

and associated system features for which better characterization would most likely improve prediction accuracy. We apply the OPS and VOII to address data collection and monitoring design issues in a ground-water model of a hydrogeologically complex regional flow system, where the predictions of interest are advective transport paths from locations of past and potential future contamination. Results suggest that collecting hydraulic-head and flow-system data at locations both far from and close to the predicted paths can be beneficial for reducing prediction uncertainty.

H41C-10 1115h INVITED

Initial Implementation of the Hanford Site-Wide Groundwater Flow and Uncertainty Analysis Framework

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Since Hanford operations began in 1943, large volumes of wastewater have been discharged into the subsurface, creating groundwater mounds (> 20m) and regional-scale contaminant plumes that will require monitoring at least through site closure. Since the cessation of wastewater disposal activities in 1988, many of the ~700 monitoring wells that previously documented mounding and contaminant movement are currently going dry. An initial implementation of the Hanford Site uncertainty methodology presented in this paper and a companion poster, investigates which of the ~700 monitoring wells are likely to go dry between now and 2050. The long-term goals of the Pacific Northwest National Laboratory effort at Hanford include the development and implementation of an uncertainty methodology with the site-wide groundwater flow and transport model.

Results are presented for two different conceptual models of the base of the unconfined aquifer. Model parameter uncertainty was determined through transient inverse modeling (1943-1996) using UCODE and ~76,000 historical observations of head. Since an analysis of model linearity using Beale's measure indicated that the model was sufficiently linear, the uncertainty in predicted future water levels was determined using linear confidence and prediction intervals. Both a steady-state and a transient case (1996-2050) were investigated in order to determine which of the current monitoring wells are likely to go dry. Results demonstrated that the uncertainty methodology can be used to evaluate the potential loss of existing monitoring wells in strategic locations, and to assist in the development of a long-term strategy for their replacement.

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URL: http://www.pnl.gov/main/publications/external/technical_reports/pnnl-13641.pdf

H41C-11 1135h

A Multipathway Model for High Explosives and Barium Transport Using GoldSim

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Outfalls from High Explosives (HE) production sites at Los Alamos National Laboratory (LANL) discharged RDX, TNT, HMX, and barium contaminated waters onto a mesa/canyon system on the western edge of the Pajarito Plateau from 1944 to 1996. HE concentrations in surface soils ranged to over 20 wt.%, and HE in waters range to over 800 ug/L. HE in water is present in springs, surface waters, alluvial waters and deep perched (> 700 ft. depth) and possibly regional (> 1200 ft depth) groundwaters. Barium concentrations range to over 4 wt.% in sediments, and to over

5000 ug/L in spring and alluvial waters. Because of the size of contaminant inventories and observations of HE in the perched zone and possibly deeper, there has been concern that there may be a long-term risk at a downgradient drinking water supply well. To address this concern, a GoldSim multipathway model was developed to simulate transport of HE and barium from source areas to the supply well. The objectives of the modeling effort were to generate a preliminary assessment of potential concentrations at the supply well and to identify any model components/parameters that require additional characterization based on model sensitivity and uncertainty. The model evaluates two main source areas, one is controlled by flow through the mesa vadose zone, and the other by flow through the canyon vadose zone. The two vadose zone modules feed into a saturated zone module that terminates at a pumping well (drinking water) module. The hydrogeology of the site is extremely complex and includes a heterogeneous, unfractured/fractured tuff vadose zone geology, ponds, springs, alluvial aquifers, a perennial stream reach, and two deep aquifers. Because of this complexity, and limited characterization and contaminant inventory information, we used a stochastic approach to quantitatively represent model/parameter uncertainties. Model parameters were developed using a variety of information including flow and transport modeling of different GoldSim modules using FEHM, various tracer experiments, borehole data, laboratory analyses, and site historical documentation. Model results will be presented as time-dependent concentration distributions for the various GoldSim modules. Results will be used to guide future characterization, monitoring, and remediation activities.

H41C-12 1150h

Colloids and Radionuclide Transport: A Field, Experimental and Modeling Effort

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Natural inorganic colloids (< 1 micron particles) found in groundwater can sorb low-solubility actinides and may provide a pathway for transport through geological aquifers. The importance of colloid-facilitated transport to the transport of low-solubility actinides, such as Pu, is still not well understood.

