothermal fluid circulation. Numerical experiments also identify the favorable hydrological conditions for the formation of the HYC deposit and evaluate the similarities and differences of modeling results between two-dimensional and three-dimensional simulations.

H11G-0920 0830h POSTER

First-order variance of solute travel time in non-stationary media

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We study solute-flux statistics in heterogeneous porous media exhibiting non-stationary covariance functions of the log-conductivity field. In particular, we investigate the cases of 1) variance scaling, in which the variance undergoes a spatial trend, 2) the blending of multiple covariance functions, including the case of zonal stationarity, 3) non-stationarity because of uncertainty in parameters describing the spatial trend of the mean log-conductivity, and 4)non-stationarity as a result of conditioning. All of these cases can be traced back to stationary covariance functions undergoing particular modifications. We calculate the first-order variance of travel time by quadratic multiplication of the discretized covariance matrix of log-conductivity fluctuations with the sensitivity matrix of the travel-time at the points of interest. The sensitivities are calculated by the adjoint-state method. The matrix-matrix multiplications are performed by Fast Fourier Transformation techniques requiring to embed the stationary counterparts of the non-stationary fields into periodic domains. The method is very efficient with respect to both computational effort and memory requirements. We apply the approach to a two-dimensional field of 1000×500 elements in which the correlation length and the variance have a spatial trend, and the parameters of the trend-model for the mean are uncertain. We include the case of conditioning on head and total-flux measurements.

H11G-0921 0830h POSTER

MIM Simulation of Cl^- and B Transport: Comparison with Measured Data from an Irrigated Field

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The mobile-immobile water (MIM) model of solute transport can provide an improved representation of solute transport in soils especially for intact soil samples or field soils. The Unsatchem model of multicomponent solute transport was upgraded to include the MIM model. A field-based test of the MIM model consisted of running Unsatchem for 45 locations within a 65 ha field in the San Joaquin Valley. Soil sampling was done for 6 depths (0-1.8 m), all locations, five different sampling periods starting in November, 1995 and ending in November, 1997. Cl^- transport was calculated for both standard uniform flow (UFM) and MIM models. The MIM model parameters, ω, the transfer coefficient, and θ_{im}, the immobile water content, were varied systematically to determine their influence on the match between the model results and measured resident chloride concentrations. The MIM model performed better than UFM with the best match occurring for the highest θ_{im} and $10^{-4} <= \omega <= 10^{-3}$.

H11G-0922 0830h POSTER

Freshwater-Saltwater Interface Configuration in a Heterogeneous Fractured Aquifer, Saturna Island, BC, Canada

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In coastal aquifers, heterogeneity due to variable fracturing introduces complexity to the configuration of the saltwater wedge and to chemical transport in the vicinity of the fresh water-salt water interfaces. Field geologic and structural mapping studies, in combination with the analysis of pumping tests and numerical simulations of flow and transport provide insight

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into the complexity of groundwater flow on the Gulf Islands in southwestern British Columbia, Canada. The islands consist of an alternating sequence of sandstone-dominant and mudstone-dominant formations, which were extensively fractured during numerous tectonic events. In contrast to typical layered porous media sedimentary aquifer systems, fine-grained rocks exhibit denser fracturing compared to coarse-grained rocks, and thus, mudstone-dominant layers and interbeds are thought to act as primary water-bearing units. Numerous pumping tests conducted in water supply wells suggest an equivalent porous media approach may be valid for representing permeability at a regional scale. A range of hydraulic conductivity (permeability) values was estimated for different geologic formations. These values were used as input in a series of models that reflect the heterogeneity of the aquifer owing to the variable fracturing of the layered aquifer system. Simulations were carried out using USGS SUTRA. Models simulations indicate that the magnitude of the permeability and the nature of layering exercise a major control of the magnitude and appearance of the freshwater-saltwater interface.

H11G-0923 0830h POSTER

Numerical Investigation of the Influence of Aquifer Heterogeneity, Reaction Kinetics, and Treatment Solution Strength on Permanganate Remediation Efficiency

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Numerical models have been developed simulating the chemical oxidation of the chlorinated solvent tetrachloroethylene using potassium permanganate. The remediation methodology modeled is the passive injection method in which the oxidant is injected to targeted locations above accumulations of dense non-aqueous phase liquids (DNAPLs) using a driven well point. Downward movement and spreading of the oxidant is caused by the initial injection pressure and by the density contrast with the groundwater. The coupled fluid flow, chemical transport, and chemical reaction equations are solved using a combination of the global implicit method and a Picard iterative scheme. The former is applied to the solution of the chemical transport and reaction equations, while the groundwater flow and chemical transport/reaction equations are solved sequentially until convergence is achieved. A partial equilibrium approach is used to model the geochemical reactions resulting from the oxidant injection. Reaction rate expressions for DNAPL dissolution and permanganate oxidation were developed based on the results of previously completed column experiments. Two and three-dimensional simulations were performed to assess the sensitivity of DNAPL destruction efficiency to oxidant concentration, reaction kinetics, and media heterogeneity. Random spatially correlated hydraulic conductivity fields were generated based on the statistical parameters of the Borden aquifer. Model results indicate that remediation efficiency was affected by solution strength, which controls the ability of the oxidant to reach the contaminant. The simulations also indicate that destruction efficiencies were insensitive to the reaction kinetics, suggesting that the DNAPL dissolution and oxidation reactions were transport controlled.

H11G-0924 0830h POSTER

Simulation of Non-Fickian Transport in Geological Formations With Variable-Scale Heterogeneities

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We study solute transport through heterogeneous media by use of continuous time random walk (CTRW) theory. Transport is governed by a joint probability density $\psi(\mathbf{s}, t)$, which characterizes tracer particle displacements $\mathbf{s}$ with associated times t. Previous work has shown the CTRW theory to be a highly effective transport framework to account for non-Fickian transport in field, laboratory and numerical experiments. Here, we introduce a number of innovations that allow for general solution of the CTRW for arbitrary $\psi(\mathbf{s}, t)$ and boundary conditions in 1-3 spatial dimensions. While in many cases, the transition times and distances are governed strictly by the flow field, they can in other cases be strongly influenced by mechanisms such as tracer diffusion into and out of "stagnant" zones of the medium and/or adsorption/desorption from the rock surfaces. All of these mechanisms, in addition to the flow field, can be specified, either implicitly or explicitly, in the determination of $\psi(\mathbf{s}, t)$, which then can account for a wide range of transport behaviors. By treating unresolved, small-scale heterogeneities (residues) probabilistically with the CTRW formalism, and large-scale heterogeneity variations (trends) deterministically, we develop and solve a Fokker-Planck equation that contains a memory term and a generalized concentration flux term. The advection-dispersion equation is a special case of this equation. The parameters defining these terms are measurable quantities. Our calculations demonstrate long tailing arising (principally) from the memory term, and effects on arrival times that are controlled largely by the generalized concentration flux term. The impact of these extensions to CTRW theory is to provide a means to calculate transport of both passive and sorbing (reactive) tracers in non-stationary geological formations.

