oration, and surplus liquid water for terrain formation. Specification of the conditions under which neither parameter changed with spatial scale enabled the derivation of an equation for long-term actual evapotranspiration (AET), $AET/P = a/(b + (P/PET))$, at scales between 2-256 km for the Columbia River Basin in the northwestern US. Here, a and b are two empirical parameters with potential hydro-ecological significance. The relationship contains a fundamental dimensionless parameter, P/PET, for hydro-ecologic and eco-hydrologic studies. This parameter was extensively used by Budyko amongst others in their eco-hydrologic investigations. This equation is similar to an equation for AET obtained by Choudhury (1999), which is given by, $(AET/P)^{\alpha} = 1/(1+(P/PET)^{\alpha})$. It predicts long-term AET at plot scales of the order of 1 sq. km for $\alpha = 2.6$, and for large drainage basins of the order of million sq. km. for $\alpha = 1.8$. Therefore, Choudhury's equation is not scale invariant. A key open problem is to investigate if these two equations can be reconciled in a scale invariant manner. This work represents first steps towards the articulation of a biophysically sound theory about coupled ecology, hydrology, geomorphology and climate of landscapes that respects a conservation law and scale invariance.

H62G MCC: 120 Saturday 1330h

Fundamental Advances in Understanding of Pore-Scale Transport Phenomena in Porous Medium Systems I

Presiding: **M Hilpert,** Johns Hopkins University**; D Zhang,** Los Alamos National Laboratory

H62G-01 1330h

Measurement of Interfacial Area per Volume on Spatially Correlated and Uncorrelated Micro-models

Jiangtao Cheng[1] (chengj@physics.purdue.edu)

Nicholas Giordano[1] (ngpPhysics.purdue.edu)

Laura J Pyrak-Nolte[1,2] (ljpn@physics.purdue.edu)

[1]Department of Physics, Purdue University 1396 PHYS Bldg, West Lafayette, IN 47907-1396, United States

[2]Department of Earth Atmos. Sciences, Purdue University, West Lafayette, IN 47907, United States

Recent theoretical developments suggest that interfacial area per volume (IAV) plays an important role in scaling theories for the flow of multiple fluid phases in a porous medium. Many investigations have shown that the values of capillary pressure (Pcap) and saturation (S) do not uniquely specify the state of the system. A single value of relative volume saturation can correspond to infinitely different distributions of two phases within the volume. IAV provides a natural yard-stick for defining the role of scale in multiphase fluid properties. The dimensional units of interfacial area per volume is a spatial frequency (inverse length) that breaks scale invariance. In this study, we investigate whether or not IAV provides a state-function-like description of the flow properties, and if so, what does this function look like.

Measurements of interfacial area per volume as a function of capillary pressure and saturation were made on micro-models of pore structures. Photo-projection lithography was used to make transparent micro-models that were 600 x 600 microns with an aperture of 1.08 microns. Two phase flow measurements were performed on the micro-models using nitrogen gas and decane for a series of drainage and imbibition cycles. The initially decane-saturated micro-models were invaded with nitrogen by the application of pressure in increments. At each pressure increment, the system was allowed to equilibrate, and the saturation and distribution of each phase was digitally imaged and analyzed.

We observed that the Pcap - S - IAV surface appears to be a smooth, single valued surface. Several measurements were made for the same, or nearly the same, values of Pcap and S, and it was observed that the geometrical arrangement of the two phases was visually quite different. However, the value of the IAV in such cases was the same, to within a typical 5% experimental error in analyzing the digital photo-micrographs. We also observed that the magnitude of IAV was significantly different between the two types of models. Correlated micro-models exhibited values of IAV that were smaller by about a factor of 2, than that found for the uncorrelated micro-model.

Acknowledgments: DOE-FE contract DE-AC26-99BC15207. LJPN wishes to acknowledge Purdue University Faculty Scholar.