In an effort to better understand the dominant geochemical mechanisms that control Pu transport, we have performed a series of sorption/desorption experiments using mineral colloids. We focused on natural colloidal minerals present in water samples collected from both saturated and vadose zone waters at the Nevada Test Site. These minerals include zeolites, clays, silica, Mn-oxides, Fe-oxides, and calcite. X-ray absorption fine-structure spectroscopy (both XANES and EXAFS) was performed in order to characterize the speciation of sorbed plutonium. The XANES spectra show that only Pu(IV) was detected (within experimental error) on these mineral surfaces when the starting Pu oxidation state was +5, indicating that Pu(V) was reduced to Pu(IV) during sorption. The EXAFS detected Pu-M and Pu-C interactions (where M=Fe, Mn, or Si) indicating Pu(IV) surface complexation along with carbonate ternary complex formation on most of the minerals tested. Although the plutonium sorption as Pu(IV) species is mineral independent, the actual sorption paths are different for different minerals. The sorption rates were compared to the rates of plutonium disproportionation under similar conditions.

The batch sorption/desorption experiments of Pu(IV) and Pu(V) onto colloidal zeolite (clinoptilolite), colloids particle size 171 ± 25 nm were conducted in synthetic groundwater (similar to J-13, Yucca Mountain standard) with a pH range from 4 to 10 and initial plutonium concentration of 10-9 M. The results show that Pu(IV) sorption takes place within an hour, while the rates of Pu(V) sorption onto the colloids is much slower and mineral dependent. The kinetic results from the batch sorption/desorption experiments, coupled with redox kinetics of plutonium in solution will be used in geochemical modeling of Pu surface complexation to colloids and reactive transport.

(This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.)

H41D WCC: 29 Thursday 1020h Groundwater Field Testing: Techniques and Results I

Presiding: S E Silliman, University of Notre Dame; Z Kabala, Duke University

H41D-01 1020h

Three-Dimensional Tidal Wave Propagation in a Coastal Aquifer

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We believe that the measured strength of groundwater response to tidal loading not only depends on how far the measured well is from the shoreline, but also depends on how deep the well screen is. Tidal amplitudes from clustered wells near a river branch of the Chesapeake Bay in Maryland were analyzed. The least square harmonic analysis was conducted on the filtered data to extract the amplitudes and epoch of the water level. There are clear exponential damping in both horizontal and vertical directions in the extracted amplitudes for different tidal constituents. The behavior of the vertical damping is similar to the horizontal damping. Therefore, we believe that predicting the groundwater response to tidal loading should consider the well screen depth. We solved the transient three-dimensional groundwater response to tidal loading in a confined aquifer analytically. We applied the exact three-dimensional analytical solution for a confined aquifer to the studied site. The groundwater response to tidal change over a period of one month based on the tidal characters was predicted. With calibration of conductivity/storativity ratio, the predicted and the filtered measured data show a reasonable match. The three-dimensional solution that considers the vertical damping of the water pressure in an aquifer is helpful in modeling the flow and geochemical interaction of soil groundwater and tidal water along a tidal creek in a marsh environment.

H41D-02 1035h

Heat Evolved During Soil Wetting Under Spontaneous and Restricted Conditions

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Heat is evolved when free water is absorbed into dry soil. When the process is conducted at constant temperature the quantity of heat evolved is known as the heat of wetting. Clay minerals have values for heat of wetting from about 5 to nearly 100 J/g. Thus, the magnitude of the effect is sufficient to be detected with modest experimental effort. Soil may also be wetted by water entering the soil at various levels of water potential, and the heat produced varies accordingly. Water entering soil at lower potential energy has less energy which can appear as heat when it absorbs to soil particles. The minimum heat evolved is associated with reversible wetting. This reversible heat is equal to the specific internal energy of adsorption.

The first law of thermodynamics and a capillary tube model were used to find an equation for heat produced during soil wetting under various conditions. Three important conditions or types of wetting were identified. They are spontaneous wetting by free water, irreversible wetting, and reversible wetting. These types should be considered when heat of wetting effects are included in mathematical models of coupled heat and water transport. Inspection of the structure of one of the major models of this type, Philip-deVries of 1957, reveals that the model treats the heat of wetting effect as independent of the details of the wetting process. In other words, the model always assumes the wetting is of the spontaneous type and it does not include work done. It appears that modification of how heat of wetting is incorporated into this model is necessary in order to satisfy the first law. For most soil types the overall model output probably would not change appreciably after modification because the magnitude of the heat of wetting effect is small compared to heat capacity of mineral soil solids and the water itself. Some models in fact do not include a heat of wetting term because it is considered relatively small. On the other hand, the effect is not completely negligible and may be quite distinct and important under special conditions, such as porous media with very low heat capacity.