H11G-0925 0830h POSTER

Stochastic boundary conditions to the convection-diffusion equation including chemical reactions at solid surfaces

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Simulations of surface chemical reactions may require complex non-linear boundary conditions to describe the flow of mass across an interface. Although stochastic methods do not suffer from the numerical diffusion that plagues grid-based methods, they typically lose accuracy in the vicinity of interfacial boundaries. We introduce new ideas and algorithms to account for mass transfer at reactive surfaces, with accuracies comparable to the bulk phase. We show how to introduce particles into the system with the correct distribution near the interface, as well as the correct flux through the interface. The algorithms have been tested in a channel flow, for which accurate numerical solutions can be independently calculated.

H11G-0926 0830h POSTER

Higher Order Time Integration and Discontinuous Galerkin Methods for Variably Saturated Groundwater Flow

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The numerical simulation of groundwater flow in the vadose zone continues to be a challenge for many problems of practical interest. Under commonly used constitutive relations, the governing equations can be highly nonlinear and produce sharp fronts in the solution variables for problems such as wetting phase infiltration into an initially dry medium. For a number of multiphase flow problems, the use of variable order and variable step size temporal discretizations has shown significant advantages. However, the spatial discretizations commonly used for variably saturated flow are dominated by low-order finite difference and finite element methods. Over the last decade discontinuous Galerkin (DG) finite element methods have received significant attention in a number of fields for hyperbolic PDE's and, more recently, for elliptic and parabolic problems. DG approaches are appealing for modeling subsurface flow since they can lead to velocity fields that are locally mass-conserving without the need for auxiliary variables or alternative meshes. Moreover, DG discretizations are inherently local and so well-suited for unstructured meshes and h-p adaption strategies. While some work has been done recently for multiphase subsurface flow, there are a range of issues related to the performance of DG methods for highly nonlinear parabolic problems that have not been investigated fully, particularly for air-water systems. In this work, we consider the combination of higher order adaptive time integration with DG spatial discretizations applied to variably saturated groundwater flow. We compare this approach to standard low order methods for a series of test problems and consider a number of issues including the methods' relative accuracy and computational efficiency.

H11G-0927 0830h POSTER

Use of Volume-Weighted Particles to Improve the Method of Characteristics

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In groundwater solute-transport models based on the traditional method of characteristics, advective transport is represented by moving particles that track concentration. This approach often leads to global mass-balance problems (even if the grid spacing is uniform) because in heterogeneous groundwater systems, particles can originate in cells having vastly different pore volumes and (or) be introduced (or removed) at cells representing fluid sources (or fluid sinks) of varying strengths. Use of weighted particles, in which the weights represent an appropriate proportional volume of water, implies that each particle, in effect, tracks solute mass. This assures that the new method will produce a negligible mass-balance error. This approach also leads to potential efficiencies by allowing the number of particles per cell to vary spatially–using high numbers of particles where concentration gradients are high and low numbers where gradients are low. The approach also eliminates the need for the model user to have to distinguish between "weak" and "strong" fluid source (or sink) cells. This is because the model automatically decides whether solute mass added by fluid sources in a cell should be represented by (1) new particles having weights representing appropriate fractions of the volume of water added by the source, or (2) distributing the solute mass added by the fluid source over all particles already in the source cell. The first option is more appropriate for the condition of a strong source. The latter option is more appropriate for a weak source. At sinks, decisions whether or not to remove a particle are replaced by a reduction in particle weight in proportion to the volume of water removed. A number of test cases demonstrate that the new method works well and conserves mass; largest improvements occur for cases involving strongly diverging or converging flow fields, such as are generated by one- and two-well tracer tests. The new algorithm is implemented as a solver option in the U.S.G.S. MODFLOW-GWT solute-transport model.

H11G-0928 0830h POSTER

A high-performance lattice Boltzmann implementation to model flow in porous media

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We examine the problem of simulating single and multiphase flow in porous medium systems at the pore scale using the lattice Boltzmann (LB) method. The

LB method is a powerful approach, but one which is also computationally demanding; the resolution needed to resolve fundamental phenomena at the pore scale leads to very large lattice sizes, and hence substantial computational and memory requirements that necessitate the use of massively parallel computing approaches. Common LB implementations for simulating flow in porous media store the full lattice, making parallelization straightforward but wasteful. We investigate a two-stage implementation consisting of a sparse domain decomposition stage and a simulation stage that avoids the need to store and operate on lattice points located within a solid phase. A set of five domain decomposition approaches are investigated for single and multiphase flow through both homogeneous and heterogeneous porous medium systems on different parallel computing platforms. An orthogonal recursive bisection method yields the best performance of the methods investigated, showing near linear scaling and substantially less storage and computational time than the traditional approach.

H11G-0929 0830h POSTER

Working Toward a Better Representation of Heterogeneities in Regional Groundwater Flow Systems: a Three Dimensional Approach

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Groundwater flow models have been increasingly used for multiple purposes, be it evaluation and management of water resources, evaluation of radioactive waste repositories, and others. However, a number of issues affecting the accuracy of obtained results have been a major source of concern and object of discussion over the years. Among these issues are problems associated with the nonuniqueness of model solutions, as well as proper representation of heterogeneities in different formations, particularly in complex regional systems. Another major question that remains unanswered is to whether 2D models are representative of real three-dimensional systems. Castro and Goblet (2003) have recently shown in a detailed 2D model study, conducted in the Carrizo aquifer and surrounding formations of south Texas, that regional groundwater flow systems present a high degree of freedom concerning hydraulic conductivity for models calibrated on measured hydraulic heads. In particular, Carrizo aquifer and overlying confining layer hydraulic conductivities that vary by up to two orders of magnitude lead to similar calculated hydraulic heads. We were interested in knowing if a more detailed representation of this regional system through a 3-dimensional model could place additional constraints and reduce the nonuniqueness problem associated with 2D models. The question of whether a 3-dimensional representation of the system can shed further light on to the degree of heterogeneity present in the different formations is also one of interest. Indeed, and like many other sedimentary sequences, the complexity of depositional processes for the Carrizo aquifer and surrounding formations in a mixture of deltaic, fluvial and marine settings has resulted in a high degree of lithologic heterogeneity. To address some of these questions, we proceeded to the expansion of the initial 2D model (Castro and Goblet, 2003) through successive projections of the initial mesh into the horizontal direction. The resulting 3D model covers an area of $\sim$ 7,000 Km^2, it comprises 233 planes, and more than 5 million elements (pentahedrals). Preliminary results show that a high degree of freedom to calibrate the model on hydraulic heads remains, confirming results previously obtained through 2D simulations. Thus, 3D models do not seem to contribute to a reduction of the nonuniqueness problem. By contrast, our results indicate that 3D models are particularly useful in better identifying the presence of heterogeneities within different formations. In particular, 3D simulations show evidence for the presence of variations in hydraulic conductivities not only along the x direction, where decreasing values from northwest to the southeast are observed, but also the presence of a distinctive corridor on the eastern part of the domain where hydraulic conductivity decreases more rapidly, possibly indicating the presence of thicker mixed-load mud-rich alluvial deposits in the area. Three-dimensional models can thus be particularly useful in identifying the presence of heterogeneities in complex regional groundwater flow systems, thus, allowing for a better representation of real systems. Castro M. C. and Goblet P. (2003), Calibration of regional groundwater flow models - working toward a better understanding of site-specific systems, Water Resources Research, 39(6), 1172, doi:10.1029/2002WR001653.

