H62A-0833 1330h POSTER

An Experimental Study of Small-Scale Drop Size Distribution Variability: Comparison with Radar Observations

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The main goal of the X-Band Polarimetric Radar on Wheels (XPOW) study is aimed at exploring the advantages of dual-polarized X-band radar systems in radar rainfall estimation. However, the design of the experiment readily facilitates investigation of variability of reflectivity at small spatial scales, specifically at scales smaller than typical NEXRAD pixels. During this two-month field experiment in Iowa City, Iowa, high-resolution polarimetric radar data from the National Observatory of Athens mobile dual-polarization X-band radar were collected over a well-instrumented ground site. The site included four disdrometers, a vertically pointing X-band Doppler radar, and several dual-gauge tipping bucket rain gauge platforms in an area about 1.0 km by 1.5 km. These instruments were used to both augment and validate the data collected by the polarimetric radar, located approximately 8 km away. The disdrometers included a two-dimensional video disdrometer, an impact-type disdrometer, a bistatic radar-based disdrometer, and an optical disdrometer. The area in which these instruments were deployed corresponds to the size of one pixel from the Davenport NEXRAD, located 80 km east of Iowa City, allowing exploration of the variability of reflectivity at such scales. We present quantitative comparisons of reflectivity and rain rates retrieved from the XPOW radar, the Davenport NEXRAD and the disdrometers. We focus primarily on characterizing the variability of the XPOW and disdrometer observations via standard methods such as scatterplots and correlation analysis, in addition to considering gradients of reflectivity.

H62A-0834 1330h POSTER

Rainfall Intensity and Drop Size Measurements with Polarimetric X-band Radar

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Most studies for developing quantitative, scanning radar estimates of rainfall have been conducted using 3-GHz (S-band, 10-cm wavelength) weather surveillance radar systems, in order to avoid attenuation effects that significantly impair reflectivity (Z) measurements at shorter wavelengths. However, the recent extension of polarimetric differential phase methods to shorter-wave systems, including X-band (9 GHz, 3-cm), now allows these generally smaller radars to also be used for quantitative rain estimations. Differential phase offers rainfall estimates that are independent of reflectivity data, as well as a way to adjust for partial attenuation effects in X-band reflectivity data. Rainfall intensity and accumulation measurements based on specific differential phase (KDP) alone offer many advantages over traditional reflectivity-based rain estimates. In this study, rain observations obtained with a polarimetric X-band scanning radar are processed with algorithms that estimate rain rate using differential phase, reflectivity, and a combination of the radar's measurements of differential phase with attenuation-corrected reflectivity and differential reflectivity (ZDR). The attenuation-corrected ZDR measurements are also used to estimate mean raindrop diameter. Demonstration measurements were obtained at Wallops Island, Virginia, in 15 storms with rain rates ranging from very light to heavy. The radar estimates are compared with measurements by tipping bucket rain gauges and raindrop disdrometers located a few kilometers away. It was found that the combined Z-ZDR-KDP estimator provided the closest agreement with gauge measurements, having an overall 22 per cent relative standard deviation of differences. The attenuation-adjusted ZDR estimates of mean drop diameter also compared well with the disdrometer measurements.

H62A-0835 1330h POSTER

Development of Research Quality Radar-Rainfall Datasets for Hydrologic Studies

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Although there is plethora of radar-rainfall data readily available, there is lack of well-documented research quality data sets over land. Two well-known and extensively studied oceanic radar-rainfall data sets are the GATE and TOGA COARE. Both are well-documented and provide high space and time resolution data. These data sets and the efforts that went into the product development are described in scientific literature. Over land the most popular data sets are the operational products generated by NOAA from the network of WSR-88D radars. Some products combine data from radars and rain gauges but leave out little information for an independent evaluation of the quality of the product. Other long-term data sets, such as the Mississippi River Basin five-year long data sets created under the auspices of the GCIP program are the results of trade-offs between feasibility and accuracy. Data sets developed for TRMM validation are limited to the tropics.

Recognizing the need for high-resolution flexible radar data sets for use in hydrologic studies of flood generation mechanism, land-atmosphere-vegetation interactions, and scaling of rainfall processes, we are developing a system that will provide such data sets. The essential characteristics of the system are: (1) ability to effectively remove non-precipitation echo; (2) flexibility in specifying the algorithm that converts the observable (i.e. radar reflectivity) into the variable of interest, i.e. rainfall on the ground according to some specific criteria; and (3) ability to describe the main features of the product uncertainty. Our system, based on the WSR-88D level II reflectivity data will possess these characteristics. It is efficient enough to generate a large (one year or more) data set of rainfall products at the resolution limited only by the raw radar data. It incorporates the quality controlled rain gauge information via a calibration process. The calibration criteria allow trade-off between different error characteristics. We present examples of the products generated using the system from data from Kansas, Oklahoma, and Iowa.

H62A-0836 1330h POSTER

Hydrometeorological Analysis of Flash Floods in the Baltimore Metropolitan Region

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We examine flood response in the Baltimore metropolitan region using high-resolution radar rainfall estimates and a distributed hydrologic model. Analyses focus on organized convective systems during the warm season. These events become an increasingly important element of regional flood hydrology with urbanization. Radar rainfall estimates are based on volume scan radar reflectivity observations and have a spatial scale of 1 km and time scale of 5 minutes. Discharge observations are taken from 26 stream gaging stations in the Baltimore metropolitan area and have time increments of 5 - 15 minutes. Stream gaging stations represent basins with drainage areas ranging from less than 0.1 square kilometers to more than 100 square kilometers and land use ranging from highly urbanized to forested. Analyses illustrate the utility of high-resolution radar rainfall estimates for quantitative hydrologic analyses of flood response in an urbanizing region. In particular, hydrologic model analyses are used to illustrate the potential for enhanced integration of radar rainfall estimates into flash flood forecasting and information systems.

H62B MCC: Hall C Saturday 1330h

Numerical Simulations of Flow and Transport in Heterogeneous Subsurface Systems Posters

Presiding: **Y Zhang,** University of Iowa**; A Tompson,** Lawrence Livermore National Laboratory

H62B-0837 1330h POSTER

A numerical approach to simulating spatially variable anisotropy, with applications in two hydrogeologic settings

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We have implemented a new method (Lee et. al., 1999) for incorporating spatially variable anisotropy in a control volume finite element setting. Flux and pressure (or head) continuity is enforced at control volume interfaces while utilizing the full permeability tensor. We describe in detail the implementation of the method. The new method has performed very well in basin scale simulations.

We present preliminary results for model applications in northern New Mexico and at Yucca Mountain, Nevada.

An important aquifer unit in the Española Basin, Northern New Mexico, is a basin-fill sedimentary rock which is strongly anisotropic due to relatively fine-scale bedding structures. Both the dip and strike of the beds vary significantly spatially. We present simulations comparing predicted heads and discharge to rivers for three conceptual models of heterogeneity: isotropic, anisotropic (orthogonal to the grid), and anisotropic (oblique to the grid and variable in space).

At Yucca Mountain, fractures produce anisotropy which is not aligned with the principal axes of the numerical grid. The new method allows for accurate representation of these effects in those parts of the domain where the anisotropy is present and naturally reverts to a simpler differencing scheme elsewhere. Thus, the method is computationally efficient.