H41D-03 1050h

Multiple Scale Fluid Mass Transfer Calibration for a Fracture Flow Model

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The objective of this research is to calibrate quantitatively the flow field of a fractured aquifer at Oak Ridge National Laboratory, Tennessee, against field measurements. The field tracer release experiments were conducted under natural gradients. Advective mass transfer parameters that characterize small scale heterogeneity and the movement of pore fluid between fractures and rock matrix are estimated. Field scale heterogeneity, e.g., major preferred flow pathways, is determined with the assistance of field observations and a preliminary solute transport calibration. A two flow-regimes subsurface flow model, conforming to the framework of MurfMd (a Multiregion flow, Multi-dimensional simulator), is used to conduct the numerical simulations necessary for the calibrations. Fundamental research questions here include: (1) relative effect of small and field scale heterogeneity on the movement of pore fluid in fractured porous media and (2) the likelihood of using field scale observations to estimate small scale mass transfer parameters. Our results indicate that advective mass transfer, or internal boundary flux of pore fluid, is relatively significant in comparison with external boundary fluxes. Pressure head variations under natural gradients, in general, do not provide data sensitive enough for small scale mass transfer parameter estimation. However, pressure head variations in upper vadose zone and around ground water table result in advective mass transfer significant enough for the estimation of mass transfer coefficients, though the sources of these variations are of diverse hydrological nature.

H41D-04 1105h

Conceptual Models of the Potentiometric Surface at Yucca Mountain, NV

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The U.S. Department of Energy (DOE) is evaluating Yucca Mountain (YM) Nevada, as the potential site for geologic disposal of high-level nuclear waste (HLW). If approved, the repository would be located approximately 244 to 305 m (800-1,000 ft) above the present water table. Total-system performance assessments consider both engineered and geologic barrier systems are one method used to evaluate whether the potential repository can meet regulatory requirements. Flow paths interpreted from the potentiometric surface in the saturated zone beneath YM are incorporated into the performance assessment codes. Therefore, it is important that our understanding of the potentiometric surface is sufficient to assess potential repository performance.

The addition of new water-level data from the Nye County Early Warning Drilling Program (EWDP) has helped constrain the conceptual model of the site-scale potentiometric surface at YM, specifically in the southern portion of the site along U.S. Highway 95. The EWDP was initiated in 1998, with the purpose of identifying the flow paths for contaminants should they egress from the proposed repository into the groundwater system. A revised site-scale potentiometric surface map for YM utilizing the new water-level data obtained from the EWDP is presented. The revised site-scale potentiometric surface map and other existing site-scale potentiometric surface maps interpreted from water-level data, are compared to structural, geophysical, and chemical data to evaluate whether consensus exists among the different data types concerning groundwater flow at YM.

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H41D-05 1120h

Sensitivity Analysis of Dipole Flow Test with Wellbore Storage

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We develop a semi-analytic non-dimensional solution for the dipole flow test (DFT) accounting for wellbore storage and conduct its sensitivity analysis by studying the logarithmic sensitivities of drawdown with respect to radial hydraulic conductivity (K_r), specific storage (S_s), and anisotropy ratio ($a^2 = K_r/K_z$) along with the plausible relative errors in these parameters and the deterministic logarithmic correlations between them. The logarithmic sensitivity for a^2 is about an order of magnitude larger than that for K_r . The logarithmic sensitivity for S_s is larger than that for the other two parameters. Due to the complexity of the system, we observe some numerical oscillations in the calculated sensitivities. The results have implications for optimal estimation of aquifer parameters from the DFT.

H41D-06 1135h

Sensitivity Analysis of Dipole Flow Test with a Tracer

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We conduct the sensitivity analysis of dipole flow test with a tracer (DFTT) for homogeneous aquifers by studying the evolution of the logarithmic sensitivities of concentration in the extraction chamber with respect to longitudinal dispersivity (α_L) and anisotropy ratio ($a^2 = K_r/K_z$) as well as the logarithmic sensitivity of steady state drawdown in the extraction chamber with respect to radial hydraulic conductivity (K_r) and the anisotropy ratio. In addition, we study the plausible relative errors in all these parameters and the deterministic logarithmic correlations between them. The results have implications for optimal estimation of aquifer parameters from the DFTT.