H11G-0930 0830h POSTER

Fate and Transport of Bacteriophage (MS2 and PRD1) During Field-Scale Infiltration at a Research Site in Los Angeles County, CA

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As the use of tertiary-treated municipal wastewater (recycled water) for replenishment purposes continues to increase, provisions are being established to protect ground-water resources by ensuring that adequate soil-retention time and distance requirements are met for pathogen removal. However, many of the factors controlling virus fate and transport (e.g. hydraulic conditions, ground-water chemistry, and sediment mineralogy) are interrelated and poorly understood. Therefore, conducting field-scale experiments using surrogates for human enteric viruses at an actual recharge basin that uses recycled water may represent the best approach for establishing adequate setback requirements. Three field-scale infiltration experiments were conducted at such a basin using bacterial viruses (bacteriophage) MS2 and PRD1 as surrogates for human viruses, bromide as a conservative tracer, and recycled water. The specific research site consists of a test basin constructed adjacent to a large recharge facility (spreading grounds) located in the Montebello Forebay of Los Angeles County, California. The soil beneath the test basin is predominantly medium to coarse, moderately sorted, grayish-brown sand. The first experiment was conducted over a 2-day period to determine the feasibility of conducting field-scale infiltration experiments using recycled water seeded with high concentrations of bacteriophage and bromide as tracers. Based on the results of the first experiment, a second experiment was completed when similar hydraulic conditions existed at the test basin. The third infiltration experiment was conducted to confirm the results obtained from the second experiment. Data were obtained for samples collected during the second and third field-scale infiltration experiments from the test basin itself and from depths of 0.3, 0.6, 1.0, 1.5, 3.0, and 7.6 m below the bottom of the test basin. These field-scale tracer experiments indicate bacteriophage are attenuated by removal and (or) inactivation during subsurface transport. To simulate the transport and fate of viruses during infiltration, a nonlinear least-squares regression program was used to fit a one-dimensional virus transport model to the experimental data. The model simulates virus transport in homogeneous, saturated porous media with first-order adsorption (or filtration) and inactivation. Furthermore, the model obtains a semi-analytical solution for the special case of a broad pulse and time-dependent source concentration using the principle of superposition. The fitted parameters include the clogging and declogging rate constants and the inactivation constants of suspended and adsorbed viruses. Preliminary results show a reasonable match of the first arrival of bacteriophage and bromide.

H11G-0931 0830h POSTER

Multi-phase Thermohaline Convection in Porous Media

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The simultaneous motion of heat and dissolved solutes by aqueous or magmatic fluids through porous or fractured media within the earth's crust is a key factor that drives many important geological processes, such as the formation of large ore deposits, cooling of newformed oceanic crust along mid-ocean ridges, metamorphism, or the evolution of geothermal systems. The motion of such crustal fluids is usually dominated by convection due to density differences within the fluids that arise from pressure, temperature and compositional variations present in the fluids. Oxygen isotope data and fluid inclusion data indicate that fluids may percolate down to 15 km depth and experience temperatures exceeding 700 ^{o}C. Although crustal fluids commonly contain various dissolved chemical components and gases, the most abundant solute is salt, i.e. NaCl. Hence, changes in the concentration of NaCl influence the density variations of crustal fluids the most. The presence of NaCl in H_2O has decisive effects on the thermodynamics and hydrodynamics of crustal fluids. NaCl-H_2O fluids can boil and separate into a high-density brine and low-salinity vapor at much higher temperatures and pressures than the critical temperature and pressure for pure H_2O. NaCl-H_2O fluids may also become saturated with respect to NaCl such that a solid NaCl phase coexists with a liquid or vapor fluid phase. Because salt advects faster than heat but diffuses slower than heat, the resulting double-diffusive and double-convective motion of salt and heat may lead to non-linear flow instabilities such as periodic or chaotic behavior. While many studies have addressed the theory of convection driven by temperature and/or salinity gradients, they were limited to a Boussinesq approximation and neglected phase separation. In this study we have numerically examined the behavior of multi-phase thermohaline convection in a porous media heated and salted from below using a novel finite element - finite volume algorithm and a new equation of state for the NaCl-H_2O system. Convection at various depths and and for temperatures up to 600 ^{o}C and salinities up to 30 wt. % NaCl was studied. The simulations show that, comparable to single-phase thermohaline convection, condition exists where the flow pattern evolves towards a convective or diffusive steady state. Flow patterns always appear to exhibit periodic behavior if the fluid starts to boil. The evolution of flow patterns, however, cannot be directly related to certain ranges of the classical descriptive dimensionless numbers such as buoyancy ratio or Raleigh number because of the complexity of the NaCl-H_2O system that does not always allow for a direct calculation of those numbers.

H11G-0932 0830h POSTER

A Numerical Study of Hydrodynamic Dispersion in Porous Media: From Tracer to High Density

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The goal of this research is to investigate the nonlinear effect of density gradients on hydrodynamic dispersion in porous media. We simulate stable upward displacements of fresh water by salt-water solutions in heterogeneous porous columns. The porous columns are heterogeneous with respect to the intrinsic permeability, which is log-normally distributed with an isotropic Gaussian correlation function. First, for the case of tracer dispersion three types of convergence were thoroughly investigated: numerical convergence, convergence of the ensemble averaging, and convergence of longitudinal dispersivity with respect to travel time. For single realizations, the observed dispersivities do not converge to the expected asymptotic value even after hundreds of correlation lengths. In the case of fluids differing in density, gravity forces stabilize the front, resulting in smaller effective dispersivities. Moreover, the uncertainty in the concentration values, averaged in the horizontal direction, reduces considerably compared to the tracer case. As a result, for high-density-gradient displacements fewer realizations are needed to obtain converged ensemble averaged results than in the tracer case.

H11G-0933 0830h POSTER

Spatially Variable Relative Permeability in Heterogeneous Multiphase Systems

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The rate of DNAPL migration through porous media is dependent, in part, on relative permeability constitutive relationships, which describe the saturation and saturation-history dependence of nonwetting phase permeability at the macroscopic scale. Gerhard and

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Kueper (2003) demonstrate that accurate prediction of DNAPL migration rates requires detailed knowledge of hysteretic relative permeability functions including their curvature and endpoints. To date, the difficulty of measuring hysteretic relative permeability functions has resulted in limited data and conflicting opinions on their shape, magnitude, and significance. This study established a database of parameters that define hysteretic relative permeability-saturation relationships for a range of porous media. Relative permeability - saturation curves were generated for sands of varying mean particle diameter using a macroscopic-scale flow cell. The relative permeability of HFE-7500 (a low solubility, low volatility, nonreactive DNAPL) was measured in a DNAPL-water system as a function of aqueous saturation and saturation history. Best-fit comprehensive constitutive relationships exhibit trends in the functional parameters that are sensitive to porous media properties. Typical numerical simulations of multiphase flow in heterogeneous porous media assume homogeneity with respect to relative permeability functions. In this study, the significance of the observed variation in the shape and endpoint locations of the relative permeability-saturation curves was examined through a series of numerical simulations. Simulations of a fixed volume DNAPL release were conducted using a spatially correlated, random permeability field. Simulations assuming homogeneity of relative permeability were compared to those employing the determined functional dependence of relative permeability on porous media properties. The results of the simulations illustrate the sensitivity of the rate of nonwetting phase migration and the ultimate extent of a DNAPL release to the spatial variability of relative permeability properties.