H62B-0838 1330h POSTER

Choices of scale and process complexity in hillslope models

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Water flow in the subsurface is a significant process participating in the response of watersheds to a variety of events, such as rainfall or irrigation. Accurately representing flow in a well-chosen fundamental geological unit of the watershed's subsurface environment is, therefore, a precondition for accurately representing the watershed response as a whole. In this work we focus on hillslopes as the fundamental geological units

of the watershed's subsurface processes, and investigate the effect of modeling decisions about scale and process complexity on the representation of hillslope hydrological response. As porous medium continuum scale models can include a high degree of process complexity and provide resolution at scales much smaller than hillslopes we first formulate a model of the hillslope unit based on the theory of porous medium continuum dynamics that incorporates the irregular three dimensional geometry of the hillslope, nonlinear and hysteretic submodels of multiphase flow processes, and the heterogeneity and anisotropy of soil parameters. We then compare the behavior of our complex, high-resolution hillslope model to a variety of simplifications in order to understand the degree to which the hillslope representation can be simplified while retaining sufficient resolution for watershed modeling applications.

H62B-0839 1330h POSTER

Effects of Field-Scale Heterogeneity on Plume Behavior and Remediation in Alluvial Aquifer Systems

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This study examines the effects of various field-scale geologic attributes on plume behavior and efficacy of remediation. Using transition probability geostatistical simulation and core descriptions available from the Lawrence Livermore National Laboratory site, we generate a spectrum of unconditional realizations representing alluvial aquifer systems with different degrees of interconnectedness (connectivity) and volumetric abundance of different facies. Both statistical and spatial measures are used to characterize degree of connectivity of high-K bodies (channel facies) in simulated K fields. The random-walk particle method is used to simulate conservative mass transport under steady-state flow conditions. Spatial and temporal analyses of simulated contaminant plumes explore the relative sensitivity of plume behavior to style of geologic complexity. Two geologic settings (one with high-K embedded in low-K materials and the other with low-K embedded in high-K) are used to evaluate a set of remedial methods for different proportions and corresponding degrees of connectivity. The remedial scenarios include ambient transport (no remediation), pump-and-treat remediation with three different rates of extraction, and two methods of enhanced remediation. Results show a percolation threshold for high-K channel bodies between channel fractions of 0.08 and 0.18. Further, as the volume fraction of high-K channel facies increases (from 0.08 to 0.68), simulated plumes show decreasingly anomalous behavior (e.g., mass holdback resulting in tailing). Results show that the architecture of high permeability units and preferential flow paths are important in controlling groundwater flow in fine-grain dominant systems, and relatively less important in coarse-grain dominant systems. Remedial experiments show total mass remaining in low-K materials after the application of remediation is always greater than the total mass in high-K channel facies at the channel facies volume fraction of 0.18. In contrast, at a channel facies volume fraction of 0.58, the total mass remaining in high-K channel facies is greater than that remaining in low-K materials. Results show that back diffusion of mass from low-K to high-K material during and after remedial efforts affects the efficiency of a remedial method more significantly in the low-K material dominant alluvial systems.

H62B-0840 1330h POSTER

Nonideal Transport of Solute and Colloidal Tracers Through Reactive Zeolite/Iron Pellets

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We conducted solute and colloidal tracer tests in laboratory columns to examine the hydraulic properties of a foamed zeolite/iron pellet material that was developed for in situ remediation of contaminated groundwater. The packed pellets had large inter-pellet pore spaces (several mm in dimension) and small intra-pellet pores (< 1 mm), with an overall porosity of 0.8. The colloidal tracer (1-micron polystyrene microspheres) transported through the columns much faster than the conservative solute tracer (tritiated water), reflecting the inter-pellet preferential flow pathways in the packed material. Flow interruption experiments with tritium and bromide showed concentration rebound of both tracers after the interruption, indicating the existence of non-advective zones inside the pellets. As expected, standard equilibrium transport models could not adequately describe the solute breakthrough curves. Physical non-equilibrium and dual-permeability models also were unable to describe the data. A model incorporating both intra-aggregate diffusion and dual permeability is required to reflect the complex transport processes in the pellets.

H62B-0841 1330h POSTER

Efficient Steady-State Solution Techniques for Variably Saturated Groundwater Flow

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We consider the simulation of steady-state variably saturated groundwater flow using Richards' equation. The difficulties associated with solving Richards' equation numerically are well known. Most discretization approaches for Richards' equation lead to nonlinear systems that are large and difficult to solve. The solution of nonlinear systems for steady-state problems can be particularly challenging, since a good initial guess for the steady-state solution is often hard to obtain, and the resulting linear systems may be poorly scaled. Common approaches like modified Picard iteration or variations of Newton's method have their advantages but perform poorly with standard globalization techniques under certain conditions.

Pseudo-transient continuation has been used in computational fluid dynamics for some time to obtain steady-state solutions for problems in which Newton's method with standard line-search strategies fails. It combines aspects of backward Euler time integration and Newton's method to select intermediate estimates of the steady-state solution. In this work, we examine the use of pseudo-transient continuation methods for Richards' equation. We evaluate their performance for steady-state problems in heterogeneous domains by comparing them with Newton's method using standard globalization techniques. We investigate the methods' performance with both direct and preconditioned Krylov iterative linear solvers. We then make recommendations for robust and efficient approaches to obtain steady-state solutions for Richards' equation under a variety of conditions.

H62B-0842 1330h POSTER

Representing the Hydraulic Conductivity Distribution in a Model Simulating Regional Groundwater Flow in a Heterogeneous Volcanic Terrane

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A regional-scale groundwater flow model has been developed for the upper Deschutes Basin in central Oregon. The basin spans the eastern side of the Cascade Range volcanic arc and the adjacent depositional basin. The geology consists of a heterogeneous assemblage of late Miocene to Holocene lava flows, vent deposits, pyroclastic materials, and volcanic sediments.

Well data and information from outcrops indicate a high degree of geologic heterogeneity in the basin at a variety of scales. However, subsurface information is inadequate to continuously map or statistically evaluate the hydraulic conductivity distribution over most of the model domain. Well data are sparse over much of the modeled area and are particularly lacking at depth. Large-scale hydraulic conductivity distribution, in contrast, can be generally mapped based on limited well tests, surface geological mapping, volcanic facies distribution, geophysical data, and inferences from hydraulic head distribution. The spatial distribution of hydraulic conductivity was represented in the model by a set of discrete zones within which values were uniform. Hydraulic conductivity zones were delineated to reflect geologic facies within the basin and refined during calibration. The complexity of the zonation scheme was constrained ultimately by the density of hydrologic data.

Inverse methods (MODFLOWP) were used for steady-state calibration. Composite scaled sensitivities and parameter correlation (calculated by MODFLOWP) and residual analysis were used for refining hydraulic conductivity zones and for ensuring that model complexity did not exceed a level supportable by available hydrologic data (head and flux observations). Transient calibration was achieved using trial and error. The goodness of fit between observed and simulated heads and flows (in time and space) varies within the model domain and is generally best in areas where hydrologic data were most plentiful. Overall, the model accurately simulates head and discharge to streams at a regional scale and their response to seasonal recharge pulses and decadal-scale climate variation.

The regional model has been used for simulating the effects of pumping and changes in artificial recharge due to irrigation canal lining. A nested model has been developed within the regional-scale model to simulate the fate and transport of septic-derived nitrate in the southern part of the basin (see Morgan et al., this session). The regional model could also be used to simulate the effects of climate change.

H62B-0843 1330h POSTER

Dispersion of Groundwater Age as a Function of Heterogeneity and Well Screen Length in Heterogeneous Media

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Four possible scenarios representing different degrees of subsurface heterogeneity of an alluvial aquifer system are developed to explore the influence of heterogeneity on dispersion of groundwater age within single water samples. Results show that every scale of geologic heterogeneity in this multi-scale heterogeneous alluvial aquifer has distinct effect on the age distribution and mean age. On the other hand, the mixture of groundwater of various ages within a single sample could cause 5.0yrs difference between CFC-11- and CFC-12- based ages because of their different historic atmospheric input curves. Secondly, a series of backward particle tracking experiments explores the role of well screen length on inferred age and on spatial variations in age along the screen in this moderately-coarse-grained aquifer. The age or age distribution of a groundwater sample, collected at different screened intervals of a single monitoring well or at the whole screen but with different screen length, depend on both the local sediment distribution around the screen and the regional-scale heterogeneity structure in the upstream aquifer zones. The sensitivity of groundwater age to well screen intervals and length might be too strong to be ignored even in a very short screen (i.e., 1.0m), when dating groundwater in typically heterogeneous media such as alluvial aquifers.