H41D-07 1150h

Identification of Potential Atmospheric Inputs Via ICP-MS and ICP-OES Analysis of Groundwater Samples From Central Benin, West Africa

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ICP-MS and ICP-OES were used to analyze major and trace element concentrations in water samples collected from a fractured crystalline rock system underlying central Benin, Africa. These samples allowed analysis of trends among: (i) element concentration and latitude, (ii) element ratios and latitude, and (iii) element ratios and element concentration. Principal Component Analysis was also applied to the data. Results indicated strong spatial trends in many of the major and minor elements. For example, Na and Sr declined with increasing latitude whereas Sr, Ti and Sc increased with latitude. Results also indicated that certain element ratios were nearly constant over latitude while other ratios showed clear trends with latitude. Among the results from the Principal Component Analysis was the identification of three primary components. The first component consisted predominantly of the major ions and was reflective of a chemical signature one might find downwind from a salt-water source. The second consisted of trace elements and appears to be consistent with the composition of dry fall-out of dust from the Sahara Desert. The third component contained Si and a number of other elements. It is anticipated that this component is related to local mineralogy and/or anthropogenic impacts. The availability of ICP-MS and ICP-OES provided, in this case, a valuable data base from which to characterize the primary chemical inputs to the recharge waters

H42A WCC: Hall D Thursday
1330h

Groundwater Field Testing: Techniques and Results II Posters

Presiding: S E Silliman, University of Notre Dame; S Bartelt-Hunt, University of Virginia; P Imhoff, University of Delaware

H42A-01 1330h POSTER

The CNWRA Three-Dimensional Groundwater Flow Model for Yucca Mountain as a Regulatory Tool to Risk Inform NRC Reviews

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To evaluate the suitability of Yucca Mountain, Nevada, as a potential nuclear waste repository, the U.S. Department of Energy (DOE) conducts total-system performance assessment analyses. The saturated zone flow and transport system is one component of the natural barriers to radionuclide transport. To include saturated zone flow and transport in total-system performance assessment analyses, DOE abstracted flow paths from their site-scale saturated zone flow model. The U.S. Nuclear Regulatory Commission (NRC) staff, with assistance from the Center for Nuclear Waste Regulatory Analyses (CNWRA) staff, are responsible for reviewing the DOE saturated zone process model and total-system performance assessment analyses abstraction to assure that the DOE approach is justified by available data, that data and modeling uncertainties are appropriately considered, and that reasonable alternative conceptual models are considered. Review of the DOE approach and the development of an independent total-system performance assessment analyses abstraction necessitates an in-depth understanding of saturated zone hydrogeology at Yucca Mountain and a means to independently evaluate model and data uncertainties and potentially important alternative conceptual models for saturated zone flow. To this end, the CNWRA staff are developing a three-dimensional groundwater flow model of the Yucca Mountain, Nevada, region. The foundation of this flow model is the CNWRA hydrogeologic framework model, which was also developed independently from the DOE model. The insights gained through such independent model development are useful for a risk-informed review of DOE models. The CNWRA flow model can be used as a tool to evaluate the potential effects of various data and model uncertainties on saturated zone flow paths. Those evaluations can then be used for comparison with the level of uncertainty considered in the DOE performance assessments resulting from factors such as groundwater specific discharge (flux) and flow path lengths through various material types. In addition, the 3D groundwater flow model provides a means for evaluating the sensitivity of simulated flow paths, groundwater travel time, and capture zones and drawdowns of pumping wells, to the underlying interpretation of geologic structures and hydrogeologic features. The CNWRA flow model provides the NRC and CNWRA staffs with a tool to help resolve key technical issues pertaining to radionuclide transport via groundwater pathways in the saturated zone.

H42A-02 1330h POSTER

Experiments to Support the Design of a Field Scale Colloid Test at the Yucca Mountain Alcove 8/Niche 3 Complex

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The Alcove 8/Niche 3 complex at Yucca Mountain is being used to study flow velocity, matrix diffusion, and fault-fracture-matrix interactions. On the conclusion of the field scale tracer test to meet the above objectives, we plan to inject fluorescent latex microspheres, as a surrogate for colloids, into the system to study their transport behavior under fractured field conditions (apertures vary between 40 - 2000 mm).