H11G-0934 0830h POSTER

Viscous Coupling Effects Of Two-Phase Flow In Porous Media

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Recent studies have revealed that the viscous coupling effects in immiscible two-phase flow, caused by momentum transfer between the two fluid phases, are important for a range of cases of porous medium flow. Generalized governing equations for coupled immiscible two-phase flow in porous media have been suggested through a formulation that includes two viscous coupling coefficients, in addition to the two conventional relative permeabilities. However, a quantitative understanding of the coupling effects and their dependence on factors including capillary number, viscosity ratio, and wettability still remain as open issues. In this work, we use a three-dimensional parallel processing version of a two-fluid-phase lattice Boltzmann (LB) model to investigate this phenomenon. A multiple-relaxation-time approximation of the LB equations is used in the simulator, which leads to stable results. We validate our model by verifying the velocity profiles in Poiseuilleu flow through channels. We then simulate co-current flow through a sphere-pack porous medium and determine the four generalized coefficients. Correlations of the coupling coefficients as a function of the fluid viscosities and wettability are investigated. The results are qualitatively consistent with experimental observations by Dullien and Dong(1996) and the numerical simulations of Langaas and Papatzacos(2001).

H11G-0935 0830h POSTER

Migration of conservative and sorbing radionuclides in heterogeneous fractured rock aquifers at the Nevada Test Site

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The Nevada Test Site (NTS) is the United States continental nuclear weapons testing site. The larger underground tests, including BENHAM and TYBO, were conducted at Pahute Mesa. The BENHAM test, conducted in 1968, was detonated 1.4 km below the surface and the TYBO test, conducted in 1975, was detonated at a depth of 765 m. Between 1996 and 1998, several radionuclides were discovered in trace concentrations in a monitoring well complex 273 m from TYBO and 1300 m from BENHAM. Previous studies associated with these measurements have focused primarily on a) plutonium discovered in the observation wells, which was identified through isotopic finger printing as originating at BENHAM, b) colloid-facilitated plutonium transport processes, and c) vertical convection in subsurface nuclear test collapse chimneys. In addition to plutonium, several other non-, weakly-, and strongly-sorbing radionuclides were discovered in trace concentrations in the observation wells, including tritium, carbon-14, chlorine-36, iodine-129, technetium-99, neptunium-237, strontium-90, cesium-137, americium-241, and europium-152,154,155. The range in retardation processes affecting these different radionuclides provides additional information for assessing groundwater solute transport model formulations. For all radionuclides, simulation results are most sensitive to the fracture porosity and fracture aperture. Additionally, for weakly sorbing Np, simulation results are highly sensitive to the matrix sorption coefficient. For strongly sorbing species, migration in the absence of colloids can only be simulated if fracture apertures are set very large, reducing the amount of diffusion that can occur. For these species, colloid-facilitated transport appears to be a more likely explanation for the measurements. This is corroborated with colloid-transport model simulations.

H11G-0936 0830h POSTER

The Role of Micromixing in Reactive Transport in Groundwater: Theory and Field Applications

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Advances in computational resources and numerical codes make possible the simulation of complex reactive transport problems involving biogeochemical reactions, sorption, and mineral dissolution-precipitation reactions. In aqueous transport systems, a thorough understanding of both chemical and hydrodynamic processes is required to attain a predictive capability. To address the issue of mixing, we apply the theory of micromixing, first introduced in the chemical reaction engineering literature, to the topic of reactive transport in groundwater. For all but the simplest linear kinetic and sorption models, the fate and transport of a reactive solute depends on the residence times and the details of small-scale mixing. The latter phenomenon, called micromixing, is important because it brings into close proximity chemical species that react, and it controls the local concentrations in a flowing system. Solutes with reaction rates or sorption isotherms that depend on species concentration will therefore be affected by micromixing. In this new theory, two models for micromixing are introduced, the minimum and maximum mixedness models, that provide bounds on the extent of reaction or retardation behavior within the constraints imposed by the residence time distribution (RTD) of a conservative solute in the same flow system. These mixing models prescribe the latest or earliest permissible mixing of parcels of fluid of different residence times. This construct provides bounds on the degree of reaction of a reactive solute for nonlinear rate laws or sorption isotherms. Simulation results using the bounding models show that micromixing effects are most important for nonlinear reactions, solute pulses of short duration, and systems with broad RTD curves. Use of these models is a straightforward and practical way to investigate the importance of a phenomenon for which data are seldom available, and whose impact on groundwater reactive transport models has not been studied to date in a systematic, bounding manner. An important requirement of any such new theory is to demonstrate its applicability to field data. In this study we use the theory to interpret interwell sorbing tracer data in fractured volcanic tuffs. Using conservative tracer data to establish the RTD, micromixing models are then used to interpret tracers undergoing nonlinear sorption. In addition to providing bounds that are useful in field test interpretation, the theory developed here may provide a practical way to incorporate complex reactive transport processes in contaminant mass flux models in a manner that factors the complexities of mixing into the analysis.

H11G-0937 0830h POSTER

Flow and Transport Simulation of Chemical Grouts in Porous Media: Shear Effects on Gelation

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Chemical grouting is emerging as a technology for containment of contaminant transport in porous media. When chemical grouts, such as sodium silicate, colloidal silica (CS), polyacrylamide and acrylates, are reacted with cross-linkers, the grout solution becomes viscous and eventually forms a gel or semi-solid depending up on CS concentration and the reaction time (age). However when the solution is flowing through porous media, gelation is retarded due to shear effects. CS, a stable dispersion or sols of discrete particles of amorphous silica, is adopted as grout in this study. The objective of the present study is to develop a code that can simulate the flow and transport of chemical grouts, subjected to shear, in porous media and analyse the effect of shear on gelation. Chemical grouting of colloidal silica solution into porous media is simulated by non-iteratively coupling MODFLOW (3-D groundwater flow simulation model) and RT3D (3-D multi-species reactive transport model) and adding modules for gelling and grout age. The flow field is calculated by MODFLOW. The grout age and concentration field determined by RT3D and shear rate (in terms of velocity) obtained in the current time step are used to calculate the viscosity of grout in the porous media as part of MODFLOW during the next time step. Gel viscosity is indirectly incorporated in MODFLOW by changing the hydraulic conductivity in each cell based on gel viscosity. The modified hydraulic conductivity is used to determine the flow field followed by concentration field for the next time step. The model may also be used for other chemical grouts by incorporating respective viscosity parameters. A three dimensional model is set up to simulate the grout curtain formation. After the completion of grouting simulation, the performance of the barrier is assessed in terms of its water tightness, by testing a MODFLOW problem of the same domain with different boundary conditions to obtain effective hydraulic conductivity of the curtain. The comparison of results, obtained when the shear is considered in gelation and when it is not considered, indicated that shear is an important property that needs to be incorporated in the gelation of chemical grouts. The grout injection process is found to be affected by shear.