H62B-0844 1330h POSTER

High-Concentration-Gradient Dispersion in Heterogeneous Porous Media: A Numerical Study

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This paper presents a numerical study of stable brine displacements in a heterogeneous porous

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medium. Computed breakthrough curves show a decrease in the apparent longitudinal dispersivity for high-concentration-gradient displacements, in accordance with experimental findings.

The objective of this study is to confirm the presumption that the non-linear dispersion effect is caused by gravity driven flow. Local heterogeneities give rise to irregularities in the initially horizontal brine front. Gravity tends to cancel out the resulting horizontal density gradients, which leads to a reduction of dispersive mixing.

The results are analyzed using the non-linear dispersion theory of Hassanizadeh and Leijnse, which involves a new dispersion parameter β. For one displacement velocity, a unique value of β is determined, with which the breakthrough curves for various density differences can be fitted. The dispersion parameter is determined for various velocities. On a log-log scale this parameter is inversely proportional to the displacement velocity.

H62B-0845 1330h POSTER

Introducing Interactive Groundwater v3.5 - A comprehensive software system for unified deterministic and stochastic groundwater modeling

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Taking advantage of the recent developments in computer technology, contaminant transport modeling, and numerical simulation techniques, we have recently developed a sophisticated combined research and educational software environment for unified deterministic and stochastic groundwater modeling. Based on a set of new efficient and robust computational algorithms, the software allows simulating complex flow and transport in aquifers subject to both systematic and "randomly" varying stresses and geological and chemical heterogeneity. Adopting a new programming paradigm, the software eliminates a major bottleneck in groundwater modeling using the traditional fragmented technologies and allows fully utilizing todays dramatically increased computing power. For the first time, the software enables real-time or near real-time groundwater modeling, visualization, analysis, and presentation.

The new software technology enriches the process of scientific discovery and professional investigation and transforms the way scientists and engineers conduct groundwater modeling.

URL: http://www.egr.msu.edu/~lishug/research/igw

H62B-0846 1330h POSTER

A Simple Numerical Method in Modeling Soil Water Dynamics During Vertical Drainage

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The change of soil water content (SWC) during vertical drainage may be divided into two parts. The maximum change of SWC, which results when there is no incoming flow, can be predicted from hydraulic conductivity. The actual change of SWC can be predicted from hydraulic conductivity and the incoming flow. A new model has been developed to simulate soil water dynamics during vertical drainage using this concept. Within this model, the maximum daily change of soil water content (SWC) was calculated using a ratio between initial SWC minus field capacity (FC, defined as SWC after 10 days of drainage) and FC. The actual daily change of SWC was obtained from multiplying the maximum daily change of SWC by a coefficient, F. The coefficient F accounts for the impact of the incoming flow on the change of SWC. The model was tested on more than 300 theoretical soils. The model SWC estimates were comparable to SWC estimates of an analytical model.

H62B-0847 1330h POSTER

Fully Implicit Temporal Integration of Index One Differential-Algebraic Equations from Nonlinear Porous Media Flow

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Time integration methods that adapt in both the order of approximation and time step have been shown to provide efficient solutions for Richards' equation. In this work, we extend the same method of lines approach to solve a set of two-phase flow formulations and address some mass conservation issues from the previous work. We analyze these formulations and the nonlinear systems that result from applying the integration methods, placing particular emphasis on their index, range of applicability, and mass conservation characteristics. We conduct numerical experiments to study the behavior of the numerical models for three test problems. We demonstrate that higher order integration in time is more efficient than standard low-order methods for a variety of practical grids and integration tolerances, that the adaptive scheme successfully varies the step size in response to changing conditions, and that mass balance can be maintained efficiently using variable-order integration and an appropriately chosen numerical model formulation.

H62B-0848 1330h POSTER

Using Results From the Yucca Mountain Drift-Scale Heater Test to Evaluate Thermohydrological Conceptual Models

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The US Department of Energy is conducting a long-term drift -scale heater test (DST) as part of a comprehensive evaluation of a proposed geologic high-level nuclear waste repository at Yucca Mountain, Nevada. The DST completed its four-year heating phase and recently began a four-year cooling phase. Results from the heating phase of the DST are available for evaluating conceptual models used to simulate heat and mass transport at the proposed repository. Conceptualizations of greatest interest include models for multiple continua, fracture representations, constitutive relations, and initial and boundary conditions. Although physical characterization (i.e., property value assignment) is not strictly considered model conceptualization, the values assigned to the model, nonetheless, have a significant affect on model outcome and were included in the evaluation.

A multiphase simulator, MULTIFLO, was used to perform the conceptual model evaluations. Conceptualizations in the model included: two- and three-dimensionality; dual continua (matrix and fracture); matrix-fracture interaction relations; van Genucthen, Brooks-Corey, and linear relative permeability functions; a range of property values (thermal conductivity and fracture permeability); and a broad range of reasonable initial (saturation) and boundary (infiltration) conditions. The evaluations identify which conceptualizations are feasible and consistent with observations from the DST, which model representations are most important for the model to agree with ambient conditions (infiltration, matrix-fracture interaction relations), and which representations are most important for the model to agree with DST heating phase results (fracture permeability and thermal conductivity).

This abstract is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC.

H62B-0849 1330h POSTER

Reactive Transport Model for the Ambient Unsaturated Hydrogeochemical System at Yucca Mountain, NV

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Reactive transport models constrain predictions of the long-term performance of Yucca Mountain (YM) as a possible high-level waste repository. These models evaluate coupled time-dependent processes controlling the composition and flux of water as it percolates through rock and waste emplacement drifts. It is difficult to quantify combined effects of inadequate model constraints, individual parameter uncertainties, and code limitations on model predictions. To increase confidence in model predictions of the thermal-hydrological-chemical response to nuclear waste emplacement at YM, it is useful first to demonstrate that the reactive transport model accurately depicts the evolution of the ambient natural system, for which site characterization provides a basis of evaluation.

We used the code MULTIFLO to simulate ambient thermal-hydrological-chemical processes and conditions occurring in a 373-meter [1224 feet] vertical column in the subsurface of YM. The model simulates two phase, non-isothermal, advective and diffusive flow and transport through one dimensional matrix and fracture continua (dual permeability) containing 10 kinetically reactive and hydrostatigraphically distinct layers. Gas-water-rock interactions include aqueous speciation, mineral dissolution and precipitation, and gas-water equilibria involving H2O and CO2. Coupled consequences of reactive transport include effects of transport on local chemical processes and effects of variations in permeability due to mineral reactions on flow and transport.

Site-specific data were used to develop a conceptual model for the ambient, unsaturated zone hydrogeochemical system at Yucca Mountain and to calibrate reactive transport simulations. Geochemical data were evaluated in concert with aqueous speciation and mineral saturation calculations to: 1) restore internal consistency to analytical data on pore water compositions; 2) identify important lithologic characteristics of individual hydrostratigraphic units; and 3) idealize thermodynamic properties of the most reactive phases to be consistent with our conceptual model.

Uncertainties in simulations were accommodated by developing calibration criteria based on the conceptual model and then adjusted using poorly constrained parameters to force the model to meet those criteria. Calibration criteria were developed from petrologic observations and thermodynamic and kinetic interpretations of analytical pore water chemistry. Model results satisfying calibration criteria reasonably represent quasi-steady state stability of water chemistry and mineralogical variations with depth and distributions between fractures and matrix. The model helps identify critical data uncertainties and provides a set of initial conditions for reactive transport modeling for the perturbed repository system.