H62G-02 1345h

The Impact of Network Structure on Pore-scale Simulation of Fluid Transport

Riyadh I Al-Raoush[1] (riyadh@lwrri.lsu.edu)

Karsten Thompson[2] (225-578-3069; karsten@che.lsu.edu)

Clinton S Willson[1] (225-578-8672; cwillson@lsu.edu)

[1]Dept. of Civil Environmental Eng., 3502 CEBA Louisiana State University, Baton Rouge, LA 70803, United States

[2]Gordon A. and Mary Cain Dept. of Chemical Engineering, South Stadium Road Louisana State University, Baton Rouge, LA 70803, United States

Network modeling techniques for subsurface transport continue to incorporate more detailed physics. Therefore, it is important for networks to reflect the true porous media structure with an appropriate level of detail. Of particular interest, is whether three-dimensional networks created from different algorithms lead to different simulated transport behavior.

In previous work, several methods were used to extract pore networks from well-defined porous media: a medial-axis-based approach (at different resolutions), a Delaunay-tessellation algorithm, and a modified-Delaunay-tessellation algorithm. While these algorithms produce statistically similar networks for a given medium, there are pore-scale differences.

In the current study, we evaluate the impact of network structure on certain transport phenomena. Quasistatic drainage and imbibition simulations were performed on simulated and real systems to obtain capillary pressure versus saturation curves. Significant differences in results are attributed to factors such as variation in local coordination number, errors in determining local pore-body and pore-throat size, and lack of uniqueness in pore location. We tie these morphologic differences to pixelization of the medium, resolution of the digital image, and logic incorporated in the network algorithms. The results provide important information regarding the use of high-resolution tomography to generate network structures.

H62G-03 1400h

Accurate and Efficient Implementation of Pore-Morphology-Based Modeling of Drainage in Totally Wetting Porous Media

Markus Hilpert[1] (410-516-5127; markus_hilpert@jhu.edu)

David Adalsteinsson[2] (919-962-2442; david@amath.unc.edu)

[1]The Johns Hopkins University, Department of Geography and Environmental Engineering, 313 Ames Hall, 3400 N Charles St, Baltimore, MD 21218, United States

[2]University of North Carolina at Chapel Hill, Department of Mathematics, CB 3250, Phillips Hall, Chapel Hill, NC 27599, United States

We present a more efficient and accurate numerical implementation of the pore-morphological approach for modeling drainage in totally wetting porous media that was recently developed by Hilpert and Miller. The new approach uses level-sets to represent the phase distribution instead of voxels arranged on a cubic lattice.

H62G-04 1415h

Fluid Interfaces at the Pore-Scale: Trying to Make Observations and Lattice-Boltzmann Simulations Meet

Marcel G. Schaap[1] (mschaap@ussl.ars.usda.gov)

Britt S.B. Christensen[2] (brc@er.dtu.dk)

Dorthe Wildenschild[3] (dw@er.dtu.dk)

Katy A. Culligan[4] (Katherine.A.Culligan.2@nd.edu)

[1]GEBJ Salinity Laboratory (USDA/ARS), 450 W. Big Springs Road, Riverside, CA 92507, United States

[2]Dept. of Environment and Resources, Danish Technical University, Lyngby, DK 2800, Denmark

[3]Dept. of Geosciences, Oregon State University, Corvalis, OR 97331, United States

[4]Dept. of Civil Engineering, University of Notre Dame, Notre Dame, IN 46556, United States

Recent advances in microtomographic imaging techniques have allowed unprecedented observations of fluid behavior and interfacial geometries at micron sized scales. At the same time, significant progress in the development of numerical models for simulating fluid mechanics allow us to compare observations and model results, potentially providing insight into the scales at which macroscopic properties emerge. One of the promising modeling techniques is the Lattice Boltzmann method that offers a relatively simple means to approximate micro-scale Navier-Stokes flow as well as fluid-fluid and fluid-solid interactions. In this presentation we compare observations of micro-scale fluid saturations and interfacial geometries with simulations of a 3D two-phase Lattice Boltzmann model. The data used in this multidisciplinary study consist of three-dimensional pore-scale images of (air-water) drainage and imbibition experiments in a glass bead porous medium. The images were obtained using the GSE-CARS microtomography beamline at the Advanced Photon Source (Argonne National Laboratory) and form a cube with approximately 300 voxels on each side with a resolution of 17 microns per voxel. The Lattice Boltzmann simulations were carried out in micro porous geometries derived from dry images using high-performance parallel computer hardware at the Danish Technical University. Besides assessing difficulties and potential pitfalls that are inherent to the Lattice Boltzmann Method, we also explore discretization effects on simulated flow and interfacial geometries.