URL: http://socr.uwindsor.ca/~boliset/agufm2003.html

H11G-0938 0830h POSTER

Lattice Boltzmann Simulations of Pulsed Field Gradient Nuclear Magnetic Resonance

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Nuclear magnetic resonance (NMR) has become a powerful well-logging tool for understanding pore space geometry of reservoir rocks in-situ. This is because, in many rocks the decay of nuclear magnetization carried by a fluid, (e.g., proton magnetization on H_2O molecules) is most strongly influenced by relaxation at the pore walls. We have developed a lattice Boltzmann computational procedure to model this process in 2-dimensions. We examine transverse magnetization by simulating Pulsed Field Gradient NMR (PFG-NMR) experiments. The decay of the transverse magnetization is described by the intermediate scattering function $G(k,t)$ from which we calculate the diffusion constant $D(t)$. Analysis of $D(t)$ at short time yields information about the surface to volume ratio S/V of the pore space. We study S/V so determined for a variety of model systems.

H11G-0939 0830h POSTER

Simulation of the Effects of Climatic Extremes on Sources of Agricultural Drain Flow, Western San Joaquin Valley, California

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Selenium loads in discharges from agricultural tile drains in the Grasslands area of the western San Joaquin Valley have exceeded regulatory thresholds after heavy rainfalls in recent years. A three-dimensional numerical ground-water flow model was developed to evaluate the effects of climatic extremes on the sources and quantities of tile drainage in the 100,000-acre Grasslands area. The model simulates transient flow in the semiconfined and confined aquifers above and below the Corcoran Clay Member of the Tulare Formation. Three-dimensional kriging of lithologic data from approximately 500 boreholes was used to approximate the spatial distribution of sediment texture in the alluvial semiconfined aquifer in eight model layers. Aquifer permeability of the semiconfined aquifer was then simulated as the weighted mean of assigned permeabilities of the variable coarse- and fine-grained lithologic end members. The confining unit and confined aquifer were each represented by a single model layer with constant permeability. Recharge and ground-water pumpage were estimated from available surface-water delivery and crop-acreage data using a water-budget model. The ground-water flow model was calibrated using hydrologic data for 1972-2000. The model is being used to evaluate causative agents that affect drain flows in the Grasslands area and to identify flow paths and contributing areas for water collected by these drains.

H11G-0940 0830h POSTER

Stochastic Modeling of Colloid-Contaminant Transport in Physically and Geochemically Heterogeneous Porous Media

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A two-dimensional model of contaminant transport in the presence of colloids is developed for heterogeneous porous media. The numerical solution of contaminant and colloids concentrations is obtained by using finite differences with a third-order total variance-diminishing (TVD) scheme for the advection terms. The model accounts for both spatially varying conductivity (physical heterogeneity), and spatially varying distribution coefficients (geochemical heterogeneity). Geochemical heterogeneity is considered for the contaminant sorption coefficient, colloids sorption (attachment) coefficient, or both. The analysis is performed within a stochastic framework using a Mont Carlo simulation technique. The model is used to investigate the impact of both physical and geochemically heterogeneity on the uncertainty associated with the contaminant movement. The effect of correlation between physical and geochemical variability is also investigated. Spatial moment and concentration variance are presented for the colloids

H11G-0941 0830h POSTER

Solution of Transient Flow in Heterogeneous Media Using Analytic Elements in Laplace Space

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A Laplace transform analytic element method (LT-AEM) is described and illustrated for the solution of transient flow problems in porous media. The solution is entirely general, retaining the mathematical elegance (in the Laplace domain) and computational efficiency of the AEM while being amenable to parallel computation. It is especially well suited for problems in which a solution is required at a limited number of points in space-time, and for problems involving materials with sharply contrasting hydraulic properties. We have illustrated the LT-AEM on transient flow through a uniform confined aquifer with circular inclusions of contrasting hydraulic conductivity and specific storage. Our results compare well with published analytical solutions in the special case of radial flow. A remaining challenge is to derive analytical expressions for additional two- and three-dimensional elements such as line sinks, doublets and dipoles satisfying the modified Helmholz equation that arises from LT-AEM.

H11G-0942 0830h POSTER

Numerical Simulations Used to Test the Effects of Lithology and Recharge Rates on Temperature Profiles Beneath Ephemeral Streams in Southern Arizona

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Recent studies conducted by the U.S. Geological Survey (USGS) have shown that deep temperature profiles, measured before and after controlled infiltration, can be used to determine infiltration rates within the unsaturated zone. In this investigation, we extend this method to deep-temperature profiles measured before and after streamflow events in two boreholes located in the channel of an ephemeral stream in southern Arizona to infer recharge rates from short-term flow events. The deep-temperature profiles were analyzed to determine vertical fluxes with the use of a one-dimensional, forward numerical computer model. Temperature profiles were collected in boreholes located in Rillito Creek, in Tucson, Arizona. The two sites are about 6 kilometers apart and were selected on the basis of their lithology and hydraulic characteristics. The lithology at the upstream site is primarily homogeneous coarse sand, and the water table is approximately 37 meters below land surface. The initial response of the water table lags the onset of streamflow by about 2 weeks, and the water-level changes are as much as a few meters depending on the magnitude of the streamflow. The lithology at the downstream site is primarily homogeneous sand, with the exception of a clay layer at 12 meters below land surface, and the water table is approximately 41 meters below land surface. The initial response of the water table at the downstream site is rapid, occurring within about a day of streamflow. The magnitude of the water table response, however, is typically less than a meter and usually on the order of a few centimeters. Basic hydrologic models were developed for each site using hydraulic and thermal properties inferred from borehole core samples and cuttings, and from laboratory-determined hydraulic parameters. Water-table elevations and stream stages were used to define hydrologic boundary conditions. Field-measured temperature profiles were used to calibrate the models. The basic numerical model constructed for each site was used to examine the effect lithology has on the recharge rate and deep-temperature profiles.

H11G-0943 0830h POSTER

Monte-Carlo Simulation of Bacterial Transport in a Heterogeneous Aquifer With Correlated Hydrologic and Reactive Properties

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It has been widely observed in field experiments that the apparent rate of bacterial attachment, particularly as parameterized by the collision efficiency in filtration-based models, decreases with transport distance (i.e., exhibits scale-dependency). This effect has previously been attributed to microbial heterogeneity; that is, variability in cell-surface properties within a single monoclonal population. We demonstrate that this effect could also be interpreted as a field-scale manifestation of local-scale correlation between physical heterogeneity (hydraulic conductivity variability) and reaction heterogeneity (attachment rate coefficient variability). A field-scale model of bacterial transport developed for the South Oyster field research site located near Oyster, Virginia, and observations from field experiments performed at that site, are used as the basis for this study. Three-dimensional Monte Carlo simulations of bacterial transport were performed under four alternative scenarios: 1) homogeneous hydraulic conductivity (K) and attachment rate coefficient (Kf), 2) heterogeneous K, homogeneous Kf, 3) heterogeneous K and Kf with local correlation based on empirical and theoretical relationships, and 4) heterogeneous K and Kf without local correlation. The results of the 3D simulations were analyzed using 1D model approximations following conventional methods of field data analysis. An apparent decrease with transport distance of effective collision efficiency was observed only in the case where the local properties were both heterogeneous and correlated. This effect was observed despite the fact that the local collision efficiency was specified as a constant in the 3D model, and can therefore be interpreted as a scale effect associated with the local correlated heterogeneity as manifested at the field scale.