This abstract is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC.

H62B-0850 1330h POSTER

The Influence of Constitutive Model Parameters on Predictions of DNAPL Migration in Heterogeneous Porous Media

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This study examines the influence of constitutive models and their parameters on predictions of the spatial and temporal distribution of a finite release of a dense, nonaqueous phase liquid (DNAPL) into a two-dimensional, spatially correlated random permeability field. The base case simulation employed a comprehensive constitutive model that was validated against relevant one-dimensional laboratory experiments. None of the nine subsequent simulations - each of which varied a single constitutive model characteristic to examine the consequences of employing more typical or more simply parameterized functions - were able to reproduce, within + or - 10%, the spatial and temporal migration characteristics of the nonwetting fluid body at late time predicted by the validated model. Capillary pressure-saturation relationships that do not incorporate specific displacement and terminal pressures are demonstrated to severely overpredict the spatial extent of nonwetting fluid advancement; this suggests that van Genuchten-based models may not be suitable for predicting DNAPL migration in saturated porous media. Not accounting for any one of hysteresis, nonwetting phase trapping, or the proper curvature or endpoint values of the nonwetting phase imbibition relative permeability curve influenced the time predicted for all nonwetting fluid movement to cease. The practical implication of this study is that a comprehensive constitutive model, characterized with the appropriate parameter values, is necessary to accurately simulate a complete DNAPL release below the watertable in both space and time.

H62B-0851 1330h POSTER

Advective-Dispersive Solute Transport using Streamlines

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We extend the streamline method to model diffusion and dispersion in solute transport problems using an operator splitting technique. The proper inclusion of dispersion is vital for the correct prediction of contaminant mixing, and is significant when this is coupled with reactive transport. Fluid is moved along streamlines ignoring dispersion, and then component concentrations are mapped onto the grid. Dispersion is included by solving the dispersive portion of the conservation equation on the underlying grid. This solution was verified by comparing with one and two-dimensional analytical solutions. We then quantified the effects of numerical dispersion and remapping of the solution from the streamline to the underlying grid. We demonstrate that using realistic values of dispersivity, dispersion can have a significant impact on the shape of contaminant plumes at the field scale. We then propose a simple formulation for reactive transport (including dispersion) and apply it to rate-limited sorption. The transfer of solute between rock matrix and water (sorbed and flowing) enters as a source/sink term in the one-dimensional transport equations along a streamline.

H62B-0852 1330h POSTER

A Finite-Volume Scheme on Unorthogonal Mesh for Ground Water Flow in Dipping-Layered Aquifers

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For groundwater flow in a heterogeneous layered anisotropic porous medium with dipping beds, we develop a computationally efficient 3-dimensional finite-volume model. This algorithm is developed applying the cell-centered finite volume method on an unorthogonal structured grid system with fully implicit time discretization. This special discretization can describe the domain and capture the boundaries accurately, especially when the domain includes vertical wells. An extra interpolation scheme is applied on the cell interface to evaluate the flux so that it is not required to transform hydraulic conductivities and average the off-diagonal entries. The results of several testing cases show that this scheme is efficient and accurate.

H62B-0853 1330h POSTER

Enhanced mapping of hydraulic conductivity field conditional to tracer test data

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A geostatistically-based sequential self-calibration (SSC) method is applied to enhance the estimation of conductivity field by conditioning on tracer test data, which contains, arguably, the most important information about the aquifer properties related to solute transport, particularly, the information about the high K flow channels embedded within the aquifer. A gradient-based technique, which requires the sensitivity coefficients of the concentrations in pumping and/or sampling wells with respect to the changes of the hydraulic conductivity field, was used to solve optimization problems. A streamline-based simulator was also presented to simulate the solute transport. The simulator allows fast calculation of sensitivity coefficients within one single simulation run. A number of points (termed as master points) within the aquifer were randomly chosen, and the optimal changes of conductivity were determined at these master points first by solving the inverse problem of minimizing the mismatch between the observed and calculated concentrations. The optimal changes of conductivity at these master points were then interpolated by kriging to all grid blocks. Promising results have been obtained to demonstrate the potential of conditioning on tracer test data to identify flow channels and to reduce the uncertainties associated with the predictions.

H62B-0854 1330h POSTER

Simulating the Development of Solution Conduits in Dualistic Karst Flow Systems

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Karst aquifers consist of highly permeable solution conduits embedded in the considerably less permeable fissured system of the adjacent rock. Hydrogeologic characterisation of these heterogeneous, dualistic flow systems requires a sound understanding of the processes involved in karstification. During the last decade numerical simulations of conduit development were frequently employed to accomplish this aim. Yet, in many of the earlier simulations the dualistic nature of the flow system and the feedback of conduit development on the hydraulic boundary conditions of the conduit system had been ignored. In this study, the dual flow system is adequately represented by a coupled continuum-pipe flow model. In order to simulate conduit development, the flow model is coupled to a module calculating dissolution rates and the corresponding widening of conduits depending on flow conditions. It is a major advantage of this modelling approach that the hydraulic boundary conditions for the conduit system do not need to be set a priori but can be obtained by a coupling to the continuum flow model representing the regional hydraulic system. This is illustrated using the example of an artesian setting, in which an unit of soluble rock is supplied with solutionally aggressive water from an aquifer below. It is demonstrated that the flow field changes both locally and at the regional scale due to solutional conduit development. These changes have to be taken into account, in order to gain adequate understanding of how the interaction of flow and dissolution processes determines the structure of the karst conduit system developing in this type of setting.

H62B-0855 1330h POSTER

Modeling Np and Pu Transport with a Surface Complexation Model and Spatially Variant Sorption Capacities: Implications for Reactive Transport Modeling and Performance Assessments of Nuclear Waste Disposal Sites

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One-dimensional (1D) geochemical transport modeling is used to demonstrate the effects of speciation and sorption reactions on the ground-water transport of Np and Pu, two redox-sensitive elements. Earlier 1D simulations (Reardon, 1981) considered the kinetically-limited dissolution of calcite and its effect on ion-exchange reactions (involving ^{90}Sr, Ca, Na, Mg and K), and documented the spatial variation of a ^{90}Sr partition coefficient under both transient and steady-state chemical conditions. In contrast, the simulations presented here assume local equilibrium for all reactions, and consider sorption on constant potential, rather than constant charge, surfaces. Reardons (1981) findings documenting the spatial and temporal variability of ^{90}Sr partitioning are reexamined and found partially caused by his assumption of a kinetically-limited reaction. In the present simulations, sorption is assumed the only retardation process controlling Pu and Np transport, and is modeled using a diffuse-double-layer-surface-complexation model. Transport simulations consider the inflow of Np- and Pu-contaminated waters into an initially uncontaminated environment, followed by the cleanup of the resultant contamination with uncontaminated water. Simulations are conducted using different spatial distributions of sorption capacities (with the same total potential sorption capacity, i.e. the same total number of sorption sites, but with different variances and spatial correlation structures). A case with a spatially uniform distribution of sorption capacities was also simulated. Results obtained differ markedly from those that would be obtained in transport simulations using constant K_d, Langmuir, or Freundlich sorption models. When possible, simulation results (breakthrough curves) are fitted to a constant K_d advection-dispersion transport model and compared to each other. Functional differences are often great enough that they prevent a meaningful fit of the simulation results with a constant K_d (or even a Langmuir or Freundlich) model, even in the case of Np, a weakly sorbed radionuclide under the simulation conditions. Functional behaviors that cannot be fitted include concentration trend reversals and radionuclide desorption spikes. Other simulation results can be successfully fitted but the fitting parameters (K_d and dispersivity) vary significantly depending on simulation conditions (e.g. infiltration vs. cleanup conditions). Notably, an increase in the variance of the specified sorption capacities results in a marked increase in the dispersion of the radionuclides, and a decrease in the fitted K_d. These results have implications for the simulation of radionuclide migration in performance assessments of nuclear waste disposal sites, for the future monitoring of those sites, and more generally for modeling contaminant transport in ground-water environments.