H62G-05 1430h

Determination of capillary pressure-saturation relation by pore-morphology-based and lattice-Boltzmann simulation

Volker Schulz[1] (volker.schulz@iup.uni-heidelberg.de)

Jonas Toelke[2] (toelke@cab.bau.tu-bs.de)

Hans-Joerg Vogel[1] (hjvogel@iup.uni-heidelberg.de)

Manfred Krafzcyk[2] (manfred.krafzcyk@tu-bs.de)

Kurt Roth[1] (kurt.roth@iup.uni-heidelberg.de)

[1]Institute of Environmental Physics University of Heidelberg, Im Neuenheimer Feld 229, Heidelberg 69120, Germany

[2]Institute for Computerapplications in Civil Engineering University of Braunschweig, Pockelsstrae 3, Braunschweig 38106, Germany

H

In this study we present two different models for the determination of the capillary pressure-saturation relation in porous media.

The first one is a pore-morphology-based model where we use methods from morphological image analysis to calculate the quasi-static primary drainage curve. Compared to previous publications in this field (Hilpert and Miller 2001), we extended the method to model trapped or irreducible wetting phase (WP). Additionally, we could optimize it in a way that the computing time is significantly reduced.

The second method to determine the capillary pressure-saturation relation is a two-phase lattice-Boltzmann (LB) model. Using a recently developed model for multi-phase flow (Tölke et al. 2001) we simulated the drainage of the porous medium by several pressure steps starting at total saturation.

As test systems, we used generated randomly sphere packages and x-ray images of a sintered borosilicate glass. Our simulations show that the capillary pressure-saturation curves from the both methods are very similar. However the morphological model is orders of magnitude faster than the LB simulation. But we point out that the good agreement strongly depends on the geometry of the investigated porous medium. Due to the model formulation, the pore-morphology-based simulation cannot be applied if the pore structure is strongly anisotropic (e. g. cracks).

References:

M. Hilpert and C. T. Miller: Pore-morphology-based simulations of drainage in totally wetting porous media, Advances in Water Resources, 24, p.243 (2001)

J. Tölke, M. Krafczyk, M. Schulz, E. Rank: Lattice Boltzmann simulations of binary fluid flow through porous media, Phil. Trans. R. Soc. Lond. A, Vol 360, Nr. 1792, p.535 (2002)

H62G-06 1445h

The Sound of Pore Filling

David A DiCarlo[1] (662-281-5705; ddicarlo@ars.usda.gov)

Jose I Gil Cidoncha[2] (jose.gil-cidoncha@ic.ac.uk)

Craig Hickey[3] (662-915-5963; chickey@olemiss.edu)

[1]USDA/ARS Natl Sedimentation Laboratory, 598 McElroy Dr, Oxford, MS 38655, United States

[2]Dept of Earth Sciences and Engineering, Imperial College, London, UK SW7 2BP, United Kingdom

[3]Natl Center for Physical Acoustics, University of Mississippi, University, MS 38677, United States

Pore-scale filling processes are often conceptually or numerically modeled, but are rarely experimentally observed. This is because of the difficulty of observing fast events at the pore scale in the interior of a porous medium. Here we measure the acoustic signal that is produced from the moving water-air interface during saturation changes in the porous medium. Traces of the magnitude of the sound versus time are obtained for different flow rates, initial condition, porous media size, and on imbibition and drainage. We show that the acoustic events are from abrupt pore-filling processes and discuss how the acoustic signals can be used to delineate particular processes in a real porous medium in-situ.