H11G-0944 0830h POSTER

Temporal Scaling and Numerical Simulations of The Hydraulic Head and River Baseflow

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Spectral analyses were conducted for hourly hydraulic head (h) data observed over a four-year period at seven monitoring wells in the Walnut Creek watershed, Iowa. The log power spectral density of the hydraulic head fluctuations verse log frequency (f) at all seven wells is shown to have a distinct slope, indicating temporal scaling in the time series of water level fluctuations. The fractal dimension (D) of the time series varies from well to well, and the spectrum for the average h over all seven wells has a fractal dimension of 1.55 and Hurst coefficient of 0.45. The log power spectral density of baseflow in the Walnut Creek and other four watersheds verse log f is shown to have two distinct slopes with a break in scaling at about 27 days. It is shown that the groundwater recharge process in a basin can be estimated from a head spectrum based on existing theoretical results. Hydraulic head in an aquifer may fluctuate as a fractal in time in response to either a white-noise or fractal recharge process, depending on how quickly the hydraulic head responds to recharge events and the physical parameters of the aquifer. The recharge process at the Walnut Creek watershed is shown to have a white-noise spectrum. The observed fluctuations of the head and baseflow are simulated numerically with a transient groundwater flow model in which the recharge rate and hydraulic conductivity are treated as a random process and/or field.

H11G-0945 0830h POSTER

Comparison of Three-Dimensional Local Grid Refinement Methods For Simulating Stream-Aquifer Interactions

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Many groundwater models require a fine grid discretization in limited areas of interest. One way of achieving greater grid resolution in a limited area of the domain is to use a method of local grid refinement. Unfortunately, accurate, fully three-dimensional local grid refinement methods are weak or unavailable in commonly used block-centered finite-difference models of groundwater flow. This work extends the previously developed two-dimensional, iterative shared-node local grid-refinement method of Mehl and Hill (2002) to three dimensions. To interpolate head boundary conditions onto the interface of the three-dimensional local grid, a new numerical interpolation technique was developed that retains the physics of the regional-grid flow. The iterative solution method adjusts the heads and fluxes of both grids to achieve equilibrium. This introduces some error into the final solution, however these errors are less than if no iterations are performed, as in a one-way coupled telescopic mesh refinement (TMR) approach. Three-dimensional, locally refined simulations of stream-aquifer interactions using the iterative shared-node method resulted in errors in stream flux less than 2%, while commonly used one-way coupled TMR resulted in errors in stream flux greater than 10%.

H11G-0946 0830h POSTER

Numerical solutions for fractal radial flow problems

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Fractional advection-dispersion equations, that model flow of a contaminant in an aquifer, are typically formulated in Cartesian coordinates. In situations where wells may act as either sources or sinks in these models, a radial model provides a more natural framework for deriving the resulting differential equations and the associated initial and boundary conditions. We provide the fractional radial flow advection-dispersion equations. Numerical models and solutions of these problems, using the finite difference approach, are provided. The behavior of the numerical approach, its accuracy and stability are examined. The hallmark of a spatially fractional-order dispersion term is the rapid transport of solute compared to the classical Fickian model. The results from the numerical method for the fractional radial flow equations are able to reproduce the early breakthrough in radial tracer tests from field experiments.

H11G-0947 0830h POSTER

Eulerian-Lagrangian Localized Adjoint Methods for Nonlinear Reactive Transport

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We consider Eulerian-Lagrangian Localized Adjoint Methods (ELLAMs) applied to nonlinear model equations governing solute transport and sorption reactions in porous media. Solute transport in the aqueous phase is modeled by standard advection and diffusion processes while sorption reactions are modeled with a local equilibrium assumption and the nonlinear Freundlich equilibrium isotherm. In this work we focus particularly on the case when the Freundlich isotherm is not Lipschitz continuous. The nonlinear parabolic equation that results can yield solutions with self-sharpening fronts under certain choices of boundary and initial data. ELLAMs were designed to circumvent the stability and accuracy limitations of standard methods when applied to advection-dominated transport equations with sharp fronts, and are thus a natural choice for this application. Indeed, for a wide range of problems in subsurface flow and transport, ELLAMs have produced accurate, non-oscillatory results for significantly larger time steps and coarser grids than is possible with standard methods such as Galerkin finite elements. The particular form of the nonlinearity in the reactive transport model we study presents a number of difficulties, which we address in the context of ELLAMs. We will present our implementations of ELLAMs to the reactive transport model as well as numerical comparisons to standard Galerkin finite elements and finite difference solutions.

H11G-0948 0830h POSTER

Mountain-Scale Transport of Radioactive Solutes and Colloids Through the Unsaturated Zone of Yucca Mountain, Nevada

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The US Department of Energy is actively investigating the technical feasibility of permanent disposal of high-level nuclear waste in an appropriate repository to be situated in the unsaturated zone (UZ) at Yucca Mountain (YM), Nevada. The objectives of this study are to evaluate the transport of radioactive solutes and colloids under ambient conditions from the potential repository horizon to the water table and to determine processes and geohydrologic features that significantly affect radionuclide transport. The radionuclide transport model considers the site hydrology, and the effects of the spatial distribution of hydraulic and transport properties in the fractured rocks of the YM subsurface. Several radionuclides (solutes and colloids) with varying properties are investigated. The results of the study indicate that the most important factors affecting radionuclide transport are the subsurface geology and site hydrology, i.e., the presence of faults (they dominate and control transport), fractures (the main migration pathways), and the relative distribution of zeolitic and vitric tuffs. Radioactive decay, diffusion from the fractures into the matrix, and subsequent sorption (for solutes) or filtration (for colloids) onto, are the main retardation processes. For solutes, arrival times at the watertable increase with the sorption distribution coefficients of the various species, and may have to account for contributions from the decay daughters of certain radionuclides. Changes in future climatic conditions can have a significant effect on transport, as increasing infiltration leads to faster transport to the water table. The transport of colloids is strongly influenced by their size (as it affects diffusion into the matrix, straining at hydrogeologic unit interfaces and transport velocity) and by the fracture attributes.