H62B-0856 1330h POSTER

Simulation of Mass Recovery of Entrapped Tetrachloroethene in Coupled Physically and Chemically Heterogeneous Porous Media

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An understanding of the transport behavior of dense non-aqueous phase organic liquids (DNAPLs) in the subsurface is a prerequisite for the accurate assessment of chemical exposures and the design of effective remediation strategies. Although a number of studies have investigated the effects of physical or chemical heterogeneity on the fate of DNAPLs, few have been undertaken to explore the influence of coupled physical and chemical variations on contaminant behavior. Results of on-going numerical studies are presented that are designed to quantify the mass recovery of entrapped residual DNAPL from coupled physically and chemically heterogeneous porous media.

For these numerical studies, tetrachloroethene (PCE) was chosen as a representative DNAPL. Permeability fields of varying heterogeneity (i.e., differing $\sigma_{ln(k)}$) were generated with sequential Gaussian simulation, based upon geostatistical parameters derived from grain size distribution measurements for a sandy glacial outwash aquifer. Using solid-phase wettability as a representative metric for chemical heterogeneity, several correlations were employed to relate organic-wet mass fraction to porous media permeability. Residual saturation distributions for a PCE spill event were then obtained for these synthetically generated parameter fields, with a multiphase flow simulator incorporating wettability-dependent constitutive relationships for capillary behavior. The simulated saturation distributions were then used as initial conditions in compositional simulations of PCE dissolution, to examine the effect of coupled wettability and permeability variations on DNAPL mass recovery.

Simulations reveal considerable differences in predicted depth of organic penetration, extent of lateral spreading, and magnitude of maximum entrapped saturation for the various modeled scenarios. These differences also correlated with observable variations in effluent concentration and mass recovery predictions in the aqueous phase flushing simulations. Representative results are presented that demonstrate the influence of the selected correlation between physical and chemical heterogeneity on the migration, entrapment, and mass recovery of DNAPLs in the subsurface.

H62B-0857 1330h POSTER

Simulation of Free Surface Dynamic in a Random Heterogeneous Porous Medium by the Method Based on Mapping the Regular Domain on the Flow Domain.

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In this paper the problem of vacuum-incompressible fluid interface moving in a porous medium by treating conductivity of a medium as a random field with known statistics is considered. The flow is described by a combination of mass conservation and Darcy law. The use of a coordinate system tied with the moving fluid allows reducing the problem to the well-explored class of problems with fixed boundaries and an effective conductivity tensor instead of the initial scalar conductivity. The hydraulic head is represented as a series in powers of effective conductivity fluctuations.

The applied procedure is close to the perturbation theory procedure in the amplitude of the hydraulic conductivity fluctuations $\tilde{K}$ when searching the solution with accuracy up to $\tilde{K}^2$. In both cases physical quantity variance is considered to be proportional to its reason: $\tilde{V} = A \cdot \tilde{K}$ (A is a linear operator). Yet unlike perturbation theory, where it is considered that A depends only on undisturbed flow parameters $A = A(\bar{K})$, in the approach being used A is considered to be dependent on averaged flow parameters $A = A\left(\bar{K}, \left\langle \tilde{K}^2 \right\rangle\right)$. Equations of the mean hydraulic head and mean flux and expressions for respective variances as well are derived in the 2-D case. For 1-D flow the derived solution agrees with the exact one within terms of σ_K^2-order at any free surface fluctuations. Within this approach the free surface moving, evolution in time of the mean hydraulic head spatial distribution, mean flux and relative correlation functions are described by the set of first-order partial differential equations.

The conjugate gradient method with preconditioning is proposed to be used as the general method of equation numerical solving to find hydraulic head statistic moments. The problem matrix symmetry and its positive definiteness serve the foundation of the method applicability. RFLOW code has been elaborated to solve this set of equations numerically. Testing data of the elaborated code and analysis results of the derived numerical solutions are presented in this report.

H62B-0858 1330h POSTER

Modeling Transport of Non-linearly and Kinetically Sorbing Solutes In Heterogeneous Porous Media.

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Transport in subsurface environments is conditioned by physical and chemical processes in interaction, the most common being advection and dispersion for the physical processes and sorption for chemical reactions. Mathematical models for solute transport were initially based on the simplified assumptions of linear and instantaneous sorption in homogeneous media. However these models don't succeed in describing solute transport observed in field-scale experiments. Growing evidences suggest that adsorption for several common sorbing solutes is non-linear and kinetically controlled. As well as the physical heterogeneity of porous media, the nonlinearity and the kinetic control of sorption processes may be partly responsible for the non-ideal reactive transport observed in experiments. As they notably cause a retardation of the solute plume center of mass, these kinetics are worth being considered in chemical transport models. In this work, we propose a method for coupling nonlinear kinetic sorption and solute advection in a three-dimensional heterogeneous porous. We assume that, at local scale, nonlinear adsorption is described by the Freundlich isotherm with the Freundlich exponent n, $0 < n < 1$. Because of the widely-scattered heterogeneity of porous media, the transport equation cannot be solved analytically, and numerical complexity even increases when taking into account nonlinear kinetics. We thus set up a flexible numerical approach based on the method of active walkers, which generalizes the particle tracking scheme for chemically active solutes. The method is rather flexible because it achieves a decoupling of the physico-chemical process at the elementary volume scale, i.e. at the lowest scale, thus enabling the modeling of virtually all possible chemical reactions. Thanks to these numerical simulations, we discuss homogenization rules that apply to such nonlinear chemical kinetics in heterogeneous flow. We have derived the relationship between the mean plume retardation coefficient and the degree of nonlinearity of chemical reactions (i.e. the Freundlich coefficient). We also describe the diffusion of the moving solute plume by analyzing the scaling rules that apply to its moments. At last, we discuss the consequences of flow heterogeneity on chemical transfer.

H62B-0859 1330h POSTER

Quantifying the Combined Effects of Chemical and Physical Heterogeneities by Combining Lagrangean Transport and the Exposure-time Concept: Inverse and Forward Solutions

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Geochemical properties of the natural subsurface play an important role in the fate and transport of contaminants. Characterization of (Eulerian) aquifer properties in general is difficult, whereas the Lagrangean approach may be more useful particularly in that it reports global variables (e.g. travel time). Passive tracers have proven useful for characterizing distributions of flux over travel time, and multiple tracer approaches have been used successfully in characterizing subsurface DNAPL distributions. We use this precedent in the design of a multiple reactive tracer approach for characterization of macroscopic geochemical variability. The technique involves a novel inverse method using data from breakthrough curves of multiple tracers undergoing first order irreversible removal. The method provides a characterization of geochemical heterogeneity in terms of distributions of flux over cumulative reactivity, which is defined roughly as the time that the solution has spent in a region of given reactivity. The distributions of flux over cumulative reactivity define the fractions of the flux that experience various exposure times to reactive regions. This concept is generalized further to describe exposure to regions of arbitrary reactivity. Via the distributions, the combined effects of physical and geochemical heterogeneity on reactive solute transport are quantitatively established without detailed knowledge of spatially distributed porous media properties. The distributions can subsequently be applied to obtain breakthrough curves of other solutes undergoing general first order reactions in similar geochemically heterogeneous configuration via the forward modified stochastic convective reactive approach (mSCR).