H62G-07 1520h

Lattice Boltzmann simulation of viscous fingering in a channel

Qinjun Kang[1,2] (qkang@lanl.gov)

Dongxiao Zhang[1] (donzhang@lanl.gov)

Shiyi Chen[2,3] (syc@jhu.edu)

[1]Hydrology, Geochemistry, and Geology Group, Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM 87545

[2]Department of Mechanical Engineering, Johns Hopkins University, 3400 North Charles Street, Baltimore, MD 21218

[3]Peking University, Haidian District, Beijing, BJ 100871, China

In this paper, we use a lattice Boltzmann (LB) multiphase model to study the flow of binary fluid with different component viscosities. We first validate the approach for a two-dimensional layered flow. The velocity profiles and the relative permeability coefficients are compared with the analytic results. We then apply this method to study viscous fingering in a two-dimensional channel where one fluid is displaced by another. The effects of viscosity ratio, capillary number, and wettability are investigated. The simulation results show that with the increase of the viscosity ratio or capillary number, both the finger width and the slipping distance of the contact lines decrease, while the finger length increases, indicating that the finger structure is truly due to viscous fingering. We also find that the finger growth is enhanced when the displacing fluid is nonwetting to the wall and that the fingering is otherwise suppressed. An indented part near the beginning of the fingers is clearly observed when a wetting fluid is displacing a nonwetting one.

H62G-08 1535h

An investigation of the parameters controlling interphase mass transfer in variable aperture fractures

Russell L Detwiler[1] (925-422-6229; detwiler1@llnl.gov)

Harihar Rajaram[2] (303-492-6604)

Robert J Glass[3] (505-844-5606; rjglass@sandia.gov)

[1]Lawrence Livermore National Laboratory, 7000 East Ave. P.O. Box 808, L-206, Livermore, CA 94551

[2]Department of Civil, Environmental, and Architectural Engineering University of Colorado, 428 UCB, Boulder, CO 80309

[3]Flow Visualization and Processes Laboratory, Sandia National Laboratories, PO Box 5800 MS 0735, Albuquerque, NM 87185-0735

In a fracture, the displacement of one immiscible phase by another (such as air or NAPL displaced by water) can result in the invading phase fully spanning the fracture with the defending phase completely surrounded or entrapped by the invading phase. During the invasion process, capillary, gravitational, and viscous forces all interact resulting in a broad range of possible entrapped phase geometries within a single fracture. The resulting geometry of the entrapped phase will play a dominant role in controlling flow, transport, and interphase mass transfer within the fracture. The dimensionless parameters that control entrapped phase geometry are the Curvature number (C - ratio of average in-plane interfacial curvature to average out-of-plane interfacial curvature), the Capillary number (Ca - ratio of viscous forces to capillary forces), and the Bond number (Bo - ratio of gravitational forces to capillary forces). In addition to entrapped-phase geometry, the Peclet number (Pe - ratio of advective to diffusive mixing) will influence interphase mass transfer rates. Using previously developed and tested computational models of immiscible displacement and entrapped phase dissolution in variable aperture fractures, we investigated the role of these dimensionless parameters on interphase mass transfer rates.

We simulated the invasion of water into a fracture initially filled with a nonwetting phase and then simulated the dissolution of the nonwetting phase as water flowed through the fracture under constant gradient. The synthetic fracture aperture fields used for these simulations exhibited a finite correlation scale (∼ 5 grid blocks) that was much smaller than the size of the domains (1024 x 2048 grid blocks). Multiple immiscible displacements were simulated using different values of C, Ca, and Bo resulting in a broad range of initial entrapped phase geometries. Subsequent simulations of entrapped phase dissolution provided estimates of saturation, mass transfer rate, and relative permeability during the dissolution of the entrapped phase. Plots of relative permeability versus saturation demonstrate that regardless of the initial phase distribution, relative permeability is strongly controlled by saturation. However, the initial geometry of the entrapped phase strongly influences the evolution of mass transfer rates during the dissolution process. The results demonstrate that an effective constitutive model of entrapped phase dissolution cannot be based solely on entrapped phase saturation and Pe. An effective model must also incorporate the role of C, Ca, and Bo in defining the entrapped phase geometry, which strongly influences dissolution rates.