H11G-0949 0830h POSTER

Modeling One-Dimensional Transport of Arsenate Through Iron Oxide-Coated Sands

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The fate and transport of metals in groundwater are commonly controlled to a significant extent by sorption reactions occurring at aqueous/solid interfaces. Traditionally, isotherms have been preferred in the groundwater literature to model sorption, since the incorporation of these models into groundwater transport equations is relatively straightforward. Alternatively, surface complexation models (SCMs) present a more mechanistic approach to sorption modeling. Due to their relative complexity and parameter requirements, however, their application in groundwater transport models has been more limited. In this work, the influence of sorption model selection on the behavior of transport predictions is explored using two alternative numerical models. Results are compared for predictions of arsenate transport experiments in columns packed with iron oxide-coated sands. The first modeling approach incorporates experimentally determined batch isotherms, that describe sorption of arsenate under constant pH conditions, in a mass-conservative finite element transport code developed for this study. In the second approach, the hydrogeochemical transport code PHREEQC-2 is employed to simulate transport of arsenate using a SCM sub-model. This SCM is based upon a self-consistent set of surface complexation parameters, developed from available titration data for arsenate sorption onto the iron oxide surfaces. Model predictions are compared with physical measurements of arsenate breakthrough under varying pH conditions. Preliminary results illustrate the promise of the SCM modeling approach, suggesting that independent batch sorption measurements can be used, within the framework of the SCM, to produce a more versatile transport model, capable of accounting accurately for temporal and spatial variations in geochemical conditions.

H11G-0950 0830h POSTER

Simulation Of An Alcohol Flushing Assisted Bioremediation System

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Bioremediation of residual DNAPL in the subsurface can be a time-consuming process due to the relatively slow mass transfer of NAPL contaminant species from the NAPL phase into the aqueous phase. It has been shown that alcohol flushing assists in raising the solubility of NAPL, thereby increasing its speed of deliverance into the aqueous phase. However, on its own, alcohol flushing does not alleviate the problem of what to do with the contaminant once it has been solubilized. It has been proposed that linking these two remediation techniques can generate an optimal system with the alcohol improving the transfer of NAPL into the aqueous phase where, in conjunction with injection of oxygen and nutrients, it can then be biodegraded readily by the existing microbes. To test this hypothesis, an existing multiphase flow and transport code was altered to accommodate the equations necessary to represent the proposed system. The species being modeled include two NAPL contaminants, oxygen, nitrogen, microbes and alcohol. Bioremediation was modeled using oxygen and nitrogen limiting Monod reaction kinetics. Constitutive relationships for the effect of the alcohol on solubility and mobility of NAPL were also added.

H11G-0951 0830h POSTER

Optimal Search Strategy for the Definition of a DNAPL Source

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Locating a DNAPL source is very difficult because of its filamentous nature and small size. This paper addresses the issue of identifying and delineating DNAPL at its source, using an optimal search strategy. A search algorithm that utilizes on-site groundwater concentration data is used to define an area where the concentration of one or more soluble DNAPL species exceeds that concentration deemed indicative of DNAPL in close proximity. The search algorithm is used to define how to achieve an acceptable level of accuracy with the least possible number of water quality samples. This computer-based strategy uses groundwater flow and transport modeling under uncertainty and a linear Kalman filter. The hydraulic conductivity realizations are generated using the Latin Hypercube Sampling technique. This search algorithm provides information about both the source location and the contaminant plume simultaneously and in real time.

H11G-0952 0830h POSTER

Determination of a Permeability-depth Curve for the Oregon Cascades Employing Numerical, Analytical, and Statistical Methods

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We employ analytical and numerical models as well as statistical methods and signal processing techniques to study both pore-fluid pressure diffusion and coupled groundwater and heat transfer in the subsurface. Both processes are used to infer the large-scale vertical permeability distribution and other hydrogeologic parameters in the Oregon Cascades volcanic arc. Multiple temperature-depth profiles and their deviations from a linear(conductive) relationship provide insight into advective heat transfer and related groundwater flow patterns and velocities. In addition, the coupled modeling approach provides background heat-flow rates of $0.080 < H < 0.130$ W/m^2 for the study region where heat flow is otherwise typically masked by cold groundwater recharge. We also infer regional scale groundwater recharge rates of about 1 m/year. Statistical, Monte Carlo, and signal processing techniques are used to investigate if seasonal groundwater recharge due to spring snow melt enhances earthquake occurrence after a pressure-diffusion related time lag, during summer. We find statistically-significant cross correlations between groundwater recharge and earthquake occurence at Mt. Hood, Oregon, with a time lag of about 151 days. This phase lag and a mean earthquake depth of about 4.5 km imply an average permeability of about 10^{-15} to 10^{-14} m^2 for a depth range of about $2 < z < 5$ km. Combining the heat-advection study, the hysroseismicity study, and other investigations allows us to infer permeability, k, as a function of depth, z. We suggest approximately log(k) = -13 to log(k)= -18.3 m^2 for z=0 to z=12 km, respectively, for the Oregon Cascades. Our results agree with values compiled by Manning and Ingebritsen (Rev. Geophys., 1999) for continental crust in general. However, we suggest an exponential k(z)-curve for $z < 0.8$ km and a power law relationship for $z > 0.8$ km.

H11G-0953 0830h POSTER

Space-Time Adaptive Solution of Richards' Equation

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Efficient, robust simulation of groundwater flow in the unsaturated zone remains computationally expensive, especially for problems characterized by sharp fronts in both space and time. Standard approaches that employ uniform spatial and temporal discretizations for the numerical solution of these problems lead to inefficient and expensive simulations. In this work, we solve Richards' equation using adaptive methods in both space and time. Spatial adaption is based upon a coarse grid solve and gradient-based error indicators, while the spatial step size is adjusted using a fixed-order approximation. Temporal adaption is accomplished using variable-order, variable-step-size approximations based upon the backward difference formulas up to fifth order. Since the advantages of similar adaptive methods in time are now established, we evaluate our method by comparison with a uniform spatial discretization that is adaptive in time for four different test problems. The numerical results demonstrate that the proposed method provides a robust and efficient alternative to standard approaches for simulating variably saturated flow.

H11G-0954 0830h POSTER

Delineation of Free Convection Pathways in a Heterogeneous Low-permeability Unit

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Study of free convection in heterogeneous geologic units poses challenges to hydrogeologists in solute transport modeling and in predicting the effective Rayleigh Number, which is the ratio of bouyancy driving forces to the viscous resistance to flow and the diffusive dissipation of solutes. Downward convection of dense fluid through heterogeneous low-permeability strata follows preferential pathways of groundwater flow and contaminant transport. In this study, the concepts of boundary layer and critical Rayleigh number are used to delineate free convection pathways in a suite of permeability field realizations. A boundary layer is formed when the upward evaporative flux stabilizes the downward groundwater movement in a saline lake environment. Onset of free convection occurs when the effective Rayleigh Number (NRa) exceeds certain value, the critical Rayleigh Number, The threshold value of permeability that permits free convection in a system where denser fluid overlies a less-denser fluid is approximately 10-14 m2 for a boundary layer of 0.315 m and a NRa of 8.5 to 10. Invasion percolation theory (an invasion process that proceeds along a path of least resistance) is used in the searching algorithm that identifies the paths for free convection in 60 different heterogeneous permeability fields. By comparing with modeling results of variable density flow through these different k-simulations, the delineation of pathways provides insight into predicting the occurrence of free convection, groundwater flow, and solute distribution in heterogeneous low-permeability systems. Individual long and wide pathways promote free convection, which indicates that local heterogeneity controls solute transport. Vertically continuous zones of high permeability form pathways that support the initiation and growth of freely-convecting solute plumes.