H62B-0860 1330h POSTER

Modeling the Effect of 3-D Multilayered Soil Topography on Preferential and Stagnant Water-Flow Zones During Infiltration

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A 16-day ponded infiltration test was carried out near the Novovoronezh Nuclear Power Plant, Russia, with measurements of the moisture content and 90Sr concentrations (used as a tracer) in several monitoring wells. Using the results of this test, we constructed a 3-D numerical model of a cylindrical flow domain (30 m in radius, 16 m in depth), reflecting a spatial heterogeneity of multiple layers of sands, clayey sands, sandy loam, and loam. Based on the solution of Richards' equation, we assessed the effect of topography and the variable thickness of soil layers on moisture content and flow-velocity distributions, as well as the creation of preferential and stagnant flow zones in unsaturated soils. Modeling was performed for both background (natural precipitation) and ponded infiltration conditions, using two types of soil layering: (1) perfectly horizontal soil layers with thickness averaged over the flow domain, and (2) soil layers of a variable thickness. The soil hydraulic properties were determined using inverse modeling. Numerical model calibration shows that despite the temporal trend of the infiltration rate, which was observed under field conditions and could be matched using the model of horizontal soil layers, this model could not simulate the formation of preferential paths and stagnant water zones. Numerical simulation of infiltration indicates that the most distinct pattern of preferential flow is observed immediately below the infiltration pond, and the preferential flow fingers extend to the bottom of the flow domain (a depth of 16 m). The soil moisture is accumulated in sand layers in depressions over the underlying loam layers, and is not increased over the top of the loam domes. Thus, numerical modeling confirms that relatively small changes in the topography of soil layers might create both preferential flow and stagnant water zones during infiltration into the vadose zone. These results should be taken into account in designing remediation activities.

H62B-0861 1330h POSTER

Positive Solution of Two-dimensional Dispersion Considering Cross Terms

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The transport of contaminants through a porous medium is usually represented by a convection-dispersion equation. There are several well-known problems associated with numerical solutions of this equation. Numerical dispersion, oscillatory solutions, poor mass conservation, and non-positive concentrations are among the main obstacles to the application of these techniques. Specifically, negative values of concentration are unphysical and produce several problems for the implementation of coupled reactive-transport models.

Several well-known studies have shown that standard treatment of the cross-dispersion terms can always lead to negative concentration. These cross terms are especially significant during non-uniform flow in heterogeneous media.

In this poster we shall explore a different approach to avoid the negative concentrations due to the cross dispersion terms. This poster will include a brief explanation of the problem of non-positive concentrations and cross dispersion terms and the numerical scheme that have been used to solve it. The proposed scheme is suitable for both Finite Difference and Finite Volume and it has been applied to explicit and implicit temporal approximations. We also present examples of application of the traditional and our new approach to simulate the dispersion process in a homogeneous and heterogeneous medium.

H62B-0862 1330h POSTER

Three-Dimensional Monte Carlo Simulations of Movement of a Contaminant Plume in Heterogeneous Aquifers

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Monte Carlo (MC) approach has been applied in studying solute transport in heterogeneous porous media. Most studies with MC simulations were either conducted in two dimensions or in three dimensions with no more than a hundred realizations or addressed only the longitudinal macrodispersion even though our understanding about the transverse macrodispersion is less satisfactory than the longitudinal macrodispersion in both ergodic and non-ergodic transport. In this study Monte Carlo approach was adopted to simulate transport of a finite solute body by steady-state groundwater flow with a uniform mean velocity in a three-dimensional heterogeneous and statistically isotropic aquifer with more than a thousand realizations. The hydraulic conductivity (K) is modeled as a random field which is assumed to be log-normally distributed with an exponential covariance. The ensemble averages of the second spatial moments of the plume about its center of mass, $\langle S_{ii}(t) \rangle$, and the plume centroid covariance, $R_{ii}(t)$ $(i = 1, 2, 3)$, were simulated for three values of the variance of log K, 0.1, 0.25, and 0.5, and a line source of different lengths normal to the mean flow. It is shown that for the small variance of 0.1 all simulated $\langle S_{ii}(t) \rangle$ and $R_{ii}(t)$ agree well with the first-order theoretical values. As the variance increases to 0.25 and 0.5, the simulated longitudinal moments, $\langle S_{11}(t) \rangle$ and $R_{11}(t)$, still agree well with the first-order theoretical results but the simulated transverse moments are significantly different from the first-order theoretical results, contrary to the assumption

that the first-order theory is generally valid for the variance of log K less than one. The simulated one-particle longitudinal displacement variance, $X_{11}(t)$, is in good agreement with the first-order theory. The simulated transverse moment, $X_{22}(t)$ and $X_{33}(t)$, are larger than the first-order values but in excellent agreement with the quasi-linear theory based on the Corrsins conjecture. We also found that more than 1000 realizations are needed in order to obtain stable second spatial moments for the variance of log K as small as 0.5, indicating the existing MC results for a much large variance with much less realizations may not valid.

H62B-0863 1330h POSTER

Effects of Model Grid Resolution and Parameter Upscaling on Predictions of Water Flow in Heterogeneous, Unsaturated Porous Media.

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Accurate prediction of water flow and solute transport in heterogeneous, unsaturated porous media is generally hampered by our inability to 1) adequately characterize the physical and hydraulic properties of the porous media, and 2) to represent these properties at the appropriate scales in our models. A methodology has recently been developed that uses both hard and soft data, geostatistical simulation methods, and scaling concepts to generate spatially distributed and upscaled estimates of soil physical and hydraulic properties, conditioned on field-measured initial water content distributions. The methodology is used to parameterize a numerical flow and transport model for simulations of a 3D subsurface water injection experiment conducted in highly heterogeneous interbedded sands and silts at the Hanford Site in southeastern Washington State. Simulated and observed results are compared, and the effects of model grid resolution and parameter upscaling are presented.

H62B-0864 1330h POSTER

Effects of Adsorption Constant Uncertainty on Contaminant Plume Migration: One and Two Dimensional Numerical Studies

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In this study, we use one- and two-dimensional (1D and 2D) reactive-transport models to numerically examine variations in predictions due to uncertainty in the adsorption constants. The study specifically focuses on the hydrogeology and mineralogy of the Naturita uranium mill tailings site in Colorado. This work demonstrates the importance of selecting the appropriate adsorption constants when using reactive-transport models to evaluate risk and pollution attenuation at contaminated sites. In our model, uranium is removed from mill tailings leachate through adsorption onto smectite, an abundant clay mineral at the Naturita site. Uranium adsorbs to specific surface sites on both the basal planes and edges of the smectite. Because uranium adsorbs predominantly to the aluminum edge surface sites [>(e)AlOH], we chose to examine uncertainty only in the equilibrium constants associated with these sites. Using the Latin Hypercube Sampling method, one-hundred pairs of adsorption constant (log K) values are selected for the surface species $>(e)AlO^-$ and $>(e)AlOUO_2{}^+$, from normal distributions of each log K. Following a grid convergence study, 1D simulation results can be identified by two distinct groups of uranium breakthrough curves. In the first group, the breakthrough curves exhibit a classical sigmoidal shape whereas in the second group the breakthrough curves display higher uranium concentrations in solution over greater distances and times. These two groups are clearly separated by two different ranges of log K $>(e)AlO^-$ values or two different ranges for the smectite point of zero charge. Preliminary 2D simulations, in both homogeneous and randomly heterogeneous aquifers demonstrate that plume geometry and migration in longitudinal and transverse directions are also influenced by the choice of adsorption constants.