H62G-09 1550h

Upscaling of Carbonate Dissolution Rates in Porous Media Using Pore-Scale Network Modeling

Li Li[1] ((609)258-5646; lili@princeton.edu)

Catherine A Peters[1] ((609) 258-5645; cap@princeton.edu)

Michael A Celia[1] ((609) 258-5425; celia@princeton.edu)

[1]Environmental Engineering and Water Resources Program, Dept. of Civil Environmental Engineering, Princeton University, Princeton, NJ 08544, United States

Geologic storage of CO_2 in sedimentary basins is an attractive option for carbon mitigation because the capacity is large and the technologies for capture, injection and monitoring are available or feasible. Basin-scale numerical modeling of CO_2 transport and reaction requires mineral reaction rate constants at a scale of meters, but laboratory measurements of such parameters are only available for the millimeter scale. Little is known about how these rate constants scale spatially. The present work addresses upscaling of mineral dissolution rates in porous media using a pore-scale network model. Calcite dissolution in the presence of aqueous CO_2 was selected as the model reaction due to the common occurrence of the carbonate mineral and its well defined and relatively fast reaction rate. The pore-scale network is constructed by random generation of pore volumes, pore cross-sectional areas, and reactive calcite surface areas. Transport and reaction of Ca^{2+} and total carbon (total concentration of $H_2CO_3{}^*$, $HCO_3{}^-$, $CO_3{}^{2-}$) are simulated as time-dependent processes; aqueous speciation reactions were considered at equilibrium. Laboratory measurements of calcite dissolution rates from the literature were assumed to describe the dissolution rate in each pore. The upscaled reaction rate may then be computed by calculating the total mass change in the whole network system, and subtracting the mass change due to advection and diffusion. Initial results indicate that model result can be compared with the reaction rate calculated by simple linear upscaling in which the system is described by its total volume and total reactive surface area. The upscaled reaction rate of the pore-scale network model is smaller than the value obtained by linear upscaling. This demonstrates the utility of pore-scale network modeling for predicting mineral dissolution rates in porous media and accounting for transport limitations in porous media. Additionally, as the model effectively describes the void structure of the porous medium, the influence of pore characteristics (volume, reactive surface area, cross sectional area between pores) on upscaled reaction rates can be investigated.

H62G-10 1605h

Spontaneous Switching of Permeability Changes in a Limestone Fracture Under net Dissolution

Amir Polak[1] (814 8659570; abp3@psu.edu)

Derek Elsworth[2] (elsworth@psu.edu)

Jishan Liu[3] (jishan@cyllene.uwa.edu.au)

Avrami S Grader[4] (grader@pnge.psu.edu)

[1]Energy Institute and Department of Energy and Geo-Environmental Engineering, Pennsylvania State University, 403 Academic Activities, University Park, PA 16802, United States

[2]Department of Energy and Geo-Environmental Engineering, 221 Walker, University Park, PA 16802, United States

[3]Center for Oil and Gas Engineering, University of Western Australia, Nedlands, WA 6907, Australia

[4]Energy Institute and Department of Energy and Geo-Environmental Engineering, Pennsylvania State University, 203 Hosler, University Park, PA 16802, United States

Results are reported for water flow-through experiments conducted on an artificial fracture in limestone at room temperature, and under ambient confining stress of 3.5 MPa. Tests are concurrently monitored for mass loss or gain and for changes in differential pressure between the inlet and outlet, throughout the 1500 h duration of the experiment. Periodic imaging by X-ray CT augments the fluid and mineral mass balance data and provides a third independent constraint on dissolution processes. The sample is sequentially circulated by water of two different compositions through the 1500 h duration of the experiment; the first 935 h by sampled groundwater, followed by 555 h of distilled water.

Large changes in the differential pressure are recorded during the duration of the experiment, for the constant flow-rate of 2 cc/m; these are used as a proxy for recorded changes in fracture permeability, under invariant effective stress conditions. Mass of Ca, Mg, and Na were net-removed throughout the experiment. During the initial circulation of groundwater, the differential pressure increased almost threefold, and is interpreted as a net reduction in permeability as the contacting asperities across the fracture are removed, and the fracture closes. With the circulation of distilled water, permeability initially reduced threefold, and ultimately increased by two orders of magnitude as a wormhole developed in the sample. This spontaneous switch from net decrease in permeability, to net increase, occurred with no change in experimental conditions of flow-rate or applied effective stress, and is attributed to the evolving localization of mass removal, triggered as free-face dissolution out-competed stress-mediated dissolution at the asperity contacts.