H11G-0955 0830h POSTER

Rare Earth Element Speciation Along Groundwater Flow Paths in Two Different Aquifer Types (i.e., Sand vs. Carbonate)

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Groundwater samples were collected in two different types of aquifer (i.e., Carrizo sand aquifer, Texas and Upper Floridan carbonate aquifer, west-central Florida) to study the concentrations, fractionation, and speciation of rare earth elements (REE) along groundwater flow paths in each aquifer. The solution complexation of REEs in these two aquifers was modeled using Humic Ion-Binding Model V. The results of the REE speciation modeling indicate that the solution complexation of REEs is controlled by pH, alkalinity, and DOC concentration. Because DOC is low (less than 0.65 mg/L) in Carrizo aquifer, organic complexation of REEs is not significant in these groundwaters. For LREEs, LnCO3+ and/or Ln(CO3)2- are the dominant species when pH is above 7.0, but when pH is below 7.0, besides LnCO3+, Ln3+ and LnSO4+ are also significant and their importance increases with decreasing pH. For HREEs, LnCO3+ and/or Ln(CO3)2- are always the dominant species, however, LnPO4o is important in some groundwaters. The similar general patterns of inorganic solution complexation of the REEs are also observed in groundwaters from the Upper Floridan aquifer. However, because of the relatively high DOC concentrations measured in the Floridan groundwaters, organic complexation of REEs, especially LREEs, is also predicted to be significant in some groundwaters. Linear correlation coefficients for total REE, Nd, Gd, and Yb concentrations, and (Yb/Nd)SN vs. pH, CO3, DOC, SO4, Fe, and Mn indicate that for the Carrizo groundwaters, REE concentrations are not correlatd to any of these factors. However, (Yb/Nd)SN is inversely related to pH and the [CO32-] concentration of these groundwaters. Because REE speciation is strongly related to pH and the [CO32-] concentration, it is reasonable to expect that REE solution complexation plays a greater role in fractionating REE than controlling absolute concentrations in the Carrizo Sand aquifer. In Upper Floridan aquifer, LREE concentrations are positively correlated to DOC and inversely related to [CO32-] and pH. MREEs do not correlate with DOC but show a weakly inverse relationship to [CO32-] and pH. The HREEs are inversely related to DOC and positively correlated with the [CO32-] concentration and pH. (Yb/Nd)SN is positively related to pH and [CO32-] and negatively related to DOC in the Floridan groundwaters. Thus, in contrast to our observations for the Carrizo Sand aquifer, REE solution complexation appears to affect both REE fractionation patterns and their absolute concentrations for groundwaters of the Upper Floridan aquifer.

H11G-0956 0830h POSTER

Fully Determined Fluid Velocity Fields for Complex 2D Media with Multi-Scaled Heterogeneity.

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Numerical schemes for fluid flow in complex rock geometries rely on comparison with existing empirical data for their validation. When available, these data are generally limited to non-unique, bulk measurements of properties such as hydraulic conductivity and permeability and are not adequate to fully validate complex numeric schemes. Here we describe an experimental system which has been developed to fully quantify velocity fields throughout synthetic two-dimensional heterogeneous media. We first create a digital image with the desired combination of matrix and fracture porosity, incorporating detail over several orders of magnitude. This image is then translated into a physical medium using either stereolithography or wire EDM machining. The result is a flow cell comprising two transparent plates with a thin section of material, identical to the digital image of the medium, between them. In order to observe and measure fluid velocity, the flow cell is integrated in a purpose built experimental rig and a controlled flow of fluid, seeded with neutrally dense micro-particles, is induced. Local velocities are then measured throughout the medium with a high-resolution digital particle image velocimetry system. Simultaneously fluid flow is simulated in these geometries using a variety of numerical schemes. Direct comparison is then made between measured and predicted velocity fields for geometries that include complex combinations of matrix and fracture flow, investigations of the effect of fracture roughness on the flow field and scaling laws in the region of the percolation threshold. Results and conclusions are presented.

URL: http://www.science.ulst.ac.uk/crg/geophys/research/nerc_fluids.htm

H11H MCC: 3022 Monday 1020h

Observations and Modeling of Land Surface Hydrological Processes II

(joint with A, B, C)

Presiding: **V Lakshmi,** University of South Carolina**; A Cahill,** Texas A&M University

H11H-01 1020h

Demonstrating the Importance of "Good" Models of Land Surface Hydrological Processes

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To reduce the uncertainty in the prediction of land surface climates, , the Atmospheric Model Intercomparison Project (AMIP) Diagnostic Subproject 12 (DSP 12) and the Project for Intercomparison of Land-surface Parameterisation Schemes (PILPS) have analysed dependence of climate simulations on the land-surface schemes (LSSs). This analysis has comprised three efforts: (i) proving that LSSs matter in coupled simulations; (ii) investigating whether improvements in LSSs have occurred over time; and (iii) searching for novel means of validating LSS predictions. In the first, Irannejad *et al.* (2003) introduce a novel method for evaluating the dependence of 19 AMIP AGCMs' LH on the LSS by excluding the impact of the atmosphere. Pseudo LSSs (PLSSs) for LH in the form of multi-variable linear models expressing mean monthly LH as a function of atmospheric forcing are developed. Analysis over three large and climatically diverse river basins shows estimates of mean annual LH from the PLSSs agreeing well with the AGCMs' simulations. RMS errors range from 0.4 to 2.2 $W\ m^{-2}$ depending on the region and the AGCM. When the PLSSs are driven by single atmospheric forcings, different LSSs behave differently, and the variability of mean annual LH among AGCMs increases. The second strand of our investigation uncovered a clear generational sequence of land-surface schemes: first generation 'no canopy'; second generation 'SiBlings'; and 'recent schemes'. We conclude that although continental surface modelling has improved over the last 30 years, full confidence remains elusive, in part due to tuning to available observations. Finally, we show that stable water isotopes challenge predictions of evaporation and condensation processes. These three-pronged findings prove that LSSs are important to AGCM and coupled climate predictions; demonstrate that new, or changed, land-surface components increase diversity among simulations; underline the need for validation data and also challenge current parameterisations with novel observations.

H11H-02 1035h

Water Availability for the Western United States: The Role for Science

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In the American West, the availability of water has become a serious concern for many communities and rural homeowners. Water of acceptable quality is harder to find because local sources are allocated to prior uses, depleted by overuse, or diminished by drought stress. Some of the inherent characteristics of the West add complexity to the task. The most rapidly growing States in population are in the Southwestthe most arid region on the continent. There is evidence that the climate is warming, which will have consequences for the Western water supplies, such as increasing minimum streamflow and earlier snowmelt events in snow-dominated basins. Endangered species are disproportionately represented in the Western States, and water availability now means sustaining riparian ecosystems