H62B-0865 1330h POSTER

Multiscale Thermohydrologic Model Analysis of Thermal-Conductivity Heterogeneity and Preclosure Operational Factors for a Repository at Yucca Mountain

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The MultiScale ThermoHydrologic Model (MSTHM) is a computationally efficient approach that accounts for thermohydrologic (TH) processes occurring at a scale of a few tens of centimeters around waste packages and emplacement drifts, and for heat flow at the multi-kilometer scale of Yucca Mountain. Presented are MSTHM simulations for the Yucca Mountain Repository that address the influence of thermal-conductivity heterogeneity and the influence of preclosure operational factors, including the following: (1) the sequence of waste-package emplacement along drifts, (2) the spatial and temporal heat-removal efficiency of drift ventilation, and (3) the duration of the ventilation period. A repository layout with multiple non-parallel emplacement planes can now be accommodated using a superposition process that combines results from two mountain-scale submodels. This superposition process is validated for several cases, including those with heterogeneous thermal-conductivity distributions. Recent improvements to the MSTHM, which better enable analysis of preclosure operational factors, include the ability to (1) predict TH conditions on a drift-by-drift basis, (2) represent sequential emplacement of waste packages along the drifts, and (3) incorporate spatial and temporal heat-removal efficiency associated with drift ventilation. We show that these improvements influence predictions of in-drift and host-rock TH conditions. We also investigate alternative approaches to addressing thermal-conductivity heterogeneity. We find that, depending on the length-scale for the heterogeneity, not all MSTHM submodels need to account for this heterogeneity. The most important parameters and factors influencing the MSTHM results for any one particular repository design include the infiltration flux, thermal-conductivity heterogeneity, waste-package sequencing, and ventilation duration.

H62B-0866 1330h POSTER

Simulation of Flow and Transport of Septic-Derived Nitrate at Multiple Scales Within a Heterogeneous Alluvial Aquifer System

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Flow and transport simulation models were developed at two scales to assess the long-term effects of on-site waste disposal systems on groundwater quality in a shallow alluvial aquifer system near La Pine, Oregon. First, a sub-aquifer scale (6 km^2 area, 30-m thickness) model was used to test concepts and estimate flow and transport parameters along a flowpath where detailed hydrogeologic and geochemical data were available from nested wells and a high-density array of direct-push samples. Then, an aquifer scale (640 km^2 area, 37-m thickness) model was calibrated assuming steady flow with transient historical nitrate loading and observed nitrate concentration data from 1960 to 2000. Groundwater age-dates and observations of hydraulic head and flux to streams were used to constrain and calibrate the models. Boundary flux conditions for the aquifer scale model were extracted using telescoping mesh refinement techniques from a regional scale flow model (11,700 km^2 area, 550-m thickness) developed in a previous investigation of the upper Deschutes basin (see Gannett and Lite, this session).

The hydrogeologic framework for the models was developed using transitional probability geostatistics. Lithologic descriptions from 390 geologic logs were categorized into three hydrofacies: gravel and coarse sand, fine-to-medium sand, and silt-clay. The three-dimensional hydrofacies model (realization) was constructed using information on volumetric proportions, mean lengths, and juxtapositional tendencies. The upper surface of an extensive low-permeability layer was mapped from well logs and merged with the geostatistical realization to complete the hydrogeologic model.

Geochemical and hydrogeologic data were collected at multiple scales to advance the understanding of $NO_3{}^-$ sources and the physical and chemical processes affecting its transport and fate. Relations between $NO_3{}^-$, Cl^-, and geochemical indicators of redox conditions, and N_2 isotope and concentration data, indicate that denitrification is an important process in the study area. The oxic / suboxic boundary within the aquifer was mapped using over 200 O_2 measurements from shallow wells; the boundary was represented in the transport model as an $NO_3{}^-$ sink. Nitrogen dynamics for this system will be described by Hinkle et al in another session at this meeting.

A simulation of the 1960-99 period shows that of the $6.1x10^5$ kg of $NO_3{}^-$ added to the system from on-site waste systems, 32 percent had been denitrified, 7 percent was discharged to streams, and the remaining 61 percent was in storage in the aquifer at the end of the simulation period. A preliminary predictive simulation shows that, assuming constant $NO_3{}^-$ loading at 1999 rates, it will take more than 160 years before this annual loading is balanced by the combined processes of denitrification and discharge to streams.

H62B-0867 1330h POSTER

Modeling a Combined Tracer and Time-Lapse Radar Imaging Test in the Heterogeneous Fluvial Aquifer at the Boise Hydrogeophysical Research Site

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Detailed characterization of aquifer heterogeneity is critical for the design and reliable monitoring of contaminant remediation systems. Traditional characterization efforts have been limited by the local nature of core measurements, and the inability to sample volumes between wells. A promising new approach for the detection and determination of fluid and solute movement involves time-lapse geophysical imaging of subsurface volumes in conjunction with borehole-based hydrogeological investigation techniques. This approach shows promise for quantifying the spatial distribution of flow and transport parameters of aquifer material between wells. A combined tracer and time-lapse radar imaging experiment was conducted in the unconfined coarse fluvial aquifer at the Boise Hydrogeophysical Research Site in August, 2001. Potassium bromide tracer was injected to form an electrically conductive plume over a 4-m interval that spanned the contact between two hydrostratigraphic units. Data from hydrogeologic and geophysical investigation methods indicate that these units: are continuous between the wells, have contrasting average permeability and porosity between units, and have variable porosity and permeability within units (i.e., heterogeneity at multiple scales from <2m to >20m). During the two-week field experiment the tracer plume traveled 6.9 m from the injection well to the extraction well, passing through a central monitoring well with 20 sampling zones over a 5-m interval spanning the injection interval. Cross borehole radar data were collected periodically on cross-sectional and longitudinal planes through the tracer plume. Two of these tomographic planes passed through the central monitoring well for quantitative calibration of radar attenuation tomograms to measured solute concentrations. Bromide breakthrough at the central well occurred first and with greatest concentration in the higher conductivity unit as expected, with significant variability in peak time and magnitude across the measured vertical dimension. We will present results from transient three-dimensional flow and transport models of the time-lapse tracer test, implemented using information from the dynamic cross-well radar tomography measurements. Preliminary modeling shows that the transport of the solute plume is strongly influenced by both small-scale aquifer heterogeneity and the geometry of hydrostratigraphic units. The dynamic plume imaging approach that we are developing should lead to a comprehensive description, characterization, and quantification of aquifer heterogeneity of the BHRS.

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

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H62B-0868 1330h POSTER

Thermally-Driven Reaction Fronts in Porous Media

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We present a mathematical model of the reaction fronts that develop when an undersaturated 'injection fluid' displaces a saturated 'formation fluid' in a chemically reactive porous medium. Flows of this kind are relevant to the geothermal and hydrocarbon industries, and are important natural geological processes. The injection and formation fluids differ both in temperature and in chemical composition. We assume that the equilibrium concentration of a reactive mineral species in the fluid is a linear function of temperature. Firstly, we consider the case where the formation fluid is isothermal at $t = 0$. We then extend this solution to the case where the formation fluid has a constant temperature gradient at $t = 0$.

The undersaturation of the incoming fluid drives a dissolution reaction and leads to the formation of a 'depletion' front. Under certain circumstances, which we describe, the temperature difference is able to drive a separate thermal reaction front. Two distinct regimes arise. If the compositional difference between the injection and formation fluids exceeds a critical value, the depletion front travels faster than the thermal front, leaving the porous medium depleted of reactant from the source to a point beyond the thermal front and no thermal reaction front develops. Conversely, if the compositional difference is smaller than the critical value, the thermal front forms downstream of the depletion front and so there is a double reaction front structure.