H62G-11 1620h

Pore Shape and Microscale Stress Distribution Effects on Soil Pore Closure Dynamics

Markus Berli[1] (860 486 3211; mberli@engr.uconn.edu)

Dani Or[1] (860 486 2768; dani@engr.uconn.edu)

[1]Markus Berli, University of Connecticut Civil and Environmental Engineering 261 Glenbrook Rd. UNIT 2037, Storrs, CT 06269-2037, United States

We study the impact of load application to wet soils of relatively high bulk density such as agricultural subsoils. An earlier model of bulk soil compaction under steady stress based on shrinkage of isolated spherical pores embedded in a homogeneous viscoplastic matrix was extended to consider spheroidal pore shapesand interactions among pores. The model describes shape evolution and rates of deformation of initially spheroidal pores as functions of macroscopic stresses and soil rheological properties. The implementation of such microscale models to real soils requires consideration of many interacting pores. We applied the Mori-Tanaka theory for interacting pores as a means for upscaling to bulk soil behavior and derived bulk soil moduli comparable to those obtained from standard geotechnical tests. Soil pore closure rates increase with higher water content (which largely controls soil rheology), and with pore size. This highlights the structural susceptibility of large pores and the significant impact of their closure on the hydrological behavior of compacted soils. Pore closure rate increases for pores with lower initial aspect ratio (i.e., oblate pores close faster than spherical pores of the same volume). Detailed pore scale stress distributions reveal formation of elastic (non-viscous) domains on a pore surface due to soil yield stress higher than the local stress. Comparisons with measurements in bulk soil will be presented.

H62G-12 1635h

Unsaturated Hydraulic Conductivity of Fracture and Capillary Networks via Lattice Boltzmann Methods

Michael C Sukop[1] (860-486-3211; msukop@engr.uconn.edu)

Dani Or[1] (860-486-2768; dani@engr.uconn.edu)

[1]University of Connecticut, Civil and Environmental Engineering 261 Glenbrook Road Unit 2037, STORRS, CT 06269-2037, United States

Modeling flow pathways and deriving constitutive relationships for unsaturated fracture and capillary networks present a challenge due to the multitude of potential invasion patterns and configurations assumed by liquid/vapor interfaces, especially at intersections of pores or fractures of unequal size. The multiphase Lattice Boltzmann Method (LBM) offers a promising tool for the computation of interface configurations

and movement in such networks and provides a means for testing previously proposed interface routing algorithms. The LBM offers a computational platform for measuring the hydraulic conductivity of unsaturated pore and fracture networks under different scenarios, including some that are not yet experimentally observable. We use a 2-D single-component multiphase LBM to simulate interface behavior at junctions where capillaries of various size and shape meet and consider the impact of changes in the capillary number on the resultant configurations. The LBM was tested using a simple bundle of capillaries in the context of a Poiseuille flow problem where flow occurs only in capillaries that remain filled at a particular fluid pressure. The unsaturated hydraulic conductivity for the equilibrium interfacial configuration in simple networks is calculated and compared with standard models based on pore size distribution and equilibrium pressure head.

H62G-13 1650h

Experimental Observations of Fluid Transport Across an Unsaturated Fracture-Intersection

Maria Ines Dragila[1] (541-737-5739; Maria.Dragila@orst.edu)

Noam Weisbrod[2] (972-8-6596901; weisbrod@bgumail.bgu.ac.il)

[1]Oregon State University, Department of Crop and Soil Science, Corvallis, OR 97331, United States

[2]Ben-Gurion University of the Negev, Department of Environmental Hydrology and Microbiology, Sde-Boqer Campus 84990, Israel

Fluid behavior in unsaturated fracture intersections was experimentally investigated in a glass fracture analog at four different flow rates. Three fractures symmetrically intersected at a single point. One of the fractures (vertical) was used to feed fluid to the intersection area and the subsequent 135 degree branches. Visualization data was collected using digital stills and video. Two flow modes were observed: film flow and capillary droplet accompanied by snapping rivulets. Distribution of film flow across the intersection was not limited to contiguous rock surfaces. The formation of a capillary bridge above the intersection allowed films to be distributed to either branch or both branches. During capillary droplet mode, two types of dynamics were observed at the intersection: (1) saturation of the intersection with continuation of droplet mode into the fracture branches; and (2) transition from droplet to film flow mode that did not saturate the intersection and resulted in film flow along both branches. Data suggests that the contact angle of the invading droplet is responsible for the mode of transport across the intersection. Rivulets where seen to stretch contiguously across the intersection and into both branches while connected to two droplet halves, a distance of 70 cm.

H71A MCC: Hall C Sunday 0830h

Conceptual Model Evaluation and Quantification of Groundwater Model Error Posters

Presiding: **T Scheibe,** Pacific Northwest National Laboratory**; M Hill,** U.S. Geological Survey

H71A-0774 0830h INVITED POSTER

Quantification of the Effect of Model Error on Groundwater Model Predictions and Risk Assessment

Petros Gaganis[1] (30-610-965220; pgaganis@terpsi.iceht.forth.gr)

Leslie Smith[2] (604-822-4108; lsmith@eos.ubc.ca)

[1]ICE/HT Foundation for Research and Technology, PO Box 1414 Stadiou Str, Platani, Patras 265 04, Greece

[2]Dept. Earth and Ocean Sciences University of British Columbia, 6339 Stores Road, Vancouver, BC V6T 1Z4, Canada

Errors arising from the imperfect mathematical representation of the structure of a hydrologic system (model error) do not necessarily have any probabilistic properties that can be easily exploited in the construction of a model performance criterion. Furthermore, the existence of parameter uncertainty imposes additional difficulties in isolating and evaluating model error because it obscures the impact of model error on model predictions. A Bayesian approach is presented for quantifying model error in the presence of parameter uncertainty. Insight gained in updating the prior information on the model parameters is used to assess the correctness of the model structure, which is defined relative to the accuracy required of the model predictions. Model error is then evaluated for each measurement of the dependent variable through an examination of the correctness of the model structure for different accuracy levels. The effect of model error on each dependent variable is quantified as a function of location and time, and represents a measure of the reliability of the model in terms of each model prediction. Through a synthetic example it is shown that this method may assist in discriminating among models in terms of the correctness of the model structure, as well as in identifying possible causes of model error. Application to a problem of 90Sr migration to water wells at Chernobyl, Ukraine, demonstrates that the Bayesian model error analysis may also offer a more informative description of the uncertainties involved in risk assessments and decision analyses, and an alternative to the practice of adopting a bias towards conservative risk estimates in decision models.

H71A-0775 0830h INVITED POSTER

Uncertainty Inherent in Geologic Data, Interpretations and Conceptual Models Used in Groundwater Flow Modeling

Donald S. Sweetkind[1] (1-303-236-1828; dsweetkind@usgs.gov)

Claudia C. Faunt[2]

Geoffrey Phelps[3]

[1]U.S. Geological Survey, MS 973, Denver Federal Center, Denver, CO 80225, United States

[2]U.S. Geological Survey, 5735 Kearny Villa Rd., Suite O, San Diego, CA 92123, United States

[3]U.S. Geological Survey, MS 989, 345 Middlefield Rd, Menlo Park, CA 94025, United States

When using MODFLOW-2000, parameter estimation and the calculation of flow model uncertainty are generally based on a static hydrogeologic framework. Although the properties of hydrogeologic units may be estimated and uncertainty ascertained during model calibration, the spatial location of the boundaries of the units are not usually modified. As such, the hydrogeologic framework is essentially viewed as absolute, and as a result having no uncertainty. In reality there are numerous types of uncertainties inherent in geologic data that could be acknowledged and accounted for. Framework models often include mixtures of quantitative geologic data, interpretations based on quantitative data, and qualitative, tacit geologic knowledge. Interpolated surfaces are created from these data and then stacked in geologic or stratigraphic modeling software to create volumetric units. In many cases, more than one geologic conceptual model may honor all available data. Because the task of building a digital 3D framework model is labor-intensive and technically difficult, it is usually not possible to construct 3D frameworks to test all possible conceptual models and decisions regarding the preferred conceptual model are often made prior to the creation of a digital model. Once a model is completed in the digital realm, the technical capabilities of the software and visual appeal can effectively mask a lack of data or flaws in the conceptual model. What is needed is a way to explicitly identify uncertainty inherent in framework models so that alternatives can be explored more efficiently, and so that the geologic and mathematical sources of error are more transparent.