When we allow for a temperature gradient in the formation fluid, the magnitude of this gradient dictates whether the depletion front speeds up or slows down over time. It is therefore possible for the depletion front to form downstream (upstream) of the thermal front but move upstream (downstream) of it over time. In the cases where the depletion front moves from one side of the thermal front to the other, we derive approximate expressions for the time at which this 'crossover' occurs.

We derive the six dimensionless parameters which control the evolution of the system and find some approximate solutions of the governing equations which are valid at long times. We illustrate the evolution of the thermal and compositional fields towards these asymptotic solutions with numerical simulations.

H62B-0869 1330h POSTER

Numerical Simulation of Non-Fickian Transport in Geological Formations with Multiple-Scale Heterogeneities

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We develop a numerical method to model contaminant transport in heterogeneous geological formations. The method is based on a unified framework that quantifies non-Fickian and Fickian transport and the transition between them over a broad range of temporal and spatial scales. As such, the method takes into account the different levels of uncertainty often associated with characterizing heterogeneities at different spatial scales. The resulting formulation leads to a Fokker-Planck equation with a memory term and a generalized concentration flux term. The former term captures the non-Fickian behavior arising from unresolved, small-scale heterogeneities, which are treated probabilistically using a continuous time random walk (CTRW) formalism. The latter term accounts for large-scale heterogeneity variations, which are included deterministically with explicit treatment at the heterogeneity interfaces. The parameters defining the small-scale and large-scale heterogeneities are measurable quantities. The advection-dispersion equation is seen to result as a special case of our unified framework. Numerical treatment of the equations involves solution for the Laplace transformed concentration by means of classical finite element methods, and subsequent inversion in the time domain. We use the numerical method to quantify transport in one- and two-dimensional domains, for a wide range of (large-scale) heterogeneity structures, (small-scale) material properties, and boundary conditions. The calculations demonstrate long tailing arising (principally) from the memory term, and the effects on arrival times that are controlled largely by the generalized concentration flux term.

H62B-0870 1330h POSTER

Non-Darcy Effects for Fluid Flow in a Rough-Walled Rock Fracture

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An experimental and computational study has been conducted of fluid flow in a rough-walled rock fracture, with emphasis on deviations from Darcy's law in the regime of Reynolds numbers greater than unity. First, profiles of a fracture in a red Permian sandstone were measured with a profilometer, to within +/- 2 microns in elevation, at intervals of every twenty microns in the fracture plane. These profiles were then used to create a three-dimensional finite element grid. The full Navier-Stokes equations were then solved over 2 cm x 2 cm regions of this grid, using no-flow boundary conditions along two opposing sides, and constant pressure boundary conditions along the inlet and outlet faces. The apparent fracture transmissivity was computed from the ratio of the total flowrate to the overall pressure drop. The simulations were carried out for a range of values of the mean aperture.

At Reynolds numbers much less than 1, the computed transmissivity is constant. Appreciable deviations from Darcy's law began to be observed when the Reynolds number (defined using the mean aperture as the length scale) exceeded unity. In the range of Reynolds numbers between 20-100, the computed transmissivities could be fit very well to a Forchheimer-type equation, in which the additional pressure drop varies quadratically with the Reynolds number. The initial deviations from linearity, for Reynolds number around 1, are consistent with the "weak inertia" model developed by Mei and Auriault (J. Fluid Mech., 1991) for porous media, and with the results obtained computationally by Skjetne et al. (J. Fluid Mech., 1999) on a two-dimensional self-affine fracture.

Flow tests are currently being conducted on this same 2 cm x 2 cm fracture region, with a mean aperture of 130 microns. The boundary conditions are the same as those used in the finite element simulations. For Re < 1, the measured transmissivity was indeed constant, and corresponded to a "hydraulic aperture" of about 71 microns. Results for higher Reynolds numbers will be compared to the predictions of the analytical weak inertia model and Forchheimer's empirical model.

H62C MCC: Hall C Saturday 1330h

Orographic Precipitation Posters

(joint with A, GC)

Presiding: **T Lang,** Harvard University; **A Barros,** Harvard University

H62C-0871 1330h INVITED POSTER

Orographic precipitation: Physics and Dynamics

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We review recent theoretical work on orographic precipitation, including several themes. 1) Studies of airmass transformation over the Alps show processes occurring on a range of scales from 10 to 100km. Parcels crossing the Alps are dried but also scrambled due to different amounts of latent heating. 2) Numerical models have been used to evaluate the use of moist stability to model the airflow dynamics. For the purpose of predicting upslope flow and blocking, the moist stability is quantitatively useful. 3) The influence of evaporating precipitation on airflow dynamics varies from case to case. In general, down-slope lee-side evaporative heating has little effect on upstream dynamics, while upslope melting or evaporation of falling hydrometeors is influential. 4) Even with latent heat, upslope flow can become non-linear and blocking can occur. This blocking leads to reverse flow driving a broad upstream arc of precipitation. 5) Clouds with significant riming, accretion or collection respond non-linearly to cloud water generation. The precipitation efficiency remains low until a certain threshold in cloud generation rate is met, whereupon, heavy precipitation occurs. 5) Horizontal scale has a profound effect upon precipitation efficiency. Small-scale hills produce patterns of ascent that extend only a short distance upward into the moist layer. Little condensation occurs. The ascent and condensation produced by broader hills may be limited too, due to wave dynamics. Precipitation from small-scale hills is also limited by condensed water advection and lee-side descent. We describe a new linear model for precipitation in complex terrain that includes 3-D dynamics and condensed water advection. The difficulty in testing models in complex terrain is discussed.

H62C-0872 1330h POSTER

Evaluation of an Upslope Precipitation Model

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A linear orographic precipitation model applicable on complex terrain for an arbitrary wind direction has been developed. The model includes mountain wave dynamics as well as condensed water advection and two micro-physical time delay mechanisms. Atmospheric input variables in the model are wind speed and direction, specific humidity, wet static stability and two conversion factors for the micro-physics. In addition, the underlying terrain is needed. Various closed-form solutions for the precipitation behavior over ideal mountains have been derived and verified with numerical mesoscale models. The model is tested in real terrain against observations. Several locations are used to evaluate the model performance (southern Norway, the Alps and the Wasatch mountains in Utah). The model results are of same magnitude as the observations, which indicate that the fundamental physics is included in the model. The ratio of condensate that is carried over the mountain crest to the amount that is left as precipitation is crucial, and the model seem to reproduce this well. When the model results are evaluated against observations with statistical measure such as correlation coefficient, it performs well overall. This requires that detailed input information such as wind direction and stability are provided and that the observations are taken frequently. Traditional observation samplings are normally unevenly distributed between valleys and mountain tops which cause a bias in objective analysis. Such an analysis can, in this case, not be held directly against model results. For the same reason, if a model for instance perform well on mountain tops, but poorly in valleys, observations will give a wrong impressions of the model performance. From our tests, the model perform well in smaller region where the input variables are representative for the whole area. Some model deficiencies are also discovered. The model performance seems to improve with slightly smoothed terrain which partly compensates for non-linear effects of flow in complex terrain.

H62C-0873 1330h POSTER

Probing Orographic Land-Atmosphere Interactions in the Himalayas During the Monsoon Using Satellite Imagery

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The linkages between the space-time variability of weather (and climate) and topography in Northern India and the Himalayas were investigated using remote sensing data. The research purpose was to test the hypothesis that cloudiness patterns are dynamic tracers of rainstorms, and therefore their temporal and spatial evolution can be used as a proxy of the spatial and temporal organization of precipitation and precipitation processes in the Himalayan range during the monsoon. The results suggest that the space-time distribution of precipitation, the spatial variability of the diurnal cycle of convective activity, and the terrain (landform and altitudinal gradients) are intertwined at spatial scales ranging from the order of a few kms (1-5 km) up to the continental-scale. Furthermore, this relationship is equally strong in the time domain with respect