Geologic error and uncertainty inherent in any digital 3D framework model might be subdivided into five general categories: (1) interpolation, the construction of surfaces between data points; (2) inference, the presence of information that constrains the location or property of a feature without being actual data from that feature; (3) extrapolation, methods for extending calculated surfaces beyond the range of the data; (4) interpretation and geologic inference that are based on data, such as geologic cross sections; and (5) paradigms, which includes elements that are constructed based on a conceptual model of the system. These five categories are not strict statistical definitions but are concepts that describe types of uncertainty within the framework model, promote understanding of the logic that went into building the model, and allow effective scrutiny of the model and possible alternatives. These subdivisions help focus attention on where the framework model has the greatest likelihood of being accurate and where alternatives are possible and therefore, where and what methods should be used to quantify error in a particular aspect of the model. By quantifying error in the framework model, model developers and users are better equipped to evaluate the use of particular aspects of the model in groundwater flow modeling.

H71A-0776 0830h POSTER

The Connection Between Conceptual Model Errors and the Capabilities of Numerical Models

Mary C. Hill[1,2] ((303) 541-3014; mchill@usgs.gov)

Steffen Mehl[1,2] ((303) 541-3078; swmehl@usgs.gov)

[1]U.S. Geological Survey, 3215 Marine St., Boulder, CO 80303-1066, United States

[2]University of Colorado, Boulder, Dept. of Civil, Env., and Arch. Engineering, Boulder, CO 80309-0428, United States

Hydrologic conceptual models consider what characteristics and processes of groundwater systems are important to predictions of interest, and provide blueprints from which analytical and numerical models can be developed to provide quantitative analyses. We often like to think that these blueprints are developed independent of the characteristics of the model we plan to use, but the limitations of the models often impact the way we think about and conceptualize a given system. For example, one of the most perplexing problems in developing models is the appropriate scale for representation of hydrologic and physical features. Scale problems can be caused, for example, by hydraulic gradients that become dramatically steeper with proximity to a pumping well, rivers with widths that are small and dynamics that are fast relative to the adjacent groundwater systems with which they interact, and small geologic features that are important to simulating areas with contaminant plumes but elsewhere are less important. As suggested by these examples, scale problems occur in representing features of a wide range of sizes.

Our inability to accommodate such scale problems is a major contributor to groundwater model errors. Contributing difficulties include inadequate data and limitations of the capabilities of commonly used models. The issue of inadequate data has been addressed most through stochastic methods because data, computer capabilities, and numerical methods have not allowed us to build models capable of representing these variations deterministically. But these limitations are changing. New field data methods are providing unprecedented representations of subsurface characteristics and computers and software are getting more powerful. Are ground-water models ready to take advantage of these opportunities? A promising way to address some of these issues is to reduce the errors associated with scale problems through local grid and time-step refinement. Local grid refinement allows model grids to represent more detailed hydraulics and features as needed. The additional model capability encourages more accurate conceptual models, but this is only an improvement if the refined models are numerically robust and do not introduce other errors.

H71A-0777 0830h POSTER

The Neglected Art of Interpretive Ground-Water Modeling

Stanley A Leake ((520) 670-6671 EXT 259; saleake@usgs.gov)

S.A. Leake, 520 N. Park Ave, Suite 221, Tucson, AZ 85719, United States

Nearly all numerical models being developed to study ground-water systems are of a type known as predictive models. These models require calibration to observations such as head, flow, and concentration, with the ultimate goal of predicting system response to some forcings. Available postaudits of predictive models have shown that predictions rarely are accurate. Among the likely reasons for this lack of success is that conceptual models of hydrologic systems are almost always incomplete and uncertain. Numerical models, however, can be used to improve conceptual models of flow systems. An approach known as interpretive modeling involves representation of a conceptual model of a system in a numerical model, and studying how the system might operate. Unlike predictive models, interpretive models are not necessarily calibrated. These models are useful to look at how well the available information on a system fits together, to test hypotheses about the way a system operates, and to study possible ranges of effects caused by changes to a system. An interpretive model, for example, could be used to study whether or not an observed inflection in a water surface could be caused by a geologic feature such as a fault or facies change. The main benefit of interpretive modeling is understanding and insight, instead of numbers, which is the goal of predictive modeling. Although the demand for predictive models by the water management community likely will remain high, we in the hydrologic sciences should strive to better educate water managers about the benefits of interpretive modeling.

H